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GROW1: A CROP GROWTH MODEL FOR ASSESSING IMPACTS OF GASEOUS POLLUTANTS FROM GEOTHERMAL TECHNOLOGIES

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GROW1: A CROP GROWTH MODEL FOR ASSESSING IMPACTS OF GASEOUS POLLUTANTS FROM GEOTHERMAL TECHNOLOGIES

ABSTRACT

A preliminary model of photosynthesis and growth of field crops was developed to assess the effects of gaseous pollutants, particularly airborne sulfur compounds, resulting from energy production from geothermal resources. The model simulates photosynthesis as a function of such variables as irradiance, CO_2 diffusion resistances, and internal biochemical processes. The model allocates the products of photosynthesis to structural (leaf, stem, root, and fruit) and storage compartments of the plant. The simulations encompass the entire growing season from germination to senescence. We describe the model conceptually and mathematically and provide examples of model output for various levels of pollutant stress. Also, we outline future developments that would improve this preliminary model and discuss its applications.

INTRODUCTION

Development of geothermal energy technology in the Imperial Valley, California, is expected to be accompanied by the release of noncondensable gases (CO_2 , H_2S , CH_4 , and NH_3) from geothermal wells. The potential of these gases for adversely affecting vegetation in the Valley, particularly crops is a source of concern. At the Lawrence Livermore Laboratory, one of the tools being developed to assess the environmental impact of such gases is a general model of photosynthesis and plant growth (GROW1). Because a model is an abstraction of a real system, its objectives determine its structural elements such as model output, important processes used to calculate output, and input variables. In our case, we wish to simulate the yield of dry matter from four morphological components of crop plants, stem, leaf, root, and fruit. We want to predict yield as a function of environmental variables (temperature, light, soil, water, soil salinity, etc.) and pollutant stress. Our model is general enough to be modified to provide a simulation of most field crops and several vegetable crops grown in the Imperial Valley.

Photosynthesis is determined by such factors as temperature, sunlight, stomatal resistance, CO_2 concentration in air, and biochemical processes in the plant. Photosynthesis is partially determined by relative humidity and plant moisture stress, both of which affect stomatal resistance. In our model, photosynthate is passed from the photosynthesis submodel to the growth submodel. A coupled set of ordinary differential equations describes allocation of photosynthate and growth during the growing season. To account for loss of photosynthesis products, these equations contain temperature-dependent expressions for respiration. The latter is modeled as two components: maintenance respiration and growth-related respiration.

A preliminary version of the model is currently implemented to run on Laboratory computers. Data primarily from corn have been included in the model, and hypothetical environmental parameters are being used to test the model and debug the computer code. These values are typical of what might be expected during the summer months in a temperate climate.

MODEL DESCRIPTION

To calculate the growth of plants, we must know the microclimate in the canopy; rate of photosynthesis (CO_2 uptake and fixation); soil-water budget, including plant uptake and transpiration; nutrient uptake,

utilization, and effect on plant processes; conversion of photosynthate and nutrients to structural material, their distribution, and respiration; and pollutant effects on plant processes. In GROW1, we considered photosynthesis in some detail, the water budget problem, distribution of photosynthesis products, pollutant effects on photosynthesis, and some aspects of the microclimate problem. Later versions will consider in greater detail the problems of microclimate, nutrient uptake, and water budget. A schematic diagram of GROW1 is presented in Fig. 1.

Fig. 1. Framework for crop growth model. The environmental variables of light, wind, CO_2 concentration, temperature, and precipitation determine plant responses. This model traces factors that determine photosynthesis, respiration, and the distribution of the products of photosynthesis. The leaf submodel is in center of diagram with leaf resistances on the left and biochemical model on the right. See Fig. 7 for more detail. Solid lines indicate flow of photosynthesis products. Dashed lines indicate functional relationships between independent and dependent variables.

Model Structure

The vegetative structure, local weather pattern, and energy from the sun interact to produce a microclimate within the canopy. In nature, there are profiles of visible light, humidity, temperature, radiant energy, latent heat, sensible heat, and wind. Profiles for visible light and wind are included in our model. During photosynthesis, CO_2 is taken up through the stomata, and incident light energy is fixed biochemically by converting CO_2 and H_2O to CH_2O and O_2 . Photosynthesis is dependent upon the biochemical processes in the plant and also on the diffusion rate of CO_2 into the plant. The diffusion rate is determined by the gradient of CO_2 concentrations from the atmosphere to the site of photosynthesis (chloroplast) and by the diffusion resistances along the CO_2 gradient. These resistances are the diffusion resistances of the canopy, and boundary layer of the leaf, the stomata, the cell wall, and the cytoplasm. Of these variables, the one most under physiological control by the plant is the stomatal resistance, which responds to light and moisture. For this discussion we take the other biological resistances (cell wall, etc.) to be constants. Stomatal resistance decreases as light intensity increases, allowing CO_2 to diffuse into the plant faster. As moisture stress increases (measured as either relative saturation deficit, leaf-water potential, or soil-moisture potential), stomatal resistance increases to prevent excessive water loss. The moisture-stress submodel must account for water uptake by roots, translocation of water through the plant, and transpiration through stomata to the atmosphere. This part of the model requires input variables such as the amount of precipitation or irrigation, resistance of the soil to water movement, soil-water potential as a function of soil-water content, energy balance of the canopy, humidity above the canopy, and leaf temperatures.

Currently there are two water-budget models under consideration. WATER1 has the less detailed resolution and is now implemented in the preliminary computer model (see Fig. 2). A more detailed model

Fig. 2. Evapotranspiration model, a modified version of a model by Curry.¹ Solid lines indicate flow of water. Dashed lines indicate casual flows of information from one variable to control another. Center portion represents leaves with variables of temperature T_L and water vapor concentration ρ_L . F is leaf-area index, which determines the number of canopy layers. Sawtooth lines are resistances (r) to water-vapor flow.

(WATER2) is being planned for future development. WATER1 accounts for soil-water content and hence soil-water potential from which we can calculate stomatal resistance. Transpiration is determined by the energy balance of the canopy (because transpiration is proportional to latent heat, which enters into the energy balance), the gradient of water-vapor concentrations from the air above the canopy to the surface of the cell walls inside the stomatal cavity, and the resistances to vapor flow along the water-vapor gradient. These resistances are to diffusion in the canopy, in the leaf boundary-layer, and through the stomata. This model is patterned after the transpiration submodel of Curry,¹ which is based partly on the work of Rijtema.² WATER1 uses transpiration and precipitation data to calculate soil-water content.

After photosynthesis products are generated, they are allocated for growth, growth respiration, and maintenance respiration of leaves, stem, fruit, and roots. We used two storage compartments: leaf storage into which these products are first introduced and main storage, which provides for growth and respiration of stems, roots, and fruits.

Fig. 3. Evapotranspiration model, a modified version of a model by Goldstein and Mankin.³ Solid lines represent the flow of water. Dashed lines represent flow of information from one variable, which controls the next. In this model, leaf potential ψ_L controls transpiration, which is set equal to water uptake.

In GROW1 we assume that the effects of pollution are to alter photosynthesis rates. This change in the rate of photosynthesis is reflected in changes in the allocation of photosynthate and in the growth of the plant. The logic of GROW1 is consistent with simulating changes in phenology as being triggered by changes in the accumulation of photosynthesis products. GROW1 does not include the effects of nutrients on growth, photosynthesis, or phenology. Instead, these effects are implicitly imbedded in the physiological parameters employed by the model. These parameters are discussed in the next section.

The GROW1 simulation follows the development of a plant during the course of a growing season. The code is now implemented to simulate the development of annual species but with the addition of an overwintering capability it could be modified to simulate the growth of perennial species also. Simulations usually begin shortly after emergence with initial values of each plant compartment specified by the user. Each day begins at midnight and continues through the day to midnight of the following night. During the daylight hours, the declination of the sun above the horizon is continuously calculated. Temperature is assumed to vary sinusoidally through the day with the daily maximum occurring at 3 p.m. and the daily minimum occurring at 3 a.m. Wind and wet bulb (or dew point) temperature can be assumed to be constant throughout the day or can be varied sinusoidally. Net radiation and soil radiation are assumed to be proportional to the declination of the sun. The coefficient of proportionality is chosen such that the integral of net radiation taken over the day is equal to the observed total for that day. The ordinary differential equations that characterize the growth of the plant compartments are integrated continuously using EPISODE, a code developed by Hindmarsh and Byrne ⁴ for the numerical integration of stiff differential equations.

