PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B BIOLOGICAL SCIENCES

Models of Integrated Photosynthesis of Cells and Leaves

G. D. Farquhar

Phil. Trans. R. Soc. Lond. B 1989 **323**, 357-367
doi: 10.1098/rstb.1989.0016

Phil. Trans. R. Soc. Lond. B **323**, 357–367 (1989)
Printed in Great Britain

Models of integrated photosynthesis of cells and leaves

By G. D. Farquhar

Plant Environment Biology, Research School of Biological Sciences, Australian National University, GPO Box 475, *Canberra City, ACT* 2601, *Australia*

The kinetics of ribulose bisphosphate carboxylase–oxygenase (Rubisco) are integrated with the stoichiometry of NADPH consumption and production in a simplified model of C_3 chloroplast photosynthesis. The extension to a leaf is discussed with reference to the gradient of irradiance that is always present within the leaf. The optimal arrangement of photosyntheic capacity is discussed in this context. Attention is then given to the effects of gradients of CO_2 concentration that sometimes occur when stomata close in a heterogeneous fashion.

Introduction

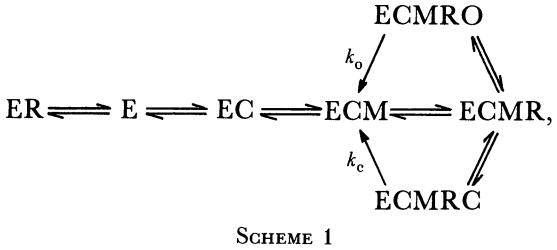
Mathematical models of photosynthesis should be used for assembling facts at one level of biological organization and making predictions at the next (Farquhar 1989).

It is perhaps a matter of taste, but I find analytical solutions, as opposed to numerical ones, more enlightening. Unfortunately the complexity of photosynthesis means that analytical descriptions can only be achieved at the expense of gross simplification. Progress in understanding photosynthesis has enabled such simplications to be made and this is revealed in the work of many, including Laing *et al.* (1974), Peisker (1974) and Hall (1979).

I review here the simplified, analytical solutions of C_3 photosynthesis developed in collaboration with S. von Caemmerer and J. A. Berry. These are basically equations describing the kinetics of the primary C_3 carboxylating enzyme linked with the stoichiometry of electron transport and NADPH consumption. I then extend this chloroplast-based (or cell-based) model to the leaf with a discussion of heterogeneity of light intensity and CO_2 concentration within the leaf. The heterogeneity of irradiance is discussed in relation to optimal allocation of protein.

Kinetics of Rubisco

The reactions of ribulose bisphosphate (RuBP) carboxylase–oxygenase (Rubisco) may be summarized as in scheme 1, where E, R, C, O, and M represent enzyme sites, RuBP, CO_2, O_2 and Mg^{2+}. ER, EC etc. represent complexes, and k_c and k_o represent the rate constants of



Scheme 1

the irreversible carboxylase and oxygenase reactions respectively (Farquhar 1979). This model assumes that the reactions with substances are ordered, with RuBP binding before either of the gases. Research on Rubisco has so far been consistent with this notion, enolization of RuBP occurring before interaction with the gaseous substrates (cf. review by Andrews & Lorimer (1987)).

The rate of carboxylation, V_c, is defined here as the rate of reaction with substrate CO_2, rather than as rate of production of product, as carboxylation produces two molecules of glycerate 3-phosphate (PGA). Farquhar (1979) showed that this could be written as

$$V_c = W_c \frac{\mathrm{CMR}}{\mathrm{CMR} + K'_e K_d \mathrm{R} + K'_r[\mathrm{CM} + (\mathrm{C} + K_e)K_d]} = W_c Z, \quad (1)$$

where W_c is the RuBP saturated, fully activated (magnesium saturated) rate. The second (complicated) factor (Z) reduces to a Michaelis–Menten dependence on R if the product CM is saturating, and to Michaelis–Menten dependence on CM if R is saturating. No satisfactory model yet exists for including the effects of Rubisco activase (Salvucci *et al.* 1985) on the parameter Z.

The above treatment was extended by von Caemmerer & Farquhar (1985) to include the binding of phosphorylated compounds other than RuBP, which increases the effective Michaelis constant for RuBP.

In turn, W_c can be written (Laing *et al.* 1974) as

$$W_c = k_c \mathrm{E_t} \mathrm{C}/\{\mathrm{C} + K_c(1 + \mathrm{O}/\mathrm{K_o})\}, \quad (2)$$

where $\mathrm{E_t}$ is the total concentration of enzyme sites, and K_c and K_o are the Michaelis constants for CO_2 and O_2, respectively.

