

Text S1

1. Vegetation Process Model Description

This section describes the formulation of the multi-layer canopy-root-soil system process model (MLCan) used to produce the simulated results presented in this paper. The symbols, units and description are summarized in Table S1. The above-ground component couples leaf-level ecophysiological (photosynthesis and stomatal conductance) and physical (energy balance and boundary layer conductance) processes that determine the fluxes of CO₂, water vapor and heat between the foliage and ambient air at each canopy level. Leaf-level conditions and forcings are determined by the structural properties of the canopy. Leaf wetness, the radiative forcing at each canopy level, the canopy environment and conditions at the soil surface are functions of the structure and density of foliage through the canopy. The interdependent nature of the leaf-level and canopy-level processes produces a tightly coupled set of physical and biological relationships that control canopy-atmosphere scalar fluxes.

The following sections begin with descriptions of leaf-level bio-physical (boundary layer conductance and leaf energy balance) and eco-physiological (photosynthesis, stomatal conductance and leaf water potential) processes that are tightly coupled. An iterative solution is required at each canopy level, separately considering sunlit, shaded and wet leaf fractions due to differences in radiative forcing and energy balance. Component models describing the canopy environment, including wind attenuation, the shortwave and longwave canopy radiation regimes, dew accumulation and throughfall, and within-canopy mixing of scalar concentrations and heat are then described. This is followed by a description of the soil surface energy balance, soil moisture transport and root moisture uptake.

1.1. Leaf-Level Biophysics

The core of the above-ground formulation is a set of coupled equations for the leaf-level eco-physiological and physical interactions that determine the exchange of CO₂, latent and sensible heat between the vegetation, or big leaf, in each layer and the surrounding air. The leaf-level model is driven by incident shortwave and longwave radiation fluxes, wind speed and local ambient environment (CO₂ concentration, humidity and air temperature) at each canopy level. Sunlit and shaded big leaves are considered at each canopy level due to the discrepancy in incident energy that the two fractions receive. Likewise, a modified energy balance for a wet leaf fraction in each layer is required to account for foliage onto which dew has formed or precipitation has fallen.

1.1.1. C3 Photosynthesis

Net leaf carbon dioxide assimilation (A_n) for vegetation that utilizes the C3 photosynthetic pathway is described by the biochemical model of *Farquhar et al.* [1980] and later modifications [*Harley and Sharkey*, 1991]. This model predicts the interactive effects of photosynthetically active radiation (Q_p), leaf temperature (T_l) and CO₂ concentration in the intercellular air space (C_i) on leaf photosynthesis. Photosynthesis is assumed to be constrained by either the rate of ribulose-1,5-bisphosphate (RuBP) regeneration (RuBP-limited photosynthesis) or RuBP carboxylase-oxygenase activity (Rubisco-limited photosynthesis). Net leaf photosynthesis is calculated as

$$A_n = \left(1 - \frac{\Gamma^*}{C_i}\right) \min[W_c, W_j] - R_d, \quad (1)$$

where the term $(1 - \Gamma^*/C_i)$ accounts for the CO₂ released by photorespiration [*von Caemmerer*, 2000], R_d is mitochondrial dark respiration, and min represents the minimum of the specified quantities. The RuBP-limited carboxylation velocity is calculated as

$$W_j = \frac{J \cdot C_i}{4.5C_i + 10.5\Gamma^*}, \quad (2)$$

where the whole-chain electron transport rate (J) is described by a non-rectangular hyperbolic function [*Bernacchi et al.*, 2003],

$$J = \frac{Q_m + J_{max} - \sqrt{(Q_m + J_{max})^2 - 4\Theta_{PSII} \cdot Q_m \cdot J_{max}}}{2\Theta_{PSII}}, \quad (3)$$

and

$$Q_m = Q_{p,abs} \cdot \Phi_{PSII,max} \cdot \beta_f \quad (4)$$

is the maximum amount of absorbed photosynthetically active radiation ($Q_{p,abs}$) available for electron transport. $\Phi_{PSII,max}$, the maximum quantum yield of photosystem II, and Θ_{PSII} , a curvature factor, are quadratic functions of T_l [*Bernacchi et al.*, 2003]. β_f is the fraction of $Q_{p,abs}$ that reaches photosystem II, and is assumed to be 0.5 for C3 plants [*von Caemmerer*, 2000; *Bernacchi et al.*, 2003]. The maximum rate of electron transport, J_{max} , is dependent on leaf temperature, with a specified value ($J_{max,25}$) at a reference temperature, ie. 25°C [*Medlyn et al.*, 2002], as described below.

