

Development of a Photosynthesis Model with an Emphasis on Ecological Applications.

IV. Wholephot – Whole Leaf Photosynthesis in Response to Four Independent Variables

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Summary. A physiologically based steady-state model of whole leaf photosynthesis (WHOLEPHOT) is detailed which describes the functional dependence of net photosynthesis in C_3 leaves on $[CO_2]$, $[O_2]$, incident radiant flux (PhAR), and leaf temperature. The model simulates among other phenomena a) observed $[CO_2]$, $[O_2]$, and temperature effects on the initial slope of light response curves, b) a C_3 type temperature response curve of net photosynthesis, c) a shift of the optimum temperature of net photosynthesis to higher temperatures with increasing light intensity, and d) observed temperature and $[O_2]$ effects on the CO_2 compensation point. Model parameters are derived from published response data of several C_3 species. Simulations also demonstrate that parameter changes based on literature data result in acclimation-like changes in net photosynthesis response with respect to light intensity and temperature. The advantages of this model are that the number of parameters is minimized in order to focus on environmental effects and that all parameters can be determined from measured net photosynthesis responses.

Introduction

Previously in this series, a general methodology was proposed for description of photosynthesis in a single C_3 leaf in response to $[CO_2]$, $[O_2]$, incident light, and leaf temperature (Tenhunen et al., 1976a). Subsequently, sub-sets of data, representing fundamental sections of the multi-dimensional response surface of photosynthesis were analyzed (Tenhunen et al., 1976b, 1977). In these analyses, clear definitions were proposed for physiologically meaningful model parameters and it was demonstrated how important parameters are obtained from measured response data. Further work (Tenhunen et al., 1979a, b, c) discussed

several problems and limitations confronted in development of such a complex model. A major difficulty is that diffusion resistances between organelles within leaf cells cannot be measured. A second problem is that photorespiratory fluxes and/or simultaneous mitochondrial CO_2 fluxes cannot be measured unaffected by photosynthetic recycling of CO_2 and cell diffusion resistances.

A pragmatic approach to solution of these problems was taken (Tenhunen et al., 1979b) resulting in what has been termed the "basic model". The significant assumptions are that the carbon fixation site and photorespiratory site within the cells are in close association (thus defining diffusion resistances between organelles and the cell wall) and that mitochondrial respiration can be extrapolated from photosynthesis responses measured at low $[\text{O}_2]$ (residual respiration; Tenhunen et al., 1976b). Nevertheless, this basic model is constructed in such a fashion that later modifications of these assumptions can easily be accommodated. The basic model is a sub-set model that applies at any constant light intensity and temperature ($[\text{CO}_2]$ and $[\text{O}_2]$ as independent variables). In the present paper, an initial version of the comprehensive model WHOLEPHOT is presented in which sub-set analyses are combined. The basic model remains a key component but light intensity and temperature dependencies of parameters are included. A calculation procedure is reported in detail which provides the simulated net photosynthesis rate for any combination of the four environmental factors (independent variables) mentioned above.

We have attempted as far as possible to base WHOLEPHOT on data from wheat reported by Jolliffe and Tregunna (1973). Newly derived parameter values thus differ somewhat from those previously reported, but study of this variation is one of the objectives of model development. The response data studied has in most cases been obtained from leaves experiencing optimal conditions of mineral nutrition and water status. It is expected that the model can also be applied to leaves experiencing sub-optimal conditions, e.g. during water stress and at different levels of applied nitrogen or other minerals, but this must yet be tested experimentally. Gaps in knowledge required to complete the comprehensive model are bridged with assumptions based on laboratory experience and on evaluation of data from the photosynthesis literature. The resulting model is tested by comparing predicted responses of net photosynthesis, particularly interactive responses to more than one environmental factor, to similar observed responses of net photosynthesis measured in the laboratory and under natural conditions.

While containing certain aspects which at this time are of a semi-empirical nature, the photosynthesis model proposed here provides an over-all framework for systematic description of net photosynthesis in response to environmental factors. A minimal number of parameters are used to describe the processes. The semi-empirical portions of the model can be improved at a later date without altering those portions that are more soundly based on physiology and biochemistry. The direction attempted in this modeling approach has been consistently toward producing a realistic guide for ecological work; realistic in that parameters and dependencies needed in the model are minimized and a guide in that it helps plan the gathering of data for leaf to leaf photosynthetic comparisons.

Method of Formulation and Description of Wholephot

Several methods of description applied to sub-sets of photosynthetic response data were discussed previously. The definitions and interpretations of individual parameters in the context of present knowledge of photosynthetic processes were also discussed. Parameter values are identified and discussed here in the order in which they enter calculations in the comprehensive model. Step by step procedures of calculation are reiterated in the appendix. The appendix, studied with reference to the publications mentioned above, provide the best means of familiarizing oneself with the details of calculation leading to all simulations presented.

1. Overview

The simplified leaf photosynthetic system treated by the model is shown in Fig. 1. The system shown considers two compartments, one at the site of carboxylation and the second at the site of decarboxylation. The compartments are separated from each other and from the air space atmosphere by diffusion resistances (Tenhunen et al., 1977, 1979b). Central to the model are Michaelis-Menten competitive kinetics controlling flow of carbon to photosynthetic and photorespiratory products at RuDP carboxylase/oxygenase. For a detailed kinetic analysis of the system shown see Peisker (1976). As discussed elsewhere (Tenhunen et al., 1979a), it may be possible in the future to equate the parameters of this model with functions of more detailed biochemical parameters considered in other models (Peisker, 1976; Hall and Björkman, 1975). The simpler parameters of Michaelis-Menten functions allow more attention to be focused on environmental aspects of the modeling problem.