Farquhar (1979) showed that the dependence of V_c on R is rather different to the dependence on free plus bound R if $\mathrm{E_t}$ is large, as is the case *in vivo*. The rate should saturate soon after the total concentration, $\mathrm{R_t}$, exceeds $\mathrm{E_t}$, unless there is low activation or there are large concentrations of compounds competing with R for binding. Measurements *in vivo* appear to show that this actually happens when concentrations reach 1.5–2 times $\mathrm{E_t}$ (von Caemmerer & Edmondson 1986; Seemann & Sharkey 1986). However, it is likely that these measurements include other RuBP which is chelated by magnesium (von Caemmerer & Farquhar 1985). There is uncertainty about stromal levels of Mg^{2+}, but when current estimates are used there is reasonable agreement between theory and observation, i.e. V_c is probably saturated when the concentration of free plus bound (but not chelated) RuBP exceeds $\mathrm{E_t}$ (von Caemmerer & Farquhar 1985), although large concentrations of phosphorylated compounds competing for RuBP binding sites can also raise the levels of RuBP required for saturation (von Caemmerer & Edmondson 1986).

The chelation of magnesium and RuBP has other theoretical implications, which have not yet been verified experimentally. When the concentration of magnesium is increased, the concentration of free RuBP should decrease, and when the concentration of RuBP is increased, that of free magnesium should decrease. This should cause a fine balance in the compromise between full activation and maintaining saturating RuBP levels, giving rise to optimal values (in terms of the effect on V_c) of $\mathrm{R_t}$ and of magnesium (von Caemmerer & Farquhar 1985). The rate of oxygenation of RuBP, V_o, is given by

$$V_o = W_o Z, \quad (3)$$

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B BIOLOGICAL SCIENCES

where $$W_o = k_o E_t O/\{O + K_o(1 + C'K_c)\}' \quad (4)$$

so that regardless of activation, or of RuBP concentration, the ratio of oxygenation and carboxylation is given by

$$V_o/V_c = k_o K_c O/k_c K_o C = 2\gamma^* O/C. \quad (5)$$

The significance of the parameter γ^* will emerge.

The events that follow oxygenation in the photorespiratory carbon oxidation cycle involve the loss of 0.5 mol CO_2 per mole oxygenation (Berry *et al.* 1978; Woo *et al.* 1978). Thus the net rate of carbon fixation by a cell, ignoring dark respiration, is

$$\begin{aligned} A &= V_c - 0.5V_o \\ &= V_c(1 - 0.5V_o/V_c), \end{aligned} \quad (6)$$

and from equation (5) (Farquhar & von Caemmerer 1982),

$$\begin{aligned} A &= V_c\,(1 - \gamma^* O/C) \\ &= V_c\,(1 - \Gamma^*/C), \end{aligned} \quad (7)$$

where Γ^* is the product γ^*O, known as the CO_2 photocompensation point (Laisk 1977). From equation (7) it is clear that A is zero at $C = \Gamma^*$, regardless of activation, RuBP or magnesium levels. When dark respiration rate, R_d, is included,

$$A = V_c\,(1 - \Gamma^*/C) - R_d. \quad (8)$$

From equation (5) it may be seen that the Rubisco specificity factor

$$V_c O/(V_o C) = 1/(2\gamma^*). \quad (9)$$

In practice the specificity factor is normally presented by taking O and C to be dissolved concentrations, but a better way is with O and C taken as equivalent gaseous partial pressures (Badger & Collatz 1977; Farquhar 1989) and this modifies the numerical value of specificity by the ratio of the Henry constants. The temperature dependence of Γ^* (and γ^*) has been measured and shown to be in good agreement with measurements of specificity factor (Brooks & Farquhar 1985). To a good approximation, $\Gamma^* = 1.7T$, when Γ^* is measured in $\mu l\ l^{-1}$ at 21 % O_2 and T is the temperature in degrees Celsius (Farquhar 1989).

Electron transport

From the modeller's viewpoint the concentrations of RuBP and Mg^{2+} are independent variables in the context of isolated Rubisco, but not when one considers functioning in the chloroplast. One knows that they must take on values that lead to fluxes no greater than those allowed by the capacity to produce ATP and NADPH, at the prevailing irradiance and temperature. With the operation of a Q-cycle (Mitchell 1976), it is thought that the electron transport required to sustain the NADPH consumption (two electrons per NADPH) by the photosynthetic carbon reduction and photorespiratory carbon oxidation cycles, given by

$$\text{electron transport} = 4V_c + 4V_o,$$

and, from equation (5),

$$\text{electron transport} = 4(1 + 2\Gamma^*/C)\,V_c, \quad (10)$$

is marginally greater than that required for ATP production. So if the prevailing potential rate of electron transport is J,

$$J \geqslant 4(1+2\Gamma^*/\mathrm{C})\, V_\mathrm{c},$$

i.e.
$$V_\mathrm{c} \leqslant J/4(1+2\Gamma^*/\mathrm{C}) = W_J, \tag{11}$$

where W_J is the rate of carboxylation allowed by the capacity for electron transport. From equation (8),

$$A \leqslant R_\mathrm{d}\, J(1-\Gamma^*/\mathrm{C})/4(1+2\Gamma^*/\mathrm{C}). \tag{12}$$

The dependence of J on absorbed irradiance, I, is given implicitly by the empirical equation

$$\theta J^2 - (J_\mathrm{max} + \tfrac{1}{2}I)\, J + \tfrac{1}{2} J_\mathrm{max}\, I = 0 \tag{13}$$

(Farquhar & Wong 1984), where J_max is the limit as I approaches infinity, and θ is a convexity factor. The solution is a rectangular hyperbola when $\theta = 0$ and two straight lines (the 'Blackman response') when $\theta = 1$.