Mathematical Expression of the Model

Light Penetration in the Canopy

The problem of light penetration and absorption in the canopy has been studied since the work of Monsi and Sacki ⁵ in 1953. They described light intensity I_L at F and height Z :

$$I_L = I_0 e^{-KF}, \quad (1)$$

where

- I_0 = light intensity at the top of the canopy, ($\text{cal cm}^{-2} \text{s}^{-1}$ or $\text{nanoeinsteins cm}^{-2} \text{s}^{-1}$)
- K = extinction coefficient,
- F = cumulative leaf area index (LAI) from Z to the top of the canopy, and
- LAI = ratio of area of leaves to unit area of ground.

Monteith ⁶ divided the canopy into layers and derived a binomial expression for the radiation distribution. He also included effects of transmittance and reflectance by leaves. Anderson ⁷ assumed a Beer's law extinction [Eq. (1)] and determined the behavior of K as a function of leaf angle. The effects of leaf angle on light intensity in a layered canopy were determined by de Wit. ⁸ Duncan *et al.* ⁹ examined the effect of the leaf angle on Beer's law [Eq. (1)], using the work of Anderson ⁷ and Warren-Wilson. ^{10,11} More recently, Monteith ¹² reviewed the light-penetration problem in some detail. A simple derivation of their results can be made by first considering a single leaf at an angle α to the horizontal. Let β be the angle of the sun above the horizon and ω the azimuthal angle between sun and leaf. To find the angle δ between sun and leaf (Fig. 4), write the unit vector in the direction of the sun as

$$\hat{s} = \sin \beta \hat{z} + \cos \beta \cos \omega \hat{x} + \cos \beta \sin \omega \hat{y}.$$

The normal to the plane of the leaf is

$$\hat{n} = \cos \alpha \hat{z} + \sin \alpha \hat{y}.$$

Fig. 4. Geometry of sun, leaf, and ground: $\hat{s}$ is the unit vector pointing toward the sun, $\hat{n}$ is the unit vector normal to the plane of the leaf, x-y is the plane of the ground, α is the angle of inclination of the leaf, β is the angle of inclination of the sun, ω is the azimuthal angle between the leaf and sun, δ is the angle between the plane of the leaf and sun, η is the angle between $\hat{s}$ and $\hat{n}$, and $\hat{p}$ is the vector projected onto leaf by $\hat{s}$.

The cosine of the angle between $\hat{s}$ and $\hat{n}$, $\cos \eta$, is equal to $\sin \delta$, since $\delta + \eta = \pi/2$ and is given by

$$\sin \delta = \hat{s} \cdot \hat{n} = \cos \alpha \sin \beta + \sin \alpha \cos \beta \sin \omega. \quad (2)$$

$\sin \delta$ is equal to the projection of the leaf in the direction of the sun. Since all leaves are randomly oriented around $\hat{z}$, we average Eq. (2) over all azimuthal angles ω to find the average projection of leaves into the direction of the sun. This average is given by

$$\begin{aligned} PL_{\alpha} &= \sin \beta \cos \alpha & \beta \geq \alpha \\ &= \frac{2}{\pi} \cos \beta \sin \alpha \sin \sigma + (1 - 2\sigma/\pi) \cos \alpha \sin \beta, & \beta < \alpha \end{aligned} \quad (3)$$

where

$$\sigma = \arccos (\cot \alpha \tan \beta).$$

Because leaves are often distributed in the angle α , we average PL_{α} over the distribution in α , $f_L(\alpha)$, to get the average PL

$$PL = \int_0^{\pi/2} PL_{\alpha} f_L(\alpha) d\alpha$$

where

$$\int_0^{\pi/2} f_L(\alpha) d\alpha = 1$$

For a spherical distribution $PL = 0.5$, for a horizontal distribution $PL = \sin \beta$, and for a vertical distribution $PL = 2/\pi \cos \beta$. For a distribution of all leaves at α , PL is given by Eq. (3).

Over an area of ground, A_g , the total flux of sunlight incident on A_g is given by $IA_g \sin \beta$ where I is the intensity of incident light. The loss by interception in a small layer of leaf area ΔA_L and absorption k is $-\Delta A_L PL I k$, which equals $\Delta I A_g \sin \beta$. Therefore, the light flux on the leaves at depth F is

$$I_L = I_0 \exp(-F PL k / \sin \beta).$$

The flux normal to the leaves at F is

$$I = PL I_L.$$

This value for I is used in calculating rates of photosynthesis.

An important point is that the total leaf area index F_{TOT} is calculated from the leaf biomass x_1 (see Fig. 1). In this scheme,

$$F_{TOT} = M_d x_1 / a_L,$$

where

- M_d = number of plants per unit area of ground (m^{-2}),
- a_L = conversion factor for leaf area to leaf dry weight (g/m^2), and
- x_1 = leaf biomass per plant (g).

Leaf Photosynthesis

Rabinowitch¹³ suggested that photosynthesis is best described by the hyperbolic function

$$P = \frac{IP_m}{I + I_m} \quad (4)$$

where I = light intensity, I_m = light intensity for P at half of its maximum value, and P_m = maximum value of photosynthesis at high light levels. Gaastra¹⁴ assembled data from many plants to use in Eq. (4). He assumed that another controlling factor of photosynthesis was the Fickian diffusion of CO_2 with air resistance, stomatal resistance, and mesophyll cell resistance in series (see Fig. 5a). Hence, he demonstrated a linear relationship of photosynthesis to atmospheric concentrations of CO_2 and introduced diffusion resistances to explain rates of photosynthesis. Thus,

$$P = \frac{C_a - C_c}{r_a + r_s + r_m}, \quad (5)$$

(a) Gaastra model (1959)

(b) Lake model (1967)

(c) Waggoner model (1969)

(d) Chartier model (1970)

Fig. 5. Historical development of CO_2 -diffusion pathways in photosynthesis models. (a) Earliest was a simple model of Gaastra,¹⁴ (b) Lake¹⁶ introduced respiration, (c) Waggoner¹⁷ introduced carboxylation resistance, and (d) Chartier¹⁸ refined model by equating diffusion rate with photochemical rate and distinguishing between intercellular and intracellular flow of respired CO_2 .

where

- P = photosynthesis rate ($\text{g/cm}^2\text{s}$),
- C_a = concentration of CO_2 in air (g/cm^3),
- C_c = concentration of CO_2 in chloroplasts (g/cm^3),
- r_a = leaf boundary diffusion resistance (s/cm),
- r_s = stomatal resistance (s/cm), and
- r_m = mesophyll cell resistance (s/cm).

Monteith¹⁵ combined both CO_2 and light dependence into one empirical expression for which he provided data from many crops:

$$P_n = \frac{C_a I}{u_1 I + v_1 C_a} \quad (6)$$

where

- P_n = net photosynthesis ($\text{g cm}^{-2}\text{s}^{-1}$),
- v_1 = inverse of slope of $P_n(I)$ at low light levels (nanoeinsteins g^{-1}), and
- u_1 = inverse of $\max(P_n(I))/C_a$ at high light levels (s cm^{-1}).

Lake¹⁶ constructed a diffusion-resistance model that explicitly introduced respiration as a variable (see Fig. 5b). Waggoner¹⁷ introduced the notion of photochemical resistance (r_c), which encompassed all biochemical reactions and was added to the end of a chain of diffusion resistances (air, stomatal, cell wall, and cytoplasmic) (see Fig. 5c). Chartier¹⁸ introduced a further sophistication (see Fig. 5d). Entering the intercellular spaces from surrounding cells is an amount of respiration CO_2 nR . CO_2 diffuses from the stomata through the mesophyll cell (r_m) to the chloroplast at concentration C_c , where an additional amount of respiratory CO_2 is generated $(1 - n)R$. Thus, at the chloroplast, the fixation rate P_g (gross photosynthesis) is

$$P_g = P_n + R. \quad (7)$$

Gross photosynthesis occurs at a rate

$$P_g = \frac{w_1 I \left(\frac{C_c}{r_c} \right)}{w_1 I + \left(\frac{C_c}{r_c} \right)}, \quad (8)$$

where

- r_c = carboxylation resistance, similar to u_1 in Eq. (6) ($\text{ppm g}^{-1}\text{cm}^2\text{s}$), and
- w_1 = constant similar to v_1^{-1} in Eq. (6) ($\text{g nanoeinsteins}^{-1}$).