With light intensity and leaf temperature constant, carbon fixation is described as a function of the system carboxylation and oxygenation characteristics and the diffusion resistances between compartments (Tenhunen et al., 1977, 1979a, b, c). Essential parameters are the maximum rate for photosynthesis, P_M ; the maximum rate of CO_2 evolution in photorespiration, W_M ; a coefficient, K_C , equal to the calculated chloroplast $[\text{CO}_2]$ at which total photosynthesis is half maximal ($[\text{O}_2] \approx 0$); a coefficient, K_{O_2} , equal to the $[\text{O}_2]$ at which photorespiratory CO_2 evolution is half maximal ($[\text{CO}_2] \approx 0$); and an effective diffusion

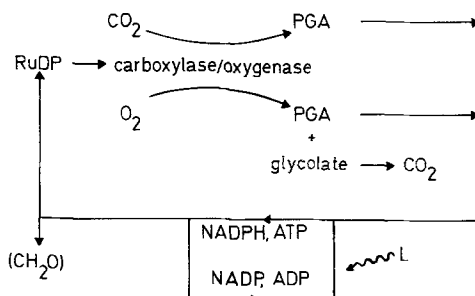


Fig. 1. Simplified scheme of leaf photosynthetic carbon metabolism from Peisker (1976) showing the components included in WHOLEPHOT. Photoproducts drive the reduction of Calvin cycle intermediates to regenerate RuDP which then undergoes carboxylation or oxygenation

resistance between the mesophyll air space and chloroplast fixation site, R_M . When light and temperature dependencies of these five parameters have been defined, the general comprehensive model of leaf photosynthesis is obtained. In other words, from defined light and temperature dependencies, specific values are obtained for each parameter valid at a specific constant light intensity and leaf temperature, and then net photosynthesis is calculated according to Tenhunen et al. (1977; see also Appendix).

2. $P_M = f(L, T_K)$

The behavior as a function of incident light (L) and absolute leaf temperature (T_K) of the maximum capacity for total photosynthesis (P_M) is relatively easily described (Tenhunen et al., 1976b). The rate of Calvin cycle processes is limited on the one hand by production of photoproducts in the light reactions (see also Prioul and Chartier, 1977; Tenhunen et al., 1979a) and on the other hand by temperature activation and denaturation of rate limiting enzymatic steps in the Calvin cycle in general.

A specific value of P_M is calculated for the present model as follows: P_{MLT} (the maximum capacity for photosynthesis at saturating $[CO_2]$, low $[O_2]$, saturating light, and optimal leaf temperature) is set at $4.0 \text{ nM CO}_2 \text{ cm}^{-2} \text{ s}^{-1}$ (an average for a variety of C_3 plants, Tenhunen et al., 1976b; Hesketh, 1963; Rabinowitch, 1951). Rates are defined on the basis of surface area, since this most advantageously interfaces leaf and environment with respect to incident light, gas exchange through stomata, and determination of leaf temperature via the energy budget. Considerable natural variation in P_{MLT} may occur depending on plants and growth conditions (Harley, unpublished; Slatyer and Morrow, 1977; Angus and Wilson, 1976).

A value of P_{ML} (at saturating $[CO_2]$, low $[O_2]$, saturating light, and a specific leaf temperature) is determined with the Johnson, Eyring, and Williams equation (Tenhunen et al., 1976b) describing over-all temperature activation and denaturation of the process. As discussed in detail previously, important parameters are the activation energy for the photosynthetic process, $\Delta H\ddagger$; the activation energy of the denaturation process, ΔH_1 ; the entropy of the denaturation process, ΔS ; and a scaling factor, C_2 . Values for these parameters included in the appendix are derived from data on wheat obtained by Jolliffe and Tregunna (1973, their Fig. 2) where $[O_2]$ is 1% and $[CO_2]$ is saturating. These data approximate rates at saturating light intensity. Parameter values are the following; $\Delta S = 153.4$ entropy units; $\Delta H\ddagger = 14,200 \text{ cal M}^{-1}$; $\Delta H_1 = 47,700 \text{ cal M}^{-1}$; and $C_2 = e^{22.47}$. Methods of analysis and comparable parameter values for *Phaseolus vulgaris* were reported previously (Tenhunen et al., 1976b).

A value of P_M (at saturating $[CO_2]$, low $[O_2]$, a specific light intensity, and a specific temperature) is obtained from the function describing a photosynthesis light dependency at constant temperature, saturating $[CO_2]$, and low $[O_2]$. If the Smith equation is used to approximate this function (Tenhunen et al., 1976a, 1979a), two parameters are important. These are the value of P_{ML} already determined above, and the value of α , the maximum light utilization

efficiency or the initial slope of the light response curve when photorespiration does not occur, e.g. at saturating $[\text{CO}_2]$ and low $[\text{O}_2]$. Alpha itself is temperature independent (Tenhunen et al., 1976 b). Alpha is set here equal to 50.0 nanomoles CO_2 fixed/microEinstein incident light, a value which agrees well with determinations of this efficiency for a variety of C_3 plants (Tenhunen et al., 1976 b; Hall, 1970; Ehleringer and Björkman, 1977).

3. $W_M = f(L, T_K)$

The behavior as a function of incident light and absolute leaf temperature of the maximum capacity for photorespiration (W_M) of the intact leaf is difficult to measure. It is our opinion that the only appropriate estimates that have been made from intact leaves for this parameter value, are those obtained by analysis of the positioning of CO_2 responses of net photosynthesis rate at 21% oxygen with respect to responses at 1% oxygen (Tenhunen et al., 1977, 1979 b). All data providing such a comparison that we have found were studied extensively according to these methods. These data include those of Ludwig (1972), Jolliffe and Tregunna (1973), Lommen et al. (1975) and Ku and Edwards (1977). Few of these families of response curves are ideal due to unmeasured stomatal resistance, non-steady-state methods, lack of replication, limited range of $[\text{CO}_2]$, or inaccurate determination of gas concentrations. Nevertheless, the following generalizations can be made.