The temperature dependence of J_max has been discussed elsewhere (Farquhar 1989). The irradiance effectively absorbed by thylakoids for photosynthesis will be less than that absorbed by the leaf because of absorption outside the chloroplasts by other pigments. The absorption depends on wavelength.

As a useful approximation, the inequality (12) can be regarded as an equation until $W_J > W_\mathrm{c}$, i.e.

$$V_\mathrm{c} = \min\{W_\mathrm{c}, W_J\}, \tag{14}$$

where min $\{x, y\}$ denotes 'the minimum of x and y' (Farquhar & von Caemmerer 1982). Of course, this ignores the limitation on flux that may be imposed at large I and C by other components of the Calvin cycle involved in the regeneration of RuBP (Farquhar *et al.* 1980).

In this model, as I increases, A therefore follows the limit imposed by equation (12), with J following the non-rectangular hyperbolic relation equation (13). However, when W_J exceeds W_c, the system becomes limited by Rubisco activity and A saturates sharply. If A were to be related to I over this whole range, then the apparent convexity, θ, would be an overestimate of that for electron transport alone. In the past, the form of equation (13) has often been used for whole-leaf assimilation rate, but the results will be difficult to interpret when conditions for $W_\mathrm{c} > W_J$ were not met, i.e. light response curves at normal ambient CO_2 concentrations. To ensure $W_\mathrm{c} > W_J$ at high light intensity, a large concentration of CO_2 should be used. A typical value for θ in describing whole-leaf photosynthesis at large C is 0.7 (Evans & Terashima (1987), data on spinach).

• Heterogeneity of light environment

Oja & Laisk (1976) showed that for a given amount of photosynthetic 'apparatus' per unit leaf area, uniform distribution of this capacity through the leaf does not give the greatest rate of photosynthesis.

This problem can be formalized. If a leaf were divided into two layers, the potential rate of the whole leaf, J, would be the sum of the potential rates for the two layers, $J = J_1 + J_2$. If the investment of limiting resources in the thylakoids (contributing to J_max) were distributed

optimally, there would be no benefit in transferring any away from one layer to the other. Taking nitrogen as being representative of this resource, the optimal condition is given when a small amount δN_1 is subtracted from layer 2, given to layer 1, and has no net effect on total flux, i.e.

$$\delta J = \delta N_1 \, \partial J_1/\partial N_1 + (-\delta N_1) \, \partial J_2/\partial N_2 = 0.$$

This occurs when

$$\partial J/\partial N = \partial J_1/\partial N_1 = \partial J_2/\partial N_2. \tag{15}$$

That is, at the optimal distribution, the response of each layer to an increase in local N and J_{max} is the same as for the other layer, and as for the whole leaf. Taking J_{max} as a measure of the resource, the optimal condition requires that

$$\partial J_T/\partial J_{max,T} = \partial J_1/\partial J_{max,1} = \partial J_2/\partial J_{max,2}, \tag{16}$$

where J_T and $J_{max,T}$ denote whole-leaf parameters. From equation (13), J is a homogeneous function (of order 1) of both J_{max} and I, i.e.

$$J(tI, tJ_{max}) = tJ(I, J_{max}). \tag{17}$$

(In words, if both J_{max} and I are doubled in equation (13), the equation is satisfied if J is also doubled.)

If the absorbed irradiances in layers 1 and 2 are in the ratio $1:t$, say, the middle term in the optimality condition (equation (16)) may be rewritten by using (17) as

$$\begin{aligned} \partial J_1 (I_1, J_{max,1})/\partial J_{max,1} &= \partial [J_1 (tI_1, tJ_{max,1})/t]/\partial J_{max,1}, \\ &= \partial J_1 (tI_1, tJ_{max,1})/\partial tJ_{max,1}, \\ &= \partial J_2 (I_2, J_{max,2})/\partial J_{max,2} \quad \text{(if and only if } J_{max,2} = tJ_{max,1}\text{)}, \\ &= \text{right-hand side of equation,} \end{aligned} \tag{16}$$

i.e. partitioning of resources is optimized if and only if J_{max} in the two layers are in the same proportion as the absorbed irradiances. In general, for n layers,

$$I_1 : I_2 : \ldots : I_n = J_{max,1} : J_{max,2} : \ldots : J_{max,n}, \tag{18}$$

and by making further use of the homogeneity properties

$$= J_1 : J_2 : \ldots : J_n. \tag{19}$$

This means that the form of the equation describing a group of layers within a leaf (e.g. the whole leaf) has the same form as for an individual layer, providing the partitioning of capacity is optimized, and both these requirements are equivalent to having the capacities in proportion to the absorbed irradiances. The results are summarized in figure 1.

