

ETc from Physiological Model (25 Oct. 2006; model has been considerably updated since then; see the extensive comment lines at the beginning of the Fortran 90 file, [http://gconsortium.com/academic\\_page/canopy\\_sim6\\_ASR\\_hspower\\_Rds.f90.txt](http://gconsortium.com/academic_page/canopy_sim6_ASR_hspower_Rds.f90.txt) )

Light interception is computed from the geometry of canopies and of solar radiation. Tree placements are specified on an arbitrary grid, taken in the current case as a square array with 9-meter spacings. Each tree has an ellipsoidal crown with semi-axes  $a_{tree}$  and  $b_{tree}$ . In the current computations, these are taken as equal (spherical crowns) and varied from 1.5 to 4.5 m. The major axis can be tilted at specified zenith and azimuth angles,  $\theta_{tree}$ ,  $\phi_{tree}$ ; these are irrelevant for spherical crowns. Foliage density within crowns is taken as constant,  $f_d$  ( $m^2 m^{-3} = m^{-1}$ ), the current model. Computations of light interception are performed on tree number 1. Light is traced through its own crown and all other crowns.

Photosynthetically active radiation (PAR) is resolved into the direct solar beam and diffuse skylight. Flux density (direct beam) and intensity (diffuse skylight) are given in quantum units ( $mol m^{-2} s^{-1}$ ) for use in photosynthesis calculations. They are readily converted to energy units for calculations of energy balance. The solar elevation, and thus the beam direction, is computed from latitude, longitude, date, and time from standard formulae (e.g., Percy, 1989). Diffuse skylight is approximated as uniform. The penetration of both components is calculated at a sampling of points within crown number  $I$ . Radii are sampled at  $n_r$  locations, chosen to give equal shell volumes for each point. Zenith and azimuthal angles, relative to the crown coordinates, are sampled at  $n_\theta$  and  $n_\phi$  locations, respectively, and locations are chosen to resolved equal solid angles.

The direct solar beam penetrates to a crown location statistically, with a probability  $P_{pen,dir} = \exp(-K*L) = \exp(-0.5*f_d*s_{tot})$ . Here,  $L$  is the leaf area index through the crowns along the ray direction and  $K$  is the extinction coefficient along the ray direction.  $K$  is simply the average cosine between leaf normals and the solar beam direction as absolute values - the factor  $G$  in formulations resolving propagation relative to vertical (Ross, 1981). It depends upon leaf angle distribution,  $LAD$ , as well as solar direction. In the current computations, we take  $LAD$  as random, thus setting  $K = 0.5$ . Leaf area index equals the foliage density multiplied by the total distance,  $s_{tot}$ , that the ray traverses in all possible crowns. This distance is computed by tracing from the canopy location of interest toward the sun, in discrete steps of size  $ds$ . At each step, a geometric calculation is performed to test if the path lies within any crown. If the result is positive,  $s_{tot}$  is incremented by  $ds$ . Accumulation of  $s_{tot}$  stops at a value  $s_{max}$ , beyond which penetration can be considered negligible. The numerical methods for path length are required in place of analytical methods (Norman and Welles, 1984) by virtue of the irregular crown center placements and crown tilts that we allow.

Fractional penetration of diffuse skylight,  $P_{pen,diff}$ , is computed as the average penetration fraction from 25 discrete directions covering equal solid angles.

