Dennis Baldocchi
Department of Environmental Science, Policy and Management
Mulford Hall
University of California, Berkeley
baldocchi@nature.berkeley.edu

March 18, 2024

AN OVERVIEW OF *CANVEG*, A CANOPY TRACE GAS FLUX MODEL

1. Introduction

CANVEG is a one-dimensional, multi-layer biosphere-atmosphere gas exchange model to compute water vapor, CO_2 and isoprene flux densities. The model consists of coupled micrometeorological and eco-physiological modules. The micrometeorological modules compute leaf and soil energy exchange, turbulent diffusion, scalar concentration profiles and radiative transfer through the canopy. Environmental variables, computed with the micrometeorological module, in turn, drive the physiological modules that compute leaf photosynthesis, stomatal conductance, transpiration and leaf, bole and soil/root respiration, as well as isoprene emission rates. We discuss the salient aspects of the model system below.

2. Principles

a. Micrometeorology

i. Sources and Sinks

The conservation budget for a passive scalar provides the foundation for computing scalar fluxes and their local ambient concentrations. If a canopy is horizontally homogeneous and environmental conditions are steady, the scalar conservation equation can be expressed as an equality between the change, with height, of the vertical turbulent flux (F) and the diffusive source/sink strength, $S(C,z)$:

$$\frac{\partial F(C,\ z)}{\partial z} = S(C,\ z) \quad (1)$$

The diffusive source/sink strength of a scalar in a unit volume of leaves is proportional to the concentration gradient normal to individual leaves, the surface area of individual leaves and the number leaves in the volume. The diffusive source strength can be expressed in the form of a resistance-analog relationship (Meyers and Paw U, 1987):

$$S(C, z) = - a(z) \frac{(C(z) - C_i)}{r_b(z) + r_s(z)} \quad (2)$$

where $a(z)$ is the leaf area density ($m^2\ m^{-3}$), $(C(z) - C_i)$ is the potential difference of scalar concentration or heat content between air outside the laminar boundary layer of leaves and the air within the stomatal cavity (mol mol^{-1}), r_b is the boundary layer resistance to molecular diffusion ($mol^{-1}\ m^2\ s^1$), and r_s is the stomatal resistance ($mol^{-1}\ m^2\ s^1$).

The light environment on sunlit and shaded leaves in a forest is very distinct and the response of many biophysical processes that light is highly non-linear. Hence, we cannot evaluate Equation 2 on the basis of the mean light environment. Rather, we must evaluate the strengths of sources and sinks at a particular level in the canopy on the basis of the radiation balance on the sunlit (p_{sun}) and shaded (p_{shade}) leaf fractions.

$$S(C,z) = f(I_{sun}, T_{sun}, q_{sun}, C_{sun}) \cdot p_{sun}(z) + f(I_{shade}, T_{shade}, q_{shade}, C_{shade}) \cdot p_{shade} \quad (3)$$

ii. Radiative Transfer

The transfer of photons through the canopy must be simulated to evaluate the probability of sunlit and shaded leaves, as well as photosynthesis, stomatal conductance, and leaf and soil energy balances. The radiative transfer model was derived from probabilistic theory (Norman, 1979). The radiative transfer model assumes that foliage is randomly distributed in space, that leaves have a spherical inclination angle distribution and the sun is

a point source. In this case the probability of beam penetration is calculated using a Poisson distribution:

$$P_0 = \exp\left(-\frac{L\,G}{\sin\,\beta}\right) \qquad (4)$$

where L is leaf area index, β is the solar elevation angle and G is the foliage orientation function. G represents the direction cosine between the sun and the mean leaf normal. For the ideal case, in which leaves have a spherical angle distribution, G is constant and equals one-half.

Native vegetation has clumped foliage. In these circumstances, the Poisson probability density function is inadequate for computing probabilities of photon transmission through vegetation. Instead, the Markov model can be employed (Myneni et al., 1989), where the probability of beam penetration is:

$$P_0 = exp\left(-\frac{L\,G\Omega}{sin\,\beta}\right) \qquad (5)$$

Ω is a clumping factor and ranges between zero and one.

Mathematically, the probability of sunflecks is equal to derivative of P_0 with respect to L times the average cosine of the leaf-sun angle (Gutschick, 1991)

$$P_b = -\frac{sin\,\beta}{G}\frac{dP_0}{dL} = \Omega \cdot exp\left(-\frac{L\,G\Omega}{sin\,\beta}\right) \quad (6)$$

The integration of equation A6 with respect to leaf area yields the sunlit leaf area.