From the outside, the diffusion rate of CO_2 (P_n , net photosynthesis) is

$$P_n = \frac{C_a - C_c - nR_m}{r_a + r_s + r_m}. \quad (9)$$

Equation (9) describes the diffusion processes, Eq. (8) describes the photochemical process, and Eq. (7) implicitly states that the rates of photochemical and the diffusion processes are equal. The C_c term can be eliminated from these equations, yielding an equation quadratic in P_n . Chartier provided data from bean plants for the solution to this equation.

Stewart's¹⁹ model explicitly equates diffusion rate to photochemical rate. His model was based on the work of Chartier¹⁸ and Rabinowitch.¹³ Stewart's diffusion equation is shown schematically in Fig. 6a. The photochemical process in Fig. 6b is equivalent to Eq. (8). The C_c and P_g terms can be eliminated from the equations representing Fig. 6, leaving an expression quadratic in P_n . P_n is then a function of I , C_a , R , and the parameters shown in Fig. 6.

In the version of the crop model being developed at this laboratory, we use a leaf-photosynthesis sub-model developed by Sinclair²⁰ and Murphy *et al.*,²¹ which is similar to a model constructed by Hall.²² The

(a) Diffusion pathway of CO_2

(b) Biochemical process

Fig. 6. Stewart's model of leaf photosynthesis.¹⁹ (a) Diffusion pathway of CO_2 and (b) Model of CO_2 biochemistry. Stewart equated these two processes.

diffusion pathway is shown in Fig. 7a with a net CO_2 diffusion rate into the leaf P_n from a concentration in air of C_a , to the intercellular air spaces with concentration C_{ia} , to inside the cell wall, C_p , and finally to a concentration at the chloroplast, C_c . Dark respiration (mitochondrial respiration, R) provides input at the C_p node also. Gross photosynthesis P_g occurs in the chloroplast, and

$$P_g = P_n + R.$$

(10)

(a) Diffusion pathway of CO_2

(b) Biochemical process model

Fig. 7. Sinclair's model of leaf photosynthesis.²⁰ (a) Diffusion pathway of CO_2 , which includes resistance of leaf-boundary layer and divides mesophyll resistance into a cell wall resistance and an average protoplasm resistance; (b) biochemical model of photosynthesis. The two loops in this model instead of one (Fig. 6b), indicate that the synergism between I and CO_2 differ in the two models.

The gaseous phase of the diffusion pathway is described by

$$P_n = \frac{C_a - C_{ia}}{r_a + r_s} \quad (11)$$

At the cell wall, CO_2 is absorbed into water; thus,

$$P_n = \frac{sC_{ia} - C_p}{r_{cw}} \quad (12)$$

where

r_{cw} = cell wall resistance, (s cm^{-1})
 s = absorption coefficient of CO_2 in water,
 r_a = boundary layer resistance, and
 r_s = stomatal resistance.

Inside the cytoplasm,

$$P_g = \frac{C_p - C_c}{r_p} \quad (13)$$

where

r_p = cytoplasmic resistance.

The biochemical reaction was modeled according to Fig. 7b. A is the CO_2 acceptor, ribulose 1,5-diphosphate (RuDP), and ACO_2 as the carboxylated product, 3-phosphoglyceric acid (PGA). CO_2 entering the cycle combines with A to form ACO_2 with a rate constant of k_1 :

In the other cycle, light absorbed by chlorophyll drives the conversion of NADP to NADPH:

Photosynthesis occurs by the enzymatic reduction of ACO_2 coupled to NADPH oxidation. This rate is given by

$$P_g = k_3[\text{ACO}_2][\text{NADPH}] \quad (16)$$

At equilibrium, Eqs. (14) and (15) are expressed as

$$[\text{ACO}_2] = k_1[A]C_c, \quad (17)$$

and

$$[\text{NADPH}] = k_2 I [\text{NADP}] . \quad (18)$$

The total amount of NADP and NADPH is assumed constant and the total amount of A and ACO_2 is assumed constant. Therefore,

$$N_o = [\text{NADPH}] + [\text{NADP}] , \quad (19)$$

and

$$A_o = [A] + [\text{ACO}_2] . \quad (20)$$

Combining Eqs. (10) through (13) and (16) through (20) leads to

$$P_n = \frac{-b - \sqrt{b^2 - 4ac}}{2a} - R , \quad (21)$$

where

$$\begin{aligned} a &= (k_2 I + 1) \quad k_1 [r_p + r_{cw} + s(r_s + r_a)] , \\ b &= -(k_2 I + 1) \quad \{s C_a k_1 + R k_1 [r_{cw} + s(r_s + r_a)] + 1\} \\ &\quad - k_1 k_2 k_3 A_o N_o I [r_p + r_{cw} + s(r_s + r_a)] , \text{ and} \\ c &= k_1 k_2 k_3 A_o N_o I \{R [r_{cw} + s(r_s + r_a)] + s C_a\} . \end{aligned}$$

Following Sinclair,²⁰ we use for r_a and r_s :

$$r_a = r_1 (D_L / U)^{1/2} ,$$

where D_L = leaf width, U = windspeed, and r_1 is a constant, and

$$r_s = \frac{\mu_1}{1 + \mu_2} + \mu_3 T + \mu_4 + \nu , \quad (22)$$

where μ_1 , μ_2 , μ_3 , and μ_4 are constants determined by fitting $r_s(I, T)$ to data obtained by varying light intensity and leaf temperature while measuring r_s . μ_1 is in units of either nanoeinsteins cm^{-3} or cal cm^{-3} , μ_2 in either nanoeinsteins $\text{cm}^{-2} \text{s}^{-1}$ or $\text{cal cm}^{-2} \text{s}^{-1}$, μ_3 in $\text{s cm}^{-1} \text{°C}^{-1}$, and μ_4 in s cm^{-1} . ν is a water stress term to be discussed below. The biochemical constants, k_1 , k_2 , k_3 , A_o , and N_o can be easily determined by examining Eq. (21) at various limits and using experimental data to fit the equation at these limits (see Sinclair²⁰ for a full discussion). Our expression for respiration is that of Waggoner¹⁷:

$$R = R_x \exp[T_x (T_x + 10) \ln Q_{10} (1/T_x - 1/T) / 10] , \quad (23)$$

where

$$\begin{aligned} R_x &= \text{base respiration rate,} \\ T_x &= \text{base temperature (}^\circ\text{K), and} \\ Q_{10} &= \text{ratio of } R(T_x + 10) \text{ to } R(T_x). \end{aligned}$$

Transpiration and Water Budgets. Currently, the basic equations and conceptualization of the water budget portion of the model are taken from Curry¹ and Curry and Chen.²³ We denote the soil-water content as the dynamic variable x_7 . The rate of change of x_7 is given by the differences between precipitation rate and transpiration rate, summing the latter over L canopy layers,

$$\frac{dx_7}{dt} = P_r H(x_{7\max} - x_7) - \sum_{i=1}^L ET(I_{ni}, G_i, T_i, e, r'_{si}, r'_{ai} + r'_{ci}), \quad (24)$$

where

$$\begin{aligned} I_{ni} &= \text{total incident radiant energy into layer } i \text{ (cal cm}^{-2} \text{ s}^{-1}\text{)}, \\ G_i &= \text{total incident radiant energy emerging from layer } i \text{ (cal cm}^{-2} \text{ s}^{-1}\text{)}, \\ T_i &= \text{temperature of layer } i, \\ e &= \text{vapor pressure of atmosphere above the canopy (mbar),} \\ r'_{si} &= \text{stomatal resistance of layer } i, \\ r'_{ai} &= \text{boundary layer resistance of leaves in layer } i, \\ r_{ci} &= \text{canopy-diffusion resistance from layer } i \text{ to a reference level where } e \text{ is measured,} \\ P_r &= \text{precipitation rate (m da}^{-1}\text{), and} \\ H(x) &= \begin{cases} 1, & x > 0 \\ 0, & x < 0. \end{cases} \end{aligned}$$

