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Main title: **Photosynthetica**

Publisher: **Ústav experimentální botaniky AV ČR**

Published in: **1967-**

Periodical volume number: **18**

Periodical item date: **1984**

ISSN identifier: **0300-3604**

SICI identifier: **nezjištěn**

Pages: **(1d), 549, 550, 552, 554, 555, 556, 557, 558, 560, 561, 562, 563, 564, 565, 566, 568, 569, 570, 571, 572, 573, 574, 576, 578, 580, 582, 584, 586, 587, 588, 590, 591, 592, 593, 594, 595**

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Photosynthesis Model for C₃ Leaves Incorporating CO₂ Transport, Propagation of Radiation, and Biochemistry

1. Kinetics and their Parametrization*

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Abstract

The steady-state biochemical model of Farquhar *et al.* (1980) is presented in a streamlined form and combined with models of CO₂ transport and propagation across the leaf thickness. Internal CO₂ gradients and photochemical rates are thus determined kinetically rather than estimated in bulk average. The significant interactions of internal CO₂ depletion and carboxylation rate are therefore represented. All parameters are physiologically determined (none are free) and approximate those for soybean (*Glycine max* L.). The model is designed to investigate evolved adaptations and agricultural potentials of leaf performance such as estimating penalties for predominantly abaxial location of stomatal conductance, identifying limiting factors, and predicting performance of mutants with altered content of chlorophyll and/or enzymes, none of which investigations are possible with separate biochemical or transport models.

Leaf photosynthesis models of increasing sophistication in treating carbon-fixation biochemistry, CO₂ transport, and irradiance gradient across the leaf thickness have been of use in ecophysiology and agronomy. In biochemistry and photochemistry *per se*, the Z-scheme (Hill and Bendall 1960) provides an outstanding synthesis and a comprehensive guide in developing detailed hypotheses for experimental tests. Models of whole-leaf phenomena for analyzing crop performance or ecological adaptations involve even more phenomena and more uncertainties in parameters. Still, modelling concepts such as resistance analysis (Gaastra 1959) have become tools of agronomists, ecologists, and physiologists.

Models would be far more useful if (1) they were more reliable quantitatively and inclusive of *interacting* kinetics of CO₂ transport, CO₂ fixation, and propagation of photosynthetically active radiation (PhAR) that are quite important in the quantitative performance of a leaf, and

* Received 2 July 1983; accepted 16 April 1984.

Abbreviations: C, C(x) — CO₂ concentration at depth x in leaf; C_a — ambient CO₂ concentration outside leaf; CF — carbon fixation; Chl — chlorophyll; FCB — Farquhar, Caemmerer, and Berry (1980); g_s — stomatal conductance; I or I_{ad}, I_{ab} — adaxial, abaxial irradiance; j, j(x) — electron transport rate [mole⁻ mol⁻¹(Chl) s⁻¹]; O — ambient O₂ concentration; OR — oxygen reduction; P_G, P_N — gross, net photosynthetic rate per leaf area; PGA — phosphoglyceric acid; PhAR — photosynthetically active radiation; r — leaf reflectivity; r_a — boundary layer resistance to CO₂ transport; r_{as} = r_a + r_s; R_D — dark respiration rate per leaf area; r_m — mesophyll resistance to CO₂ transport; r_s — stomatal resistance; RuBP — ribulose 1,5-bisphosphate; RuBPCO — ribulose bisphosphate carboxylase oxygenase; t — leaf transmissivity; x — depth in leaf, from top; Φ — ratio of oxygenation rate to carboxylation rate. All other parameters are defined in the Section, "Estimating Parameter Values and Solving the Full Equation Set".

(2) they were specified in fully physiological, unambiguously measurable parameters, *e.g.*, biochemical contents and not phenomenological resistances that are not independent of each other. Models so upgraded could greatly enhance the information extractable from experiments; they could also help to design experimental programs to get deeper and more definitive views on how photosynthetic performance is limited, both in the wild and in agriculture. [For example, one can inquire about optimal chlorophyll (Chl) content, optimal stomatal conductance (g_s) and its adaxial/abaxial distribution, *etc.*] The model developed here is a step toward these goals. In Section 2 of the following paper, the model is tested for realism of its predicted detailed responses of gross photosynthetic rate (P_G) — and of intermediate functions such as stomatal resistance (r_s) — to irradiance and to CO_2 and O_2 concentrations. Then the model is applied to diverse ecological and agricultural problems.

No physiological (nonphenomenological) models currently treat simultaneously all three principal kinetic aspects — biochemistry, CO_2 transport, radiation transport — even though important couplings among the three are identifiable. Models that are principally biochemical (*e.g.*, Farquhar *et al.* 1980) have synthesized diverse biochemical data well and have some predictive capabilities, but they are partly indeterminate. They cannot evaluate the internal CO_2 concentration, which is drawn down across the mesophyll transport resistances (r_m) during rapid photosynthesis. By using fixed bulk average CO_2 concentrations, they distort the curves relating P_G to irradiance (I), as also the estimated PhAR-use efficiency with its ecological implications. The ecologically and agriculturally optimal distributions of g_s (adaxial/abaxial) and other traits cannot be estimated. Models treating CO_2 transport only (such as Parkhurst 1977) or adding biochemistry and I -dependence only phenomenologically do reveal some important adaptive designs in stomatal and mesophyll three-dimensional geometric structure. However, they cannot address I response, adaptations to I history, or relative performance importance of enzyme and Chl contents. Virtually all models ignore the usually strong gradient of I across the leaf thickness. This gradient strongly shapes the I response and overall PhAR-use efficiency (see Fig. 1 in Gutschick 1984). No quantitative estimate has been published for the performance reduction attached to CO_2 and PhAR entering from opposite sides of the leaf, contrary to efficiency considerations. Even Lařsk's (1969) model of PhAR gradients in the leaf ignored the top-to-bottom CO_2 gradient and also used a crude estimate of the PhAR gradient that ignored scattering phenomena. One may ask if the bottom of the leaf really contributes to carbon assimilation.

Coupled biochemistry and CO_2 transport are routinely treated in highly phenomenological resistance models introduced by Gaastra (1959) and refined by many researchers (*cf.* Lommen *et al.* 1971, Jones and Slatyer 1972). Arbitrary assumptions of CO_2 concentration at the assimilating site (zero, especially) compromise the value of these models. With these models, limitations on leaf performance by physiological or quasiphysiological traits (examples respectively are r_s and "excitation resistance") are analyzed to compare cultivars (Treharne 1972) or to follow ontogenetic patterns (řesták *et al.* 1975, Tichá *et al.* 1980) but with many pitfalls (Jarvis 1971) or unresolvable ambiguities (Prioul *et al.* 1975). This ambiguity and the added problem of poor definability of lumped resistances in terms of physiological traits frustrates agronomic utility. [The simple correlation of r_m to carbonic anhydrase enzyme content (Prioul *et al.* 1975) is an exception, but anhydrase content is not agronomically limiting.] For example, qualitative arguments can be advanced for increasing yield by judicious reduction of Chl content or alterations of enzyme contents of leaves (see Gutschick 1984), yet the consequent changes in resistances and hence final leaf performance cannot be predicted; a physiological model is required. Agronomists, justifiably wary of pitfalls of modelling, proceed without a coherent model for a guide, using statistical correlations of one or a few parameters with P_G (Treharne 1972, Wallace *et al.* 1972). Results of experimental analyses are rarely definitive, and correlations of leaf traits and even of P_G to final yield are even more discouraging (Elmore 1980, Gifford and Evans 1981; but see Zelitch 1982). Models to relate leaf traits and performance — distributed differentially

bottom (but not lateral) gradients in all these biochemical concentrations; however, I generally assume uniformity and I find that gradients in general make few and narrow differences in performance. As a first approximation, I have dropped FCB's dark respiration term, R_D , except when calculating CO_2 compensation concentration. R_D is not readily localized in depth as are carbon fixation and oxygen reduction. Also, if it is nearly constant, independent of I as FCB assume, it may be added later as almost a simple shift of all curves. Alternatively, it may be negligible above modest I , being suppressed by PhAR itself (Lommen *et al.* 1971, Epel 1973); this is contradicted by the review of Graham (1980), and this disagreement argues for leaving R_D details for later refinement. Lastly, I add calculations of intermediate variables of PhAR-use efficiency, carbon fixation and oxygen reduction efficiencies, in order to pinpoint "leverage" points in functional design.

Further biochemical detail of the FCB model deserves discussion. The carbon fixation (CF) cycle is represented as RuBP carboxylation (with binding, reaction steps) and reduction of phosphoglycerate (PGA) product by photogenerated NADPH. The first step has Michaelis-Menten kinetics with a concise accounting for limitations by pool sizes (their original parameters R_p , N_t) and by the chain of intermediate electron transfer reactions (their parameter m). The photorespiratory or oxygen reduction (OR) cycle is represented as RuBP oxygenation to PGA plus phosphoglycolate, further oxidation of the latter to glycine with CO_2 liberation, stoichiometric reduction of glycine (less the recycled amino group) into PGA, and reduction of pooled PGA by photogenerated NADPH. The stoichiometric hypothesis, leaving no net glycine synthesis, is an inflexibility and shortcoming discussed later.

The FCB model as I modify it here is not definitive even within the realm of major environmental factors. I have dropped all the information in the original model on temperature dependence of processes, though such information exists for most of the CO_2 transport dynamics as well. My interest in these two papers lies in effects with origins outside of the temperature dependence of kinetics, and the addition of large numbers of Arrhenius-like parameters is then more of a burden than an aid. In the future, I do hope to address some temperature-dependent phenomena. Second, I retain simplified photophysical kinetics. The spectral composition of incident radiation is ignored, though in reality this affects absorption rate, carotenoid-to-Chl photoexcitation transfer efficiency, and ability of photosystems 1 and 2 to cooperate *via* a "spillover" (Butler 1978, Chow *et al.* 1981). A partial remedy, calculating spectral composition by depth in the leaf or canopy, is simple, because to a very good approximation all spectral components propagate and are absorbed independently. There is only minor interconversion by fluorescence, at least in unstressed systems (Goedheer 1972). The calculation of spillover adequacy as a function of spectral composition and environmental conditions is more difficult and has not been done in a model; however, variations are not strong generally. The net effects of spectral composition variability with depth in the leaf or a canopy, such as adaptive developmental variation of the Chl-to-carotenoid ratio, are probably modest* and are not addressed here.

(1) Carbon Assimilation Rate

The external environmental conditions are defined by O = oxygen concentration [mol m^{-3}], C = carbon dioxide concentration [mol m^{-3}], and I = irradiance on leaf normal surface [$\text{mol m}^{-2} \text{s}^{-1}$]. For present purposes (see above), I assume a constant temperature of 25°C . P_G per volume of leaf tissue [$\text{mol CO}_2 \text{ m}^{-3} \text{s}^{-1}$] is expressible as

$$A_v = A_c q_c, \quad (1)$$

* The variation in excitation transfer efficiency is probably restricted to the range 0.5 (only auxiliary pigment absorbing) to 0.59 ("white light").

rate is a direct function of the PhAR absorption rate at depth x in the leaf,

$$j = j(x) = 0.5a(x) \eta_t. \quad (9)$$

Here

$a(x)$ = local rate of photon absorption per Chl unit $[\text{mol}(\text{photon}) \text{mol}^{-1}(\text{Chl}) \cdot \text{s}^{-1}]$, i.e.,

$$= b(x)/\varrho_c(x) = (\text{local volume rate of photon absorption } [\text{mol m}^{-3} \text{s}^{-1}]) / (\text{Chl concentration } [\text{mol Chl m}^{-3}]), \quad (10)$$

and η_t = quantum efficiency of transfer of photoexcitation from all pigments to Chl reaction centers; approximate value 0.5–0.6. The coefficient 0.5 in Eq. (9) reflects the stoichiometry of two photons, one for each photosystem 1 and 2, per electron transported noncyclically. In principle, $b(x)$ is directly related to ϱ_c and a cross-section per pigment (expressed as per Chl), but this is prone to some problems; see Section C of the PhAR-propagation model.

Electron transport is limited to a maximal rate, $j \leq j_{\max}$, as discussed by FCB. They used a simple, sharp cutoff or a parametrically smoothed function to impose this limitation. The RuBP-pool-limited rate follows the development by FCB (their Appendix 2) and is very simply

$$v_{cP} = k'_c R_p, \quad (11)$$

where k'_c is as in Eq. (3) and R_p = total (free plus bound) RuBP concentration $[\text{mol RuBP mol}^{-1} \cdot (\text{Chl})]$. Lastly, the NADP^+ -reduction-limited rate is

$$v_{cH} = m/(2 + 1.5\Phi), \quad (12)$$

based on a stoichiometry of $(2 + 1.5\Phi)$ mol of PGA cycled per mol of RuBP that gets carboxylated. Here, m is an effective rate of NADP^+ reduction composed from many linked reactions. FCB estimated m as equal to at least $2k_c E_t$, (unprimed k_c , note). This couples photoreductant generation strongly but plausibly to CF and OR cycles; see the discussion by FCB after their Eq. (25).