The Rubisco-limited carboxylation rate is calculated as

$$W_c = \frac{V_{cmax} \cdot C_i}{C_i + K_c \left(1 + \frac{O}{K_o}\right)}, \quad (5)$$

where the the maximum rate of carboxylation (V_{cmax}) varies, similarly to J_{max} , as an exponential function of T_l that requires the specification of a reference value ($V_{cmax,25}$) determined by leaf-level observation. O represents the oxygen concentration (210 mmol mol⁻¹), and K_c and K_o are the Michaelis-Menten constants for CO₂ and O₂, respectively.

Generic temperature response functions derived from *in vivo* observations of leaf gas exchange are used here to describe the variation of $P_i \in [V_{cmax}, R_d, \Gamma^*, K_c, K_o, J_{max}]$ with T_l [*Bernacchi et al.*, 2001, 2003].

$$P_i = P_{i,25} \exp \left[c_i - \frac{\Delta H_i}{R \cdot T_l} \right] \quad (6)$$

Here $P_{i,25}$ are the parameter values at the reference temperature (25°C) and R is the molar gas constant. The scaling constants (c_i), activation energies (ΔH_i) and the subset of reference values [$R_{d,25}, \Gamma_{25}^*, K_{c,25}, K_{o,25}$] have been determined through *in vivo* observations by *Bernacchi et al.* [2001, 2003]. $V_{cmax,25}$ and $J_{max,25}$ are known to vary widely between species [*Medlyn et al.*, 2002; *Wullschlegel*, 1993] and seasonally within species (ie. *Ellsworth* [2000]; *Wilson et al.* [2000]; *Xu and Baldocchi* [2003]). In this application, half-hourly average values taken from field observations are used (see Table S1). Photosynthetic capacity is assumed to decline exponentially with cumulative leaf area from the top of the canopy (ξ) following *Leuning et al.* [1995], where

$V_{cmax,25}(0)$ is the canopy top value and k_n is the decay coefficient for leaf nitrogen concentration.

$$V_{cmax,25}(\xi) = V_{cmax,25}(0) \exp[-k_n \cdot \xi] \quad (7)$$

1.1.2. C4 Photosynthesis

The C4 photosynthetic pathway [Hatch and Slack, 1966] is characterized by structural and biochemical specialization that concentrates CO_2 within the bundle sheath cell at the site of Rubisco [Hatch, 1987; von Caemmerer and Furbank, 2003]. CO_2 is supplied to the bundle sheath by way of C4 acid decarboxylation in the mesophyll [Hatch, 1987; Ghannoum, 2009]. These structural and biochemical augmentations to the C3 pathway act to maintain internal CO_2 concentrations at levels near saturation under current atmospheric conditions [Ludlow and Wilson, 1971; Ghannoum et al., 2000]. These changes, in turn, inhibit oxygenation and reduce photorespiration [von Caemmerer and Furbank, 1999]. C4 photosynthesis is modeled here following Collatz et al. [1992], which simplifies the intercellular transport model of Berry and Farquhar [1978]. Net photosynthetic CO_2 uptake is determined by three potentially limiting rates, representing limiting light intensities (J_i), low CO_2 concentrations (J_c) and the capacity for CO_2 fixation by Rubisco (J_e).