Irradiance, or intercepted flux density,  $I_L$ , on a given leaf is composed as the sum of 1) the projection of the direct solar beam, at flux density  $I_{00}$ , onto the leaf multiplied by the cosine of the angle between (flat) leaf normal and solar direction,  $X_{LS}$ , as an absolute value, and 2) the intensity of diffuse skylight,  $D_0$ , which equals the top-of-canopy flux,  $D_{00}$ , multiplied by  $P_{pen,diff}$  at the leaf location. We neglect second interceptions of the modest amount of scattered PAR. The value of  $D_0$  is taken as constant, independent of leaf orientation and without significant statistical variation, following the results of Gutschick (1984). The contribution from the direct beam at any location is either zero (shaded leaves) or  $I_{00}X_{LS}$  because the penetration of the direct beam is statistical. For canopies with random LAD, the distribution of direct-beam irradiances is uniform from zero to  $I_{00}X_{LS}$  (Gutschick and Wiegel, 1988). Consequently,  $I_L$  has a single, deterministic value,  $D_0 = D_{00}P_{pen,diff}$ , for shade leaves. For sunlit leaves, it has a statistical distribution uniformly from  $D_0$  to  $I_{00} + D_0$ . Because photosynthesis responds very nonlinearly to irradiance, it is inappropriate to use an average intensity. For practical computations, we must resolve  $I_L$  in a limited number,  $n_{bins}$ , of intervals between zero and the maximum,  $D_{00} + I_{00}$ . In a further simplification, the probabilities of each  $I_L$  interval are accumulated over the whole canopy; computations of leaf photosynthesis and transpiration are performed for each discrete  $I_L$  value (bin central value) and summed by weighting with the total bin probability. This method neglects variations between

canopy locations in environmental variables other than irradiance that determine energy balance; generalizations are possible, with significant increases in computation time.

The magnitudes of direct-beam flux density and diffuse skylight radiance vary with solar elevation and sky conditions. They are computed from total solar energy flux density,  $Q_{sol}$ , on a horizontal sensor, as recorded in standard weather records, and from the solar zenith angle,  $\theta_s$ . Energy flux density is converted to quantum flux density in the PAR,  $I_s$  (NIR flux densities are approximated later). From the solar zenith angle, one readily computes the approximate air mass,  $m_a$ , traversed by the direct beam. From this, one computes an expected value of  $D_{00} = D_{000}m_a^{-0.3}$ ; we use  $D_{000} = 200 \mu\text{mol m}^{-2} \text{s}^{-1}$ . With a clear sky, the expected value of  $I_s$  is  $D_{00} + I_{00}\cos\theta_s \exp(-am_a)$ . The last factor accounts for direct-beam scattering;  $I_{00}$  is taken as  $2000 \mu\text{mol m}^{-2} \text{s}^{-1}$ . If  $I_s$  is less than this value, we apportion the time interval into a fraction of clear sky and a complementary fraction of overcast, and we compute leaf conditions separately for both cases.

Leaf photosynthetic rate,  $A_L$  (or  $A$ , for short), and transpiration rate,  $E_L$  or  $E$ , are computed from four simultaneous equations, all but one nonlinear: 1) enzyme kinetics of  $\text{CO}_2$  assimilation; 2) stomatal control; 3) diffusion through stomata and the leaf boundary layer; and 4) energy balance. Enzyme kinetics are formulated following Farquhar *et al.* (1980 *ff.*). At low irradiances,  $\text{CO}_2$  assimilation rate,  $A$ , is stoichiometric with photon use:  $A_{LL} = Q_0 I_L$ . The “initial quantum yield” depends upon leaf temperature,  $T_L$ , and  $\text{CO}_2$  partial pressure,  $C_i$ , in the leaf interior (actually, at the chloroplast, a distinction ignored here but of modest significance: Gutschick, 2006). It is computed as  $Q_0 = Q_{00} (C_i - \Gamma)/(C_i + 2\Gamma)$ , where  $\Gamma$  is the  $\text{CO}_2$  compensation partial pressure computed from temperature by the formula of Farquhar *et al.* (1980) as  $3.69 + 0.18(T_L - 25) + 0.0036(T_L - 25)^2$ , in Pa. At high  $I_L$ ,  $A$  saturates to the rate limited by activity of the Rubisco enzyme:  $A_{sat} = V_{c,max}(C_i - \Gamma)/(C_i + K_{co})$ . Here,  $V_{c,max}$  is the rate at both light- and  $\text{CO}_2$ -saturation, set by enzyme investment, and  $K_{co}$  is the effective Michaelis constant for  $\text{CO}_2$  binding in the presence of  $\text{O}_2$ . Farquhar *et al.* (1980) show that  $K_{co} = K_c(1 + \text{O}/K_o)$ , with  $K_c$  and  $K_o$  as binding constants for  $\text{CO}_2$  and  $\text{O}_2$  as known functions of temperature taken as universal among plant species (but see Bernacchi *et al.*, 2003). At intermediate values of  $I_L$  is a transition zone with  $A$  described as the solution of  $\Theta A^2 - A(A_{LL} + A_{sat}) + A_{LL}A_{sat}$ . For  $\Theta=1$ ,  $A=A_{LL}$  or  $A=A_{sat}$  (a sharp Blackman curve); a typical value is 0.8 (Leverenz, 1994), giving a slightly smoothed transition.