In those cases where measurements appear to be reliable and where $[\text{CO}_2]$ is increased into the saturation range for photosynthesis, W_M was found to be more or less the same order of magnitude as P_M . Setting W_M equal to or proportional to P_M is theoretically supportable if the system is validly described by Fig. 1 (Peisker, 1976). Light affects the recycling of substrates which then affect similarly either reaction at the carboxylase/oxygenase. Temperature affects either recycling of substrates or the fixation enzyme itself and a similar effect should be seen on photosynthesis and photorespiration. Temperature activation energies for W_M and P_M derived from the Jolliffe and Tregunna data are approximately equal. Activation energies of the carboxylation and oxygenation functions of RuDP carboxylase/oxygenase *in vitro* are known to be approximately equal (Laing et al., 1974; Badger and Collatz, 1977). In other words, the general behavior of the two processes theoretically should be similar and experimentally appears to be similar with respect to light and temperature. If W_M is equal or proportional to P_M , simulation of this behavior is achieved.

If W_M is set equal to P_M , the analysis still results in a good description of observed data (Tenhunen et al., 1979 c). The consequences are that a parameter is eliminated from the model, that K_{O_2} is altered in value for a particular data set to compensate for the restriction on W_M , and that K_{O_2} is primarily responsible for the amount of inhibition of photosynthesis occurring in the presence of oxygen. It was decided to set $W_M = P_M$ since these consequences are not particularly negative, at least until further data are gathered that allow reevaluation of the assumption.

$$4. K_C = f(L, T_K); K_{O_2} = f(L, T_K)$$

The lack of appropriate data for study of W_M discussed above also creates similar difficulties in defining the light and temperature dependencies of K_C , K_{O_2} , and R_M . Results of all analyses for K_C from 1% oxygen CO_2 response curves were discussed by Tenhunen et al. (1979c). The estimates are extremely scattered. Nevertheless, for what has been termed the basic model (fixation and photorespiratory sites close together), the order of magnitude of K_C is around 0.1 to 1.0 nM cm⁻³. Estimates of K_C from the wheat data of Jolliffe and Tregunna (mean for 80 seedlings) suggested a temperature dependency for K_C similar to that reported for the enzyme affinity constant for CO_2 of RuDP carboxylase/oxygenase by Laing et al. (1974; verified by Badger and Collatz, 1977). Insufficient information was obtained from extant leaf data to estimate the temperature dependency of K_{O_2} , but the magnitude obtained for data from Jolliffe and Tregunna with the basic model is approximately 9% oxygen.

Based on the similar temperature dependency in K_C values from Jolliffe and Tregunna and enzyme data mentioned above and because such temperature dependencies offer an explanation for observed increase in oxygen inhibition of photosynthesis at higher temperatures in intact leaves (Jackson and Volk, 1970; Chollet and Ogren, 1975), temperature dependencies for carboxylase/oxygenase affinities for CO_2 and O_2 were used to define temperature dependencies for K_C and K_{O_2} . The magnitude of K_C and K_{O_2} is determined by the diffusion relations within leaf cells assumed in the analysis. For the basic model, mean values for K_C of 0.435 nM CO_2 cm⁻³ and for K_{O_2} of 9% oxygen are obtained from analysis of the Jolliffe and Tregunna data.

These mean values were used to define K_C and K_{O_2} at the mean temperature of measurement, 30°C. Values at other temperatures were obtained by multiplying

by a factor $\frac{K_m(CO_2)_t}{K_m(CO_2)_{30}}$ or $\frac{K_m(O_2)_t}{K_m(O_2)_{30}}$. $K_m(CO_2)$ and $K_m(O_2)$ are the affinity

constants found for CO_2 and O_2 with RuDP carboxylase/oxygenase by Laing et al. (1974) in soybean at temperatures t (variable) and 30°C respectively.

The temperature dependent value of K_C in nM cm⁻³ is thus described with Eq. (1):

$$K_C = -1478.9 + 15.361 T_K - 0.053188 T_K^2 + 0.61405 \times 10^{-4} T_K^3 \quad (1)$$

Further, the temperature dependent value of K_{O_2} expressed as a volume fraction (9% O_2 is indicated by a value of 0.09) is given by Eq. (2):

$$K_{O_2} = 0.29068 - 0.67253 \times 10^{-3} T_K \quad (2)$$

No data exist from which light dependencies of K_C or K_{O_2} may be determined. Required are families of CO_2 responses at different light intensities. However, since there is no evidence indicating a direct light effect on the properties of fixation enzymes, light is assumed to have no influence on K_C and K_{O_2} .

5. $R_M = f(L, T_K)$

R_M is determined from the initial slope of the CO_2 response curve at 1% oxygen. How this slope changes over a wide temperature range is uncertain. Study of available data resulted again in a large scattering of estimates of R_M at different temperatures. In some cases such scatter may be due to the phenomenon of photoinhibition in leaves exposed to extremely low $[\text{CO}_2]$ in the presence of oxygen (C.B. Osmond, personal communication) and further careful experimentation is needed.