For optimal use of nitrogen by a leaf it is also important that transition from limitation of V_c by W_J to that by W_c^* also occurs for all layers at the same leaf irradiance. This means that Rubisco activity should also scale with light absorption. The present analysis does not specify how much nitrogen should be invested into proteins for light harvesting, as opposed to that for photosynthetic capacity.

Experiments by Terashima & Inoue (1985) qualitatively confirm the predictions that both electron transport and Rubisco capacities decrease with depth into the leaf. The results are analogous to those seen for leaves within a canopy (Field 1983; Hirose & Werger 1987). Field

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B BIOLOGICAL SCIENCES

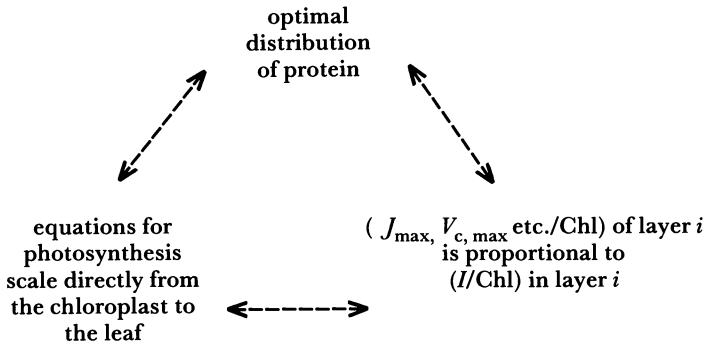


FIGURE 1. For a leaf that has a fixed internal pattern of light absorption, i.e. each layer (i) always absorbs the same proportion of the absorbed light, the above results hold *provided that* the equation relating J to J_{max} and I (the absorbed irradiance) is homogeneous, of order one, and does not change its form with depth.

(1983) predicted that this should be the case with computer simulations. He subsequently presented the condition for optimality,

$$\partial A_{day}/\partial N = \lambda, \tag{20}$$

where λ is an unspecified Lagrange multiplier that changes with canopy structure and total nitrogen investment (Field, 1988). This is analogous to equation (15). (This was, unfortunately, erroneously published as $A_{day}/N = \lambda$ (Field, personal communication).)

The equivalent optimization problem for a leaf is: maximize

$$\int_0^Z J(J_{max}(z), z)\,dz$$

subject to

$$\int_0^Z J_{max}(z)\,dz = \text{constant}, \tag{21}$$

where z is a measure of depth in the leaf, Z is the thickness, and J is again a function of J_{max} and I, but I depends only on depth, z. There is a formal analogy with the problem: maximize

$$\int_0^T A(E(t), t)\,dt$$

subject to

$$\int_0^T E(t)\,dt = \text{constant}, \tag{22}$$

where E is evaporation rate, t is time, and T is the length of the day. The solution (Cowan & Farquhar 1977) is

$$\partial A/\partial E = 1/\lambda', \tag{23}$$

a different constant from that in equation (20), provided $\partial^2 A/\partial E^2 < 0$. It may also be shown that

$$\partial \int_0^T A\,dt/\partial \int_0^T E\,dt = 1/\lambda'. \tag{24}$$

Similarly, then, the solution to the present problem is

$$\partial J(z)/\partial J_{\max}(z) = K, \tag{25}$$

say, and

$$\partial J_T/\partial J_{\max,T} = K, \tag{26}$$

where again J_T and $J_{\max,T}$ denote whole-leaf parameters. The solution is an optimal one because $\partial^2 J/\partial J_{\max}^2 < 0$ for equations such as equation (13). Note that the value of K depends on the overall irradiance. This should also be the case with equation (20).

However, just as one cannot always say A/E is constant, one cannot, in general, say A/N or $J/J_{\max}$ is constant. The latter result depends on the relation $J = J(J_{\max}, I)$ being homogeneous of order unity, as discussed earlier. The homogeneity is lost, for example, if θ changes with depth. Terashima & Saeki (1985) iteratively modelled the effects of changes of capacity with depth and concluded that, in their model, maximal efficiency occurred when capacity and light absorption were in constant ratio among layers (present equation (18)). They also used equation (13), which does satisfy the homogeneity condition. They chose a convexity (θ) of 1, which should have meant that the whole leaf also had $\theta = 1$ for the appropriate partitioning, although this was not demonstrated. The authors did show how less optimal arrangements decreased the convexity.