The resistances to water vapor diffusion that are discussed in this section differ from the resistances to CO_2 diffusion by constant factors because of the different diffusivities of CO_2 and H_2O . (The prime indicates H_2O .) Our model differs from Curry's in that he uses soil-water potential as an input. Also, we sum over canopy layers, whereas Curry uses a single transpiration surface. As noted above, stomatal resistance r_s is a function r_1 of light and temperature as well as water stress ν , so that

$$r'_s = r'_1 + \nu'.$$

Curry gives ν' as a function of soil-water potential ψ_s :

$$\nu' = \frac{r_{w1}}{r_{w2} + \psi_s(x_7, C_s)} - \frac{r_{w1}}{r_{w2} + \psi_s(x_{7\max}, 0)} \quad (25)$$

where the soil-water potential is a function of soil-water content and soil salt concentration.

$$\psi_s(x_7, C_{\text{soil}}) = -r_{w3}e^{-r_{w4}x_7} - R_G T_r C_{\text{soil}}, \quad (26)$$

where

$$\begin{aligned} R_G &= \text{gas constant (} 83.14 \times 10^3 \text{ mbar cm}^3 \text{ mol}^{-1} \text{ }^\circ\text{K}^{-1}\text{)}, \\ T_r &= \text{temperature of soil (}^\circ\text{K), and} \\ C_{\text{soil}} &= \text{concentration of salt in soil (mol cm}^{-3} \text{ solute).} \end{aligned}$$

The empirical constants, r_{w1} and r_{w2} are obtained by fitting Eq. (25) to data of r'_s vs ψ_s . r_{w1} is in units of mbar-s/cm and r_{w2} in units of mbar. By fitting data of ψ_s vs soil water content, x_7 , we obtain r_{w3} and r_{w4} . r_{w3} is in units of mbar and r_{w4} in units of m^{-1} . The transpiration term ET is calculated from a modified Penman equation.²⁴

$$ET = \frac{\Delta(I_n - G) + \rho c[e_s(T) - e]/(r'_a + r'_c)}{\lambda \{ \Delta + \gamma [1 + r'_s/(r'_a + r'_c)] \}} 864, \quad (27)$$

where

$$\begin{aligned} ET &= \text{transpiration (m da}^{-1}\text{)}, \\ e_s(T) &= \text{saturation vapor pressure at temperature T (mbar),} \\ \rho c &= \text{volume heat capacity of dry air (} 290 \times 10^{-6} \text{ cal cm}^{-3} \text{ }^\circ\text{K}^{-1}\text{),} \\ \gamma &= \text{psychrometric constant (0.66 mbar }^\circ\text{K}^{-1}\text{),} \\ \lambda &= \text{latent heat of evaporation (585 cal g}^{-1}\text{),} \\ \Delta &= de_s/dT; \end{aligned}$$

and $e_s(T)$ and Δ are calculated by the computer code using the Clausius-Clapeyron equation. The derivation of Eq. (27) uses three factors. The first factor is Fick's law of diffusion for water vapor:

$$ET = \frac{\rho_{Ls} - \rho_Z}{r'_{si} + r'_{ai} + r'_{ci}}, \quad (28)$$

where

$$\begin{aligned} \rho_{Ls} &= \text{saturation-vapor density at the leaf, and} \\ \rho_Z &= \text{vapor density at reference height Z.} \end{aligned}$$

The next factor is the energy balance for the leaf

$$I_{ni} = \lambda ET + H + G_i, \quad (29)$$

where

$$\begin{aligned} H &= \text{rate of sensible heat transfer from leaf,} \\ I_{ni} &= \text{net flux radiant energy into layer i from above, and} \\ G_i &= \text{net flux of radiant energy out of layer i below.} \end{aligned}$$

The third factor is the rate of sensible heat transfer from the leaf:

$$H = \frac{\rho c (T_L - T_Z)}{r'_{ai} + r'_{ci}}. \quad (30)$$

Then Eq. (27) is derived by combining Eqs. (28), (29), and (30), and using the ideal gas law (Goldstein and Mankin).³

Curry uses Eq. (25) because he did not need hourly changes in stomatal resistance for his purposes. However, the equation is not detailed enough to estimate pollutant effects accurately. Stomatal resistance is modeled in Eq. (25) as a function of soil-water potential, but soil-water potential changes very slowly during the day. Stomatal resistance is a function of leaf-water potential, which changes drastically during the course of a day, thus changing stomatal resistance. This occurs because the plant undergoes water stress from its energy load $(I_n - G)$ during the middle of the day when evaporation rates are high. When this occurs, the stomata close. This midday closure is not reflected in Eq. (25) since ψ_s changes very little in the course of a day. As a refinement necessary to take these effects into account, we propose the adaptation of the work of Goldstein and Mankin.³ Because of the *a priori* importance of this refinement (WATER2), we discuss its implementation (Fig. 3), which we propose for future work.

For Fig. 3 there are three state variables: rooting-zone water x_7 , soil-surface water x_8 , and canopy-storage water x_9 . Note that for this brief discussion we change the units convention by using the unit weight basis. Thus, for example, water potential is in units of length (m). The coupled differential equations that follow the rates of change of these compartments with time are

$$\frac{dx_7}{dt} = \frac{\psi_8 - \psi_7}{r_{\text{soil}}} H(x_{7\text{max}} - x_7) - \sum_i \frac{\psi_7 - \psi_{Li}}{r_{\text{sp}}} \quad (31)$$

$$\frac{dx_8}{dt} = [P_2 + P_1 H(x_9 - x_{9\text{max}})] H(x_{8\text{max}} - x_8) - \frac{\psi_8 - \psi_7}{r_{\text{soil}}} - ET(G, 0, T, e, 0, r_{\text{gnd}}) \quad (32)$$

$$\frac{dx_9}{dt} = P_1 H(x_{9\text{max}} - x_9) - \sum_{\substack{\text{canopy} \\ \text{layers} \\ i=1}}^L ET(I_{n_i}, I_{n_{i+1}}, T, e, 0, r'_{ai} + r'_{ci}) \quad (33)$$

Our model differs conceptually from Goldstein and Mankin's in that we sum over canopy layers, while they use a single evapotranspiration surface.

In Eq. (31), we balance the rate of change of the rooting-zone water with the water moving down from the surface and the transpired water. We assume that the flow is accurately modeled by an electrical analog of potential differences divided by resistances.

- ψ_8 = soil-water potential of surface-soil water (m),
- ψ_7 = soil-water potential of rooting-zone water (m),
- ψ_{Li} = leaf-water potential of leaves in layer i (m),
- r_{soil} = resistance of soil to water flow (da), and
- r_{sp} = resistance to flow between soil and plant leaves (da).

In Eq. (32),

- P_2 = precipitation striking ground without interception (m da^{-1}), and
- P_1 = precipitation intercepted by leaves (m da^{-1}).