Certain studies that have considered the temperature dependence of mesophyll resistance, suggest that R_M decreases to a minimum between 25° and 35° C and then increases rapidly (Doley and Yates, 1976; Neilson et al., 1972). The resistance determined in these cases, however, is determined at 21% oxygen and contains a photorespiratory component. In the present studies, R_M is treated more simply as a constant equal to 5.86 s cm^{-1} or as a linear function of temperature (described in results section) to study possible resistance effects on the photosynthesis response. The value 5.86 was obtained as a mean resistance value for wheat from analysis of the data of Jolliffe and Tregunna. Other constant values were also used as described in the results section.

Mesophyll resistance may be dependent on light intensity. Chloroplast re-orientation, for example, might result in change in this parameter value. Due to lack of quantifiable information, R_M is assumed to be independent of light intensity.

6. The Photosynthesis Rate

As described previously for the basic model (Tenhunen et al., 1977, 1979 b), a parameter M describing the geometric arrangement of cell organelles is set equal to 100 (chloroplast and photorespiratory sites in close association). An iterative solution is performed to obtain the photosynthesis rate including residual respiration. Residual respiration (Tenhunen et al., 1976 b) was estimated from 1% oxygen CO_2 response curves at six temperatures from the Jolliffe and Tregunna data. These estimates result in the following equation for residual respiration after regression analysis according to the Arrhenius equation.

$$W = J \cdot e^{(25.19 - (13,000 / (1.987 \times T_k)))} \quad (3)$$

where: W is the residual respiration rate in picomoles $\text{cm}^{-2} \text{ s}^{-1}$

J provides the proper units = 1 picomole $\text{cm}^{-2} \text{ s}^{-1}$

The correct net photosynthesis rate is obtained by subtracting residual respiration from the photosynthesis rate including residual respiration. Net photosynthesis responses were simulated for various combinations of CO_2 , O_2 , light intensity, and temperature as described below.

Results of Simulations

The behavior of WHOLEPHOT was studied by simulating general types of responses of net photosynthesis as discussed in the following sub-sections. These simulations are used as an initial test of the model by comparison to known behavior of C_3 leaf net photosynthesis. The comparison is qualitative since WHOLEPHOT represents a generalized plant leaf in which resistance is constant at values discussed below. This single resistance can be considered as the mesophyll resistance entirely with stomatal resistance zero or as a lumped resistance of mesophyll and stomatal components that is constant. Of interest is how the photosynthetic components respond when observed external to the leaf and as the environmental conditions are altered.

Light Response of Photosynthesis

At a constant temperature, predicted light response curves of net photosynthesis are obtained by varying light intensity with $[CO_2]$ and $[O_2]$ in the intercellular air space (input conditions for the model – see appendix) at set values. The only effect of light intensity is on $P_M = W_M$. Typical simulation results are shown in Fig. 2. Curve A is obtained at $40 \text{ nM } CO_2 \text{ cm}^{-3}$ (approximately 1,000 ppm), $[O_2] = 0.01$ (1% oxygen), and 25°C ; curve B at 13.5 nM cm^{-3} (330 ppm), $[O_2] = 0.21$ (21% oxygen), and 25°C . High $[CO_2]$ and/or low $[O_2]$ are found to prevent a strong photorespiratory effect on photosynthesis and the initial slope of the light response approximately equals α ($50.0 \text{ nM per } \mu\text{E}$; see also Tenhunen et al., 1979a). In case B, photorespiration and an altered competitive situation lead to inhibition of net photosynthesis and a change in the shape of the light response in a manner which has been described in detail for *Beta vulgaris* by Hall (1970) and for other C_3 species.

As seen in Fig. 2, the simulated initial slope of the light response curve decreases as photorespiration significantly alters the response. This initial slope is thus a function of $[CO_2]$ and $[O_2]$ with the maximum value of $\alpha = 50.0 \text{ nM}/\mu\text{E}$. Shown in Fig. 3 are the predicted effects of $[CO_2]$ between zero and approximately $40 \text{ nM cm}^{-3} CO_2$ (1,000 ppm) at 1 and 21% oxygen ($[O_2] = 0.01$ and 0.21 respectively) and 30°C . At 1% oxygen, photorespiration does not occur and the initial slope approaches α at all $[CO_2]$. Only at very low $[CO_2]$ is the initial slope decreased. At 21% oxygen, an inhibition of the initial slope with respect to 1% oxygen is seen. The inhibition, as a percent of the 1% oxygen initial slope, is large at low $[CO_2]$ and decreases rapidly to approximately 15% at $13.2 \text{ nM cm}^{-3} CO_2$ (330 ppm) and then decreases more slowly. Figure 3 reproduces very closely in simulation the observed data from *Encelia californica* at 30°C reported by Ehleringer and Björkman (1977, their Fig. 2).

The initial slope of the light response can also be studied with respect to temperature. In Fig. 4, the simulated initial slope is shown for 2 degree steps in leaf temperature at 330 ppm CO_2 ($[CO_2]$ in nM cm^{-3} is temperature dependent) and 1% and 21% oxygen. At 1% oxygen, photorespiration is essentially zero. A slight influence of photorespiration is seen on the initial slope

Fig. 2. Light response curves of net photosynthesis simulated with WHOLEPHOT at 40 nM CO₂ cm⁻³ (1,000 ppm) and 1% oxygen (curve A) and at 13.5 nM cm⁻³ (330 ppm) and 21% oxygen (curve B). Gas concentrations are outside a mesophyll and/or stomatal resistance of 5.86 s cm⁻¹. Leaf temperature is 25° C