The results in figure 1 are most likely to be applicable to horizontal leaves, or, more precisely, to those leaves that receive light from either side in a fixed proportion. For leaves that can receive light from either surface at *different* times, there will always be capacity used ineffectively. There should be greatest concentration near the surfaces and less in the centre of the leaf (Kirschbaum 1987). This also means that the form of the whole-leaf equation relating J to I differs from that for the local layer, with convexity, θ, being less.

Heterogeneity of CO_2 concentration

Having discussed heterogeneity in the light environment within a leaf I now consider heterogeneity in the partial pressure of CO_2 (p_{CO_2}). If there were rapid diffusion within the leaf air spaces there would be no problem, provided the liquid phase resistance in the complicated pathway involving cell walls cytoplasm and stroma (Evans 1983; Evans *et al.* 1986) is also small. However, with the packing of cells that obtains in the leaf, diffusion over distances more than, say, 2 mm is likely to be slow. This estimate derives from observations of the difference in p_{CO_2} across a leaf when CO_2 is supplied to the abaxial surface only and the concentration is then determined for the substomatal cavities of the adaxial surface (Parkhurst *et al.* 1988). This presumably corresponds to the supply of CO_2 across mesophyll tissue to active sinks (where I is greatest). The observations were that the differences were typically 35 μbar†, for leaves with thicknesses of about 0.35 mm. The effect should be exacerbated in the case where cells all along the path are actively photosynthesizing, and adjacent stomata are closed. Such will be the case when groups of stomata are more closed in one region than in the other. The mathematical solution for a real leaf is obviously complicated, but an idea of what happens is obtained by considering a collection of regions on a leaf, sufficiently large for there to be minimal diffusion from one to the other. The size of each region, or patch, will be greater for open-structured leaves than for close-packed leaves, and probably also for leaves lacking bundle-sheath extensions (Terashima *et al.* 1988).

† 1 μbar = 10^{-1} Pa.

Consider a leaf (or perhaps a portion of a leaf) divided into, say, one hundred such patches of equal size. The leaf conductance to the diffusion of CO_2, g, will be given by the arithmetic mean of the hundred conductances per unit area:

$$g = (g_1 + g_2 + \ldots + g_{100})/100, \tag{27}$$

where the subscript denotes the individual patch. Similarly, the CO_2 assimilation rate will be

$$A = (A_1 + A_2 + \ldots + A_{100})/100. \tag{28}$$

The linkage between these two gas-exchange parameters is provided by the intercellular concentration of CO_2, C_i, in

$$A = g(C_a - C_i), \tag{29}$$

where C_a is the ambient concentration. Solving for C_i,

$$C_i = C_a - A/g \tag{30a}$$

$$= C_a - (A_1 + A_2 + \ldots + A_{100})/(g_1 + g_2 + \ldots + g_{100}). \tag{30b}$$

Using equation (29) for the individual patches, equation (30*b*) becomes

$$C_i = C_a - \frac{g_1(C_a - C_{i,1}) + g_2(C_a - C_{i,2}) + \ldots + g_{100}(C_a - C_{i,100})}{g_1 + g_2 + \ldots + g_{100}}$$

$$= C_a - (g_1 + g_2 + \ldots + g_{100})\, C_a/(g_1 + g_2 + \ldots + g_{100}) + (g_1 C_{i,1} + g_2 C_{i,2} + \ldots + g_{100} C_{i,100})/(g_1 + g_2 + \ldots + g_{100}). \tag{30c}$$

$$C_{i,g} = (g_1 C_{i,1} + g_2 C_{i,2} + \ldots + g_{100} C_{i,100})/(g_1 + g_2 + \ldots + g_{100}). \tag{31}$$

In other words, the C_i so calculated is the conductance weighted value, averaged over all the patches. I denote this $C_{i,g}$. Note that equation (30*b*) and the equations that follow assume that there is no lateral diffusion of CO_2 within the leaf between patches. The value of $C_{i,g}$, calculated this way, is appropriate for linking transpiration and assimilation rates of a leaf. On the other hand, for interpreting changes in A in terms of underlying mesophyll metabolism, a relation between A and C_i is needed. Consider the simplest such relation,

$$A = k(C_i - \Gamma), \tag{32}$$

where k is the 'carboxylation efficiency' and Γ is the CO_2 compensation point. Rearranging equation (32),

$$C_i = \Gamma + A/k, \tag{33a}$$

and applying equation (32) to individual patches,

$$C_i = \Gamma + [k_1(C_{i,1} - \Gamma) + k_2(C_{i,2} - \Gamma) + \ldots + k_{100}(C_{i,100} - \Gamma)]/100k \tag{33b}$$

$$= \Gamma - (k_1 + k_2 + \ldots + k_{100})\Gamma/100k + (k_1 C_{i,1} + k_2 C_{i,2} + \ldots + k_{100} C_{i,100})/100k. \tag{33c}$$