The carboxylation capacity of RuBPCO at ambient C and O levels, k'_c , is related to its maximal velocity, k_c , by well-established Michaelis-Menten kinetics (see Farquhar 1979 for review):

$$k'_c = \frac{k_c}{1 + \frac{K_c}{C} \left(1 + \frac{O}{K_o}\right)}, \quad (13)$$

where K_c, K_o = Michaelis binding constants for CO_2 , O_2 , respectively $[\text{mol m}^{-3}]$, and one assumes effective activation by CO_2 , Mg^{2+} , etc. Likewise,

$$k'_c = \frac{k_o}{1 + \frac{K_o}{O} \left(1 + \frac{C}{K_c}\right)}. \quad (14)$$

The partition ratio between oxygenation and carboxylation, Φ , as introduced in Eq. (8), is now expressible in final variables and parameters as

$$\Phi = \frac{k'_o}{k'_c} = \frac{k_o}{k_c} \frac{O/K_o}{C/K_c}. \quad (15)$$

(B) Electron Transport Rate and Relation to Pigment Absorptions

In Eq. (9) and below it, the electron generation rate was related to the volume rate of photon absorption, $b(x)$. This rate of absorption by all pigments combined depends on Chl volume concentration, the spectral photon fluence, and pigment cross-sections as

$$b(x) = \varrho_c(x) \int d\lambda I(\lambda, x) \sigma_c(\lambda) + \varrho_a(x) \int d\lambda I(\lambda, x) \sigma_a(\lambda), \quad (16)$$

where $I(\lambda, x)$ = photon fluence rate per unit wavelength interval at depth x in leaf [$\text{mol m}^{-2} \text{s}^{-1} \cdot \text{m}^{-1}$], $\varrho_c(x)$, $\varrho_a(x)$ = Chl or auxiliary pigment volume concentrations [mol m^{-3}], and $\sigma_c(x)$, $\sigma_a(x)$ = Chl or auxiliary pigment absorption cross sections at wavelength λ [$\text{m}^2 \text{mol}^{-1}$]. For narrow spectral bands where σ and I are approximately constant, we have

$$b(x) = [\varrho_c(x) \sigma_c(\lambda) + \varrho_a(x) \sigma_a(\lambda)] I(\lambda, x) \quad (17)$$

$$\equiv kI(\lambda, x). \quad (18)$$

Here, k is the linear attenuation (Beer's law) coefficient at wavelength λ [m^{-1}]. It is the quantity that is readily measured for leaves (in a narrow waveband or averaged over the PhAR band), along with $\varrho_c(x)$; see the light propagation model. I use this as a primary parameter and not σ_c , σ_a and ϱ_a , ϱ_c , all of which show some complex features *in vivo* (Katz and Norris 1973) and give little advantage in modelling.

The value of η_t must still be estimated. The total rate of photoexcitation transfer to reaction centers is similarly expressible,

$$b(x) \eta_t = \varrho_c(x) \eta_c \int d\lambda I(\lambda, x) \sigma_c(\lambda) + \varrho_a(x) \eta_a \int d\lambda I(\lambda, x) \sigma_a(\lambda), \quad (19)$$

where η_c , η_a = quantum efficiencies of excitation transfers, respectively Chl \rightarrow reaction trap, auxiliary pigment \rightarrow Chl \rightarrow reaction trap. We can develop Eq. (19) to an analog of Eq. (17) and use estimates of η_c , η_a (Goedheer 1969, 1972). However, this estimate of η_t is very sensitive to the ratio of green: (red + blue) radiation at the location of interest. This latter ratio is a strong function of position in the leaf, and it is difficult to choose a meaningful average without resolving wavebands explicitly. It is more fruitful to estimate η_t from the quantum yield of photosynthesis at low I (see below), and I use only such an estimate in the model. [The dependence of η_t on the $\varrho_c : \varrho_a$ ratio would be of interest in considering mutants or variants. However, the Chl-deficient mutants of primary interest in this work (Gutschick 1984) have virtually the same ratio as do the wild type plants — *e.g.*, in soybean (Keck *et al.* 1970).]

(C) Definition of Efficiencies of Electron Use (Photon Use)

Efficiencies of using photons for carbon fixation, oxygen reduction, and P_G can be defined, and they give insight into photosynthetic performance limitations as affected by leaf geometry and biochemical composition. The saturated rate of electron consumption per Chl, *i.e.*, the rate never exceeded but only approached, is

$$j_s = 4E_t(k'_c + k'_o).$$

It is a function of depth x in the leaf, because C is a function of depth, hence k'_c , k'_o also. Thus, the degree of photochemical saturation is a useful intermediate variable,

$$S(x) = j(x)/j_s(x), \quad (20)$$

with limits zero in the dark and exceeding unity at the leaf top at high I .

The efficiency of electron flow to carboxylation relative to its minimum, $4v_c$, is simply

$$\eta_{cF}(x) = 4v_c(x)/j(x), \quad (21)$$

where v_c is the actual carboxylation rate at depth x determined by C , O , I , and biochemical parameters. Similarly, the efficiency of electron flow to oxygenation is

$$\eta_{OR}(x) = 4v_o(x)/j(x), \quad (22)$$

and the efficiency of electron flow for P_G is

$$\eta_{net} = 4(v_c - 0.5v_o)/j. \quad (23)$$

At low I , these attain the following limits, independent of x .

$$\eta_{cF} \rightarrow 1/(1 + \Phi) \quad (24)$$

$$\eta_{OR} \rightarrow \Phi/(1 + \Phi)$$

$$\eta_{net} \rightarrow (1 - 0.5\Phi)/(1 + \Phi)$$

$$\Phi \rightarrow \frac{k_o}{k_c} \frac{O/K_o}{C_f/K_c},$$

where C_f is the ambient CO_2 concentration in the substomatal space.

CARBON DIOXIDE TRANSPORT MODEL

CO_2 is transported sequentially through air spaces, cytosol (and cell wall), and chloroplast. The largest resistance lies in the first step, covering the greatest physical distance (Jarvis 1971, Raven and Glidewell 1981). Transport is almost exclusively by isothermal diffusion, with negligible effects of convection or mass flow. In air-space diffusion, CO_2 concentration is a function of position within the leaf, in three dimensions; denote it as $C(r)$. A local diffusion coefficient is defined as $D(r)$. A very good approximation for steady-state diffusion is then

$$\nabla(D \nabla C) - A_v = 0, \quad (25)$$

where A_v is the reaction sink term of Eq. (1) (minus the respiratory source term, if present).

Because the air spaces are tortuously connected, C is defined only in a complicated subspace that excludes the space occupied by cells. In the latter space, one can define an equivalent gas-phase C as that in equilibrium with the dissolved CO_2 . I average out the structure to a continuous medium, wherein the major variation in C is in one dimension x , that normal to the leaf surface. [Within the continuous-medium picture, there still are significant variations in between stomatal entry sites (Parkhurst 1977); these variations have additional implications for leaf functional design that I do not address here.]

The diffusion equation becomes

$$\frac{d}{dx} \left(D(x) \frac{dC(x)}{dx} \right) - A_v(x) = 0 \quad (26)$$

and simplifies when the diffusion coefficient is x -independent to

$$D \frac{d^2 C(x)}{dx^2} - A_v(x) = 0. \quad (27)$$

I use both constant and x -varying diffusivity in the model calculations. Most realistically, D increases toward the bottom of the leaf where cell packings are looser and large substomatal chambers occur.

In my model, the air-space CO₂ concentrations $C(x)$ are used as carboxylation-site concentrations. This is not fully accurate because concentrations drop across additional liquid-phase resistances. Estimates of the latter for normal mesophytes lie in the range 0.3–1.5 s m⁻¹ (Jarvis 1971, Sinclair *et al.* 1977), implying that at peak photosynthetic rates per leaf (not mesophyll cell) area, say, 20 μmol m⁻² s⁻¹, there is an additional drop of the order of 1 mmol m⁻³ or 2.5 Pa. This is significant quantitatively, but I still have accounted for the major CO₂ drop (to as little as 1/2 atmospheric CO₂ content, see Gutschick 1984) and for its selective occurrence near the leaf top that is significant for leaf design (see discussion of cost of "hypostomaticity" in leaves, Gutschick 1984). This accounting is a significant addition to the FCB model, which assumes that C is everywhere equal to its value in substomatal chambers. While the more sophisticated resistance models account for the CO₂ gradient in x and resolve liquid-phase transport (review by Cooke and Rand 1980), they are inherently phenomenological and much cruder in the biochemistry and always ignore PhAR-propagation effects. I propose inclusion of liquid-phase resistances for future modelling; this will allow investigation and prediction of leaf internal morphology effects on performance such as Holmgren (1968) observed. Such inclusion will require firmer information on resistance magnitudes than is available now from experiments (Jarvis 1971) or models (Sinclair *et al.* 1977). (The models are useful for single cells, but averaging over highly varied leaf structure between mesophyll, parenchyma, *etc.* is difficult to formulate.)

(A) Boundary Conditions and Stomatal Resistance Functions

For hypostomatous leaves, there can be no flux across the top of the leaf:

$$J(x) = -D \frac{dC}{dx} [\text{mol m}^{-2} \text{s}^{-1}] \quad (28)$$

$$\rightarrow 0 \quad \text{at} \quad x = 0.$$

At the bottom of the leaf in the substomatal chamber ($x = L$, the leaf thickness), there is an (area-averaged) flux which equals P_G of the leaf and which determines the drop between outside air CO₂ concentration C_a and substomatal concentration $C(L)$:

$$J(L) = -DC'(L) = (C(L) - C_a)/r_{as}. \quad (29)$$

Of course, $J(L)$ is negative because the flux is up, toward decreasing x . Here, r_{as} is r_s plus the boundary layer resistance r_a [s m⁻¹]. Thus we have a two-point boundary value problem to solve for $C(x)$, where the form of $A_p(x)$ cannot be specified analytically. The entire equation is solved numerically as described below.

The resistance varies over a large range, being sensitive to numerous environmental variables (Burrows and Milthorpe 1976, Farquhar and Sharkey 1982). It is a function in particular of substomatal CO₂ concentration $C(L)$, thus yielding a further consistency condition. This sensitivity may be the major determinant of the apparent dependence of r_s on I (Scarth 1932, Meidner and Mansfield 1965, but see Farquhar and Sharkey 1982). The ability of r_s on the leaf bottom to respond with broad similarity to both adaxial I and poorly-transmitted abaxial I (Raschke *et al.* 1978) is an additional argument for this causal connection.

My model requires an explicit form for r_s as a function of $C(L)$. Very complex models have been derived (*cf.* Penning de Vries 1972). Because even these show only semi-quantitative agreement with experiment, I use the Takakura *et al.* (1975) simplification of the Penning de Vries

(1972) model. Control of r_s is by a ramp function,

$$\begin{aligned} r_{as} &= r_{\min}, \quad \text{if } C(L) < C_{\min} \\ r_{as} &= r_{\max}, \quad \text{if } C(L) > C_{\max} \\ r_{as} &= r_{\min} + \frac{(r_{\max} - r_{\min})}{(C_{\max} - C_{\min})} (C_{\max} - C), \quad \text{if } C(L) \text{ is inbetween.} \end{aligned} \quad (30)$$

This model has four parameters, r_{\min} , r_{\max} , C_{\min} , C_{\max} , which have been extracted by Takakura *et al.* (1975) for *Phaseolus vulgaris*, and surely resemble those for *Glycine max*, my target species. Basically, $C(L)$ tends to be entrained strongly between 8.8 and 9.2 mmol m⁻³ (22 and 23 Pa), much as FCB assumed. (For evidence against such simplicity, see Ramos and Hall 1982 and the discussion in Gutschick 1984 of consequent model weaknesses.)

For any given species and cultivar of plant, the formulations of r_{as} as dependent on I or on $C(L)$ are largely equivalent or interconvertible. The difference is of some importance for predicting performance of mutants. I have modelled the performance of Chl-deficient mutants assuming that r_{as} depends upon $C(L)$ exactly as in the wild type (Gutschick 1984). A contrary assumption of dependence on I directly might imply that mutants require significantly higher I than the wild type to achieve the same r_{as} , if Chl content of the mutants' guard cells drops to the same relative degree as in mesophyll cells. Unfortunately, no measurements of either guard-cell Chl content or the I -dependence of r_s exist for the mutants.

For amphistomatous leaves, there are CO₂ fluxes into both abaxial and adaxial surfaces:

$$J(0) = -DC'(0) > 0. \quad (31)$$

This yields a second consistency requirement between substomatal concentration and flux, this time for the adaxial surface ($C(0)$ and $J(0)$), analogous to Eq. (29) for the abaxial surface. The mathematical problem remains a two-point boundary value problem, while the efficient solution method changes (see below). If one assumes control of r_{as}^{ad} and r_{as}^{ab} independently by $C(0)$ and $C(L)$ respectively, one now has eight parameters. The simplifying assumption I use is that C_{\min} and C_{\max} values are the same for top and bottom, while minimum and maximum r_{as} values are simply proportional, the values for the top being about four times larger than those for the bottom.