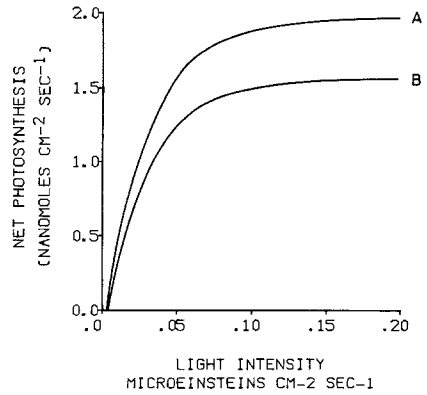


Fig. 3. Initial slope of the light response curve of net photosynthesis as affected by CO₂ concentration at 1 and 21% oxygen simulated from WHOLEPHOT. The inhibition of slope at 21% oxygen as a percent of the slope at 1% oxygen is also shown. Leaf temperature is 30° C

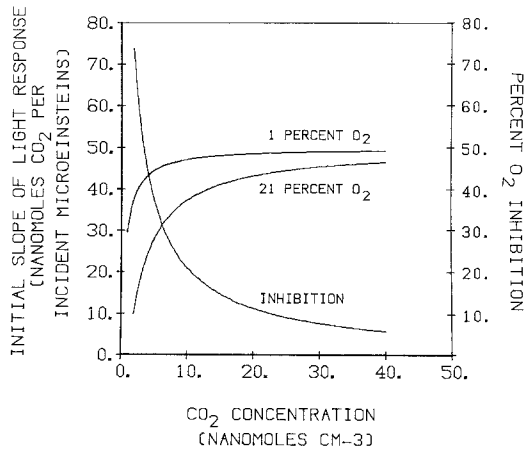
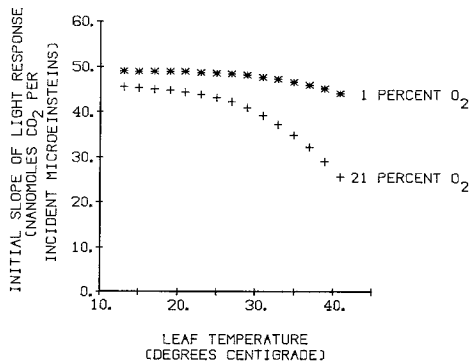


Fig. 4. Initial slope of the light response curve of net photosynthesis as affected by leaf temperature at 1 and 21% oxygen simulated from WHOLEPHOT. CO₂ concentration is 330 ppm (temperature dependent when expressed in nM cm⁻³)



of the light response at very high temperature due to rapid increase in K_C . At 21% oxygen, increased inhibitory effect of oxygen on net photosynthesis decreases the initial slope by approximately one third at 35° C. The results shown in Fig. 4 reproduce very closely in simulation the observed data on *Encelia californ-*

nica reported by Ehleringer and Björkman (1977, their Fig. 3). The simulated 1% oxygen response in Fig. 4 is essentially the same as that reported for the C_4 plant *Atriplex rosea* by the same authors. The only difference is that for simulated C_3 leaves at 1% oxygen a greater initial slope occurs at all temperatures since C_4 leaves require more ATP for two CO_2 fixation steps in series.

Temperature Responses of Photosynthesis

It is instructive to consider components of the predicted temperature response curve from WHOLEPHOT. Following the example of Hesketh and Baker (1967, their Fig. 2) and Larcher (1969, his Fig. 5), the curves shown in Fig. 5 were simulated. Light intensity is high ($=0.18 \mu E \text{ cm}^{-2} \text{ s}^{-1}$). Curve A demonstrates the type of net photosynthesis response obtained from WHOLEPHOT at $[CO_2]$ of 40 nM cm^{-3} (1,000 ppm) and 1% O_2 . This potential net photosynthesis response is observed in C_3 leaves under non-photorespiratory conditions (Tenhunen et al., 1976b) and resembles the temperature response of C_4 leaves which are able to effect non-photorespiratory conditions.

Curve B is the net photosynthesis response curve obtained when $[CO_2]$ is decreased to 330 ppm ($[CO_2]$ temperature dependent). Photorespiration (shown as curve E) and change in the effective carboxylation affinity constant leads to a decrease in photosynthesis from A to B. Curve C is obtained with an increase in $[O_2]$ to 21% (ambient air in the intercellular air space, i.e. 330 ppm CO_2). Photorespiration (curve D) increases and is activated more strongly by increasing temperature between 25° and 35° C. This temperature activation overcomes more fully the increase in net photosynthesis due to temperature activation of the photosynthetic maximum and shifts the optimum temperature to a much lower temperature than seen in either curve A or B.

The predicted interaction of light intensity with the leaf temperature response (with ambient air outside the resistance) is shown in Fig. 6. At low light intensity ($0.01 \mu E \text{ cm}^{-2} \text{ s}^{-1}$), the temperature optimum is at a rather low temperature (21–23° C). As light intensity increases the optimum shifts to higher temperatures. Figure 6 reproduces in simulation a similar shift in temperature optimum long observed in C_3 leaves, cf. Pisek et al. (1973, their Fig. 3).

CO₂ Compensation Point Behavior

A common characteristic measured for plant leaves is the CO_2 compensation concentration at which respiratory processes balance photosynthesis resulting in zero net photosynthesis. It was previously shown that the model correctly described the compensation point as a function of $[O_2]$ at 25° C based on analysis of the data of Ludwig (Tenhunen et al., 1977). The compensation point is also affected by temperature and the predicted behavior from WHOLEPHOT is shown in Fig. 7. Figure 7 reproduces in simulation, responses of this type observed in wheat by Jolliffe and Tregunna (1973, their Fig. 9).