$$A_n = \min[J_i, J_c, J_e] - R_d \quad (8)$$

The light-limited rate is determined by

$$J_i = \alpha_r \cdot f \cdot Q_{p,abs} \quad (9)$$

where α_r is the intrinsic quantum yield of C3 photosynthesis and f the fraction of absorbed photons used by C3 reactions. The formulation used here combines the quantity $\alpha_r \cdot f$ into a single constant value of $0.067 [\text{mol mol}^{-1}]$ [Collatz et al., 1992]. The CO_2 limitation for C4 plants typically occurs under very low CO_2 concentrations at which photosynthesis varies linearly from the compensation point to the rate saturation level

$$J_c = C_i \cdot k / P_a \quad (10)$$

where k is a constant that accounts for leakage of CO_2 from the bundle sheath to the mesophyll intercellular space and a linear growth of photosynthesis with C_i , and P_a is the atmospheric pressure. At high CO_2 concentrations and saturating light levels, Rubisco-limited photosynthesis is equal to the CO_2 fixation capacity of Rubisco for saturating substrate concentrations (V_{max}). The pair of nested quadratic equations described in Appendix B of Collatz et al. [1992] is used to calculate gross photosynthesis (A) as a function of C_i , T_l and $Q_{p,abs}$. We refer to Appendix B of Collatz et al. [1992] for the T_l dependencies of $[V_{max}, R_d, k]$, given as functions of reference values of the respective variables $[V_{max,4}, R_{d,4}, k_4]$.

1.1.3. Stomatal Conductance

The Ball-Berry [Ball and Berry, 1982] equation relates stomatal conductance to vapor (g_s) to the net uptake of CO_2 , as well as the leaf surface relative humidity (h_s) and CO_2 concentration (C_s).

$$g_s = f_{sv} \cdot m \frac{A_n \cdot h_s}{C_s} + b \quad (11)$$

This model, while empirical in origin, has been demonstrated to be robust in capturing the response of g_s to environmental conditions across a range of C3 and C4 vegetation species [Ball et al., 1987; Leuning, 1990; Lloyd, 1991]. Its apparent simplicity belies the implicit dependencies on leaf

states such as $Q_{p,abs}$ and T_l , through the dependence of A_n on these variables [Leuning, 1995]. The slope (m) and intercept (b) parameters are vegetation-specific. The factor f_{sv} represents stomatal sensitivity to leaf water potential (Ψ_l) and varies from 1 (no change in stomatal conductance) to 0 (total loss of conductance) (see Figure 4) as Ψ_l decreases to the critical water potential [Tuzet et al., 2003; Sperry et al., 1998]. This function depends on a species specific reference potential (Ψ_f) and sensitivity parameter (s_f) [Tuzet et al., 2003], determined for soybean and maize from data presented by Bunce [2004] who showed no significant change in the relationship under elevated CO_2 .

$$f_{sv} = \frac{1 + \exp[s_f \cdot \Psi_f]}{1 + \exp[s_f(\Psi_f - \Psi_l)]} \quad (12)$$

Leaf water potential at each canopy layer is calculated using an Ohm's law analog relating the transpiration flux (T_r) to the potential difference between the root system water potential ($\Psi_{r,wgt}$) and Ψ_l and the resistance to flow through the plant (R_p) [van den Honert, 1948; Jones et al., 1982; Jones, 1992].

$$T_r = \frac{\Psi_{r,wgt} - \Psi_l}{R_p} \quad (13)$$

An exponential dependence of R_p on soil water potential ($\Psi_{r,wgt}$) was derived from the observations of Blizzard and Boyer [1980]. $\Psi_{r,wgt}$ is a weighted average over the root fraction r_f in each of the n_s soil layers.

$$\Psi_{r,wgt} = \sum_{i=1}^{n_s} \Psi_{r,i} \cdot r_{f,i} \quad (14)$$

1.1.4. Leaf Surface and Intercellular Conditions

At the leaf surface, within the boundary layer formed by air flow across the leaf surface, the concentration of CO_2 (C_s) is determined from a one-dimensional Fick's Law diffusion formulation [Campbell and Norman, 1998]

$$C_s = C_a - A_n \frac{1.37}{g_{bv}}, \quad (15)$$

where g_{bv} is the vapor conductance across the leaf boundary layer. The CO_2 concentration within the stomatal pore (C_i) is likewise determined using a one-dimensional diffusion relationship.

$$C_i = C_s - A_n \frac{1.6}{g_s} \quad (16)$$

The factors 1.37 and 1.6 account for the ratio of the diffusivities of CO_2 and water vapor through the leaf boundary layer and through the interface between the intercellular space and the leaf surface [Cowan and Troughton, 1971], respectively.