PhAR PROPAGATION MODEL

PhAR propagation inside a leaf is complicated because the leaf medium is strongly scattering, each scattering event is anisotropic, and the structure of the leaf itself is anisotropic (*e.g.*, denser and less strongly scattering at the top). The leaf optical phenomena cannot be specified in detail with a few parameters. Detailed models generally involve assuming an explicit geometry for a whole leaf section, as in the pioneering work of Willstätter and Stoll (1918). For our purposes, one needs a simple representation that accounts for gross properties of net reflection and transmission and of the approximate pattern of I with depth x . One such model is that of Kubelka and Munk (1931) which ignores lateral variations and assigns local (isotropic) scattering and absorption coefficients. [Within such assumptions, an exact solution is possible, such as Gutschick and Wiegel (1984) used for a canopy, but it is generally not significantly different, and thus it is not worth the computational effort in a model making small approximations in all other phenomena.] The Kubelka-Munk formulation is the only simple way to predict PhAR interception and ultimately photosynthesis for arbitrarily varied Chl content and leaf thickness.

ESTIMATING PARAMETER VALUES AND SOLVING THE FULL EQUATION SET

(A) Biochemical and Morphological Parameters

(1) L = leaf thickness: 0.2 mm is a representative value appropriate for expanded soybean leaves grown in full sunlight (Jarvis and Slatyer 1970; my own occasional measurements confirm this).

(2) q_c = Chl volume concentration: one can derive the average concentration from reported areal concentrations divided by L . Hesketh *et al.* (1981) reported areal concentrations for soybean cultivars clustered fairly closely about $0.6 \text{ g m}^{-2} \approx 0.66 \text{ mmol m}^{-2}$. Thus,

$$q_c \approx 3.3 \text{ mol m}^{-3}.$$

The distribution of Chl by depth is far from uniform. A profile of $q_c(x)$ can be estimated from soybean leaf sections (Breece and Holmes 1971), and the effect of the profile on photosynthetic performance can be modelled (Gutschick 1984).

(3) E_t = RuBPCO octamer concentration [$\text{mol RuBPCO mol}^{-1}(\text{Chl})$]: Hesketh *et al.* (1981) reported areal concentrations of total soluble protein as clustered about 7 g m^{-2} for soybean cultivars. I assume that 50% by mass is RuBPCO, as typical for strong photosynthetic performers such as soybean (Ku *et al.* 1979). This converts to 6 kg RuBPCO per kg Chl, as Farquhar *et al.* used in their model as a baseline value. Using a gram molecular mass of 550 000 for the octamer (Jensen and Bahr 1977), one estimates

$$E_t = 0.01 \text{ mol RuBPCO mol}^{-1}(\text{Chl}).$$

(This differs from the FCB definition of E_t , which is monomer sites per gram Chl.)

(4) k_c = maximal carboxylation velocity of RuBPCO: the brief survey by Farquhar *et al.* (1980) for their model yielded the most probable value at 25 °C of

$$k_c = 20 \text{ mol CO}_2 \text{ mol}^{-1}(\text{RuBPCO}) \text{ s}^{-1}$$

in the normal activation state *in vivo*. The assay and incubation conditions most relevant to activity *in vivo* are still being refined (Mächler and Nösberger 1980); k_c values at least as large as assumed here are expected, and indeed are necessary to explain the observed rates of photosynthesis (see Gutschick 1984).

(5) k_o = maximal oxygenation velocity of RuBPCO: the ratio of oxygenase to carboxylase activities is a favored measurement; the FCB model uses $k_o/k_c = 0.21$ at 25 °C, implying

$$k_o = 4.2 \text{ mol O}_2 \text{ mol}^{-1}(\text{RuBPCO}) \text{ s}^{-1}.$$

(6, 7) K_c, K_o = Michaelis constants for CO_2, O_2 substrate-dependences of reaction velocities: again, the survey for the FCB model yields, as gas-phase concentration equivalents at 25 °C

$$K_c = 0.0184 \text{ mol m}^{-3} \text{ (or 46 Pa in air at 25 °C)}$$

$$K_o = 13.2 \text{ mol m}^{-3} \text{ (or 33\% in air at 25 °C)}$$

(8) j_{\max} = maximal electron transport rate: FCB refer to measurements on barley by Nolan and Smillie (1976). Converting the latter data directly, I obtain for 25 °C the value

$$j_{\max} = 0.253 \text{ mol e}^- \text{ mol}^{-1}(\text{Chl}) \text{ s}^{-1}.$$

This is a high rate which never limits photosynthesis in my calculations, and thus I have dropped consideration of it hereafter. FCB and also Farquhar and Caemmerer (1981) argue that j_{\max} -limitation of assimilation can occur at high I and CO₂ levels. Measured performance of *Phaseolus vulgaris* cited in the latter study supports their contention. One good indication is a breakpoint in photosynthetic rate *versus* intercellular CO₂ concentration, with reduced slope above the breakpoint. Growth conditions certainly affect the relative import of limiting factors and complicate the arguments. I cite (Gutschick 1984) some studies where there is no consistent evidence of breakpoint behavior, and I leave the question of j_{\max} -limitation for future experimental resolution.

(9) η_t = quantum efficiency of photoexcitation transfer to reaction centers: an initial estimate of 0.59 was developed above. A more directly experimental determination relates η_t to the initial quantum yield per absorbed photon at low I , $dP_G/dI \equiv Q'$. The latter is the product of the number of electrons generated per photon, $0.5\eta_t$, and CO₂ fixed per electron transported, $0.25(1 - 0.5\Phi)/(1 + \Phi)$, according to the discussion near Eq. (24). Ehleringer and Björkman (1977) measured this quantum yield for a number of C₃ species, finding an average value of $0.0524 \text{ mol CO}_2 \text{ mol}^{-1}(\text{photon})$ at 30 °C and 32.5 Pa external CO₂ concentration. I use their Fig. 2 data to extract a value of 0.047 in these same units for $C_a = 23 \text{ Pa}$. I further correct this to 0.505 at 30 °C, using their Fig. 3 data which indicates a rise in Q of 5–10% for this decrease in temperature. Then, using the values of k_c , k_o , K_c , and K_o noted above, I derive $\Phi = 0.267$ for this same temperature and C_a level. Thus,

$$Q_{25^\circ\text{C}} = \frac{\eta_t (1 - 0.5\Phi)}{8 (1 + \Phi)} = 0.0505 \quad (39)$$

$$\approx 0.0855\eta_t$$

and this implies

$$\eta_t = 0.59$$

as estimated previously.

(10) R_p = RuBP pool size: again I follow the FCB model, setting R_p to $300 \text{ mmol kg}^{-1}(\text{Chl})$ or

$$R_p = 0.273 \text{ mol RuBP mol}^{-1}(\text{Chl}).$$

This value was derived from an alga, there being no equivalent measurement for soybeans or related higher plants.

(11) m = maximal rate of NADP⁺ reduction of PGA: Farquhar *et al.* (1980) derived an estimate of $436 \text{ mmol PGA kg}^{-1}(\text{Chl}) \text{ s}^{-1}$, which converts to

$$m = 0.40 \text{ mol PGA mol}^{-1}(\text{Chl}) \text{ s}^{-1}.$$

(12) Other potentially useful parameters include the auxiliary pigment: Chl molar ratio and specifications of top-to-bottom gradients in q_c , E_t , R_p , and m (also D of the CO₂ transport model). I have made preliminary estimates in applying the model (Gutschick 1984).

(B) CO₂ Transport Parameters

(1) D = diffusion coefficient: this is difficult to derive from leaf photosynthesis measurements unobscured by dubious assumptions about chloroplast CO₂ concentrations or liquid-phase resistances (Jarvis 1971). A simple estimation from diffusion-path geometry is that D equals the free-air value (about $7 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$) reduced by the fractional cross-sectional area open to air

(about $1/5$ in the mesophyll) and by a tortuosity factor which is the ratio of the shortest path to the average path in air channels between any two points (about $1/2$). Thus,

$$D \approx 7 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}.$$

Parkhurst (1977) used D estimates in a broad range about this value. A check is provided by converting experimental interpretations of effective mesophyll diffusion resistances, r_m (Jarvis 1971),

$$r_m \approx L/D \approx 150 \text{ to } 300 \text{ s m}^{-1}$$

to D values. Using $L = 0.2 \text{ mm}$, one obtains D in the range $7 \text{ to } 15 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$.

(2) $r_{as} = r_a + r_s$: first, I assume that r_a is minimal, of the order of 50 s m^{-1} as appropriate to moderately good air circulation at the leaf, because my focus is on internal physiological limitations rather than whole-canopy effects. For r_s I use as a minimal value

$$r_{s,\min} \approx 150 \text{ s m}^{-1} \rightarrow r_{as,\min} \approx 200 \text{ s m}^{-1}.$$

Such values are observed for soybeans and allied C_3 species (Takakura *et al.* 1975, Hesketh *et al.* 1981).

For r_s controlled by substomatal CO_2 concentration, I estimate the three additional parameters as

$$r_{as,\max} \rightarrow r_{\max} \approx 1000 \text{ s m}^{-1}$$

$$C_{\min} \approx 8.8 \text{ mmol m}^{-3}$$

$$C_{\max} \approx 9.2 \text{ mmol m}^{-3}.$$

The last two parameters have been discussed above. My choice of r_{\max} as 5-fold higher than r_{\min} matches data on *Phaseolus vulgaris* by Takakura *et al.* (1975), from which C_{\min} and C_{\max} were taken. This choice does not apply at very low I where r_{as} rises even higher in all species (Pospíšilová and Solárová 1980). Farquhar and Sharkey (1982) review additional semiquantitative information.

For amphistomatous leaves, I must specify in addition the adaxial r_{\min} and r_{\max} values. For proper comparison to hypostomatous models, I set the total conductance

$$1/r_{\min} = 1/r_{\min,ad} + 1/r_{\min,ab}$$

to the value of $1/r_{\min,ab}$ alone of hypostomatous leaves. Then I assume a ratio, typically 4 : 1 between adaxial and abaxial values of both r_{\min} and r_{\max} .

(C) Leaf Optical Parameters

(1) α = linear attenuation coefficient due to scattering: this parameter is estimated simply (Breece and Holmes 1971) from gross leaf transmittance and reflectance at non-absorbed infrared wavelengths, where

$$t \rightarrow 1/(1 + \alpha L)$$

$$r \rightarrow \alpha L/(1 + \alpha L).$$

As both t and r tend to 0.5 here, this yields

$$\alpha \approx 1/L = 5000 \text{ m}^{-1}.$$

Fukshansky's (1981) more sophisticated analyses support a slightly lower value.

(2) k = linear attenuation coefficient due to pigment absorptions: this is related in principle to q_c and the pigment absorption cross sections. The values of the latter are less certain *in vivo* than *in vitro* (Katz and Norris 1973) because of environmental shifts and broadenings. More significantly, the average cross-section per pigment molecule is decreased by pigment clumping into chloroplasts, leaving non-absorbing space in between (the sieve effect: Rabinowitch 1951, Fukshansky 1981). Thus, I have chosen a k value that reproduces typical t and r values when used in the Kubelka-Munk model. The value

$$k = 2.5\alpha = 1.25 \times 10^4 \text{ m}^{-1}$$

yields $r = 0.146$, $t = 0.034$. The sum of the latter is appropriate for the average over the PhAR band (Breece and Holmes 1971), though the ratio $r : t$ is slightly high (and is only increased by realistic gradients in α and k : Gutschick 1984).

(D) Method of Solving the Set of Kinetic Equations

One must specify the four basic environmental conditions, C_a , O , I_{ad} , and I_{ab} . The latter two completely determine the profile $I(x)$ in the leaf, hence also the potential rate of electron generation per volume, $j(x)$.

For hypostomatous leaves, one guesses the CO₂ concentration at the top of the leaf, $C(0)$, which sets the assimilation rate $A_p(0)$ and hence the second derivative $C''(0)$. The first derivative, $C'(0)$, is zero, by Eq. (28). One then integrates to the next finite step, $x = dx$, computing new values of $C(x)$ and its derivatives. I typically use 1000 steps to reach $x = L$, where the calculated values $C^*(L)$ and $C'^*(L)$ are provisional, *i.e.*, they may not correspond to the correct C_a . They imply a provisional value

$$C_a^* = C^*(L) + r_{as}[DC'^*(L)],$$

where the bracketed quantity is the predicted photosynthetic rate per unit leaf area. If C_a^* is too small (large), one guesses a larger (smaller) value of $C(0)$ and re-solves the equations. Eventually one narrows the range of $C(0)$ and interpolates to the proper value. The entire search is readily automated.

For amphistomatous leaves, it is most efficient to specify an estimate of the derivative, $C'(0)$, or equivalently, the adaxial portion of $P_G = DC'(0)$. This then sets $C(0)$ as $C_a - r_{as}DC'(0)$. One integrates numerically to $x = L$ as before, and iterates C_a^* to agreement with C_a . This approach is better than estimating $C(0)$ directly because small shifts in $C(0)$ can imply gradients $C'(0)$ too large for numerical stability.