Fig. 5. Temperature dependencies of metabolic and gas exchange processes in the leaf simulated with WHOLEPHOT. Net photosynthesis at $[CO_2]=40 \text{ nM cm}^{-3}$ (1,000 ppm) and 1% oxygen (curve A); at 330 ppm CO_2 and 1% oxygen (curve B); and at 330 ppm CO_2 and 21% oxygen (curve C). Predicted photorespiration rate occurring with curve B (curve E) and with curve C (curve D). Light intensity equal to $0.18 \mu\text{Einstein cm}^{-2} \text{ s}^{-1}$

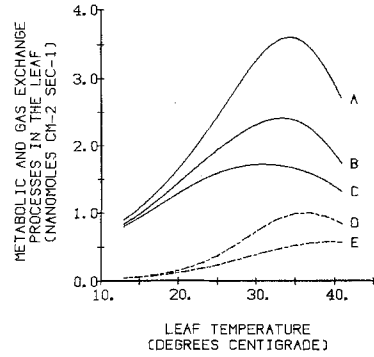


Fig. 6. Temperature dependencies of net photosynthesis simulated with WHOLEPHOT at three light intensities (0.01; 0.02; and $0.18 \mu\text{Einsteins cm}^{-2} \text{ s}^{-1}$) and at 330 ppm CO_2 and 21% oxygen. Temperature optimum shifts to higher temperature with increase in light intensity

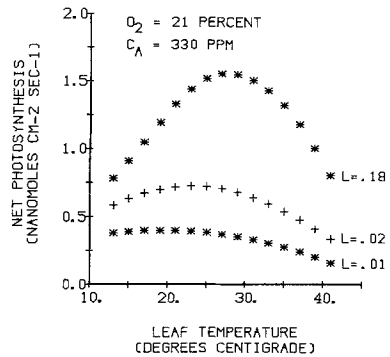
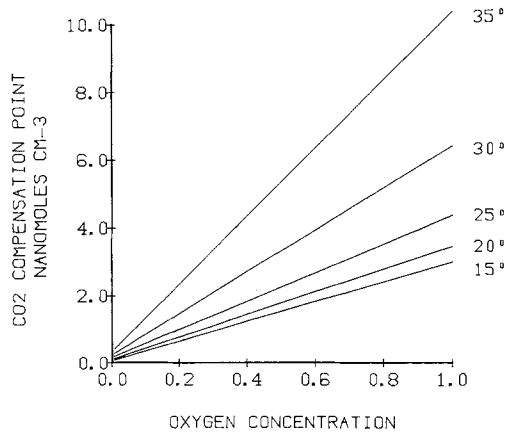


Fig. 7. Carbon dioxide compensation point obtained from simulations with WHOLEPHOT as a function of oxygen concentration and leaf temperature in degrees C. Light intensity is $0.18 \mu\text{Einstein cm}^{-2} \text{ s}^{-1}$



Photosynthetic Acclimation to Temperature

One application of WHOLEPHOT is in the study of leaf photosynthetic acclimation and adaptation. Strain et al. (1976) point out the many studies made with a wide variety of plants demonstrating consistent shifts in the photosynthetic optimum temperature to higher or lower temperatures depending on higher

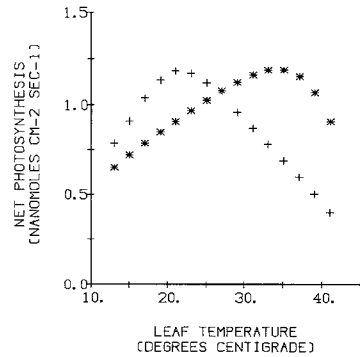
or lower growth temperatures respectively. Such shifts occur within 24 h (Mooney and Harrison, 1970; Mooney and Shropshire, 1967) and are complex, e.g. leaves show altered dark respiration, stomatal resistance, mesophyll resistance, etc. Further experience will show whether applying WHOLEPHOT to temperature pre-treated plants will allow a quantified determination of change in one or several component parameters effecting the ambient net photosynthesis response. Because of the method of parameter evaluation and subsequent calculation, it may be possible to resolve some aspects of the interactive effects of environmental factors on photosynthesis.

Simulations were undertaken to determine whether WHOLEPHOT possessed the capacity to reproduce acclimation-like responses. Varying any of several parameters, within a range of physiologically realistic values, results in a shift of the temperature optimum of 10° to 15° C. For example, increasing the total diffusion resistance from 1.0 s cm⁻¹ to 20.0 s cm⁻¹ shifts the ambient leaf temperature optimum in WHOLEPHOT at high light intensity and with ambient air from 30° C to 20° C. Increased resistance in the mesophyll and/or due to altered stomatal reaction have been reported for cold-treated *Encelia californica* by Mooney and Harrison (1970). The shift in optimum to lower temperature due to increase in resistance with the model is due to change in [CO₂] at the fixation site, altered competitive relationships with respect to CO₂ external to the leaf and to oxygen, and change thereby in the photosynthesis to photorespiration ratio. That increased resistance leading to more photorespiration may in fact occur is supported biochemically by observations of Sawada and Miyachi (1974a, b) of proportionally more labelling of photorespiratory products in wheat leaves grown at cold temperatures.

Possible reasons for increased resistance to CO₂ diffusion in response to cold temperature treatment may be altered cytoplasm consistency (higher sucrose, Sawada and Miyachi, 1974a) or changes in membrane permeability to CO₂. Starch increases dramatically in response to a single cold night treatment in some plants (Hilliard, 1975). Such starch build-up due to low temperature might affect chloroplast permeability or diffusion relationships within the chloroplast. Smith and Struckmeyer (1974) indicate that "chloroplasts in cool-temperature [grown alfalfa] leaflets could not be identified readily because of the large accumulation of starch."