The probability of diffuse radiation penetration is computed by integrating equations 4 or 5 over the sky's hemisphere.

$$P_{diffuse} = 2\int_0^{\pi/2} P_0\,cos\,\theta\,sin\,\theta \cdot d\theta \quad (7)$$

The scattering of light was computed for the visible and near infrared wavebands using the slab, 'adding' approach of Norman (1979). Downward-directed diffuse light (D_i), at layer i for a given waveband, is a function of the downward directed diffuse radiation that was transmitted from the upper layer ($T_n D_{i+1}$) and the upward directed radiation that is reflected ($R U_i$):

$$D_i = R_l \cdot U_i + T_n D_{i+1} \quad (8)$$

Similarly, the upward directed diffuse sunlight (U_{i+1}) is a function of that radiation which is transmitted through the layer and the reflected downward radiation:

$$U_{i+1} = R_u \cdot D_{i+1} + T_n U_i \quad (9)$$

Since we are considering the transmission and reflectance of sunlight through layers of vegetation (Δf) rather from the surface of planes of leaves, the layer transmission and reflectance coefficients are defined as:

$$T_n = exp(\frac{-\Delta f \cdot G \cdot \Omega}{sin\,\beta}) + (1 - exp(\frac{-\Delta f \cdot G \cdot \Omega}{sin\,\beta}))\tau \quad (10)$$

$$R_u = (1 - exp(\frac{-\Delta f \cdot G \cdot \Omega}{sin\,\beta}))\rho_u \quad (11)$$

$$R_l = (1 - exp(\frac{-\Delta f \cdot G \cdot \Omega}{sin\,\beta}))\rho_l \quad (12)$$

The subscripts *u* and *l* refer to the upper and lower sides of the leaves, ρ is the leaf reflectance and τ is the leaf transmittance for the specific waveband.

iii. Turbulence Closure

The interdependence between sources and sinks (*S(C,z)*) and scalar concentrations (*C(z)*) requires the use of a turbulent diffusion model. We used a Lagrangian random

walk model to evaluate turbulent diffusion in the vertical directions, above and within a plant canopy using a Lagrangian framework (see Thomson, 1987 ; Raupach, 1988).

The principles of Lagrangian diffusion modelling for a horizontally homogeneous canopy under steady conditions, where only vertical diffusion is of interest is outlined in this sub-section.. The concentration field of a scalar is related to the statistics of an ensemble of dispersing marked fluid parcels. The ensemble mean concentration, C(z,t), at a given vertical location (z) and time (t) equals:

$$\mathbf{1}\, C(z,t) = \iint P(z,t|z_0,t_0) S(z_0,t_0) dz_0 dt_0 \quad (13$$

where S is the diffusive source/sink strength of a scalar from a unit volume of leaves. $P(z,t|z_0,t_0)$ is the probability density function that defines whether a fluid parcel released from a point in space (z_o) at time t_o is observed at another location and time (z,t). This approach valid as long as the diffusivity of the turbulent field far exceeds the molecular diffusivity of the scalar (Sawford, 1985; Wilson, 1989).

Inside a plant canopy, turbulence is inhomogeneous and non-Gaussian. In other words, the mean wind velocity and its statistics vary appreciably with height and the probability density functions of velocity fluctuations are skewed and kurtotic (Wilson et al., 1982; Baldocchi and Meyers, 1988; Raupach, 1988). The probability density function, $P(z,t|z_o,t_o)$, cannot be specified analytically in non-Gaussian, inhomogeneous turbulence. Yet, $P(z,t|z_o,t_o)$ can be determined numerically by using a Markov sequence model; $P(z,t|z_o,t_o)$ can be estimated by calculating the trajectory of an ensemble of fluid parcels and determining what proportion of fluid parcels (released from z_o) reside at a given height as they travel for a given time span (Raupach, 1989).