DISCUSSION

The complex model presented here synthesizes knowledge about three important kinetic aspects of photosynthesis. It is fully physiological with no adjustable parameters. Parameter values are all extracted from physiological measurements on *Glycine max* or the most closely related species for which data are available. Only one of the parameters of modest significance for leaf performance is moderately uncertain (D). The model is quantitatively accurate (Gutschick 1984) — not authoritatively so, but sufficient for utility and credibility in testing hypotheses of ecological function and agricultural crop performance. Even its deficiencies provide opportunities for experiments of broader significance.

Some of the biochemical simplifications need further discussion. Foremost, the photorespira-

tory cycling back to the Calvin cycle is presented as total, without net glycine or serine synthesis. Zelitch (personal communication) rightly regards this as a deficiency. Variations in the fraction of glycolate recycled would lead to calculable changes in the direct quantum yield of photosynthesis, as Peisker (1976) discussed along with additional effects of varied final oxidation states (glycine/serine or all the way to CO_2). Varied oxidation states of gross photosynthesis must be rectified in dark respiration; the quantum yield in net photosynthesis is then less sensitive to the recycling ratio. At high I , complete CO_2 recycling within the leaf has an added effect on quantum yield, beyond stoichiometry; it raises the internal CO_2 operating point of the leaf and raises Q quantitatively (Eq. 39). Biochemical data on the extent of recycling and the oxidation level of the recycled products would be very desirable, especially regarding possible dependence on I , C_a , O , and status of amino acid biosynthetic demand in the plant.

A second simplification deserving comment concerns the stoichiometry between electron transport and RuBPCO catalysis. I have used the FCB model option wherein NADPH production by electron transport is matched by consumption of NADPH in carboxylation and oxygenation. Farquhar *et al.* noted that matching ATP production and consumption produces a modestly different stoichiometry and hence a modestly different initial quantum yield, *etc.* (their Eq. 37). Farquhar and Caemmerer (1981) resolve the discrepancy in favor of the ATP-stoichiometry formulation, with cyclic photophosphorylation allowing ATP throughput to exceed NADPH throughput. The predicted change in photosynthetic performance is modest. Initial quantum yield is reduced up to 10%. At high I , where potential electron supply exceeds biochemical usability for either ATP or NADPH production, photosynthesis is little affected unless j_{\max} -limitation is possible (not the case with our estimated parameter values).

A third simplification, most difficult to assess, is lack of representation of source-sink regulation of photosynthesis. While partitioning of photoproducts into various biosynthetic pathways has seen some experimental and theoretical study (Bassham 1971), the regulation of total carboxylation rate of a mature leaf to levels below those set by I , C_a , and O is poorly understood. The sensitivity of enzyme activities to allosteric factors may be relatively unimportant (*e.g.*, Dvořák and Sel'kov 1980). Regeneration of inorganic phosphate as substrate (especially in ATP synthesis) may be an important control (Herold 1980), but only crude "black box" studies of gross environmental responses have been done. Crude negative feedback mechanisms such as disruption of chloroplast membrane structure by starch accumulation have been suggested by experimental results (*e.g.*, Thorne and Koller 1974). A mechanistic description of source-sink regulation is not yet feasible.

One last simplification warranting discussion is the lack of accounting for CO_2 transport resistances between photorespiratory CO_2 -liberating sites and photosynthetic sites. These sites and the intercellular air spaces are all linked to each other through resistances and thus operate at CO_2 concentrations that are offset from one another, depending on inter-site fluxes and resistance values. This coupling is described well by Lommen *et al.* (1971). The model here, not accounting for these offsets, is slightly decreased in quantitative accuracy, mostly in representing photosynthesis at elevated O_2 levels.

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Photosynthesis Model for C₃ Leaves Incorporating CO₂ Transport, Propagation of Radiation, and Biochemistry

2. Ecological and Agricultural Utility*

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Abstract

The previous paper developed the combination of the biochemical model of Farquhar *et al.* (1980) with models of CO₂ transport and propagation of radiation across the leaf thickness. Here I present the model's quantitative predictions of gross photosynthetic rate (P_G) as a function of irradiance (I), CO₂ and O₂ concentrations, leaf chlorophyll (Chl) and enzyme contents, and stomatal distribution and behavior pattern. Using parameter values appropriate to wild-type cultivars, the model approximates measured performance of soybean (*Glycine max* L.) fairly well. The model indicates that the gradient in I across the leaf thickness is a stronger determinant of I -dependence and maximal P_G than is the CO₂ gradient or stomatal control. Modest discrepancies in modelling CO₂ and O₂ dependences of P_G suggest opportunities to get new information on photorespiration and on stomatal control. The performance penalty for predominantly abaxial

* Received 2 July 1983; accepted 16 April 1984.

Abbreviations: A_v or $A_v(x)$ — net CO₂ assimilation rate (carboxylation — 1/2 oxygenation) per area or per volume at depth x ; $C(x)$, $C'(x)$ — CO₂ concentration, derivative at depth x ; \bar{C} — average of C_{\min} , C_{\max} ; C_a — ambient CO₂ concentration outside leaf; C_f — CO₂ concentration in substomatal chamber; C_{\min} , C_{\max} — CO₂ concentration limits for stomatal control; Chl — chlorophyll; D_{CO_2} — diffusion coefficient for CO₂ inside the leaf; E_t — RuBPCO concentration, mol per mol Chl; FCB — Farquhar, Cammerer, Berry (1980); g_s — stomatal conductance; I , $I(x)$ — irradiance, within leaf at depth x ; I_{ab} , I_{ad} — abaxially, adaxially incident irradiance; I_s — effective saturating irradiance (Eq. 5); k_c , k_o — maximal carboxylation, oxygenation velocities of RuBPCO; K_c , K_o — RuBPCO Michaelis constants for CO₂, O₂; L — leaf thickness; LAI — leaf area index; m — maximal rate of NADP⁺ reduction per Chl; N_c , N_e , N_D , N_α — leaf top-to-bottom ratios in Chl content, RuBPCO content per Chl, CO₂ diffusivity optical scattering power; O — ambient O₂ concentration; P_{adax} — adaxial flux of CO₂ into leaf; P_c — canopy photosynthetic rate per ground area; P_G or $P_G(\text{area})$, $P_G(\text{mass})$, $P_G(I)$ — gross photosynthetic rate per leaf area, per leaf mass, as function of irradiance; P_{\max} — maximal gross photosynthesis; PhAR — photosynthetically active radiation; Q , Q' — low-irradiance quantum yield per absorbed, incident photon; $Q(C)$ — Q as a function of CO₂ concentration; Q_{\max} — maximal value of $Q(C)$; r — leaf reflectivity; R_D — dark respiration rate; R_p — ribulose biphosphate pool size, mol per mol Chl; r_s — stomatal resistance; RE — relative quantum efficiency of using abaxial *vs.* adaxial irradiance; RuBPCO — ribulose biphosphate carboxylase oxygenase; S_a — sensitivity of P_G to increase in parameter a (Eq. 9); SLM — specific leaf mass; t — leaf transmissivity; x — depth in leaf; α — optical scattering power of leaf tissue; Γ_{CO_2} , Γ_o — CO₂ compensation concentration, with zero dark respiration; $\eta_{nt}(x)$ — net efficiency of using electrons to fix CO₂ at depth x ; ϱ_c — chlorophyll volume concentration; Φ — ratio of oxygenation rate to carboxylation rate.

rather than adaxial location of stomatal conductance appears to be small. Gradients in the structure of the leaf, and indeed the lower portion of the leaf itself, appear to be only weakly relevant to leaf-total photosynthetic rates and primarily relevant to minimizing transpiration and to mechanical support. The model allows estimates of sensitivity of photosynthesis to each physiological parameter, as well as interpretations of these sensitivities in terms of adaptive value. In conjunction with a canopy radiation interception model, the leaf model predicts narrow agricultural utility for mutants of decreased Chl content. However, the model suggests that alternative improvement routes of higher promise do exist, as in optimizing ontogenetic patterns of leaf thickness, and it can help guide the necessary experimental physiological studies.

The preceding paper (Gutschick 1984a) presents a leaf photosynthesis model that uniquely combines biochemical and photochemical kinetics, CO_2 transport in the leaf, and internal propagation of photosynthetically active radiation (PhAR). This combination remedies important limitations of the component models used separately. For example, the biochemical and photochemical model of Farquhar *et al.* (1980; denoted here as FCB) which I incorporate is itself a sophisticated, explicit kinetic formulation of photosynthetic performance as dependent on irradiance (I), CO_2 and O_2 levels, and about ten major, measurable physiological parameters: contents of carboxylating enzyme, chlorophyll (Chl), ribulose biphosphate...; carboxylation parameters; *etc.* However, it cannot determine the internal CO_2 concentration that varies with depth in the leaf and that is drawn down to progressively lower levels at higher I and gross photosynthetic rates (P_G) by virtue of air-space and other transport drags. More phenomenological resistance models (Gastra 1959 and many sophisticated modern derivatives) account for such dynamic interaction but poorly and distantly reflect carboxylation kinetics and other crucial physiological data. CO_2 transport models such as Parkhurst's (1977) that resolve detailed geometric diffusion path features are valuable but must depend on the physiological accuracy of the biochemical and photochemical description and have never been used with sophisticated models of the latter. Lastly, the strong leaf-depth dependence of light flux, $I(x)$, has been investigated by Laisk (1969) and Oya and Laisk (1976) for its importance in scaling photosynthetic performance *versus* external I . It is also important for performance per unit enzyme investment, *etc.*; it has not been evaluated with very accurate biochemistry or concurrent depth-dependence of CO_2 concentration.

A verified combined model can address many ecological and agricultural questions. For my own interests, the model has given useful predictions and has suggested analysis methods for experiments on canopy photon-use efficiency in Chl-deficient mutants. The model also yields insights into evolved ecological functioning and into potential crop improvements, as presented below. Examples include estimates of how adaxial:abaxial partition of stomatal conductance (g_s) affects leaf photosynthetic performance, new lines of evidence for stomatal control, estimates of contributions of the lower leaf to P_G *vs.* to transpiration, and assessments of limiting factors both physiological and environmental.

To establish the reliability and utility of the model for such inquiries, it must be verified against a wide range of experimental data without adjusting its kinetic parameters, which were determined physiologically to represent a soybean leaf — fully expanded, adequately nourished, and adapted to full sunlight and normal CO_2 levels. The model must accurately predict P_G as a function of the major environmental variables (irradiance I , ambient CO_2 and O_2 concentrations C_a and O ; I do not treat temperature here, however) and of the leaf physiological constitution. Quantitative data on the latter are minimal but will be increasingly important for crop improvement. These model tests are reported in the next Section and they yield constructive criticisms of formulations of carboxylation and oxygenation kinetics, stomatal behavior models, and the degree and functional significance of the attenuation of photosynthetically active radiation (PhAR) across the leaf thickness.

COMPARISON TO EXPERIMENTS: MODEL STRENGTH AND DEFICIENCIES

Values of P_G (as a function of I , C_a , O , or some combination) are given for soybeans by Dornhoff and Shibles (1970) and Hesketh *et al.* (1972) for extensive ranges of cultivars, and by Egli *et al.* (1970) and Bowes *et al.* (1972) for more specific cultivars, variously for single leaves or whole canopies and at varied (or even variable) temperature. More limited correlations to environment can be discerned in field data as of Kanemasu and Hiebsch (1975) or Tenhunen *et al.* (1980). Ludwig (1972) studied detailed C_a - and O -dependences of P_G in sunflower, a comparable high-performance C_3 species, and his data are also used here. *Phaseolus vulgaris*, another model species, was studied by Caemmerer and Farquhar (1981) for P_G at many C_a and O levels and several I , as well as under varied N-nutritional status, *etc.* Only Hesketh *et al.* (1981) provided extensive physiological data on Chl and protein contents, ribulose biphosphate carboxylase/oxygenase (RuBPCO) activities, *etc.*

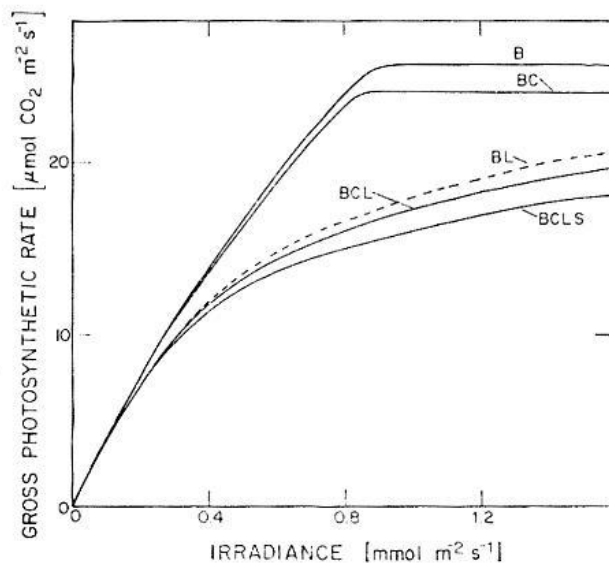


Fig. 1. Photosynthesis calculated by models of varying completeness: (*B*) biochemistry only; set $C(x) = 23$ Pa everywhere; D infinite; photon absorption rate $a(x)$ is uniform and reproduces total absorption of full model; (*BC*) biochemistry and CO_2 -transport only; as "*B*", except set $C(0) = C(L) = 23$ Pa; C at other x set by diffusion equation with standard $D = 7 \times 10^{-7} \text{ m}^2 \cdot \text{s}^{-1}$; (*BL*) biochemistry and radiation-penetration only; as "*B*", except photon absorption rate $a(x)$ set by nonuniform irradiance $I(x)$ calculated by Kubelka-Munk model; (*BCL*) biochemistry, CO_2 -transport, and radiation-penetration only; full model except stomatal control replaced by simple setting of $C(0) = C(L) = 23$ Pa; (*BCLS*) full model, with stomatal control submodel (Gutschick 1984a).