Vapor pressure at the leaf surface (e_s) is derived from the diffusion principles used for CO_2 ,

$$e_s = \frac{g_s \cdot e_i + g_{bv} \cdot e_a}{(g_s + g_{bv})} \quad (17)$$

where the intercellular space is assumed to be saturated such that e_i is equivalent to the saturation vapor pressure at leaf temperature [Nikolov et al., 1995], computed using Tetens formula [Campbell and Norman, 1998].

1.1.5. Boundary Layer Conductance

Boundary layer conductance can play a significant role in modulating the coupling between stomata and their ambient environment [Collatz et al., 1991]. Flow over plant

foliage and buoyancy driven by temperature differences between foliage and the ambient environment can be factors affecting boundary layer conductance. Following *Nikolov et al.* [1995], we consider both free and forced convection in determining the boundary layer conductance of each foliage layer. Forced-convective leaf boundary layer conductance is computed as

$$g_{bf} = c_f T_{lk}^{0.56} \left[(T_{lk} + 120) \frac{U}{d_o P_a} \right]^{0.5} \quad (18)$$

where d is the characteristic dimension of a leaf (leaf width). The free-convective leaf boundary layer conductance to vapor is calculated as *Nikolov et al.* [1995]

$$g_{br} = c_e T_{lk}^{0.56} \left(\frac{T_{lk} + 120}{P_a} \right)^{0.5} \left(\frac{|T_{lv} - T_{av}|}{d_o} \right)^{0.25} \quad (19)$$

where $T_{lv} - T_{av}$ is the virtual temperature difference between foliage and the local air [*Monteith and Unsworth*, 1990]. The leaf boundary layer conductance to vapor transport is taken to be the maximum of g_{bf} and g_{br} . The boundary layer conductance to heat is calculated as $g_{bh} = 0.924 g_{bv}$ [*Nikolov et al.*, 1995].

1.1.6. Leaf Energy Balance

The energy balance of the leaves determines T_l , and hence the partitioning of energy between latent and sensible heat as well providing a control on leaf photosynthesis. Absorbed energy from both sides of a leaf (R_{abs}) is dissipated through latent and sensible heat exchange with the local atmosphere, long-wave radiation emission and metabolic storage (M_e) [*Nikolov et al.*, 1995]

$$R_{abs} = \frac{L_v g_{vt}}{P_a} (e_s(T_l) - e_a) + c_p g_{bh} (T_l - T_a) + 2\epsilon\sigma T_{lk}^4 + M_e \quad (20)$$

where the four right-hand side terms represent energy dissipated by latent and sensible heat fluxes with the atmosphere, outward longwave flux and the energy consumed in photosynthesis, respectively. M_e is assumed to be 0.506 [J ($\mu\text{mol CO}_2$) $^{-1}$] [*Nikolov et al.*, 1995].

The total vapor conductance of dry leaves is computed as

$$g_{vt} = \frac{g_s \cdot g_{bv}}{g_s + g_{bv}}. \quad (21)$$

For wet leaves $g_{vt} = g_{bv}$, and all available energy is assumed to be used for evaporation, resulting in no sensible heat flux from the wet leaf fraction.

To facilitate an accurate solution for T_l that does not require linearization of the leaf energy balance, a fourth-order polynomial approximation for $e_s(T_l)$ is used [*Nikolov et al.*, 1995].

1.2. Canopy Radiation Regime

The vertical resolution of the shortwave radiative regime through the canopy considers photosynthetically active and near-infrared bands separately. As sunlit and shaded vegetation fractions are resolved through the canopy for accurate flux calculations, the beam and diffuse fractions of the incident shortwave radiation are calculated. The longwave radiation solution is complicated by both sources and sinks at each canopy level in which foliage exists, in addition to sky and soil fluxes, producing a dependence on leaf and soil energy balances.

1.2.1. Shortwave Radiation

Incoming shortwave radiation is separated according to the standard assumption that approximately half is in the photosynthetically active (Q_p) range of the spectrum, with

the remainder being near-infrared (Q_n) [*Campbell and Norman*, 1998]. The diffuse fraction of the downwelling shortwave is determined from algorithms described in *Spitters* [1986], based on solar zenith angle, day of year and the theoretical clear-sky incoming shortwave radiation. The solar zenith angle is determined from time of day and site location as described by *Campbell and Norman* [1998].