But, as may be seen from the case where all C_i of the various patches are equal, for equations (33*a*) and (33*b*) to be consistent,

$$k = (k_1 + k_2 + \ldots + k_{100})/100, \tag{34}$$

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B BIOLOGICAL SCIENCES

and so equation (33*c*) becomes

$$C_{\mathrm{i,k}} = \frac{k_1 C_{\mathrm{i},1} + k_2 C_{\mathrm{i},2} + \ldots + k_{100} C_{\mathrm{i},100}}{k_1 + k_2 + \ldots + k_{100}}. \tag{35}$$

Here the relevant C_i is the average weighted by carboxylation efficiency (i.e. by photosynthetic capacity), which I denote as $C_{\mathrm{i},k}$. In the special case where each of the patches has the same carboxylation efficiency, k, then $C_{\mathrm{i},k}$ becomes the spatially averaged valued of C_i. In contrast, where each of the patches has the same conductance, $C_{\mathrm{i},g}$ is the spatial average.

Equations (31) and (35) contrast in other ways. A patch with closed stomata, but with healthy mesophyll cells underneath at a concentration of Γ, contributes nothing to the C_i relevant for relating transpiration and assimilation, namely $C_{\mathrm{i},g}$. This measure is weighted towards those patches with wide open stomata. However, this patch reduces the effective value of $C_{\mathrm{i},k}$, that measure for C_i which is required for maintaining a fixed relation between A and the 'capacity' for photosynthesis, such as the amount of active Rubisco or electron transport capacity. A patch with open stomata, but containing no viable mesophyll chloroplasts, contributes nothing to $C_{\mathrm{i},k}$, because this measure is weighted by capacity. Nevertheless it increases the effective value of $C_{\mathrm{i},g}$.

An interesting question is what is the most appropriate weighting for C_i as it affects carbon isotope discrimination. This is the process by which the carbon assimilated by plants contains less $^{13}\mathrm{C}$, as a proportion of the total carbon, than occurs in $\mathrm{CO_2}$ in the atmosphere. It can be measured during gas exchange (Evans *et al.* 1986) and depends on $C_\mathrm{i}/C_\mathrm{a}$. Putting the question in a more practical way, will simultaneous measurements of discrimination and gas exchange enable us to detect 'apparent' changes in capacity, caused by $C_{\mathrm{i},g}$ exceeding $C_{\mathrm{i},k}$ because of stomatal heterogenity?

The simplest equation for discrimination, Δ, by leaves of $\mathrm{C_3}$ species is (Farquhar *et al.* 1982)

$$\Delta = a + (b-a)\, C_\mathrm{i}/C_\mathrm{a}, \tag{36}$$

from which

$$C_\mathrm{i} = (\Delta - a)\, C_\mathrm{a}/(b-a). \tag{37}$$

Now Δ for a whole leaf will be the assimilation rate weighted values of Δ for the individual patches, i.e.

$$\Delta = (A_1 \Delta_1 + A_2 \Delta_2 + \ldots + A_{100}\, \Delta_{100})/(A_1 + A_2 + \ldots + A_{100})$$

and, using equation (36) for the individual patches,

$$\begin{aligned}\Delta &= \frac{A_1[a + (b-a)\, C_{\mathrm{i},1}/C_\mathrm{a}] + \ldots + A_{100}\,[a + (b-a)\, C_{\mathrm{i},100}/C_\mathrm{a}]}{A_1 + A_2 + \ldots + A_{100}} \\ &= a + [(b-a)/c_\mathrm{a}]\frac{A_1 C_{\mathrm{i},1} + A_2 C_{\mathrm{i},2} + \ldots + A_{100} C_{\mathrm{i},100}}{A_1 + A_2 + \ldots + A_{100}}\end{aligned}$$

and substituting in equation (37),

$$C_{\mathrm{i},A} = (A_1 C_{\mathrm{i},1} + A_2 C_{\mathrm{i},2} + \ldots + A_{100} C_{\mathrm{i},100})/(A_1 + A_2 + \ldots + A_{100}). \tag{38}$$

The value of C_i obtained here is that weighted by local assimilation, which I denote as $C_{\mathrm{i},A}$.

Now, for one isolated patch, assimilation rate is a saturating function of conductance, so in general $C_{\mathrm{i},A}$ will be less than $C_{\mathrm{i},g}$, but not so low as $C_{\mathrm{i},k}$. Formally, $C_{\mathrm{i},k} < C_{\mathrm{i},A} < C_{\mathrm{i},g}$. Under stressed conditions where A is more nearly linearly dependent on g, the $C_{\mathrm{i},A}$ determined from on-line discrimination measurements are likely to be more similar to $C_{\mathrm{i},g}$ determined by gas exchange than to $C_{\mathrm{i},k}$, the value wanted for interpretation of possible effects on capacity.