Dependence of P_G on I at normal C_a and O is a crucial test. My model's predictions (Fig. 1) were not corrected for leaf respiration (see discussion in Gutschick 1984a). Curve 'BCLS' represents the full, integrated model, and it has a qualitatively accurate shape. There are few consistent data on the full curve, $P_G(I)$, so I examine a few discrete features. An important feature is maximal photosynthetic rate per leaf area, P_{\max} , at maximal terrestrial $I \approx 1.6 \text{ mmol m}^{-2} \text{ s}^{-1}$. The model predicts $P_{\max} = 18.2 \text{ } \mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ at 25°C , raised to $21.3 \text{ } \mu\text{mol m}^{-2} \text{ s}^{-1}$ upon setting the stomatal resistances more realistically to 800 and 200 s m^{-1} (adaxially and abaxially, respectively) and positing 10% abaxial I as is common in canopies or measuring chambers. Dornhoff and Shibles (1970, Fig. 1) measured a range of 18.6 to $27.4 \text{ } \mu\text{mol m}^{-2} \text{ s}^{-1}$ for

many cultivars, with an average near 22, for a comparable $T = 26^\circ\text{C}$ and a time-varying C_a averaging 28.2 Pa. Bowes *et al.* (1972, Fig. 1) obtained $P_{\max} \approx 29 \mu\text{mol m}^{-2} \text{s}^{-1}$ at 30°C for the high-performing Wayne cultivar, which we may correct to $26 \mu\text{mol m}^{-2} \text{s}^{-1}$ at 25°C using the temperature scaling of the full FCB model (their Fig. 9, dashed curve). Hesketh *et al.* (1981) found P_{\max} near $29.7 \mu\text{mol m}^{-2} \text{s}^{-1}$ for the high-performing Amsoy cultivar at 30°C , correctible to $24.7 \mu\text{mol m}^{-2} \text{s}^{-1}$ at 25°C ; correcting my model to their probable $C_a = 33$ Pa gives $22.6 \mu\text{mol m}^{-2} \text{s}^{-1}$. Thus the model is plausible, if slightly low. I ascribe this lowness to deficiencies in representing stomatal behavior and perhaps also to a low estimate of exciton transfer efficiency, η_t ; both are discussed below.

A second major test of the model is its ability to reproduce the initial quantum yield per absorbed photon,

$$Q = \left. \frac{\partial P_G}{\partial I} \right|_{I \rightarrow 0}. \quad (1)$$

Ehleringer and Björkman (1977) found Q to be virtually universal for C_3 plants. Within close limits, one can argue that Q reflects only RuBPCO kinetic parameters and photorespiratory stoichiometry, and the former at least are fairly comparable among all C_3 species (Delaney *et al.* 1978, Yeoh *et al.* 1980; but see Ranty and Cavalie 1982). At low I , internal CO_2 concentration stabilizes and Q simplifies greatly (FCB, their Eq. 37; Gutschick 1984a, Eqs. 15 and 24):

$$Q \rightarrow \frac{1}{8} \frac{(1 - 0.5\Phi)}{(1 + \Phi)} \eta_t \quad (2)$$

The value of Φ , the ratio of oxygenation to carboxylation rates, is predicted from our chosen RuBPCO parameters to be 0.267 at 25°C , 23 Pa CO_2 (intercellular), and 21% O_2 . The value of Q at 25°C is about 0.052, corrected (see Ehleringer and Björkman 1977, Fig. 3) 10% upward from its measured value of about 0.047 at 30°C . The measured and predicted Q are consistent if $\eta_t = 0.61$, close to my estimated value.

At 2% O_2 , Φ becomes essentially zero and Q is predicted to be $\eta_t/8$. Q is measured (at 30°C , though temperature is fairly irrelevant at low O_2) as 0.081, requiring $\eta_t = 0.65$, fairly consistent with the previous estimate.

The dependence of Q on intercellular CO_2 concentration, C , is problematic in the FCB model, hence my model also. At low I , Φ is modelled as simply inversely proportional to C . In terms of the RuBPCO parameters (FCB 1980),

$$\Phi = \frac{k_o}{k_c} \frac{O/K_o}{C/K_c}, \quad (3)$$

and Q can be rewritten as

$$Q = Q_{\max} \frac{C - \Gamma_o}{C + 2\Gamma_o} \quad (4)$$

much as Peisker and Apel (1981) showed. Here $\Gamma_o = k_o K_c O / (2k_c K_o)$ is the limit of the CO_2 compensation concentration, Γ_{CO_2} , when dark respiration is zero. The kinetics of the FCB model and the best values for k_c , k_o , K_c , and K_o yield $\Gamma_o = 3.07$ Pa at 25°C , or 3.59 Pa at 30°C . The latter value can be used in the last equation to calculate $Q(C)$ for comparison to measurements, and Fig. 2 shows that the fit is poor. If the Michaelis-Menten kinetic structure is not wrong, one can revise the RuBPCO parameter values to give $\Gamma_o \approx 5.0$ Pa and get a good fit to the data of Ehleringer and Björkman (1977, Fig. 2). However, Γ_o is a lower limit to Γ_{CO_2} but 5.0 Pa is too

high an estimate for the latter. It is difficult to conceive of a mechanism (alternative photorespiratory path or otherwise) that is consistent with a single set of RuBPCO parameters and that depresses Q more than it increases Γ_{CO_2} . This is a problem for photosynthesis research in general, beyond the modelling here.

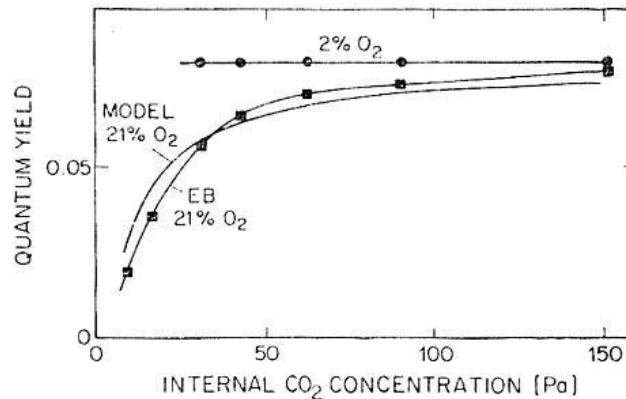


Fig. 2. Initial quantum yield at 30 °C. Curves labelled “2% O₂” and “EB 21% O₂” are results of Ehleringer and Björkman (1977) for a C₃ plant, *Encelia californica*. Curve “MODEL 21% O₂” is calculated from Eq. (4) of text using RuBPCO enzyme parameters of Farquhar *et al.* (1980) adjusted to 30 °C, with limiting Q (at 2% O₂) adjusted to match curve “2% O₂” by choice of η_i .

A third test of the model is the “shape” of P_G between low and high I , typically approximated as a hyperbola,

$$P_G \approx P_{\max} \frac{I}{I + I_s}. \quad (5)$$

This form has deficiencies, of course. One can constrain it to give the proper initial quantum yield per incident photon, $Q' = P_{\max}/I_s$, which induces a poor fit to high- I behavior where many more kinetic phenomena enter (CO₂ transport drags, photochemical saturation) that are unrelated to Q' . Alternatively, one can choose P_{\max} and I_s to fit $P(I)$ over a broad range, which generally distorts Q' (I found 10–15% errors for fits to experimental data and model results).

With an awareness of these deficiencies, one can do a least-squares fit of $P(I)$ to the last equation to derive a rough value of I_s , which reflects complex saturation kinetics. The data of Hesketh *et al.* (1981) on high-performing Amsoy cultivar give $I_s \approx 0.83 \text{ mmol m}^{-2} \text{ s}^{-1}$; the data of Bowes *et al.* (1972) on average-performing Wayne cultivar fit $I_s \approx 0.41 \text{ mmol m}^{-2} \text{ s}^{-1}$. My model calculations fit $I_s \approx 0.46 \text{ mmol m}^{-2} \text{ s}^{-1}$, implying that the model incorporates reasonable saturation kinetics. Better experimental data are highly desirable.

A fourth test of the model is its reproduction of the CO₂-dependence of P_G at moderate to high I , where stomatal control, internal diffusive drags, and RuBPCO capacity limitations enter into performance. Dornhoff and Shibbes (1970) give P_G values near maximal I (about $1.54 \text{ mmol m}^{-2} \text{ s}^{-1}$) for 22-cultivar averages at four external CO₂ concentrations, C_a . Relative to performance at $C_a = 30 \text{ Pa}$, the performances at 10, 20, 30, and 38.6 Pa (all at 26 °C) are 0.22, 0.63, 1.00, and 1.10. Using the basic stomatal control model (Gutschick 1984a), my comparable results are 0.32, 0.71, 1.00, and 1.06, in moderately good agreement. Other data at C_a significantly above 30 Pa, however, indicate problems. Egli *et al.* (1970) measured total canopy photosynthesis up to $C_a = 60 \text{ Pa}$ and found only slight saturation as a function of C_a at the highest values. In my comparable model estimates (Fig. 3), P_G rises with significantly lower slope above about 25 Pa CO₂ than below this value. The cause is the “entrainment” of substomatal CO₂ concentra-

tion $C_f = C(0)$ or $C(L)$ to 22–23 Pa that my stomatal model tries to enforce. Other evidence discussed soon also indicates flaws in the stomatal behavior model.

I have thus pursued two routes, the first being a test of the model exclusive of stomatal function. I compare photosynthetic rate as a function of C_f between the model and two detailed experimental studies on comparably high-performing species, those by Caemmerer and Farquhar (1981) on *Phaseolus vulgaris* and those by Ludwig (1972) on sunflower. The species differences should not be too significant, as I focus on CO_2 -saturation kinetic only. Fig. 4 presents the model calcu-

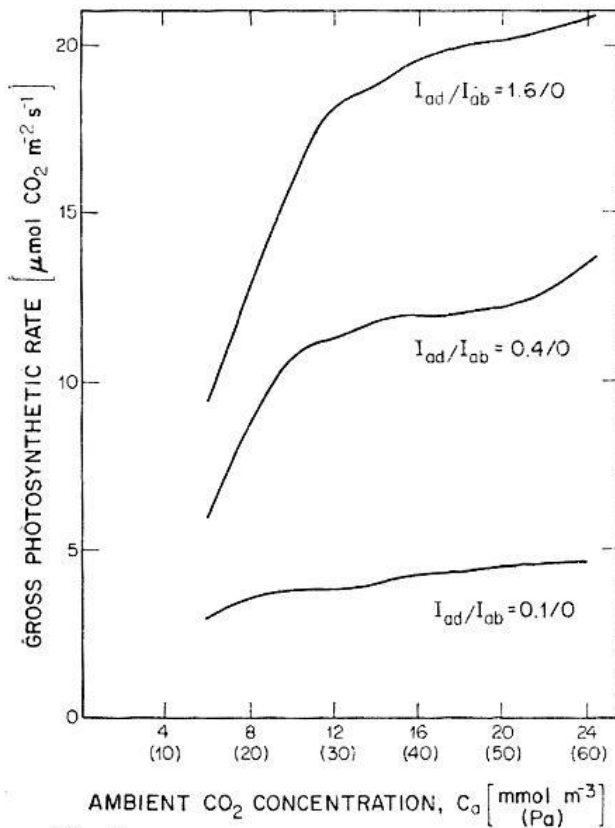


Fig. 3.