The vertical trajectory of a fluid parcel depends on its vertical position and velocity. The vertical displacement of fluid parcels was computed as a function of time:

$$dz = w \cdot dt \qquad (14)$$

where *w* is the Lagrangian vertical velocity and *dt* is differential time increment. Incremental changes in vertical velocity were computed with the Langevin equation, an algorithm that is weighted by a deterministic forcing (which is a function of the fluid parcel's previous velocity) and a random forcing term (Thomson, 1987). The vertical position of each fluid parcel, z, is determined by integrating vertical velocity (w) with respect to time:

$$z(t) = z(t_0) + \int_{t_0}^{t} w(t')dt' \quad (15$$

The vertical velocity of fluid parcels is calculated from the Langevin equation, a stochastic differential equation for the acceleration of a velocity component (Sawford, 1985; Raupach, 1988). The Langevin Equation calculates acceleration as a function of the memory of its velocity and a random forcing:

2

$$\frac{dW}{dt} = -\alpha W + \beta d\Omega(t) \quad (16$$

∀ and ß are coefficients and dΣ(t) is a Gaussian "white noise" process. The random forcing function dΣ(t) has a mean of zero, a variance of one and a covariance of zero between subsequent random events (Sawford, 1985; Raupach, 1988).

When the vertical velocity variance increases with height, a downward drift of fluid parcels occurs in random walk models based on the Langevin Equation (Legg and Raupach, 1982; Wilson et al. 1981a; Leclerc et al., 1988). An artificial accumulation of matter occurs in heterogeneous turbulence because fluid parcels entering into a lower region with a decreased vertical velocity scale have a reduced probability of leaving that region (Raupach, 1988; Sawford, 1985). This drift is undesirable because it violates the thermodynamic constraint that an initially uniform distribution of material must be maintained (Sawford, 1985; Thomson, 1987).

Several attempts have been made to develop random-walk models that remove this unrealistic accumulation of matter near the surface. One approach introduces an additional force term into the Langevin equation, which becomes a mean upward drift velocity in the Markov sequence (Wilson et al., 1981b; Legg and Raupach, 1982). A second approach is based on an expression for the higher moments of the random term in the Markov sequence (Thomson, 1984). This second approach allows non-Gaussian random forcing. However, Thomson's 1984 approach has received criticism by Thomson (1987), among others , because non-Gaussian forcing yields unrealizable solutions. Thomson (1987) starts his derivation with this form of the differential form of the Langevin equation:

$$dw = a(z,t,w)dt + b(z,t,w)d\xi \qquad (17)$$

The coefficients *a(z,t,w)* and *b(z,t,w)* are non-linear functions of w and are defined to account for inhomogeneous turbulence. The term $d\xi$ defines a Gaussian random forcing with a mean of zero and a variance of *dt*. The terms *a(z,t,w)* and *b(z,t,w)* are derived from the budget equation for the Eulerian probability density function of *w* (the Fokker-Planck equation) (Thomson, 1987). For the one-dimensional case, where velocity fluctuations and gradients occur only in the vertical direction, equation 3 becomes:

$$dw = (-\frac{w_L}{T_L} + \frac{1}{2}\left[1 + \frac{{w_L}^2}{\sigma_w^2}\right]\frac{\partial\sigma_W^2}{\partial z})dt + \sqrt{\frac{2\sigma_W^2}{T_L}}d\xi \qquad (18)$$

This algorithm has gained acceptance, theoretically, for it meets the model criteria proposed by Sawford (1985) and Thomson (1987), including the well-mixed criterion.

For the numerical calculations performed here, the finite difference algorithm of Luhar and Britter (1989) is used, which expresses the random operator in terms of an increment (i) that has a mean of zero and a variance of one (dΩ):

$$w_{i+1} = w_i + (-\frac{w_i}{T_L} + \frac{1}{2}\left[1 + \frac{w_i^2}{\sigma_w^2}\right]\frac{\partial \sigma_w^2}{\partial z})\Delta t + \sqrt{\frac{2\sigma_w^2}{T_L}\Delta t}\, d\Omega \qquad (19)$$

Equations 18 and 19 do not consider the impact of non-Gaussian and skewed statistical properties on the movement of fluid parcels, although these are distinct characteristics of canopy turbulence (Raupach, 1988; Wilson, 1989; Raupach et al., 1996). The rationale for neglecting the impact of non-Gaussian turbulence statistics on Equations 18 and 19 is based on information in a recent article by Wilson and Sawford (1996). They report that Lagrangian models, which considered the effect of non-Gaussion turbulence on fluid element movement, perform worse than Thomson's 1987 model, which assumes Gaussian and Eulerian turbulent statistics.