A characteristic simulated shift in photosynthetic optimum is shown in Fig. 8. In this case, an imposed change in the linear temperature dependency of mesophyll resistance (R_M) as opposed to a discrete change in R_M , is responsible for the change in the ambient temperature response curve (see figure caption; see also Tenhunen et al., 1979a, Fig. 15). When the temperature optimum shifts to lower temperature, a stimulation of the magnitude of photosynthesis at low temperatures occurs. The simulations thus reproduce a phenomenon described clearly by Strain et al. (1976, Fig. 1) for *Pinus taeda*. Both in that study and in this simulation, no change in the magnitude of photosynthesis at optimum temperature occurs. Few studies have as yet considered changes in the temperature dependency of R_M with temperature treatment. Doley and Yates (1976) and Neilson et al. (1972) indicate that the mesophyll resistance temperature dependency may be altered in response to growth temperature. However, their

Fig. 8. Simulated shift in the temperature dependency and temperature optimum of net photosynthesis. In this particular case, shift occurs due to change in mesophyll resistance. Optimum shifts to higher temperatures (* symbols) when resistance decreases from 15 s cm^{-1} to 5 s cm^{-1} across the temperature range shown and shifts to lower temperatures (+ symbols) when resistance increases from 5 s cm^{-1} to 15 s cm^{-1} . Carbon dioxide concentration is 330 ppm; oxygen concentration is 21%; and light intensity is $0.18 \mu\text{E cm}^{-2} \text{ s}^{-1}$.



dependencies are not measured under conditions (1% oxygen) which eliminate photorespiratory effects and are thus difficult to relate to R_M .

Changes in K_C or K_{O_2} obviously affect the relationship of photosynthesis to photorespiration and thereby the temperature optimum. Such effects are not considered here since so little in general is known about these parameters. Changes in mitochondrial and residual respiration probably occur but are not discussed at this time. More interesting is that change in the magnitude of the maximum capacity for photosynthesis (P_{MLT}) significantly alters the temperature optimum. As P_{MLT} changes, P_M and W_M change equally ($P_M = W_M$) but the effect on photorespiration and photosynthesis changes in a more complex manner regulated by the competitive interplay at carboxylase/oxygenase. If P_{MLT} is increased, for example, from 4.0 to $8.0 \text{ nM cm}^{-2} \text{ s}^{-1}$ with a total resistance of 10.0 s cm^{-1} , the optimum temperature shifts from 25°C to 19°C , or with a resistance of 20 s cm^{-1} , shifts from 19°C to 13°C . By such a change in P_{MLT} , photorespiration is favored at high temperatures and photosynthesis at low temperatures. The results obtained due to an increase in P_{MLT} are also represented by Fig. 8, i.e. the magnitude of photosynthesis at the optimum temperature remains essentially the same. P_{MLT} may be influenced in nature by the concentration of carboxylase/oxygenase present. Concentration of carboxylase/oxygenase has been shown in some plant populations of *Dactylis glomerata* (Treharne and Eagles, 1970) to increase greatly when plants are grown under cold temperatures. On the other hand, results from *Larrea divaricata* (Mooney et al., 1977) indicate that shift in the temperature optimum may in some cases occur without change in P_{MLT} or concentration of carboxylase/oxygenase.

The results obtained by Sawada and Miyachi (1974a) from wheat indicate that shift of the optimum to lower temperature may be accompanied by a decrease in magnitude of photosynthesis at the optimum in contrast to the situation found in *Pinus taeda*. With WHOLEPHOT this case is found when P_{MLT} and resistance increase simultaneously. The most interesting thing to note with respect to temperature acclimation is that while several factors might possibly change, an increase in mesophyll and/or stomatal resistance is expected to contribute in a major way to the final response. This does not seem to be the case for light acclimation.

Photosynthetic Acclimation to Light

Light acclimation has most often been shown as an increase in capacity for photosynthesis (at ambient $[\text{CO}_2]$ and $[\text{O}_2]$ and light saturation) associated with increased dark respiration (Björkman et al., 1972). A reasonable assumption is that P_{MLT} is dependent on growth light conditions, i.e. maximum capacity of the over-all system increases. This is supported by light curves measured at 1.5% oxygen in *Atriplex patula* ssp. *hastata* by Medina (1971, Fig. 55). It should be apparent from the discussion of temperature acclimation, however, that change in P_{MLT} alone does not result in dramatic increases in photosynthesis rates at the ambient air photosynthesis temperature optimum. Increasing P_{MLT} with everything otherwise constant only increases photosynthetic capacity in ambient air below the optimum and simultaneously lowers the optimum. Thus in plants with a high optimum temperature, the effect of an increase in P_{MLT} would be more likely translated into an increase in photosynthesis rates under ambient conditions in general.

Relatively high temperature optima are predicted with WHOLEPHOT for C_3 leaves with low mesophyll resistance (and/or stomatal resistance). Such leaves will profit most from an increase in P_{MLT} but also link high realization of photosynthetic capacity to those C_3 plants able to obtain abundant water. C_4 plants (K_{O_2} infinitely large) have extremely high temperature optima and will profit much more readily from an increase in P_{MLT} . To increase photosynthesis at the optimum temperature, increase in P_{MLT} must be linked with a decrease in mesophyll and/or stomatal resistance. Such an effect is seen in *Atriplex patula* ssp. *hastata* (Medina, 1971, Table 29). Increase in concentration of carboxylase/oxygenase and altered leaf structure may both contribute to effecting this lower mesophyll resistance (see Boardman, 1977). Finally, the results of Medina (1971, Fig. 55) suggest that α may increase in leaves grown under high light intensity. This may be due to increase in components of the light reactions (Björkman et al., 1972).