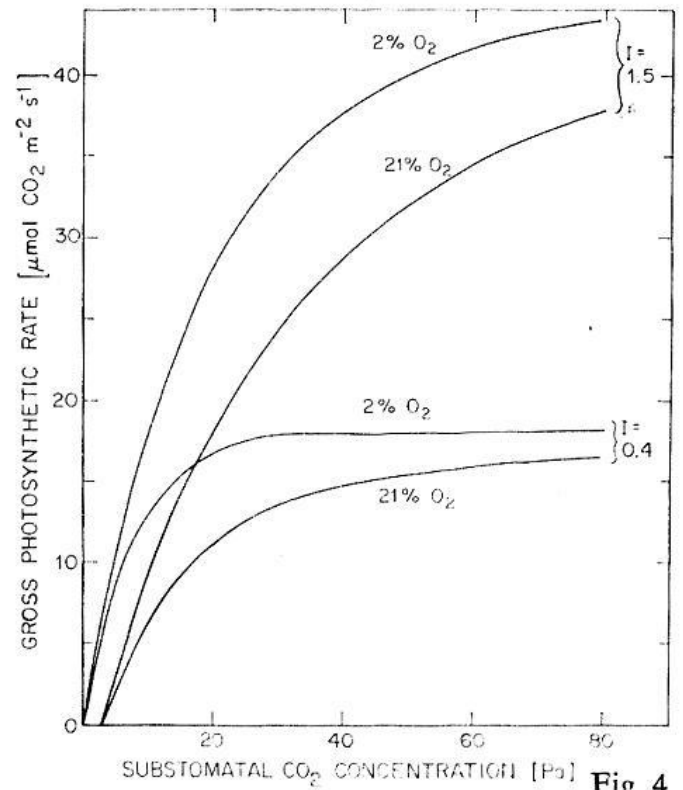


Fig. 4.

Fig. 3. Gross photosynthetic rates calculated by standard model as a function of ambient CO_2 concentration, C_a , at three different irradiances, I (specified in $\text{mmol m}^{-2} \text{s}^{-1}$, adaxial/abaxial).

Fig. 4. Calculated gross photosynthetic rate as a function of chosen substomatal CO_2 concentrations, at moderate ($0.4 \text{ mmol m}^{-2} \text{s}^{-1}$) and high ($1.5 \text{ mmol m}^{-2} \text{s}^{-1}$) irradiances (I). The model is standard as in Gutschick (1984a), except for stomatal control which is bypassed here.

lations for two I values, $0.4 \text{ mmol m}^{-2} \text{s}^{-1}$ (presumed comparable to $0.5 \text{ mmol m}^{-2} \text{s}^{-1}$ for the late-saturating sunflower) and $1.5 \text{ mmol m}^{-2} \text{s}^{-1}$ (as in the *Phaseolus* studies). At the higher I , *Phaseolus* attains half-maximal performance at approximately 9.0 Pa CO_2 in 1.9% O_2 or at 16.0 Pa CO_2 in 20% O_2 . The model shows half maximum at approximately 13.3 and 25.6 Pa CO_2 for comparable O_2 levels of 2% and 21%. At lower I , sunflower attains half-maximal performance at approximately 6.7 and 20.0 Pa CO_2 in 2% and 21% O_2 , respectively. My model yields 6.7 and 15.5 Pa, respectively. Thus the model is in only fair agreement with these experiments. (However, the *Phaseolus* data also show a decline in photosynthesis with increasing CO_2 at low O_2 , which is hard to explain in any kinetic scheme.)

The second route is replacing the stomatal behavior model with the probably more realistic model of Bell (1982), wherein C_f is held to a constant fraction of C_a . In Table 1, I used the value

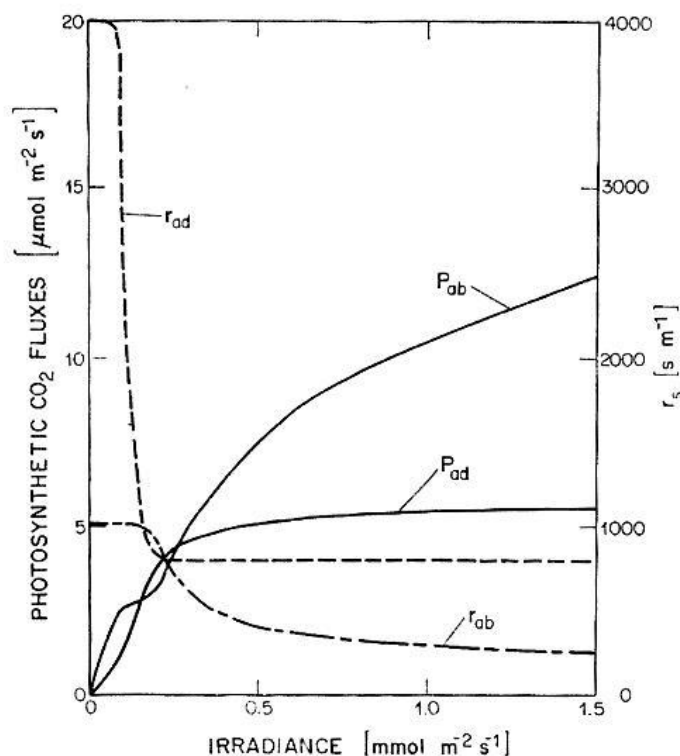


Fig. 5. Behavior of standard model as a function of adaxial irradiance. P_{ad} , P_{ab} , $r_{s,ad}$, $r_{s,ab}$ are respectively photosynthetic CO_2 fluxes into adaxial (top) and abaxial (bottom) surfaces of leaf, and corresponding stomatal resistances.

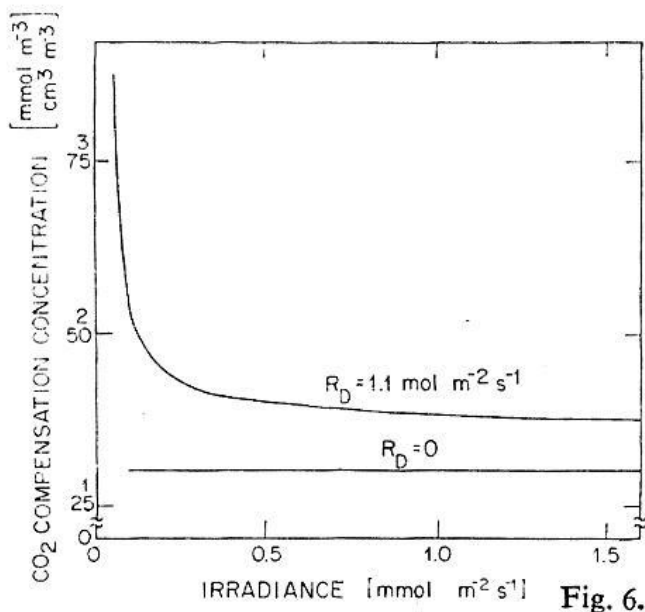


Fig. 6.

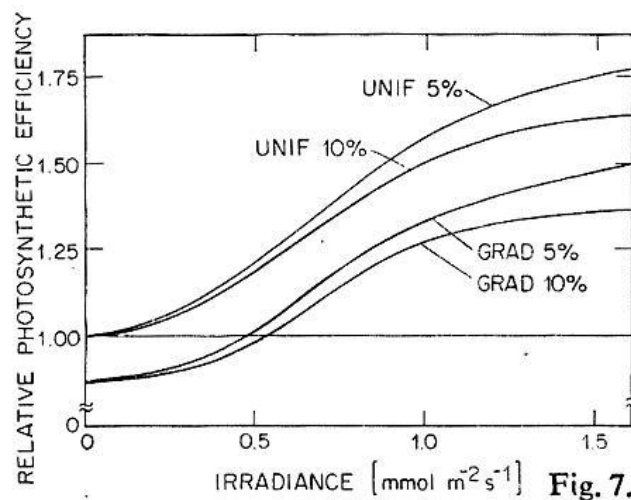


Fig. 7.

Fig. 6. Calculated CO_2 compensation concentration in standard model with and without internal dark respiration, R_D , presumed to be distributed uniformly over whole volume of leaf.

Fig. 7. Calculated relative efficiency of bottom (abaxial) irradiance I vs. top I in driving photosynthesis. Curves "UNIF" and "GRAD" refer respectively to uniform-structure and gradient-structure models of the leaf. Curves labelled "5%" and "10%" are respectively for bottom I equalling 5% or 10% of the top I (abscissa).

1982, especially pp. 326 and 331). It is very desirable to develop models that properly correlate stomatal behavior changes with changes or mutations in other physiology, such as in Chl content. If one accepts that stomatal control is exercised largely by guard cell photosynthesis affected by CO_2 depletion, then control may change fairly significantly when (if) Chl-deficiency mutations in the bulk leaf are also reflected in the guard cells.

A sixth test of the model is the accuracy of the predicted CO_2 compensation concentration, Γ_{CO_2} . The RuBPCO and photorespiratory kinetics (and some problems therein) that underlie the formulation of Γ_{CO_2} have been covered earlier, in the discussion of Q . The model, assuming no dark respiration, predicts $\Gamma = 3.07 \text{ Pa CO}_2$ at 25°C . Dark respiration increases Γ , particularly at low P_G (low I); Fig. 6 here and Fig. 6 in FCB (1980) show $\Gamma(I)$ for assumed constant dark respiration, R_d . Experimental curves are even flatter with increasing I (see Zelitch 1971), indicating a progressive suppression of R_d . Whatever the degree of suppression, Γ is given by the model as being between 3.07 and 3.6 Pa CO_2 at 25°C . Forrester *et al.* (1966) measured 3.5 Pa at 25°C , while Dornhoff and Shibbes (1970) found a mean of $4.01 \pm 0.34 \text{ Pa}$ at 26°C for a sample of 20 cultivars. Thus, the model agrees reasonably well with experimental data.

A seventh and last set of tests for the model concerns the realism and the consequences of internal PhAR-propagation phenomena. The Kubelka-Munk (1931) PhAR propagation submodel predicts reflection and transmission coefficients $r = 0.1457$ and $t = 0.0342$ for soybean leaves of normal Chl content. (The model cannot predict dependence on angle of incidence.) Experimental data on soybeans or similar leaves vary significantly, perhaps from instrumental differences (sensitivity to infrared, *etc.*). Breece and Holmes (1971) reported extensive measurements on soybeans with varied angles of incidence and collection. One must integrate over the latter angle,

$$r = \int d\Omega_{\text{coll}} \cos \theta_{\text{coll}} \varrho'(\theta_{\text{coll}})$$

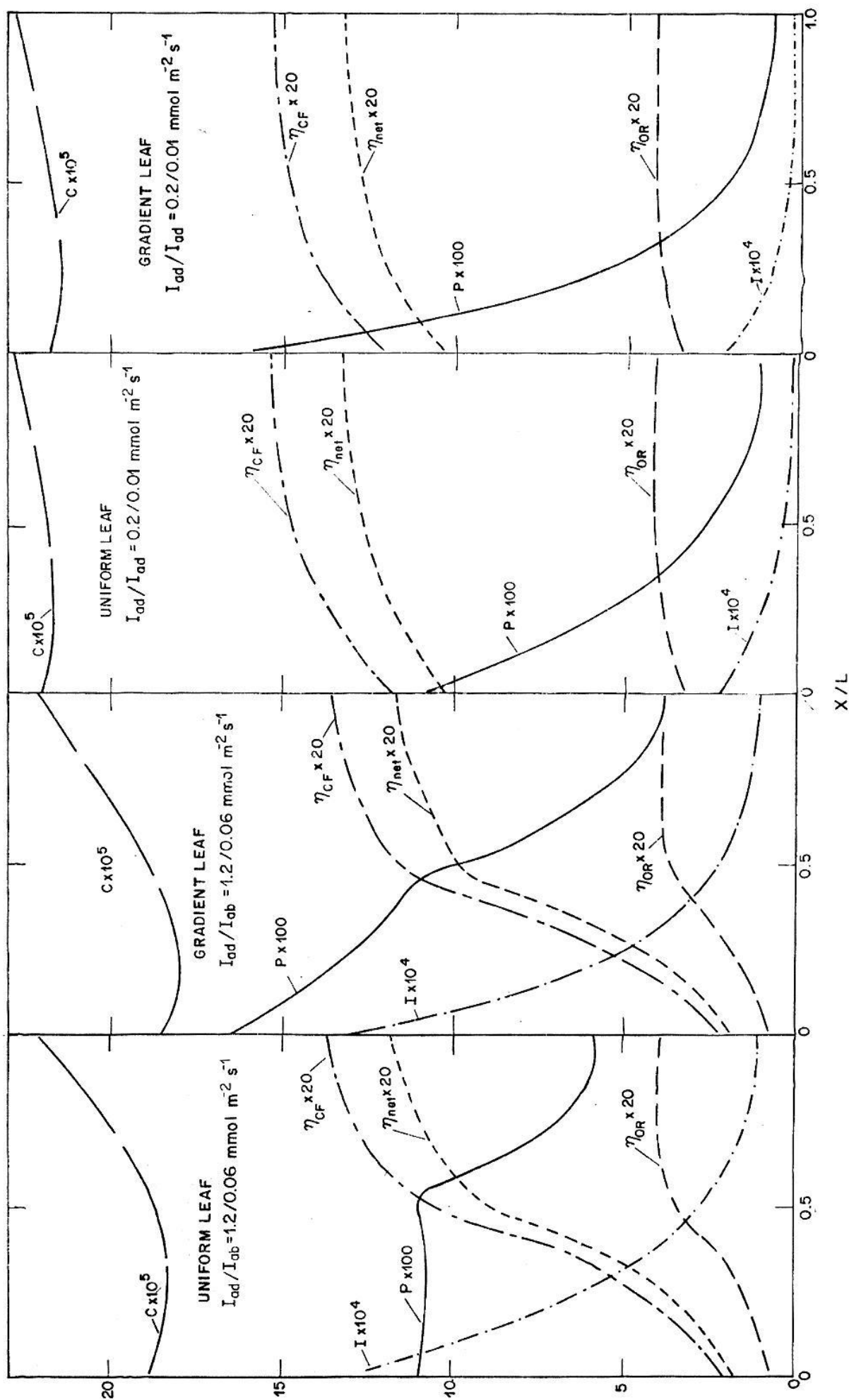
and similarly for t . A rough estimate from their Fig. 7, also averaging over the 400–700 nm region, gives an average $\varrho' \approx 0.05$, implying $r \approx 0.15$. Similarly, one derives $t \approx 0.05$. Both values are quite close to the model's. Fukshansky (1981) measured *Phaseolus* leaves, obtaining for r and t averaged over the 400–700 nm region the values 0.13 and 0.065, as estimated from his Fig. 2a. The pioneering work of Gates *et al.* (1965) on varied species gave the smallest of all reported ratios of r/t , well below 2.0 and below the ratio in the more recent studies. Overall, one can say that the model is fairly realistic for r and somewhat too low for t . Perhaps the estimated scattering strength α is too high. I used $\alpha L \approx 1.0$ while Fukshansky (1981) derived $\alpha L \approx 0.7$ in *Phaseolus*. This disparity may also explain why the model predicts significant differences in r for top and bottom incidence when one incorporates realistic gradients (Eq. 12 below) in the leaf structure, while Breece and Holmes (1971, p. 122) measured only about 5% relative differences.