If surface-soil storage is saturated ($x_8 = x_{8\max}$), then excess input runs off. In Eq. (33), if leaf-surface storage is saturated, excess falls to the ground. We balance input to leaf surfaces with direct evaporation to the atmosphere in Eq. (33). Following Goldstein and Mankin, we calculate the soil resistances with

$$r_{\text{soil}} = \frac{d_8}{2K(x_8)} + \frac{d_7}{2K(x_7)}, \quad (34a)$$

and

$$r_{\text{sp}} = \frac{d_7}{2K_r} + \frac{d_7\delta}{fK(x_7)A}, \quad (34b)$$

where

- d_i = thickness of soil layer i (m),
- δ = ratio of cross-sectional area of roots in x_7 to area of x_7 ,
- f = fraction of root surface area through which water is absorbed,
- A = ratio of total root surface area to area of ground, and
- K_r = conductivity of plant tissue (m/da);

and we calculate soil potentials using

$$\psi_7 = d_8 + \frac{d_7}{2} + \left(\frac{\theta d_7}{x_7} \right)^{1/u},$$

and

$$\psi_8 = \frac{d_8}{2} + \left(\frac{\theta d_8}{x_8} \right)^{1/u} \quad (35)$$

Soil conductivities are calculated, using

$$K(x_i) = \frac{K_{\text{soil}}}{\left(\frac{\psi_i}{w} \right)^v + 1}, \quad (36)$$

where v and u are empirical constants easily determined by log-log fits of soil water potential versus soil water content and

- K_{soil} = soil conductivity at soil potential equal to 0,
- θ = volumetric water content at which matric potential is equivalent to a pressure of 1 m of water, and
- w = value of soil potential at which soil conductivity has fallen to half maximum.

Equation (35) states that the total soil potential is the sum of the gravitational potential ($d_8 + d_7/2$ or $d_8/2$) plus the matric potential $(\theta d_i/x_i)^{1/u}$. This is a well known description of soil water potential.²⁵ The form for the matric potential as $(\theta d_i/x_i)^{1/u}$ was suggested by Gardner et al.²⁶ Equation (36) was first proposed by Gardner.²⁷

The calculation of ψ_{Li} is the qualitative difference between this model (WATER2) and WATER1. The calculation of ψ_{Li} is the central improvement of WATER2 over WATER1. To calculate ψ_{Li} , we equate the flow to the leaf layer i with the transpiration flow out of the leaf:

$$\frac{\psi_7 - \psi_{Li}}{r_{sp}} = ET (In_i, In_{i+1}, T, e, r'_{si}, r'_{ai} + r'_{ci}) . \quad (37a)$$

Stomatal resistance (of H_2O) of the i^{th} foliage layer is given by

$$r'_{si} = r'_{li} + (r_o - r'_{li}) \exp[(\psi_c - \psi_{Li})m] , \quad (37b)$$

where

- r_o = critical or maximum resistance attained when $\psi_{Li} = \psi_c$ ($s\ cm^{-1}$),
- ψ_c = critical potential (mbar), and
- m = slope of resistance with respect to change in ψ_{Li} at ψ_c ($mbar^{-1}$).

Substituting Eq. (37b) into Eq. (37a), we note that the latter is an implicit equation for ψ_{Li} . This equation is solved at discrete time steps and results in variation in ψ_{Li} , hence, variation in r'_{si} .

Calculation of Canopy Resistance. Dividing the canopy into L layers, we denote the wind above the canopy to be U_o and the wind in layer i to be U_i . The resistance in the canopy between layer i and the top of the canopy is given by

$$r_{ci} = \int_0^{Z_i} \frac{dZ}{D(Z)} , \quad (38)$$

where

- Z = distance of layer i measured from the top of the canopy, and
- $D(Z)$ = diffusivity in canopy ($cm^2\ s^{-1}$).

Following Waggoner and Reifsnnyder,²⁴ we assume $D(Z_i)$ is proportional to U_i or

$$D(Z_i) = D_o U_i / U_o . \quad (39)$$

If wind data is lacking, the computer code calculates

$$U(Z) = U_o \exp[-k_\alpha F(Z)] , \quad (40)$$

where

- k_α = decay constant of wind velocity with canopy depth, and
- $F(Z)$ = cumulative LAI at Z .

According to Waggoner and Reifsnnyder,²⁴ if we introduce the differential LAI designated as f ,

$$f(Z) = \frac{dF(Z)}{dZ} ,$$

we find that $f(Z)$ is often best fit as a normal distribution,

$$f(Z) = f_{\max} \exp[-d(Z - Z_{\text{TOT}}/2)^2] ,$$

where

Z_{TOT} = depth of the canopy (cm),

d = inverse of square of standard deviation of distribution describing spread of foliage in the canopy (cm^{-2}), and

$f_{\max}$ = maximum density of leaves in the canopy (cm^{-1}).

However, for simplicity as a first-order estimate, we take $f(Z) = h'$, to be a constant where $h' = F_{\text{TOT}}/Z_{\text{TOT}}$ where F_{TOT} is the total LAI. Combining Eqs. (38-40), we calculate

$$r_{\text{ci}} = \frac{1}{D_o k_{\alpha} h'} [\exp(k_{\alpha} h' Z) - 1] . \quad (41)$$

Calculation of Photosynthesis Under Pollutant Stress. At low levels, sulfur-containing pollutants often have a fertilizing effect on the growth of plants (e.g., SO_2 as shown by Faller and Kuhn²⁸ and Cowling *et al.*²⁹). Shinn *et al.*³⁰ showed that a simulated geothermal gas consisting of CO_2 , H_2S , CH_4 , and N_2 increases photosynthesis in lettuce. At higher levels, this mixture depresses photosynthesis strongly. Therefore, as a tool to expedite model development, we make the preliminary assumption that above a threshold level S_o photosynthesis is depressed linearly, and below S_o photosynthesis is enhanced quadratically. Thus,

$$\begin{aligned} P_p &= P_n \left[1 + \frac{c_1}{r_s} \left(S_o \frac{r_s}{r_b} - S \right) \right] , & S > S_o , \\ &= P_n \left[1 + \frac{c_1}{r_s^2} \frac{S r_b}{S_o} \left(S_o \frac{r_s}{r_b} - S \right) \right] , & 0 < S < S_o , \end{aligned} \quad (42)$$

where

c_1 = reduction in photosynthesis for a unit increase in pollutant at one unit of diffusion resistance, ($\text{s cm}^{-1} \text{ ppm}^{-1}$),

r_s = stomatal resistance (s cm^{-1}),

S = concentration of pollutant (ppm), and

r_b = stomatal resistance at which S_o was determined.

This submodel is not a complete or satisfactorily accurate portrayal of the effect of H_2S on photosynthesis, but rather it is qualitatively correct. It is used here to demonstrate properties of the allocation model at altered levels of photosynthate production. Work is currently underway to improve this submodel by

examining the interaction of sulfur compounds with the photosynthetic process at the biochemical level. We note that r_g can be a function of pollutant stress. However, the preliminary evidence³⁰ indicates that r_g is not highly dependent upon geothermal pollutants. Therefore, most of the effect seems to be on the photosynthetic process itself.

Respiration, Allocation, and Growth. There is strong evidence^{31,32} that respiration can be divided into two components. Maintenance respiration is proportional to standing crop or living biomass, and growth respiration is proportional to the rate of growth. We define growth as the transfer of photosynthate from a storage compartment (x_2 leaf storage or x_3 main storage) to a structural compartment (x_1 leaf, x_4 stem, x_5 fruit, or x_6 root). When this transfer occurs, there is a concomitant loss from the storage compartment resulting from growth respiration. Leaf maintenance respiration is already accounted for as a reduction in photosynthate increment added to the leaf-storage compartment (see Fig. 1). Maintenance respiration losses of the leaf-storage compartment are subtracted from the total of that compartment.