Both PAR and NIR wavebands are attenuated through the canopy according to a Beer's Law relationship in which the fraction of radiation penetrating through the top ξ units of LAI is given by

$$\tau = \exp[-K_b \cdot \Omega \cdot \xi]. \quad (22)$$

Ω is a clumping coefficient that accounts for the reduction in ground coverage by vegetation not randomly distributed [*Campbell and Norman*, 1998]. Q_p and Q_n are considered separately as green foliage exhibits differential absorption between the two bands [*Goudriaan*, 1977]. Absorptivities for each waveband are specified, and reflection coefficients are calculated from [*Campbell and Norman*, 1998]

$$\rho_{[p,n]} = \frac{1 - \sqrt{\alpha_{[p,n]}}}{1 + \sqrt{\alpha_{[p,n]}}} \quad (23)$$

where the subscripts $[p, n]$ designate reflection coefficients (ρ) or absorptivities (α) for PAR or NIR, respectively. Radiation incident on vegetation is either absorbed, reflected or transmitted. The extinction coefficient for beam radiation (K_b) represents the fraction of the leaf area projected onto a horizontal plane from the sun's zenith angle (ϕ).

$$K_b = \frac{\sqrt{x^2 + \tan^2 \phi}}{x + 1.774(x + 1.182)^{-0.733}}, \quad (24)$$

The leaf angle distribution parameter x can be varied to specify a range of canopy geometries, with $x = 1$ commonly used to specify a spherical leaf angle distribution [*Campbell*, 1986].

Equation 22 is also applied for the attenuation of diffuse radiation through the canopy, with the diffuse extinction coefficient K_d specified separately from considerations of the isotropic nature of diffuse radiation [*Leuning et al.*, 1995; *Campbell and Norman*, 1998]. Direct and diffuse radiation fractions are considered separately as sunlit leaves, defined as those receiving direct radiation, are subject to significantly greater radiation forcing during the course of a day and thus require separate consideration with respect to energy balance as well [*De Pury and Farquhar*, 1997]. The sunlit leaf fraction (f_{sun}) is equivalent to τ calculated in Equation 22, and the shaded fraction $f_{shade} = 1 - f_{sun}$.

For each canopy layer, radiation incident from above accounts for solar direct beam and diffuse radiation that was not intercepted by overlying vegetation, as well as transmitted and downward reflected radiation from overlying vegetation. Upward incident radiation includes unintercepted reflected radiation from underlying vegetation and the soil surface. The numerical solution iterates over the entire canopy, from top to bottom, until at least 99% of the shortwave radiation at the top of the canopy is accounted for as either absorbed by the canopy or soil, or reflected out of the system.

1.2.2. Longwave Radiation

The longwave radiation regime through the canopy is a function of downward longwave from the sky (R_{lw}) and the longwave emission by each layer of the foliage and the soil. For periods when R_{lw} observations were not available the downward flux was calculated as

$$R_{lw} = \epsilon_a \sigma T_{ak}^4, \quad (25)$$

where sky emissivity is determined from [Brutsaert, 1982] 2004].

$$\epsilon_a = 1.72 \left(\frac{e_a}{T_{ak}} \right)^{1/7}. \quad (26)$$

Sunlit and shaded leaf fractions are considered separately with respect to leaf energy balance and generally have different temperatures due to the greater incident shortwave flux density on sunlit leaves. The longwave emission of vegetation and soil layers was calculated using the Stefan-Boltzmann Law with an emissivity to account for deviation from the emission of an absolute blackbody. For each canopy layer, the longwave emission is the weighted sum of the two-sided emission from sunlit and shaded leaves. Thermal absorptivity was considered to be equal to emissivity for both foliage and the soil surface. Similar to the solution for the shortwave radiation regime, the longwave regime was computed by iterating downward and upward through the canopy until at least 99% of the incident and emitted radiation was accounted for either by absorption by the canopy and soil or as outgoing flux.