There are no reported r and t values for the mutant soybeans for comparison to the model's predictions (without gradient accounting) of 0.2305 and 0.126, respectively. It is of note that the increase of t is significantly less than when one uses a Beer's law approximation, ignoring scattering, in which case

$$t(\varrho_c/2) = \sqrt{[t(\varrho_c)]}, \quad (6)$$

implying that for the mutant $t = 0.185$.

The functional significance of the great difference in photon flux (up + down) between the top and bottom of the leaf (30-fold in the model for adaxial-only irradiance) is suggested by Fig. 1. Curve „B“ represents the basic biochemical behavior ($D_{\text{CO}_2} \rightarrow \infty$, or uniform C ; total photon absorption rate adjusted to same value as in full model but made uniform throughout the leaf volume). It is very similar to the original FCB curve (their Fig. 10), and it is far too angular. Accounting for the finite CO_2 diffusivity makes C a function of depth x in the leaf and yields curve „BC“, only slightly different from „B“; nonuniform distributions of D_{CO_2} and biochemical



Lacking such data, one may use the model's predictions as first indications; they are shown in Fig. 8. At the higher I (1.2 and 0.06 in our units, adaxially and abaxially, respectively), the most apparent feature in $C(x)$ is the disparity of adaxial and abaxial limits, $C(0)$ vs. $C(L)$, discussed above briefly. Further, the minimum in midleaf is as low as 18 Pa, which increases the oxygenation:carboxylation ratio 28% above its value at the nominal operating point of 23 Pa modelled by Farquhar *et al.* (1980); the depression of local $A_p(x)$ is comparable. This "conclusion" obtains for both the uniform and gradient approximations to leaf structure (see Eq. 12 for gradients used). Again at $I_{ad}/I_{ab} = 1.2/0.06 \text{ mmol m}^{-2} \text{ s}^{-1}$, the photon flux $I(x)$ varies strongly, about 12-fold from $x = 0$ to $x = L$. Levelled by the photochemical supersaturation characteristics, the resultant variation in net assimilation rate A_p (carboxylation — $1/2$ oxygenation) is about 2-fold across the leaf depth (uniform structure approximation; about 4.3-fold with realistic gradients accounted). Both structural models imply that A_p reexpressed on a mass basis is about 2-fold higher at the top than at the bottom, with a fairly sharp break at mid-depth. This assimilation per unit mass is even more sharply varied with depth at the nonsaturating $I_{ad}/I_{ab} = 0.2/0.01 \text{ mmol m}^{-2} \text{ s}^{-1}$. This trend, combined with the studies (below) estimating a low rate of gain in P_G with increasing leaf thickness, suggests that the lower portion of the leaf has primarily an indirect role in photosynthesis. Mechanistic considerations by Pickard (1982) imply that the lower leaf serves to locate substomatal chambers of sufficiently large dimensions to optimize the ratio of transpiration to CO_2 flux. The predominantly abaxial placement of stomatal conductance supports this view.

A question of some fascination is, "Why are leaves predominantly hypostomatous?" While ontogenetic variations in degree of hypostomaticity occur (review: Tichá 1982), their value for unravelling the effect on photosynthetic performance is clouded by simultaneous variations in leaf constitution. With the model one can consider performance as a function of g_s distribution at fixed total adaxial + abaxial g_s . Fig. 9 presents the most definitive comparison: total hyperstomaticity, which intuitively appears optimal because CO_2 has best access to the area of greatest photon absorption; total hypostomaticity, as the opposite extreme; and a 1 : 4 ratio in g_s , as typical of many plants. Even this last shift of 20% of g_s to the adaxial surface brings performance very near that of the first case; it is even superior at highest I values. Thus, largely abaxial stomatal placement costs little or nothing in photosynthetic performance, and other considerations favored by abaxial placement, such as easier mechanical closure during wilting or lessened dust and pathogen interception, can be met uncompromised. Fig. 10 shows, for two selected I , a continuous survey of performance vs. g_s distribution. Two total g_s are represented, and give very similar behavior. Photosynthesis is optimized near $2/3$ adaxial placement, but the optimum is broad. Most gain occurs with a small adaxial placement, and the optimum-to-minimum contrast is only 1.15-fold at high I , 1.095-fold at the lower I .

A third inquiry is assessing the optimality of leaf dimensions, particularly total leaf thickness L , which is clearly closely proportional to specific leaf mass, SLM . In normal SLM ranges, P_G is an increasing function of SLM (Hesketh *et al.* 1981, Gourdon and Planchon 1982); P_G also correlates well with quantities related to SLM such as leaf content of nitrogen, protein, or Chl per area (Murata 1961, Buttery and Buzzell 1977). However, Nichiporovich (1980, especially p. 695) and Parkhurst (1977) have argued that an asymptote is reached or even that a peak is passed at high SLM , because diffusive drags in CO_2 transport accumulate in thick leaves. Takano and Tsunoda (1971) measured a curvilinear and presumably saturable correlation of P_N with leaf nitrogen content in wheat (SLM not reported).

In searching with the model for a peaking of P_G , I assume that RuBPCO content as moles per area is directly proportional to L (i.e., $q_c E_t$ is constant; similarly for R_p and m). I assume that Chl per area ($q_c L$) acts similarly until it becomes constant above $L = 200 \mu\text{m}$ (else, the extra thickness of the leaf has such low photon flux as to be useless). I assume that the optical scattering strength α and the CO_2 diffusion coefficient D_{CO_2} are constant, reflecting only an unvaried density

environmental factors regarding $P_G(\text{area})$. A first estimate for the degree of limitation of P_G by any factor a is a sensitivity or logarithmic slope,

$$S_a = \frac{d \ln P_G}{d \ln a} \quad (9)$$

High values imply significant limitation. Table 3 presents the model's estimates. There are few surprises in rank order. The most limiting factors all relate to RuBPCO kinetics or its concentration. However, these S estimates neglect necessary couplings between parameters. For example, an attempt to improve P_G by increasing E_t will require a thicker leaf (larger L) or a denser one (smaller D_{CO_2}) or both. The algebraically combined S value may be low. Second, nonlinearities or saturation phenomena, as discussed for q_c and L earlier, are not included. Even in the simplest estimates, some factors have S near zero or optimal: α , L , D_{CO_2} , r_s , etc. In the gradient leaf model, there are few changes in rank and no major differences.

Table 3

Sensitivity of calculated photosynthesis to increases in physiological parameters and environmental variables. Definition of sensitivity is in Eq. (9) of text; for practical difference calculations, a 10% increase in the chosen parameters was used. The standard model and its parameters are defined in Gutschick (1984a). The gradient model has a graded depth-distribution defined by Eq. (8).

Parameter	High irradiance [$1.6 \text{ mmol m}^{-2} \text{ s}^{-1}$]			Low irradiance [$0.1 \text{ mmol m}^{-2} \text{ s}^{-1}$]		
	rank	Sensitivity		rank	Sensitivity	
		uniform	gradient		uniform	gradient
k_c	1	+0.74	+0.76	5	+0.33	+0.33
K_c	2	-0.63	-0.64	3	-0.35	-0.35
E_t	3	+0.52	+0.54	14	0.00	0.00
O	4	-0.38	-0.38	4	-0.35	-0.35
K_o	5	+0.37	+0.36	6	+0.33	+0.33
\bar{C} (note a)	6	+0.35	+0.31	7	+0.27	+0.29
k, q_c	7	+0.32	+0.35	9	+0.22	+0.19
k_o	8	-0.22	-0.21	2	-0.35	-0.35
C_a	9	+0.22	+0.22	8	+0.25	+0.19
η_t	10	+0.21	+0.19	1	+0.89	+0.90
α	11	-0.11	-0.08	11	-0.10	-0.06
L	12	+0.10	+0.15	10	+0.12	+0.14
D	13	+0.09	+0.10	16	0.00	0.00
$r_{s,\text{top}}$	14	-0.06	-0.09	14	-0.01	-0.01
m	15	+0.04	+0.04	12	+0.06	+0.06
$r_{s,\text{bottom}}$	16	-0.01	-0.01	13	-0.02	-0.01
slope (note b)	17	-0.01	-0.01	17	0.00	0.00
R_p	18	0.00	0.00	15	0.00	0.00

^a $\bar{C} = 1/2 (C_{\min} + C_{\max})$, the midpoint of the stomatal control range.

^b slope = $C_{\max} - C_{\min}$, the span of the stomatal control range.

1980). The FCB model was a limited exception, as the leaf nitrogen-leaf performance correlation was treated. The leaf model here is more complete and somewhat more accurate for predictive use. By "predictive" I intend no indication that it is quantitatively authoritative nor that it replaces many experiments. Rather, it allows one to explore hypotheses about performance under well-defined physiological variations unobscured by other linked variations occurring in all experiments. One can then choose the most promising hypotheses to test experimentally and also design clearer and more definitive experiments.

To date, breeders have not used such detailed and mathematically complex models, for numerous good reasons — *e.g.*, they wish to avoid a great imbalance in effort on the few photosynthetic traits *vs.* the remaining hundreds of traits of agronomic interest; they justifiably mistrust model predictions resembling the tenuous empirical correlations (as between short-term P_G and yield discussed earlier); lastly, other "high technology" applications to agriculture, such as genetic introduction of N_2 fixation into nonsymbionts, have been oversold recently. Given these caveats, the model will be useful and attractive to breeders only in conjunction with experimental designs and only if a potential user need not get excessively involved in modelling details; to assure the latter, the details must be reasonably well verified before attempting agricultural application.

My first agricultural application of the model is assessment of the whole-canopy photosynthetic potential of variants (mutants) having a reduced Chl content. I have hypothesized that Chl decreases could increase the quantum efficiency, hence the photosynthetic rate, for the canopy as a whole by redistributing photons to Chl's that are less supersaturated photochemically. This redistribution would be from leaves at the top of the canopy, which would have increased r and t , to the leaves of the middle canopy, which consequently would receive the enhanced diffuse light transmitted and reflected by the top leaves.

A morphological strategy for redistributing photons and enhancing efficiency was proposed by Boysen Jensen (1932), namely, greater erectness of leaves to give a smaller average cosine of the angle between leaf normals and the direct solar beam. Monsi and Saeki (1953), de Wit (1965), Duncan *et al.* (1967), Loomis and Williams (1969), and Duncan (1971) quantified the proposal more fully. Some crop modifications were successful, as reviewed by Trenbath and Angus (1975). The performance gains have some constraints: (1) restriction to narrow-leaved, mostly gramineous species with low physical hindrance to denser leaf packing (however, Kokobun and Watanabe 1981 had some success with soybeans); (2) relative narrowness of the range of solar elevations over which the radiation redistribution is significant; and (3) some penalty in early growth rate because leaf erectness delays canopy closure and thus total radiation interception, which is important for whole-season performance (Thorne 1971, Watson 1971). A potentially more flexible morphological solution is leaf heliotropism (Ehleringer and Forseth 1980). This generally holds leaves at angles for maximal or minimal PhAR interception. The former is best for total canopy photosynthesis, P_c , at low LAI , the latter is best at high LAI . However, plants are observed to alter their heliotropism only as a function of water stress and not LAI .