With regard to the Lagrangian model, concentration differences between an arbitrary level (C_z) and a reference level (C_r) (located above a plant canopy) were computed by summing the contributions of material diffusing to or from different layers in the canopy (Raupach, 1988). Numerically, this relation is expressed as:

$$C_z - C_r = \sum_{j=1}^{N} S_j(C_j) D_{z,j} \Delta z_j \qquad (20)$$

The dispersion matrix ($D_{z,j}$) has units of s m^{-1} and was calculated using the random walk algorithm of Thomson (1987). The dispersion matrix is calculated by following the trajectory of an ensemble fluid parcels, whose source strength is prescribed and is uniform with height.

To minimize excessive computational overhead, energy balance and canopy photosynthesis model runs were performed using dispersion matrices which were scaled to measured friction velocities. The data shows that the mean ratio between the dispersion matrices at two different friction velocities increases by 1.90 as u* increases by 2.11. The difference between these two ratios is only 11%, a tolerable error in scaled D(i,j) values.

In practice the source-sink function, S, is dependent on local concentration, c, and vice versa. Raupach (1988) devised a scheme that computes the interdependence between S and c. The concentration difference between an arbitrary level (c_i) and reference level (c_r located above a plant canopy can be expressed as by summing the contributions of material diffusing to or from layers in the canopy (denoted by the subscript j):

$$c_i - c_r = \sum_{j=1}^{N} S_j(c_j) D_{i,j} \Delta z_j$$

The dispersion matrix ($D_{i,j}$) is solely a function of the turbulence statistics and can be computed by uniformly releasing fluid parcels from each canopy level.

$$D_{ij} = \frac{C_i - C_r}{S_j \Delta z_j}$$

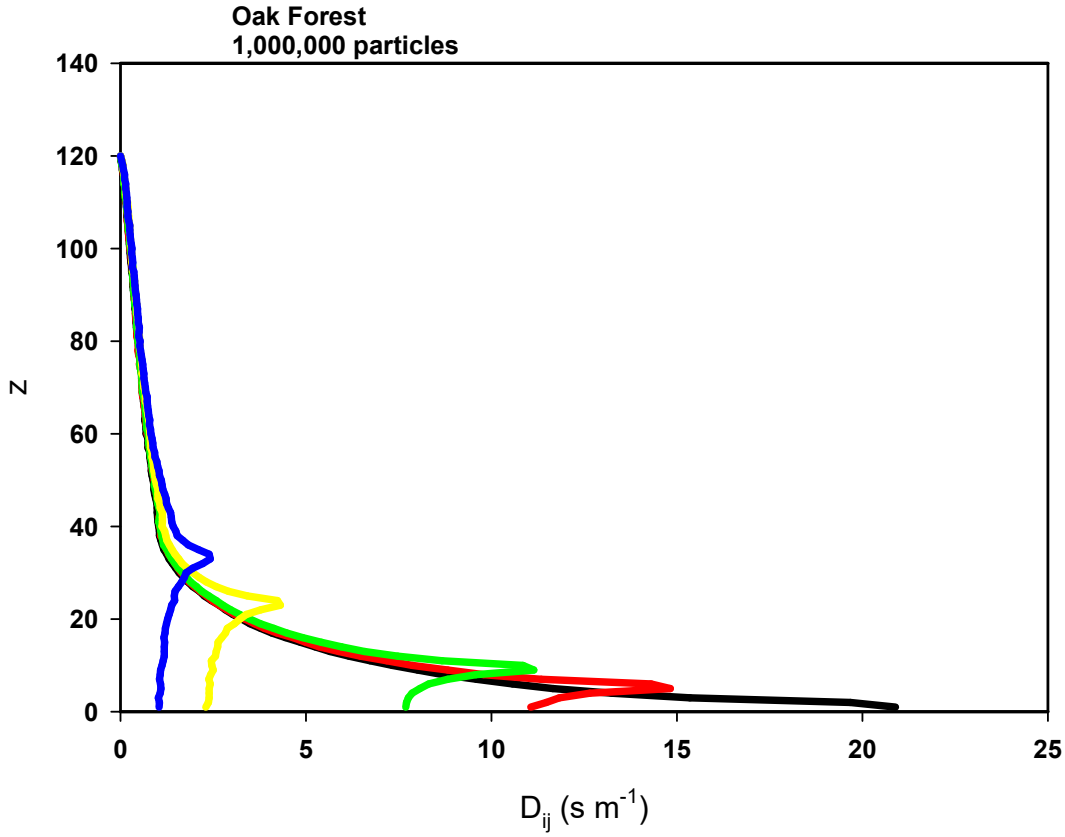

Figure 1 Dispersion matrix as a function of height and release height.