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B BIOLOGICAL SCIENCES

Gross effects of heterogeneity have been demonstrated experimentally. Laisk (1983) showed that conventional gas exchange gave a changing relationship between A and $C_{i,g}$ in leaves of barley when they were excised. From observations of how the statistical distribution of stomatal aperture changes with mean conductance (Laisk *et al.* 1980), he was able to show that photosynthetic capacity had not changed. In terms of the present analysis, the relation between A and $C_{i,k}$ was unaffected. Terashima *et al.* (1988) showed that the apparent non-stomatal inhibition of photosynthesis by abscisic acid was an artefact of the same type.

There is an obvious need to build better models that include realistic levels of lateral diffusion, as the above analysis makes the oversimplification that there is no such diffusion. Nevertheless the above effects must occur to some extent and demand reassessment of those gas exchange experiments in which stress appears to have reduced both conductance and photosynthetic capacity. It also is an important caveat in the interpretation of the relation between 'on-line' carbon isotope discrimination, Δ, and $C_{i,g}$ (Evans *et al.* 1986): Δ will appear to be less than expected.

Conclusion

Models of photosynthesis can be useful aids to understanding (and for prediction), but are also potential hazards when the simplifications involved are forgotten. The treatment of C_i as a lumped parameter is an example of such a hazard because under certain conditions the value obtained by conventional gas exchange will exceed that required for modelling photosynthesis. Sometimes, however, Nature appears to be kinder. The treatment of absorbed irradiance may be such a case, for if the leaf tends to optimize its use of nitrogen, the equations of photosynthesis tend to become simpler, as shown in figure 1.

The work leading to figure 1 was done while the author held a Carnegie Fellowship and a Senior A.A.E.F. (Fulbright) Fellowship at the Carnegie Institution of Washington Plant Biology Department, Stanford in 1982, and the work on heterogeneity of CO_2 concentration was done while the author held a Bursary from the French Ministry of Research and Teaching at the Paris-Sud University in 1987. Discussions with Dr J. R. Evans and Professor I. R. Cowan at R.S.B.S. were appreciated.

References

Andrews, T. J. & Lorimer, G. H. 1987 Rubisco: structure, mechanisms and prospects for improvement. In *The biochemistry of plants* (ed. M. D. Hatch & N. K. Broadman), vol. 10, pp. 131–218. Orlando, Florida: Academic Press.

Badger, M. R. & Collatz, G. J. 1977 Studies on the kinetic mechanism of ribulose-1,5-bisphosphate carboxylase and oxygenase reactions, with particular reference to the effect of temperature on kinetic parameters. *Carnegie Instn Wash. Yb.* **76**, 355–361.

Berry, J. A., Osmond, C. B. & Lorimer, G. H. 1977 Fixation of $^{18}O_2$ during photorespiration. *Pl. Physiol.* **62**, 954–967.

Brooks, A. & Farquhar, G. D. 1985 Effect of temperature of the CO_2/O_2 specificity of ribulose-1,5-bisphosphate carboxylase/oxygenase and the rate of respiration in the light. Estimates from gas-exchange measurements on spinach. *Planta* **165**, 397–406.

Cowan, I. R. & Farquhar, G. D. 1977 Stomatal function in relation to leaf metabolism and environment. *Symp. Soc. exp. Biol.* **31**, 471–505.

Evans, J. R. 1983 Nitrogen and photosynthesis in the flag leaf of wheat (*Triticum aestivum* L.) *Pl. Physiol.* **72**, 297–302.

Evans, J. R. & Terashima, I. 1987 The effects of nitrogen on electron transport components and photosynthesis in spinach. *Aust. J. Pl. Physiol.* **14**, 59–68.

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B BIOLOGICAL SCIENCES

Evans, J. R., Sharkey, T. D., Berry, J. A. & Farquhar, G. D. 1986 Carbon isotope discrimination measured concurrently with gas exchange to investigate CO_2 diffusion in leaves of higher plants. *Aust. J. Pl. Physiol.* **13**, 281–292.

Farquhar, G. D. 1979 Models describing the kinetics of ribulose biphosphate carboxylase–oxygenase. *Archs Biochem. Biophys.* **193** (1), 456–468.

Farquhar, G. D. 1989 Models relating subcellular effects of temperature to whole plant responses. *Symp. Soc. exp. Biol.* **42**. (In the press.)

Farquhar, G. D. & Wong, S. C. 1984 An empirical model of stomatal conductance. *Aust. J. Pl. Physiol.* **11**, 191–210.

Farquhar, G. D., von Caemmerer, S. & Berry, J. A. 1980 A biochemical model of photosynthetic CO_2 assimilation in leaves of C_3 species. *Planta* **149**, 78–90.

Farquhar, G. D., O'Leary, M. H. & Berry, J. A. 1982 On the relationship between carbon isotope discrimination and the intercellular carbon dioxide concentration in leaves. *Aust. J. Pl. Physiol.* **9**, 121–137.