Conclusion

The results presented above demonstrate that the model WHOLEPHOT includes sufficient detail to provide a general description of behavior of leaf net photosynthesis. Simulations shown in Fig. 2 through 8 were chosen as test criteria due to the relatively frequent discussion of such phenomena. The real advantage of WHOLEPHOT is that all parameters are obtainable from standard types of steady-state photosynthesis measurements (Tenhunen et al., 1976b, 1977). Within present limitations of our knowledge of leaf physiological processes, all parameters can be interpreted in a physiological sense. Reinterpretation of parameter meaning can be expected, but the advantage gained with WHOLEPHOT in planning data gathering will not be affected by such reinterpretation. The number of parameters which must be evaluated as affected by light and temperature and then according to growth treatment and age are minimal.

While it is apparent that interpretation of leaf photosynthesis data with a model such as WHOLEPHOT offers a new viewpoint for understanding acclimation and adaptation of metabolic processes, it is equally apparent that new studies must be conducted in order to obtain data which allow plant to plant comparisons of parameters. The most interesting photosynthesis data (measured under ambient conditions of CO_2 and O_2) can be predicted only indirectly from such a model. Measurement of photosynthesis under "non-ecological" extreme conditions allows parameter determination and such measurements have seldom been made. That these parameters are relevant to steady-state laboratory photosynthesis measurements is apparent from the results presented above. A following paper in this series will demonstrate that they are equally relevant to field measured photosynthesis where light, leaf temperature, and leaf internal CO_2 concentration fluctuate.

Future investigations based on this comprehensive model may demonstrate that simpler versions of the model can also be used, thus allowing the emphasis during measurement to be placed on variation in fewer factors than discussed here. This would be extremely desirable from many standpoints. On the other hand, the need for further development of a comprehensive model that allows simultaneous study of many photosynthetic characteristics is apparent from the large number of unanswered questions arising from study of photosynthesis in plants grown under different light and temperature conditions.

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Appendix

Detailed Calculation Procedure of WHOLEPHOT

Net photosynthesis rate as a function of four independent variables is calculated in WHOLEPHOT in the following manner. Input to the model are values of absolute leaf temperature (T_K) in degrees K , incident light intensity (L) in $\mu\text{Einstein cm}^{-2} \text{ s}^{-1}$, $[\text{CO}_2]$ in nM cm^{-3} (C_w), and $[\text{O}_2]$ as a volume fraction (see equation 2 of text). The gas concentrations are understood to be measured in the intercellular air space, i.e. outside a resistance component in the cytoplasm (R_M). R_M is set at a constant value, here initially = 5.86 s cm^{-1} . A second diffusion factor also influences photosynthesis rate but is expressed in terms of R_M and a ratio M (arbitrarily set equal to 100 in the "basic model") which is the diffusion resistance from cell wall to chloroplast divided by the diffusion resistance from photorespiratory site to chloroplast (see Tenhunen et al., 1977). One can also think of the input resistance value (R_M) as a lumped value for mesophyll plus stomatal resistance, although a small error is thereby introduced. This is discussed further in a subsequent publication.

Constant values must be known from previous study for the following parameters: $\Delta H \ddagger = 14,200 \text{ cal M}^{-1}$; $\Delta H_1 = 47,700 \text{ cal M}^{-1}$; $\Delta S = 153.4$ entropy units; $C_2 = e^{22.47}$; $P_{MLT} = 4.0 \text{ nM cm}^{-2} \text{ s}^{-1}$; R (gas constant) = $1.987 \text{ cal } ^\circ\text{K}^{-1} \text{ M}^{-1}$; and $\alpha = 50.0 \text{ nM } \mu\text{E}^{-1}$ (see text and Tenhunen et al., 1976a, b). The maximum value for photosynthesis rate under particular light and temperature conditions is then obtained.

$$P_{ML} = \frac{P_{MLT}}{100} \times \frac{C_2 \cdot T_K \cdot e^{-\Delta H^*/RT_K}}{1 + e^{-\Delta H_1/R \cdot T_K} \cdot e^{\Delta S/R}} \quad (\text{A.1})$$

$$P_M = \frac{\alpha L}{[1 + (\alpha^2 L^2 / P_{ML}^2)]^{1/2}} \quad (\text{A.2})$$

As discussed in the text, $W_M = P_M$; and K_C and K_{O_2} are found from text Eqs. (1) and (2) respectively. Three equations must be balanced to obtain the photosynthesis rate. The iteration is necessary because the chloroplast $[CO_2]$ which influences photorespiration rate is not known. An initial value of chloroplast $[CO_2]$ (C_c) is chosen and used to calculate the rate of photorespiration (W_p).

$$W_p = \frac{W_M [O_2]}{[O_2] + K_{O_2} \left(1 + \frac{C_c}{K_C}\right)} \quad (\text{A.3})$$

Then W_p is used in the net photosynthesis equation:

$$P = \frac{AA - [(AA)^2 - BB]^{1/2}}{2R_M} \quad (\text{A.4})$$

where:

$$AA = C_w + K_C \beta + R_M (P_M - W_p) - W_p \left(\frac{R_M}{1 + M}\right)$$

$$BB = 4R_M \left[\left(C_w - W_p \frac{R_M}{1 + M} \right) (P_M - W_p) - W_p K_C \beta \right]$$

$$\beta = \left(1 + \frac{[O_2]}{K_{O_2}} \right)$$

The values obtained for W_p and P are used in Fick's Law equation to calculate a new C_c compatible with these fluxes.

$$C_c = C_w - PR_M - W_p \left(\frac{R_M}{1 + M}\right) \quad (\text{A.5})$$

The second estimate of C_c is compared to the first and used again in Eq. (A.3) until the change in C_c between iteration steps is acceptably small.

The corrected net photosynthesis rate is obtained by subtracting residual respiration.

$$P_N = P - (W/1000) \quad (\text{A.6})$$

where: W is obtained from Eq. (3) in the text.

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