1.3. Canopy Wetness

Water accumulates on foliage from both precipitation interception and dew formation. The total H₂O storage capacity of a canopy layer (S_t [mm]) is given by the product of the leaf area of the layer, the maximum storage capacity of a leaf (S_m [mm LAI⁻¹]) and the fraction of the foliage that can hold water. During a precipitation or dew event, the incident water (S [mm]) intercepted by the i 'th vegetation layer with LAI L_i is given by

$$S_i = S \cdot (1 - \exp[-0.2\Omega \cdot L_i]). \quad (27)$$

If S_i is less than the available storage capacity of each layer, given by ($S_t - S_o$) where S_o is the amount of water currently stored on the layer, then S_i is added to the storage of the layer. Otherwise, $S_t - S_o$ is added to the layer storage, and the remainder continues downward through the canopy toward the soil surface. Water stored on foliage is removed through evaporation, requiring a separate energy balance for the fraction of each canopy layer holding water, as discussed above.

1.4. Canopy Micro-Environment

The vertical distributions of wind speed, air temperature and CO₂ and water vapor concentrations through the canopy are required for the gradient flux calculations that determine foliage states and the net scalar exchange between the canopy and the atmosphere. A variety of models have been proposed for the calculation of wind and scalar concentration distributions through plant canopies. Here we utilize formulations that, while remaining relatively simple, have been experimentally validated to reproduce experimental observations. Wind and scalar profiles through the canopy are computed from the mean momentum and scalar transport equations, using a K-theory closure and assuming horizontal homogeneity of the canopy foliage. The wind profile is computed from the mean momentum equation [Poggi et al., 2004]

$$-K_m \frac{d^2 u}{dz^2} - \frac{dK_m}{dz} \frac{du}{dz} + \frac{1}{2} C_d L U |U| = 0, \quad (28)$$

where K_m is the eddy diffusivity, C_d the drag coefficient and L leaf area density. A no-slip boundary condition is applied at the ground surface, with an upper boundary condition determined from the observed canopy-top wind speed. The eddy diffusivity (K_m) is derived from a simple variant of the von Karman-Prandtl mixing-length theory [Katul et al.,

$$K_m = l_m^2 \left| \frac{du}{dz} \right| \quad (29)$$

The mixing length (l_m) through the depth of a dense canopy is described by a linear function of the canopy height (h)

$$l_m = \alpha \cdot h, \quad (30)$$

which can account for several of the known properties of canopy turbulence such as the generation of von Karman streets [Poggi et al., 2004; Katul et al., 2004]. The factor α is calculated as $k_v/3$, assuming the displacement height is equal to 2/3 of the canopy height [Katul et al., 2004]. Turbulent transport of scalar quantities (heat, vapor and CO₂) is similarly computed using the temporally averaged conservation of mass equation assuming negligible scalar storage within the canopy [Poggi et al., 2004; Dreury and Albertson, 2006], given below for a scalar c .

$$-K_m \frac{d^2 c}{dz^2} - \frac{dK_m}{dz} \frac{dc}{dz} + S_c = 0 \quad (31)$$

The scalar source strength (S_c) is determined from the flux density (per unit ground area) as described above in the sections on leaf-level ecophysiology and energy balance. Upper boundary conditions are taken from canopy-top observations of scalar concentrations and lower boundary conditions are derived from calculated soil scalar fluxes (described below). The dependence of the scalar profile solution on the vertical distribution of flux densities, and the corresponding dependence of photosynthesis and energy partitioning on the local environment experienced at each canopy layer, necessitates iteration for a consistent solution of the leaf-level biophysical and ecophysiological states and fluxes and the microenvironmental states [Gu et al., 1999].

1.5. Soil Surface Fluxes

The total energy absorbed at the soil surface ($R_{abs,s}$) accounts for the energy flux conducted between the soil surface and subsurface (G), soil longwave emission ($LW_{out,s}$) and sensible (H_s) and latent (LE_s) heat exchanged between the soil surface and the overlying layer of air.

$$R_{abs,s} = G + H_s + LE_s + LW_{out,s} \quad (32)$$

Soil surface sensible heat flux is calculated as a function of wind speed at the bottom of the canopy and the gradient in temperature between the bottom canopy layer ($T_{a,1}$) and the soil surface temperature ($T_{s,1}$) [Hinzman et al., 1998].