This value of  $A$  is gross assimilation. Observed  $A$ , or net  $A$ , incorporates a debit for leaf respiration,  $R_d$ . Respiration responds to leaf temperature approximately as  $R_d = R_d(T_{mean}) \exp(0.7(T - T_{mean}))$ . Here,  $T_{mean}$  is the temperature to which the leaf is acclimated, taken as mean temperature in the photoperiod of the previous 2 weeks (a simple approximation to formulae of Wythers *et al.*, 2005). The base value is typically  $R_d(T_{mean}) = f_{Rd} A(T_{mean})$ , with  $A(T_{mean})$  being the assimilation rate at  $T_{mean}$  and  $f_{Rd}$  a constant near 0.08.

The value of  $C_i$  is determined by  $\text{CO}_2$  series transport through the leaf boundary layer (conductance  $g_b$  for water vapor,  $g_b' = 0.77 g_b$  for  $\text{CO}_2$ ) and stomatal pores (conductance per area  $g_s$  for water vapor,  $g_s' = 0.62 g_s$  for  $\text{CO}_2$ ). The net conductance is  $g_{bs} = 1/(1/g_s + 1/g_b)$  for water vapor and analogously for  $\text{CO}_2$ , denoted  $g_{bs}'$ . We have  $A = g_{bs}'(C_a - C_i)/P_a$ , using modern molar units of conductance (Ball, 1987); here,  $C_a$  is the  $\text{CO}_2$  partial pressure in external air beyond the boundary layer and  $P_a$  is total air pressure. Stomatal conductance responds to environmental variables and to  $A$  itself. A good approximation (Gutschick and Simonneau, 2002) is the Ball-Berry equation (Ball *et al.*, 1987),  $g_s = m A h_s / C_s + b$ . Here,  $m$  and  $b$  are empirical constants that vary mildly with species and more so with water stress, which is assumed absent in present calculations. The variables  $h_s$  and  $C_s$  are, respectively, the relative humidity and  $\text{CO}_2$  partial pressure at the leaf surface, beneath the leaf boundary layer. They are computed from transport equations as  $h_s = (g_b e_a / e_i + g_s) / (g_b + g_s)$  and  $C_s = C_a - A P_a / g_b$ . Here,  $e_a$  and  $e_i$  are the water-vapor partial pressures in external air and inside the leaf, respectively;  $e_i$  is set at the saturated vapor pressure at leaf temperature, ignoring a very small correction for leaf water potential.

The final equation is energy balance. Leaves have very low thermal capacity and thus are approximated as being in steady state:

$$\text{Net energy gain} = 0 = Q_{SW}^+ + Q_{TIR}^+ - Q_{TIR}^- - Q_E - Q_{CC} \quad (\text{XX})$$