Note how the dispersion matrix varies with depth and the nose reflects the combined impacts of the local source strength and degree of local and distant turbulent mixing. Dispersion matrics are near zero for well-mixed flows. The advantage of using a numerical model as opposed to an analytical one is that one is able to incorporate as much information as necessary on local source sink distributions and how turbulence is affected by stability and the distribution of foliage.

Our calculations have shown that we need to compute D for different stability classes.

iv. Random-Walk Model Parameters and Turbulence Statistics

To compute fluid parcel trajectories, we must specify the canopy's attributes, the model domain size, the number of released fluid parcels, their travel duration, the duration between time steps. Optimal values for these parameters were determined from sensitivity tests performed by van den Hurk and Baldocchi (1990). For computations of the dispersion matrix, the canopy was divided into 40 layers. Subsequently, 5000 fluid parcels were distributed equally among each canopy layer and released. The vertical domain over which parcels traveled contained 120 equally spaced layers and extended up to 3 times canopy height. It was assumed that parcels leaving the top of the domain never re-entered. Fluid parcels intercepting the soil surface were perfectly reflected upward. Fluid parcel trajectories were followed for travel times up to 2000 s. Longer trajectories were unnecessary because equilibrium concentration profiles were attained by this time (van den Hurk and Baldocchi, 1990). Markov sequence calculations used time-steps equalling 5% of the integral time scale (T_L) at canopy height. Random numbers were computed with the rejection technique (Spanier and Gelbard, 1969).

The calculation of parcel trajectories also depends on how turbulence statistics are parameterized. Values of T_L were computed with the formulation of Raupach (1988). T_L was regarded as constant in the canopy and equal to 0.3 h/u*. Above this height T_L was computed as $T_L(z) = T_L(h)\ (z/h)^{0.5}$. The standard deviation of the vertical velocity (Φ_w) was parameterized to increase linearly with canopy height. Its value ranged between 0.187 u* at z equal zero and 1.25 u* at canopy height (h) (Raupach, 1988). Above the canopy Φ_w was assumed to be constant with height. These turbulence parameter values are representative of near-neutral atmospheric stability conditions and agree very well with observations within and above a crop canopy (Raupach, 1988).

Within vegetation, σ_w/u_* and σ_u/u_* were approximated to decrease linearly with depth (Raupach, 1988) using:

$$\sigma_{w,u}/u_* (z) = a_0 + (a_1 - a_0)\ z/h \qquad (21$$

The coefficient, a_1, was assumed to equal 1.25 for σ_w/u_* and 2.39 for σ_u/u_*. The coefficient, a_0, ranges between 0.1 and 0.5 (Raupach, 1988). The vertical variation in the covariance between w and u (*wu*) was prescribed to decrease exponentially with depth into the canopy (Uchijima and Wright, 1964).

For most circumstances Lagrangian time scale (T_L) was assumed to be invariant with height, within vegetation (Raupach, 1988, 1989), and was approximated as:

$$T_L = 0.3\ h\ /\ u_*. \qquad (22$$

However, there are data in the literature showing T_L u*/h to be as low as 0.1 (Amiro, 1990). In the surface boundary layer T_L was approximated, under near neutral stability, as (see Raupach, 1989):

$$T_L = k\ (z\text{-}d)/(1.25\ u_*) \qquad (23$$

Probability statistics were computed by releasing a large ensemble of fluid elements (> 5000) from the canopy; the algorithms for parcel movement were coded in C, compiled with a 32 bit compiler, and run on a Pentium-class personal computer. The trajectory of each fluid element was tracked and the number of elements that crossed specified heights, after a given travel distance, were counted. The sum of fluid elements captured, at each bin, was normalized by the source strength. Normalization insured that the integral, with respect to distance (x) at each level, equaled one when integrated between zero and infinity.

Several boundary conditions were specified for the random walk calculations. The time step of each incremental movement was equal to 0.025 T_L(h). Fluid elements reaching the forest floor were reflected perfectly, an *ad hoc* approach that is valid for Gaussian turbulence (Sawford, 1985; Wilson and Sawford, 1996). With regard to wind

profile calculations, the zero plane displacement (d) was set at 0.6h and the roughness parameter (z_o) was 0.1h. Friction velocity was assumed to equal 1 m s^{-1}.