$$H_s = c_p \rho_a D_h (T_{s,1} - T_{a,1}) \quad (33)$$

Latent heat flux from the soil surface is likewise modeled through a gradient relationship between the vapor pressure at the bottom of the canopy airspace ($e_{a,1}$) and that of the soil surface layer ($e_{s,1}$).

$$LE_s = L_v \rho_a D_w \left(\frac{0.622}{P_a} \right) (e_{a,1} - e_{s,1}) \quad (34)$$

The soil surface vapor pressure is calculated using the soil surface temperature and relative humidity Noilhan and Planton [1989]. These convective and evaporative heat transfer relationships rely on the assumption that the exchange coefficients (D_h and D_w , respectively) are equal to the exchange coefficient for momentum [Hinzman et al., 1998]

$$D_h = D_w = \frac{U_1 k_v^2}{(\ln[z_1/z_o])^2}, \quad (35)$$

where u_1 is the wind speed at the lowest canopy level, z_1 is the height of the lowest canopy level and z_0 is the average soil surface roughness. Outgoing longwave radiation from the soil surface is a function of the temperature of the surface soil layer ($T_{sk,1}$), taken from observations at the Bondville site

$$LW_{out,s} = \epsilon_s \sigma T_{sk,1}^4, \quad (36)$$

where ϵ_s is the soil emissivity. Heat conducted into the soil is determined from the thermal conductivity of the surface soil layer ($K_{T,1}$) and the temperature gradient between the soil surface and the near-surface air

$$G = K_{T,1} \frac{T_{s,1} - T_{a,1}}{dz_1} \quad (37)$$

where dz_1 is the thickness of the near-surface air layer [Hinzman et al., 1998].

The efflux of CO_2 from the soil surface is determined using a simple model to account for the known temperature dependence of soil respiration [Janssens and Pilegaard, 2003].

$$F_{c,s} = R_o Q_{10}^{\frac{T_{s,1}-10}{10}} \quad (38)$$

While this formulation neglects factors such as soil moisture that partially control microbial decomposition rates and hence soil respiration [Porporato et al., 2003; Purnanen et al., 2003; Palmroth et al., 2005], a lack of data to constrain the dependencies of $F_{c,s}$ on other factors prohibited the use of a more complex formulation.

1.6. Soil Moisture Transport and Root Water Uptake

Soil moisture transport through the soil column is modeled using the Richards equation with a sink term ($S_r(z)$) representing moisture extraction by the root system.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K_{sh} \left(\frac{\partial \Psi_s}{\partial z} - 1 \right) \right] - S_r \quad (39)$$

Here $\theta(z)$ represents the volumetric soil moisture content, $K_{sh}(z)$ the soil hydraulic conductivity, $\Psi_s(z)$ soil matric potential and z is the vertical coordinate. Soil hydraulic properties, including hydraulic conductivity and matrix potential, are calculated as functions of saturated hydraulic conductivity, matrix potential and soil moisture content [Clapp and Hornberger, 1978; Oleson et al., 2004; Amenu and Kumar, 2008]. These functions require the fractional sand (f_s) and clay (f_c) contents of the soil, taken here to be uniform through the soil column. The sink term is expressed as

$$S_r = r_f \left(\frac{\theta - \theta_d}{\theta_s - \theta_d} \right) T_r, \quad (40)$$

where $\theta_d(z)$ is the soil moisture at dryness (ie. soil moisture beyond which extraction is not possible) and $\theta_s(z)$ is the porosity. Here $r_f(z)$ is the distribution of root conductivity through the soil column determined from the logistic dose function of Schenk and Jackson [2002] using 50th and 95th percentile rooting depths.

The sink term can also be formulated as [Amenu and Kumar, 2008]

$$S_r = K_r (\Psi_s - \Psi_r). \quad (41)$$

Combining equations (40) and (41), the root pressure potential ($\Psi_r(z)$) can be determined as

$$\Psi_r = \Psi_s - \frac{r_f T_r}{K_r} \left(\frac{\theta - \theta_d}{\theta_s - \theta_d} \right), \quad (42)$$

where the total root system radial conductivity ($K_{r,tot}$) is distributed through the rooting zone according to the vertical root profile [Amenu and Kumar, 2008].