The maintenance respiration of all other compartments is subtracted from the main storage compartment. This approach is the same as in Goldstein's model of forest growth.³³

The equations describing the rate of change of the state variables x_1 through x_6 with time are shown pictorially in Fig. 1 and are described mathematically as:

$$\frac{dx_1}{dt} = T_1, \quad (43a)$$

$$\frac{dx_2}{dt} = \frac{S_L P_T H(P_T)}{S_L + x_2/x_1} + H(-P_T) P_T - [1 + r_g(T)] T_1 - T_3 - r_n(T)x_2, \quad (43b)$$

$$\frac{dx_3}{dt} = T_3 - (1 + r_g) (T_4 + T_5 + T_6) - r_n(T_r) x_6 - r_n(T) (x_3 + x_4 + x_5), \quad (43c)$$

$$\frac{dx_4}{dt} = T_4 - r_n(T) x_4 H(a_4 x_4^\mu - x_3), \quad (43d)$$

$$\frac{dx_5}{dt} = T_5 - r_n(T) x_5 H(a_4 x_4^\mu - x_3), \quad (43e)$$

and

$$\frac{dx_6}{dt} = T_6 - r_n(T_r) x_6 H(a_4 x_4^\mu - x_3), \quad (43f)$$

where

$$P_T = B_c \int_0^F P_p(F) dF / M_d,$$

$r_g(T)$ = growth-respiration rate with a dependence on T as R above,

$r_n(T)$ = maintenance-respiration rate with a dependence on T as R above,

T = temperature of above-ground parts ($^{\circ}K$),

T_r = temperature of roots ($^{\circ}K$),

- μ = exponent of x_4 for calculating the fraction of x_4 used in growth,
 a_4 = empirical parameter,
 S_L = ratio of leaf storage to leaf structural tissue at which photosynthesis is at half its maximum value,
 P_T = added biomass (g dry wt da⁻¹ plant⁻¹),
 B_c = conversion factor from gCO₂ cm⁻² s⁻¹ to g dry wt m⁻² da⁻¹ (4.69×10^8), and
 T_i = transfer flux to compartment i, i = 1, 3, 4, 5, 6

The coefficient, $S_L/(S_L + x_2/x_1)$, is used because there is some evidence of the inhibition of photosynthesis by starch accumulation.^{34,35} This is controversial but we have included the coefficient in the event that more supportive evidence is found. The plant uses structural material for stem, fruit, and root respiration when x_3 falls below the critical level $a_4(x_4)^\mu$ as described by Eqs. (43d-43f). The transfers, T_1 , T_3 , T_4 , T_5 , and T_6 , contain the actual dynamics for growth. The expressions for these transfers are hypothetically:

$$T_1 = e_1 x_1 \left\{ k_n [H(D_d - t) + H(T - D_s)] + k_d H(t - D_d) H(D_s - t) \right\} \frac{x_2/x_1}{c_2 + x_2/x_1} (1 - M_d x_1/a_L F_0), \quad (44a)$$

$$T_3 = T_{rs} x_2 \left(\frac{a_1 x_2}{x_1 + x_2} - \frac{b_1 x_3}{x_3 + x_4 + x_5 + x_6} \right) H \left(\frac{x_2}{x_1 + x_2} - S_p \right), \quad (44b)$$

$$T_4 = e_4 \xi_1 x_4^\mu H(x_3 - a_4 x_4^\mu) \frac{x_3 - a_4 x_4^\mu}{b_4 + x_3 - a_4 x_4^\mu}, \quad (44c)$$

$$T_5 = H(\tau - \tau_0) e_4 \xi_2 x_5 H(x_3 - a_4 x_4^\mu) H(\tau_1 - \tau), \quad (44d)$$

and

$$T_6 = e_6 x_6 \frac{x_3 - a_4 x_4^\mu}{b_4 + x_3 - a_4 x_4^\mu} H(x_3 - a_4 x_4^\mu). \quad (44e)$$

In Eq. (44a), we assume that the growth demand by leaves on leaf storage for photosynthate is proportional to leaf biomass, that it is diminished by factors to account for depletion of storage, and that it is diminished by a factor $(1 - M_d X_1/a_L F_0)$, which vanishes as the leaf area index approaches a maximum value. The model accepts this optimal value as input data or calculates a value by optimizing net photosynthesis. In Eq. (44b), we assume that the needs of the leaves for growth are met first, that the flow between storage compartments is always towards main storage, and that the flow is proportional to the size of the donor compartment. Furthermore, we assume that the flow is proportional to the difference between the relative concentration of storage in the leaf, $x_2/(x_1 + x_2)$, and relative concentration of storage in the rest of the plant, $x_2/(x_3 + x_4 + x_5 + x_6)$. In Eq. (44c), we assume that the transfer to stem is proportional to the living tissue of the stem, which we take to be a power of x_4 with μ as the exponent. The factor,

$$H(x_3 - a_4 x_4^\mu) (x_3 - a_4 x_4^\mu)/(b_4 + x_3 - a_4 x_4^\mu),$$

in both Eqs. (44c) and (44d) indicates that the storage system maintains a reserve storage equal to a fraction a_4 of the living tissue of the stem. This factor indicates that as the value for reserve storage is approached by x_3 , the transfers to stem and root are cut off gradually. In Eq. (44d), after a physiological time τ_0 is passed (degree-days or heat units), fruit growth commences and is terminated at τ_1 . While this growth occurs, it is proportional to standing fruit crop x_5 with $e_4 \xi_2$ a growth constant. In Eq. (44e), root growth is proportional to

root size and inversely proportional to water stress. The parameters, e_1 , T_{ms} , e_4 , and $\bar{e}_6$ are growth constants and are in units of da^{-1} . The constants, k_d and k_n , are unitless and distinguish relative growth differences between day and night, while ξ_1 and ξ_2 are dimensionless and distinguish between stem growth and fruit growth. The times of sunrise and sunset are D_d and D_s , respectively.

MODEL INPUTS

The model requires four types of data:

- Climatic data, including latitude, incident light levels, total radiation into the canopy, total radiation absorbed by the ground, air temperature, precipitation, wind above the canopy, and wet bulb temperature;
- Plant data, including those to calculate stomatal resistance as a function of light, temperature, and water stress; data to calculate the turbulent diffusion resistance of the canopy, the wind profile, leaf boundary-layer resistance; values of cell-wall and protoplasm-diffusion resistance of mesophyll cells; measurements of photosynthetic processes; respiration rate of leaves at a base temperature and Q_{10} value; maintenance-respiration rate per unit biomass; growth-respiration rate per unit biomass added per unit time; total leaf-area index of maturing plants; growth of leaf, stem, fruit, and root; data on the effects of leaf storage on photosynthesis; and data describing the movement of photosynthate from leaf to main storage;
- Soil data, including soil temperature, soil salinity, data for calculating soil-water potential from soil-moisture content, soil conductivity from soil-moisture content, and soil resistance from soil conductivity, depth of soil compartment, and root resistance to water flow;
- Pollution data including daily maximum, diurnal distribution, and parameters for calculating photosynthesis reduction or enhancement as a function of pollutant load.

PRELIMINARY RESULTS

Figure 8 shows a typical output of the current model, running under conditions with no pollution. Data from Sinclair,²⁰ Stewart,¹⁹ and Curry and Chen,²³ which is valid primarily for corn, are used along with respiration values from cotton. In Fig. 9, we show the model output with the pollution level of SO_2 at 10 pphm (parts per hundred million) and in Fig. 10, the output with 50 pphm SO_2 . The data providing the

Fig. 8. Output of model showing total growth, and the growth of leaf, stem, fruit, and root during a growing season. This case had no input from pollution stress.

Fig. 9. Output of model with a constant pollutant stress of 10 pphm SO_2 with data on stress effects from barley and alfalfa. The SO_2 exerted a slight fertilization effect on plant growth.

Fig. 10. Output of model with a constant pollution stress of 50 ppm SO_2 . In this case the SO_2 exerted a deleterious effect on growth. The effect was greatest on stem, fruit, and root parts.

pollution effect are from barley and alfalfa.³⁵ Notice the enhanced growth at 10 ppm (Fig. 9) and the deleterious effects at 50 ppm (Fig. 10). With fertilization, total growth increased by 2%, fruit by 5%, and stem growth 3%, while the shoot:root ratio decreased by 3%. With stress treatment total growth decreased by 7%, fruit by 4%, and stem growth by 13%, while the shoot:root ratio increased by 11%. A comparison of shoot:root ratios is in qualitative agreement with the work of Bennet and Oshima,³⁷ who studied the effect of ozone on carrots.

FUTURE RESEARCH

Validation

Our immediate concern is to acquire data and validate the model for sugar beets, one of the most important crops in the Imperial Valley. The five most important crops in the Imperial Valley are lettuce, alfalfa, wheat, sugar beets, and cotton. For a simulated crop we need empirical estimates for the model parameters (translocation, respiration, etc.). To validate the model, we must compare results from our model to photosynthesis, allocation, and growth studies under nominal field conditions. As an additional check on the performance of the water-budget submodel, comparison can be made with evapotranspiration studies. The final validation would be a comparison with fumigation studies in which plants are stressed by pollutants under field conditions.