In our upcoming versions we have converted the higher order closure model of Meyers and Paw U to Matlab and are running it with new information on canopy structure. This will give us theoretically based profiles of wind velocity and the standard deviation of w within the vegetation.

Leaf boundary layer resistances for molecular compounds were computed using flat plate theory (Schuepp, 1993). In principle such resistances, under forced convection, are a function of a leaf's length scale (l), molecular diffusivity (d) and the Sherwood number, Sh.

$$r_b = \frac{l}{d \cdot Sh} \qquad (24).$$

In this form r_b has units of s m^{-1}, but it can be converted into units of mol m^{-2} s^{-1} with gas law conversion factors to be consistent with the inputs of the stomatal conductance and photosynthesis algorithms.

To simulate wind speed within the vegetation, which is required to assess Sh, we applied the logarithmic wind law above the canopy and the exponential wind profile within it. Within vegetation, U was computed from an exponential relation, first proposed by Cionco (1965):

$$U(z) = U(h)\exp(-\alpha(1-\frac{z}{h})) \qquad (25)$$

where h is canopy height and α is the canopy wind velocity attenuation coefficient. The attenuation coefficient typically ranges between 0.5 and 5, and tends to increase as

canopy density progresses from sparse to dense (Cionco, 1978). The logarithmic wind law was applied to calculate horizontal wind velocity above the vegetation:

$$u = \frac{u_*}{k} \ln\left(\frac{z-d}{z_0}\right) \qquad (26$$

where u_* is friction velocity, k is von Karman's constant (0.4), d is the zero plane displacement height and z_0 is the roughness length. The reader should note that Equation 13 applies only for conditions of near-neutral, thermal stratification.

Under free convection, we computed the Sherwood number as a function of the Grasshof number and the leaf to air temperature difference (see Schuepp, 1993).

Leaf temperature was calculated to determine enzymatic rates associated with carboxylation, electron transport, and respiration and to evaluate transpiration, sensible heat fluxes and infrared emission. A quadratic equation, defining the difference between leaf and air temperature (ΔT), was derived from the leaf energy balance relationship so an analytical solution could be used to compute leaf temperature (Paw U, 1987):

$$a\,\Delta T^2 + b\,\Delta T + c = 0 \qquad (27)$$

The coefficients are defined as:

$$a = 12 \cdot \varepsilon \cdot \sigma \cdot T_k^2 + \frac{\rho_a \lambda G_c m_v}{2 m_a P} \frac{d^2 e_s(T)}{dT^2}$$

$$b = 8 \cdot \varepsilon \cdot \sigma \cdot T_k^3 + \frac{\rho_a \lambda G_c m_v}{m_a P} \frac{de_s(T)}{dT} + 2\rho C_p G_h$$

$$c = 2 \cdot \varepsilon \cdot \sigma \cdot T_k^4 + \frac{\rho_a \lambda G_c m_v (e_s(T) - e_a)}{m_a P} + 2\rho C_p G_h - Q$$

where ε is emissivity, σ is the Stefan-Boltzman constant, ρ_a is air density, λ is the latent heat of vaporization, T_k is absolute temperature (K), G_c is the canopy surface conductance

(m s^{-1}), G_h is the aerodynamic conductance for sensible heat transfer (m s^{-1}), C_p is the specific heat of air, Q is absorbed energy (incoming short and long wave radiation, minus reflected shortwave radiation; W m^{-2}), m_v and m_a are the molecular weights of vapor and dry air (g mol^{-1}), P is pressure (kPa), e_s is saturated vapor pressure (kPa) and e_a is the ambient vapor pressure (kPa). The leaf energy balance can also be used to derive a quadratic equation for latent heat exchange (λE; W m^{-2}):

$$a\,LE^2 + b\,LE + c = 0 \qquad (28)$$

The coefficients for A19 are:

$$a = \frac{\rho_a \lambda G_c m_v}{8 m_a P(\rho_a C_p G_h + 4\sigma\varepsilon T_k^3)} \frac{d^2 e_s(T)}{dT^2}$$

$$b = -4 \cdot \varepsilon \cdot \sigma \cdot T_k^3 - \frac{\rho \lambda G_c m_v}{2 m_a P} \frac{de_s(T)}{dT} - \rho C_p G_h + \frac{\rho_a \lambda G_c m_v}{2 m_a P(\rho_a C_p G_h + 4\sigma\varepsilon T_k^3)} \frac{d^2 e_s(T)}{dT^2} \left[\frac{-Q}{2} + \sigma\varepsilon T_k^4 \right]$$