Farquhar, G. D. & von Caemmerer, S. 1982 Modelling of photosynthetic response to environmental conditions. In *Encyclopedia of plant physiology, new series* (ed. O. L. Lange, P. S. Nobel, C. B. Osmond & H. Ziegler), vol. 12*b*, pp. 549–587. Heidelberg: Springer-Verlag.

Field, C. 1983 Allocating leaf nitrogen for the maximisation of carbon gain: leaf age as a control on the allocation program. *Oecologia* **56**, 341–347.

Field, C. B. 1988 On the role of photosynthetic responses in constraining the habitat distribution of rainforest plants. *Aust. J. Pl. Physiol.* **15**, pp. 343–358.

Hall, A. 1979 A model of leaf photosynthesis and respiration for predicting carbon dioxide assimilation in different environments. *Oecologia* **143**, 299–316.

Hirose, T. & Werger, M. J. A. 1987 Nitrogen use efficiency in the instantaneous and daily photosynthesis of leaves in the canopy of a *Solidago altissima* stand. *Physiologia Pl.* **70**, 215–222.

Kirschbaum, M. U. F. 1987 A model of photosynthesis for isobilateral leaves incorporating biochemical constraints and the light gradient within the leaf. In *Progress in photosynthesis research* (ed. J. Biggens), vol. 4, pp. 261–264. Dordrecht: Martinus Nijhoff.

Laing, W. A., Ogren, W. & Hageman, R 1974 Regulation of soybean net photosynthetic CO_2 fixation by the interaction of CO_2, O_2 and ribulose-1,5-diphosphate carboxylase. *Pl. Physiol.* **54**, 678-685.

Laisk, A. 1977 Modelling of the closed Calvin cycle. In *Biophysikalische Analyse pflanzlicher Systeme* (ed. K. Unger), pp. 175–182. Jena: Fischer.

Laisk, A. 1983 Calculations of leaf photosynthetic parameters considering the statistical distribution of stomatal apertures. *J. exp. Bot.* **34**, 1627–1635.

Laisk, A., Oja, V. & Kull, K. 1980 Statistical distribution of stomatal apertures of *Vicia faba* and *Hordeum vulgare* and the *Spannungsphase* of stomatal opening. *J. exp. Bot.* **31**, 49–58.

Mitchell, P. 1976 Possible molecular mechanisms of the proton-motive function of cytochrome systems. *J. theor. Biol.* **34**, 1627–1635.

Oja, V. M. & Laisk, A. 1976 Adaptation of the photosynthesis apparatus to the light profile in the leaf. *Soviet Pl. Physiol.* **23**, 381–386.

Parkhurst, D. F., Wong, S. C., Farquhar, G. D. & Cowan, I. R. 1988 Gradients of intercellular CO_2 levels across the leaf mesophyll. *Pl. Physiol.* **86**, 1032–1037.

Peisker, M. 1974 A model describing the influence of oxygen of photosynthetic carboxylation. *Photosynthetica* **8**, 47–50.

Salvucci, M. E., Portis, A. R. & Ogren, W. L. 1985 A soluble chloroplast protein catalyzes activation of ribulose bisphosphate carboxylase/oxygenase *in vivo*. *Photosynth. Res.* **7**, 193–201.

Seemann, J. R. & Sharkey, T. D. 1986 Salinity and nitrogen effects on photosynthesis, ribulose-1,5-bisphosphate carboxylase and metabolite pool sizes in *Phaseolus vulgaris* L. *Pl. Physiol.* **82**, 555–560.

Terashima, I. & Inoue, Y. 1985 Vertical gradient in photosynthetic properties of spinach chloroplasts dependent on intra-leaf light environment. *Pl. Cell Physiol.* **26**, 781–785.

Terashima, I. & Saeki, T. 1985 A new model for leaf photosynthesis incorporating the gradients of light environment and of photosynthetic properties of chloroplasts within a leaf. *Ann. Bot.* **56**, 489–499.

Terashima, I., Wong, S. C., Osmond, C. B. & Farquhar, G. D. 1988 Characterisation of non-uniform photosynthesis induced by abscisic acid in leaves having different mesophyll anatomies. *Pl. Cell Physiol.* **29** (3), 385–394.

von Caemmerer, S. & Edmondson, D. L. 1986 The relationship between steady-state gas exchange, *in vivo* RuP_2 carboxylase activity and some carbon reduction cycle intermediates in *Raphanus sativus*. *Aust. J. Pl. Physiol.* **13**, 669–688.

von Caemmerer, S. & Farquhar, G. D. 1985 Kinetics and activation of Rubisco and some preliminary modelling of RuP_2 pool sizes. In *Proceedings of the 1983 Conference at Tallinn* (ed. J. Vill, G. Grishina & A. Laisk), pp. 46–58. Estonian Academy of Sciences: Tallinn.

Woo, K. C., Berry, J. A. & Turner, G. 1978 Release and refixation of ammonia during photorespiration. *Carnegie Instn Wash. Yb.* **77**, 240–245.

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B BIOLOGICAL SCIENCES