The gain of shortwave energy is  $Q_{SW}^+ = a_{PAR}E_{PAR} + a_{NIR}E_{NIR}$  for leaf absorptivities  $a_{PAR}$  and  $a_{NIR}$  in the respective wavebands and corresponding energy flux densities  $E_{PAR}$  and  $E_{NIR}$ . We allow  $a_{PAR}$  to be set by the user and we set  $a_{NIR}=0.35$ . Energy flux density is computed from quantum flux density,  $I_L$  (which is in the PAR), multiplied by the average energy per mole in the PAR, 220 kJ/mol.  $E_{NIR}$  is equated to  $E_{PAR}$ , which is valid at the top of the canopy but less so in the crown interior because NIR is more weakly absorbed and penetrates farther. Thermal infrared energy is gained at the rate  $Q_{TIR}^+$  by absorbing TIR from the sky and from surrounding vegetation. These have energy flux densities, respectively, of  $E_{TIR,sky} = \sigma T_{sky,abs}^4$  and  $\varepsilon\sigma T_{veg,abs}^4$ , where  $abs$  indicates Kelvin temperature. A fraction of leaf area  $P_{pen,diff}$  is exposed to sky TIR and a fraction  $2-P_{pen,diff}$  (the remainder of the 2 sides) is exposed to vegetation TIR. We approximate vegetation temperature as  $T_L$  of the leaf in question.

The last three terms in Eq. (XX) depend upon leaf temperature, which is iterated to balance the equation. TIR loss,  $Q_{TIR}^-$ , equals  $2\varepsilon\sigma T_{L,abs}^4$ . Transpirational cooling,  $Q_E$ , equals the molar heat of vaporization multiplied by the leaf transpiration rate in molar units,  $E = g_{bs}(e_l - e_{air})/P_{air}$ , using quantities defined earlier. Convective-conductive cooling,  $Q_C$ , equals the product of the temperature difference between leaf and air (at  $T_a$ ), the boundary-layer conductance  $g_b$ , and the molar heat capacity of air. The value of  $g_b$  in  $\text{mol m}^{-2} \text{s}^{-1}$  is approximated as  $0.264(u/d_{leaf})^{1/2}$ , where  $u$  is the windspeed in m/s and  $d_{leaf}$  is characteristic leaf dimension.

Efficient simultaneous solution of all four equations is iterative. One sets search limits in  $g_s$  and performs a binary search. At each value of  $g_s$ , the energy-balance equation is readily solved for  $T_L$ , enabling the computation of temperature-activated values of enzyme-kinetic parameters, as well as  $e_l$  and  $h_s$ . The enzyme-kinetic expression for  $A$  is equated to the transport expression of  $A$ , giving a quartic equation for  $C_i$  that is solved iteratively. This enables computation of a self-consistent value of  $A$ . An error function to use in the binary search is then defined as  $g_s$  minus the Ball-Berry expression.

Partial pressures of  $\text{CO}_2$  and water vapor in free air, above the canopy, are prescribed as  $C_a^0$  and  $e_{air}^0$ , the latter from weather data. Leaves in the canopy are exposed to partial pressures  $C_a$  and  $e_a$ , which are offset by amounts proportional to canopy-total  $A$  and  $E$ :  $C_a = C_a^0 - P_a A/g_{a,can}$  and  $e_a = e_a^0 + P_a E/g_{a,can}$ . The canopy aerodynamic conductance,  $g_{a,can}$ , is estimated from windspeed as  $u/C$ , with  $C$  being a constant dependent upon canopy leaf-area index and its vertical distribution; formulas are given by Sellers *et al.* (1996). Because  $A$  and  $E$  themselves depend upon  $C_a$  and  $e_a$ , the entire computation of  $A$  and  $E$  must be iterated. Constraints on increments are imposed to avoid unstable solutions. Each iteration yields an error estimate, e.g., for water-vapor pressure, it is in the current iteration minus the quantity  $e_a^0 + E*P_a/g_{a,can}$ . If more than three iterations are required, their error values are used to estimate the partial derivatives of  $A$  and  $E$  with respect to  $e_a$  and  $T_a$ . In turn, these are used to solve for improved estimates of  $e_a$  and  $T_a$ . After solutions have converged at all levels, all computed quantities are reported and a total accounting of photon fates is made, including a test of conservation of energy.

The full Fortran program, incorporating copious explanatory comments, is posted on the Website <http://biology-web.nmsu.edu/vince>. Also posted are sample data sets and lists of program variables with their units and purposes.

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