$$c = (\rho_a C_p G_h + 4\varepsilon \cdot \sigma \cdot T_k^3) \frac{\rho_a \lambda G_c m_v (e_s(T) - e_a)}{m_a P} + \frac{\rho_a \lambda G_c m_v}{m_a P} \frac{de_s(T)}{dT} \left(\frac{Q}{2} - \varepsilon \cdot \sigma \cdot T_k^4 \right) + \frac{\rho_a \lambda G_c m_v}{2 m_a P(\rho_a C_p G_h + 4\sigma\varepsilon T_k^3)} \frac{d^2 e_s(T)}{dT^2} \left[\frac{Q^2}{4} + (\sigma\varepsilon T_k^4)^2 - Q \cdot \sigma\varepsilon T_k^4 \right]$$

(29)

Soil constitutes the lowest boundary of a canopy-scale, water vapor, CO_2 and trace gas exchange model. Flux densities of convective and conductive heat transfer and evaporation at the soil/litter boundary and soil temperature profiles were computed using a ten layer numerical soil heat transfer model (Campbell, 1986). Surface energy fluxes were computed using an analytical solution to a surface's energy balance. Soil evaporation was computed using an algorithm reported in Mahfouf and Noilhan (1991):

$$E_s = \frac{\rho_a}{Rsoil}(\varphi \cdot q_{sat}(T) - q_a) \quad (30)$$

where R_{soil} is the resistance of the soil to evaporation, φ is the relative humidity of the soil matrix, q_a is the mixing ratio of the air and q_{sat} is the saturated mixing ratio. For these calculations we assumed R_{soil} was 1500 s m^{-1} and that the vapor pressure at the evaporating site was 80% of the saturation vapor pressure ($\varphi q_{sat}(T)$).

b. Eco-Physiology: photosynthesis, respiration and stomatal conductance

The biochemical equations for the carbon exchange processes are taken from Farquhar et al., (1980). Leaf photosynthesis (A) is a function of the carboxylation (V_c), oxygenation (V_o, photorespiration) and dark respiration (R_d) rates of CO_2 exchange between the leaf and the atmosphere (all have units of μmol m^{-2} s^{-1}).

$$A = V_c - 0.5V_o - R_d \quad (31)$$

The term: V_c - 0.5 V_o is expressed by Farquhar et al. (1980) as:

$$V_c - 0.5V_o = \min[W_c, W_j](1 - \frac{\Gamma}{C_i}) \quad (32)$$

Adopting the minimum value between W_c, the rate of carboxylation when ribulose bisphosphate (RuBP) is saturated, and W_j, the carboxylation rate when RuBP regeneration is limited by electron transport assesses equation A22. The variable, Γ, is the CO_2 compensation point in the absence of dark respiration (mol mol^{-1}) and C_i is the intercellular CO_2 concentration (mol mol^{-1}). Evaluating Equation 32, in terms of C_i, implicitly assumes that the mesophyll conductance is infinite.

If W_c is minimal, then:

$$V_c - 0.5V_o = W_c = \frac{V_{C\max}(C_i - \Gamma)}{C_i + K_c(1 + \frac{[O_2]}{K_o})} \quad (33)$$

In this case V_{Cmax} is the maximum carboxylation rate when RuBP is saturated and K_o and K_c are the Michaelis-Menten coefficients for O_2 and CO_2.. If W_j is minimal, then:

$$V_c - 0.5\ V_o = W_j = \frac{J(C_i - \Gamma)}{4C_i + 8\Gamma} \qquad (34)$$

where J is the potential rate of electron transport (μmol e^- m^{-2} s^{-1}). J is evaluated as a function of incident. photosynthetic photon flux density (I):

$$J = \frac{\alpha I}{\sqrt{1 + \frac{\alpha^2 I^2}{J_{max}^2}}} \qquad (35)$$

The variable, α, is the quantum yield (mol e- mol^{-1} quanta) and J_{max} is the maximum rate of electron transport.