My strategy of reducing Chl content may have fewer restrictive conditions for gains. I assume that RuBPCO content per area of leaf will remain unchanged and thus normal $P_G(\text{area})$ for top-most canopy leaves will be retained. This retention is observed for low-Chl mutant peas (Highkin *et al.* 1969) and tobacco (Schmid and Gaffron 1967a, b, Zelitch and Day 1968, Okabe *et al.* 1977). Mutant soybeans probably act similarly, but only partial reactions of phosphorylation and electron transport have been investigated (Keck *et al.* 1970a, b). A caveat is that most of these mutants are heterozygous and segregating. For commercial use, one would need to transfer a homozygous trait, perhaps the y_9 gene from the outmoded soybean cultivar, Illini (R. Nelson, Univ. of Illinois; personal communication). Another caveat is that the mutants often show a lag in developing grana (Schwarz and Kloppstech 1982) and thus also in attaining full photosynthetic competence.

While short-term P_G has been measured in these mutants, season-long vegetative growth and

yield have not. In advance of such measurements I have done detailed predictive modelling in order to (1) derive rapid estimates before undertaking a large experiment and (2) identify complex yield-relevant factors to include in the experimental design — planting density, seasonal insolation patterns, *etc.* — and aid in quantitative analysis of the field trials. A combined optical-biochemical model such as mine is required in order to account simultaneously for altered $P_G(I)$ behavior and changes in leaf reflectivity and transmissivity. Fig. 12 presents the $P_G(I)$ simulations for normal and mutant leaves, using three distinct assumptions about important yet-unmeasured

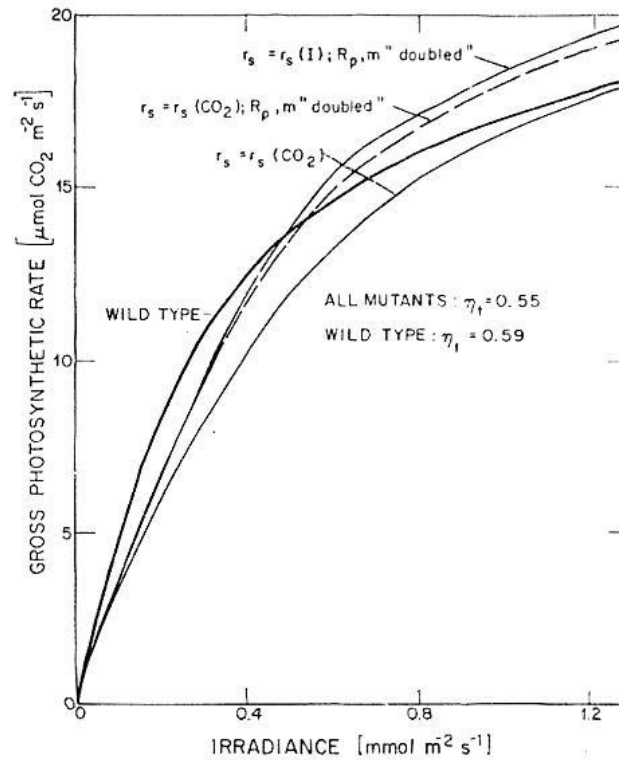


Fig. 12. Calculated photosynthesis of wild type soybeans and reduced chlorophyll mutants. Standard model of uniform-structure leaf is used for wild-type curve. Three possible curves for the mutant all use a reduced exciton-transfer efficiency, η_t , because mutants absorb a greater fraction of radiation in less-efficient pigments. Two curves, labelled " $r_s = r_s(\text{CO}_2)$," use the standard submodel of stomatal control according to internal CO_2 concentration. The topmost curve, labelled " $r_s = r_s(I)$," uses a submodel of stomatal control according to irradiance (minimum resistances 800 and 200 s m^{-1} , adaxial and abaxial; exponential increase with decreasing irradiance, doubling at 0.15 and 0.25 $\text{mmol m}^{-2} \text{s}^{-1}$ respectively). The topmost two curves also assume that parameters R_p , m are normal on a per-volume basis, or doubled on a per-chlorophyll basis.

physiological traits of the mutants. Note that the most likely behavior is superior to the wild type at all I above 0.65 $\text{mmol m}^{-2} \text{s}^{-1}$; relative performance ranges between 1.066 at 1.6 $\text{mmol m}^{-2} \text{s}^{-1}$ and a low of 0.86 at low I . Predicted values of r and t increase from 0.1457 and 0.0342 in the wild type to 0.2305 and 0.1260 in the mutant.

These results must be incorporated into an accurate model of canopy PhAR interception in order to predict the canopy photosynthetic rate, P_c . Leaf irradiance contributed by first interceptions of solar radiation depends upon leaf depth in the canopy, solar elevation, direct: diffuse ratio, and leaf angle distribution (reviews: Lemeur and Blad 1974, Bunnik 1978). The last factor also causes leaf-received I to be statistically distributed over a wide range; ignoring the distribution can cause sizeable errors in P_c (Gutschick 1984b). Lastly, leaf I has a diffuse contribution, quite

Table 4

Calculated whole-canopy photosynthesis, P_c , by wild type and chlorophyll-deficient mutant soybeans. Canopy temperature is 25 °C, leaf area index 4.0; isotropic leaf orientations. Soil reflectance is 5%. Solar irradiances are specified in $\mu\text{mol m}^{-2} \text{s}^{-1}$ (horizontal projection) for a collimated direct beam I_o at elevation θ_s above the horizon and hemispherically isotropic diffusive beam D_o . For comparison, full sunlight with the sun overhead in a clear sky is approximately $I_o/D_o = 1.2/0.4$ in the units. F_{abs} = fraction absorbed by canopy.

Sky condition $I_o(\theta_s)/D_o$	F_{abs}	Wild type P_c [$\mu\text{mol m}^{-2} \text{s}^{-1}$]	F_{abs}	Mutant P_c [$\mu\text{mol m}^{-2} \text{s}^{-1}$]	Relative "gain" by mutant
Hazy day 0.4 (60°)/0.4	0.875	24.60	0.812	25.03	+1.8[%]
Full overcast 0/0.4	0.871	15.53	0.825	14.49	-6.7[%]
Partial overcast 0.4 (60°)/0.2	0.870	19.49	0.807	19.57	+0.4[%]
Clear sky 0.8 (60°)/0.4	0.870	29.72	0.807	32.08	+7.9[%]
Low sun 0.3 (30°)/0.15	0.916	14.94	0.847	15.13	+1.3[%]
Clear sky, low sun 0.5 (30°)/0.25	0.916	20.59	0.847	21.95	+6.6[%]

important in comparing high $r + t$ mutants to normal plants, from secondary and higher interceptions with intervening reflections and transmissions at other leaves (or soil). I have used Gutschick and Wiegel's (1984) exact integral equation for canopy radiation propagation, with isotropy as a reasonable first approximation for the soybean leaf angle distribution.

It is important to develop P_c estimates for a variety of solar elevations, direct:diffuse ratios, and LAI values. The first two affect single-leaf I , as noted above. Also, diffuse sky radiation such as predominates on cloudy days penetrates less deeply into the canopy than does the direct beam. This decreases the extent of PhAR redistribution and thus also the potential P_c gain of the mutants. LAI is important because the mutants capture fewer photons at single leaves than do the wild types. Total canopy PhAR interception is comparable between mutants and wild type only at high LAI . At high insolation rates, the interception discrepancy becomes mostly irrelevant to relative canopy performance, but at low insolation rates P_c becomes proportional to interception.

Table 4 presents the model results for six different sky conditions, all at $LAI = 4$. The predicted P_c gain of the mutants is modest, not exceeding 8%. With an overcast sky, the mutants may even operate at significant penalties, such as the 6.7% in the second case. Surprisingly, the mutant canopy shows photosynthetic gains even at low insolutions where single mutant leaves are inferior to wild-type leaves (the third and fifth cases). Any estimate of season-long performance, of course, must weight the frequencies of sky conditions and account for LAI history. Performance gains or losses must be compounded; *e.g.* a 5% gain in P_c becomes a 28% gain over five doubling times.

Briefly, the mutants may be expected to show modest superiority in geographical regions with a high proportion of clear days. Cloudy days exact greater penalties early in the season (at low LAI) than later. An additional benefit in total crop performance with the mutants in the favored

bute to control. Current knowledge is largely restricted to leaves at early nodes. While experimental knowledge develops, modelling may at least be solving some problems of what to measure and when, in an economical assay.

Other potential applications for physiological modelling are apparent. A great challenge is identifying optimal physiological patterns (for photosynthesis, water use, or other performance goals) under the ever-present fluctuations in temperature. Certainly, plants adapt photosynthetic capacities and partial-reaction capacities to the longer temperature *trends* (e.g., Berry and Björkman 1980, Turner and Kramer 1980). They cannot adapt to faster fluctuations, and so one may ask, "What is the optimal set point (in RuBPCO or total N investment in the leaf, for example) in a fluctuating environment?" The time-averaged temperature is not a good indicator in general. If it is well below the lowest adapted optimum temperature of the plant, then most photosynthesis will be done during the positive temperature fluctuations, weighting them highly. A performance-weighted average temperature is most relevant for optimization. Some photosynthesis models such as the FCB model resolve the component and net process temperature dependences, and are therefore usable for such optimization. Of course, while modelling may *define* the optimum, one needs experimental data on the mechanistic controls responsive to T , δT that achieve some (usually lesser) degree of optimization. An added complication is the consideration of risk of damage. In an obvious case, that of freezing-injury risk, one realizes there is a balance between carbon gain from developing leaf area and the stochastic risk of carbon loss by freezing or (regenerable) leaves. The drive for maximal leaf area can decrease long-term carbon gain if damaging fluctuations are frequent enough. No physiological models currently incorporate risk.

Another application is the study of plant performance under the greatly increased atmospheric CO_2 concentration apparently destined by fossil-fuel use (Baes *et al.* 1977, Siegenthaler and Oeschger 1978). The CO_2 changes will be accompanied by climatic changes (increased temperature and cloudiness, decreased rainfall in the Northern temperate zone? — Manabe and Wetherald 1975). Together these climatic changes will alter the developmental patterns in many physiological functions — RuBPCO activity, g_s , root nutrient uptake (by changed soil water availability), *etc.* — and will induce adaptations in many integrated functions — leaf expansion, branching patterns, *etc.* (see Hicklenton and Jolliffe 1980, Kramer 1981). These changes are complex and not universal among species or even cultivars. The net effects on performance are often striking. Frequently the vegetative growth rates and final biomass are increased, while the vegetative-to-reproductive shift is delayed (determinate) or the partition decreased (indeterminate), leading to a decrease in reproductive yield. These effects have not been evaluated at high population densities, where source-sink balances shift to favor the sink (Loomis *et al.* 1971, p. 452) and may alleviate the problem, and where canopy density alters the penetration of solar fluence components important for growth (PhAR region), morphogenesis (red, far red, blue), and heat balance (thermal infrared). To interpret future experiments on adaptations and performance changes, the leaf photosynthetic model and the canopy model may be augmented by deterministic physiological models of CO_2 adaptations and other morphogenetic behavior. The latter models are not yet developed and pose a big challenge, as does the task of designing and performing critical experiments.

One can list still more potential applications of physiological leaf photosynthesis modelling. Water-use efficiency and its optimization is an important task; both field management procedures (Bolton 1980) and breeding (Fischer 1980) are relevant to improving performance. Here the leaf model is still significant but admittedly mostly peripheral to the task: (1) very few physiological changes in photosynthesis affect the transpiration ratio (Cowan and Farquhar 1977, Fischer and Turner 1978); an exception is Chl content, as discussed earlier; altered stomatal control is a possibility evaluable in the model, but generally it should be *deoptimizing* for photosynthesis per unit water use. (2) The physiological changes most significant for water-use efficiency are at higher levels not described in the leaf model — e.g., ability to photosynthesize at lower water potential

has been important in improving soybean performance (Boyer 1982), and diaheliotropic behavior of the leaf angle may help water-use efficiency directly in future breeding (Ehleringer and Forseth 1980). For both these examples, the leaf model can help to evaluate "secondary" effects. Other potential applications of the leaf model, properly extended, concern the optimization of mesophyll CO_2 resistance (the partition between air and liquid-phase portions), or of total-plant nitrogen-use efficiency considered for fertilizer input costs rather than plant growth itself.

CONCLUSIONS

The leaf photosynthesis model has been developed for its physiological, predictive capability. It has been largely verified against limited experimental data on soybean (or related species) photosynthesis as dependent on I and on CO_2 and O_2 concentrations. Some weaknesses were indicated in the description of stomatal control and of the stoichiometry of photorespiration. These weaknesses are opportunities for experimental investigations of broader significance. The model appears to be a relatively powerful tool to supplement studies where experiments are difficult or intrinsically obscured by other effects — *e.g.*, evaluating the significance of alternative g_s distributions between top and bottom of the leaf, or assigning functional significance to the structural variation from top to bottom in the leaf.

A major effort in this paper was assessing a potential route to increased whole-canopy photosynthesis by a particular physiological alteration, one that is demonstrably genetically feasible. While the prediction was for modest gains, the modelling suggested new routes of crop improvement where additional modelling could help in designing and interpreting experiments. Other, less-developed capabilities of the model for ecological and agricultural studies are also suggested here.

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