Model Development

A number of modifications will improve the usefulness and accuracy of the model. The WATER2 submodel discussed above is an important example. This submodel would simulate stomatal resistance as a function of leaf-water potential so that stomatal resistance will respond to daily variations in water stress. When averaged over a month, such changes make little difference in the absence of pollutants or pollutant fluctuations. However, changes in stomatal resistance can affect plant sensitivity to pollutant stress. Therefore, diurnal changes in stomatal resistance are important for the understanding of the effects of diurnal variations in pollutant levels.

Because so many processes are dependent on leaf temperature or microclimate, the model should be altered to include microclimate properties that are important in determining plant behavior, i.e., profiles of radiation, sensible heat, humidity, air temperature, and leaf temperature. Currently, some very simple assumptions are made for these environmental variables.

Attention should be given to improving the simulation by the model of the effects of stress on phenology or physiology. For example, under stress, plants often enter the flowering stage earlier than normal. Our model currently does not address such problems. The model predicts qualitatively the results of Bennet and Oshima,³⁷ who found that ozone stress reduced root biomass rather than altering leaf biomass. However, stress on roots such as due to soil salinity is not accurately predicted by our model. The phenomenological effects of pollutants on photosynthesis are incorporated into our model. However, we feel that the submodel should be reformulated to include the effect of pollutants on actual physiological and biochemical processes. This biochemical approach is now under investigation.

Another aspect of modeling plant growth is the effect of nutrients, which is beyond the scope of GROW1. Future models should incorporate the knowledge in this area. We would prefer to simulate these effects by the mechanisms involved rather than phenomenologically. Future modeling efforts should include synergisms between pollutants and interactions between pollutants and nutrients. If we are successful in developing mechanistic models of pollutant effects and nutrient effects separately, then the task of simulating synergistic interactions should be easier.

Sensitivity Analysis

A sensitivity analysis is important in establishing either the properties or the usefulness of any model. The changes in model output caused by varying model parameters indicate parameters that are most important and that, therefore, must be specified most accurately. Also, these sensitivities are useful in estimating the confidence level of the results from the model.

Applications

The model will provide an assessment of the effects of gaseous pollutants on one of the five most important crops in the Imperial Valley, which will be an overall, valley-wide estimate of affected acreage and the degree of effect by acreage. This assessment will be made for various levels of geothermal development.

Because the water-budget model is a tool for estimating crop water usage in management studies, it has strong potential for future assessment of water resources.

Dose-yield curves may be useful in an assessment of pollutant effects on crop yield. These curves could be constructed as multidimensional yield curves, using environmental variables such as soil salinity, soil moisture parameters, average temperature during the growing season, plant density, length of time to harvest, CO₂ level, etc. Other advanced models could generate curves as functions of such parameters as levels of other pollutants present (ozone), nutrients, etc. Thus, besides providing calculations for assessments, a well-established, validated model is a potential management tool in balancing acceptable levels of pollutants with other compensatory or antagonistic activities.

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APPENDIX A. LIST OF SYMBOLS

This table contains a list of all the symbols used in this report. Some of these symbols are relevant input data for the example cases in the text. Units under Description do not always correspond to units under Value. In these cases, the computer code internally converts values to appropriate units of the Description.

Symbols	Description	Page	Value used in examples
a_L	Conversion factor for changing LAI to leaf dry weight (g/m^2)	7	33
a_1	Coefficient determining translocation of photosynthate	21	1
a_4	Coefficient determining amount of storage to be held in reserve (g)	20	1
A_0	Total concentration of PGA and RuDP ($\text{mol } \ell^{-1}$)	13	see k_3
A	Ratio of total root-surface area to area of ground	17	
b_1	Coefficient determining translocation of photosynthate	21	1
b_4	Parameter determining slope of function that cuts off flow of photosynthate out of main storage as main storage level approaches a critical value	21	0.1
B_c	Converts $\text{g CO}_2/\text{cm}^2\text{s}$ to $\text{g dry wt}/\text{m}^2\text{da}$	20	4.69×10^8
c_1	Reduction in photosynthesis for unit increase in pollutant with one unit of diffusion resistance ($\text{s cm}^{-1} \text{ ppm}^{-1}$)	19	0.7125
c_2	Inverse slope of function cutting off flow of photosynthate from leaf storage to structural leaf as $x_2/x_1 \longrightarrow 0$	21	0.05
C_a	Concentration of CO_2 in air (g/cm^3)	7	310 ppm
C_c	Concentration of CO_2 at chloroplast (g/cm^3)	7	
C_{ia}	Concentration of CO_2 in pore (g/cm^3)	11	
C_p	Concentration of CO_2 in protoplasm (g/cm^3)	11	
C_{soil}	Concentration of salts in soil (mol/cm^3)	14	0
d	Inverse of square of standard deviation of foliage density (m^{-2})	19	

Symbols	Description	Page	Value used in examples
d_7	Thickness of rooting zone layer in soil (m^{-1})	17	
d_8	Thickness of surface zone layer of soil (m^{-1})	17	
D	Diffusivity in the canopy ($cm^2 s^{-1}$)	18	
D_d	Time of dawn (da)	21	
D_L	Leaf width (cm)	13	7
D_o	Turbulent diffusivity in air ($cm^2 s^{-1}$)	19	300
D_s	Time of sunset (da)	21	
e	Vapor pressure (mbar)	14	
e_s	Saturation-vapor pressure (mbar)	15	
e_1	Leaf-growth constant (da^{-1})	21	0.137
e_4	Growth constant for stem and fruit (da^{-1})	21	2.44
e_6	Growth constant for root (da^{-1})	21	0.15
ET	Evapotranspiration ($m da^{-1}$)	14,15,16	
$f(Z)$	Density of leaves in the canopy as a function of Z	19	
$f_L(\alpha)$	Angular distribution of leaves	6	
F	Leaf area index LAI (area of leaves/area of ground)	5,7	
F_o	Maximum allowed LAI in simulation	20	5.6
F_{TOT}	Total LAI	19	
G_i	Net flux of radiant energy out of layer i in the downward direction ($cal cm^{-2} s^{-1}$)	14	
h'	Ratio of F_{TOT} to total canopy depth Z_{TOT} (cm^{-1})	19	0.025
H	Unit step function (Heaviside function); rate of sensible heat transfer from the leaf	15,16,20	
I	Flux of light or light intensity normal to the leaf at canopy depth F (nanoeinstens $cm^{-2} s^{-1}$ or $cal cm^{-2} s^{-1}$)	7	
I_L	Light flux reaching F from the direction of the sun	5	

Symbols	Description	Page	Value used in examples
I_m	Light intensity at photosynthesis half maximum	7	
I_n	Net radiation into the canopy ($\text{cal cm}^{-2}\text{s}^{-1}$)	14	
I_o	Light flux at top of canopy in the direction of the sun ($\text{cal cm}^{-2}\text{s}^{-1}$)	5	.02
k_1	Equilibrium constant for conversion of CO_2 and RuDP to PGA (cm^3/g)	12,13	2.28×10^8
k_2	Equilibrium constant for light conversion of NADP to NADPH (cm^2/cal or $\text{cm}^2/\mu\text{einstein}$)	12,13	$21.9 \text{ cm}^2/\text{cal}$
k_3	Coefficient for maximum photosynthesis for high CO_2 and high light ($\text{g cm}^{-2}\text{s}^{-1}\text{mole}^{-2}\ell^2$)	12,13	$k_3 A_o N_o = 500 \text{ mg dm}^{-2}\text{hr}^{-1}$
k_d	Relative rate of growth during day	21	1
k_n	Relative rate of growth during night	21	1
k_α	Decay constant for reduction of windspeed in canopy	19	0.44
K_{soil}	Maximum value of soil hydraulic conductivity (weight basis, m da^{-1})	17	
$K(x_i)$	Hydraulic conductivity of the soil (m da^{-1})	17	
K	Extinction coefficient of light in the canopy	5	
L	Number of layers in canopy	14	10
M_d	Number of plants per unit area (m^{-2})	7,21	5
$\hat{n}$	Normal to the plane of the leaf	6	
N_o	Total concentration of NADP and NADPH ($\text{mol } \ell^{-1}$)	13	see k_3
P	Photosynthesis ($\text{g cm}^{-2}\text{s}^{-1}$)	7	
P_g	Gross photosynthesis ($\text{g cm}^{-2}\text{s}^{-1}$)	9	
P_m	Maximum values of photosynthesis at high light levels	9	
P_n	Net photosynthesis	9	
P_r	Precipitation (m da^{-1})	14	
P_1	Precipitation intercepted by leaves (m da^{-1})	16	
P_2	Precipitation striking ground without interception (m da^{-1})	16	