A simple conductance relation is employed to express C_i:

$$C_i = C_s - \frac{A}{g_s} \qquad (36)$$

where C_s is the surface CO_2 concentration and g_s is stomatal conductance (mol m^{-2} s^{-1}). Stomatal conductance was computed with the algorithm of Collatz et al. (1991), which couples it to leaf photosynthesis and relative humidity.

$$g_s = \frac{m\ A\ rh}{C_s} + g_0 \qquad (37)$$

The coefficient m is a dimensionless slope, rh is relative humidity at the leaf surface, g_0 is the zero intercept, and A (μmol m^{-2} s^{-1}) is leaf photosynthesis. Finally, the system of equations and unknowns, for computing leaf photosynthesis, is closed by expressing the CO_2 concentration at the leaf's surface (C_s) in terms of the atmosphere's CO_2 concentration (C_a) and the conductance across the laminar boundary layer of a leaf (g_b):

$$C_s = C_a - \frac{A}{g_b} \qquad (38)$$

The variables, C_a and g_b, are external inputs to the leaf biochemistry model and are determined from the micrometeorology of the canopy. Either numerical or analytical solutions for the coupled leaf photosynthesis-stomatal conductance model can be used to compute these fluxes.

The evaluation of some photosynthetic model parameters merits further comment. The coefficients for J_{max}, V_{Cmax} and Γ, K_{O2}, K_C and R_d are strong, non-linear functions of temperature (Johnson and Thornley, 1985; Harley and Tenhunen, 1991). One temperature function used for J_{max} and V_{Cmax} is:

$$f(T) = \frac{\exp\left(E_a \cdot (T_l - T_{opt}) / (R \cdot T_l \cdot T_{opt})\right)}{1 + \exp\left(\frac{\Delta S \cdot T_l - \Delta H)}{R \cdot T_l}\right)} \qquad (39)$$

E_a is the activation energy, R is the universal gas constant, T_l is leaf temperature and T_{opt} is the optimum temperature. The terms ΔH and ΔS represent changes in enthalpy and entropy. The Arrenhius temperature function is used to describe temperature dependencies for Γ, K_{O2}, K_C and R_d, with respect to a reference temperature (T_{ref})

$$f(T) = \exp\left(E_a \cdot (T_l - T_{ref}) / (R \cdot T_l \cdot T_{ref})\right) \qquad (40)$$

Respiration provides energy for metabolism and synthesis. At the leaf level, Collatz et al. (1991) and Amthor (1994) model dark respiration as a function of $V_{Cmax.}$—a typical value being R_d equals 0.015 times V_{Cmax}. Their assumption implies that R_d is a function of leaf nitrogen.

Soil respiration was computed with a relation based on the Arrhenius equation (see Hanson et al., 1993).

c Model Inputs and Parameters

An objective of this work is to examine how well a leaf to canopy integration model can simulate water vapor, sensible heat and CO_2 exchange rates over a range of environmental conditions using simple input variables and constrained parameters. Variable model inputs include photosynthetic photon flux density, air temperature, humidity, wind speed and soil temperature at a deep reference point. CO_2 concentration is required for the photosynthesis model. For cases when CO_2 data was not available we assumed it equaled 350 ppm. The key extrinsic plant input parameters are leaf area index and V_{Cmax}. Other model parameters are scaled to these two parameters, or they are representative of the vegetation's functional type (e.g. roughness length, zero plane displacement, canopy height).

The maximum carboxylation rate (V_{cmax}), the maximum rate of electron transport (J_{max}), dark respiration rate (R_d) are needed at a reference temperature to compute leaf photosynthesis and stomatal conductance. These data were derived from a prior study on oak leaves (*Quercus alba*). Information on the leaf photosynthesis model parameters at the oak-maple site is reported in Harley and Baldocchi (1995). Parameterization of the photosynthetic model used for the aspen was achieved with data collected by Dr. Joe Berry (Carnegie Institution of Washington) at the same boreal aspen stand (see Table 2).

Evaluation of the Lagrangian dispersion matrix requires information on the vertical variation in the standard deviation of vertical velocity (σ_w). Algorithms and parameters presented by Raupach (1988) were used to calculate the dispersion matrix for a given friction velocity. Dispersion matrices for other conditions were scaled to friction velocity.

For aerodynamic calculations, the roughness parameter was set at 10% of canopy height. We assumed that the zero plane displacement (d) was 60% of canopy height for the crops and conifer stand. For the deciduous forest, d was set at 85% of canopy height. An exponential relation was employed to calculate wind speeds within the canopy. The attenuation coefficient was set at 2.5, a reasonable assumptions for canopies with leaf area indices ranging between two and six and having a zero plane displacement equal to 60% of canopy height (Periera and Shaw, 1980).