Symbols	Description	Page	Value used in examples
PL	Average cosine of projection of sunlight onto leaf for all leaves	6	
PL _α	Average cosine of projection of sunlight onto leaves at angle α	6	
Q ₁₀	Ratio of respiration at (T _x + 10)°K to respiration at T _x °K, where T _x is a reference temperature	13	2
r _a	Leaf-boundary-layer resistance (s cm ⁻¹)	7	
r _c	Carboxylation resistance	7	
r _{ci}	Turbulent diffusion resistance from canopy layer i to top of canopy (s cm ⁻¹)	18	
r _{cw}	Cell-wall-diffusion resistance (s cm ⁻¹)	12	0.126
r _g	Specific growth-respiration rate	20	0.35 at 25°C
r _l	Stomatal resistance due to all factors except water stress (s cm ⁻¹)	13	
r _m	Mesophyll-cell resistance (s cm ⁻¹)	7	
r _n	Specific maintenance-respiration rate	20	0.006 at 25°C
r _p	Protoplasm resistance to CO ₂ diffusion (s cm ⁻¹)	12	1.0
r _s	Stomatal-diffusion resistance (s cm ⁻¹)	12	
r _{soil}	Resistance to hydraulic flow of water in the soil (da, weight basis)	16	
r _{sp}	Resistance to flow of water between soil and the plant (da, weight basis)	16	
r _{w1}	Parameter proportional to slope of curve of stomatal resistance as a function of water stress (soil-water potential) (bar s cm ⁻¹)	14	5.004
r _{w2}	Value of ψ _s at which stomatal resistance is singular (bar)	14	-15
r _{w3}	Soil-water potential at a soil-water content of 0 (bar)	14	-267
r _{w4}	Logarithm of the ratio of the soil-water potentials with one unit of soil-water-content difference between them (m ⁻¹)	14	85.67

Symbols	Description	Page	Value used in examples
r_o	Critical or maximum stomatal resistance attained when ψ_{Li} is maximum	18	
r_l	Leaf-boundary-layer resistance when $D_L = 1 \text{ cm}$ and $U = 1 \text{ cm s}^{-1}$ (s cm^{-1})	13	1.3
R	Respiration (usually leaf) ($\text{g cm}^{-2}\text{s}^{-1}$)	11,13	
R_G	Gas constant (bars $^{\circ}\text{K}^{-1} \text{mol}^{-1}\text{cm}^3$, or $\text{cal mol}^{-1}\text{K}^{-1}$)	14	$8.314 \text{ J mol}^{-1}\text{K}^{-1}$
R_x	Dark leaf respiration at 25°C ($\text{g cm}^{-2}\text{s}^{-1}$)	13	$2.5 \text{ mg dm}^{-2}\text{h}^{-1}$
$\hat{s}$	Unit vector in direction of the sun		
s	Absorption coefficient of CO_2 in water	12	0.756 at 25°C
S	Air-pollutant concentration (ppm)	19	
S_o	Threshold for depressant effect of pollutant (ppm)	19	20 pphm
S_L	Ratio of leaf storage to leaf structural tissue at which photosynthesis is at half maximum	20	
S_p	Reserve concentration of leaf storage photosynthate that the leaf retains	21	0.1
t	Time (da)	20	
T	Temperature, usually of air ($^{\circ}\text{K}$)	13,20	
T_i	Transfer flux to compartment i from storage ($\text{g m}^{-2}\text{d}^{-1}$)	20	
T_r	Root or soil temperature ($^{\circ}\text{K}$)	20	
T_{rns}	Transfer coefficient for movement between leaf storage and main storage (da^{-1})	21	3.0
T_x	Reference temperature for calculating respiration ($^{\circ}\text{K}$)	13	25°C
u	Inverse of exponent that transforms soil content to soil potential	17	
u_1	Inverse of $\max [P_n(I)]/C_a$ at high light levels ($\text{ppm g}^{-1}\text{cm}^2\text{s}$)	9	
U	Windspeed (cm s^{-1})	13,18	

Symbols	Description	Page	Value used in examples
v	Exponent of soil potential used to calculate soil conductivity from soil potential	17	
v_1	Inverse of slope of $P_n(I)$ at low light levels (nanoeinsteins g^{-1})	9	
w	Value of soil potential at which soil conductivity has fallen to half maximum (m)	17	
w_1	Inverse of slope of $P_g(I)$ at low light levels (nanoeinsteins g^{-1})	9	
x_1	Biomass (dry wt) of structural leaf material (g)	7,20	
x_2	Biomass (dry wt) of leaf material in storage (g)	20	
x_3	Biomass (dry wt) of main storage (g)	20	
x_4	Stem biomass (dry wt) (g)	20	
x_5	Fruit biomass (dry wt) (g)	20	
x_6	Root biomass (dry wt) (g)	20	
x_7	Soil water in the root zone (m)	14	
x_8	Soil water in the soil-surface zone (m)	16	
x_9	Water in the leaf-interception storage (m)	16	
x_{7max}	Maximum water content of the root zone (m)	14	0.12
Z	Vertical distance usually measured from the top of the canopy (m)	18	
Z_{TOT}	Thickness of the canopy (m)	19	
α	Angle of the leaf to the horizon	5	
β	Elevation of the sun	5	
γ	Psychometric constant (mbar $^{\circ}K^{-1}$)	15	0.66
δ	Angle between the sun and the leaf	6	
Δ	Derivative of saturation vapor pressure with respect to temperature (mbar $^{\circ}K^{-1}$)	15	
η	Angle between the sun and the normal to the leaf	6	
θ	Volumetric water content at which matrix potential is equivalent to a pressure of 1 m of water	17	

Symbols	Description	Page	Value used in examples
λ	Latent heat of vaporization (cal g ⁻¹)	15	558
μ	Power of x_4 used to calculate biomass of x_4 capable of growth	20	1.0
μ_1	Coefficient proportional to slope of $r_s(I)$ (s ² cm cal ⁻¹)	13	1.3×10^{-3}
μ_2	Coefficient inversely proportional to square root of slope of $r_s(I)$ at $I = 0$ (nanoeinsteins cm ⁻² s ⁻¹ or cal cm ⁻² s ⁻¹)	13	3.33×15^{-6} cal cm ⁻² s ⁻¹
μ_3	Slope of $r_s(T)$ (s cm ⁻¹ °K ⁻¹)	13	0.5
μ_4	r_s at 0.0°C, infinite light levels, and no water stress (s cm ⁻¹)	13	-7.0
ν	Water-stress component to stomatal resistance	13	
ξ_1	Relative growth constant for stem	21	2.0
ξ_2	Relative growth constant for fruit	21	0.0346
ρ_{Ls}	Saturation concentration of water vapor at the leaf	15	
ρ_Z	Concentration of water vapor at reference height Z	15	
ρ_c	Volume heat capacity of air (cal cm ⁻³ °K ⁻¹)	15	290×10^6
σ	Function of α and β used in calculating PL_α	6	
τ_0	Physiological time for initiation of fruit growth (degree-da)	21	800
τ_1	Physiological time for termination of fruit growth (degree-da)	21	2500
Ψ_c	Critical water potential at which r_s attains its maximum value (m, weight basis)	14 21	
Ψ_s	Soil-water potential (bars)	16	
Ψ_{Li}	Leaf potential for layer i (m, weight basis)		
Ψ_7	Soil-water potential for root-zone layer (m, weight basis)	16	
Ψ_8	Soil-water potential for soil-surface layer (m, weight basis)	18	
ω	Azimuthal angle between sun and leaf	5	