$$K_r = r_f \cdot K_{r,tot} \cdot \frac{\theta}{\theta_s}. \quad (43)$$

The total radial conductivity of the root system ($K_{r,tot}$) is determined using the radial conductivity observations presented by Huang and Nobel [1994]. The radial conductivity per unit fine root area ($K_{r,unit}$), averaged across the agricultural species they analyzed, was $1.52 \cdot 10^{-9} \text{ [s}^{-1}\text{]}$. A budget of fine root area index (R_{fr}) across a range of biomes was presented by Jackson et al. [1997]. As agricultural species were not explicitly considered in this budget analysis, we use the value given for “temperate grasslands” to determine the total root system radial conductivity

$$K_{r,tot} = R_{fr} \cdot K_{r,unit}. \quad (44)$$

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Table S1. Symbols, Units and Descriptions

Variable Description	Symbol	Units
subscript denoting soil variable	s	
subscript denoting atmospheric variable	a	
subscript denoting first canopy or soil level	1	
vertical coordinate	z	m
layer thickness	dz	m
<i>Ambient States</i>		
solar zenith angle	ϕ	°
CO ₂ concentration	C_a	ppm
vapor pressure	e_a	kPa
vapor pressure deficit	VPD	kPa
air temperature	T_a	°C
air temperature in Kelvin	T_{ak}	K
virtual air temperature	T_{av}	°C
wind speed	U	m s ⁻¹
air pressure	P_a	kPa
precipitation	P	mm s ⁻¹
density of dry air	ρ_a	mol m ³
<i>Photosynthesis: C3</i>		
leaf photosynthetic rate	A	μmol m ⁻² s ⁻¹
net leaf photosynthetic rate	A_n	μmol m ⁻² s ⁻¹
Rubisco-limited carboxylation rate	W_c	μmol m ⁻² s ⁻¹
RuBP-limited carboxylation rate	W_j	μmol m ⁻² s ⁻¹
mitochondrial respiration in light	R_d	μmol m ⁻² s ⁻¹
CO ₂ compensation point	Γ^*	μmol mol ⁻¹
electron transport rate	J	μmol mol ⁻¹
maximum rate of electron transport	J_{max}	μmol m ⁻² s ⁻¹
maximum Q available for electron transport	Q_m	μmol m ⁻² s ⁻¹
maximum rate of Rubisco-limited carboxylation	V_{cmax}	μmol m ⁻² s ⁻¹
maximum quantum yield of photosystem II	$\phi_{PSII,max}$	-
Michaelis-Menten constant for CO ₂	K_c	μmol mol ⁻¹
Michaelis-Menten constant for O ₂	K_o	mmol mol ⁻¹
oxygen concentration	O	mmol mol ⁻¹
curvature factor	Θ_{PSII}	-
temperature dependent parameter value	P_i	parameter dependent
reference parameter value at 25°C	$P_{i,25}$	parameter dependent
scaling constant	c_i	-
energy of activation	ΔH_i	kJ mol ⁻¹
<i>Photosynthesis: C4</i>		
light-limited photosynthetic uptake rate	J_i	μmol m ⁻² s ⁻¹
CO ₂ -limited photosynthetic uptake rate	J_c	μmol m ⁻² s ⁻¹
Rubisco-limited photosynthetic uptake rate	J_e	μmol m ⁻² s ⁻¹
<i>Conductances</i>		
stomatal conductance to vapor	g_s	mol m ⁻² s ⁻¹
boundary layer conductance to vapor	g_{bv}	mol m ⁻² s ⁻¹
boundary layer conductance to heat	g_{bh}	mol m ⁻² s ⁻¹
forced-convective boundary layer conductance to vapor	g_{bf}	mol m ⁻² s ⁻¹
free-convective boundary layer conductance to vapor	g_{br}	mol m ⁻² s ⁻¹
total leaf conductance to vapor	g_{vt}	mol m ⁻² s ⁻¹
<i>Leaf States</i>		
leaf temperature	T_l	°C
leaf temperature in Kelvin	T_{lk}	K
leaf virtual temperature	T_{lv}	°C
leaf surface CO ₂ concentration	C_s	μmol mol ⁻¹
leaf surface relative humidity	h_s	-
leaf surface vapor pressure	e_s	kPa
internal CO ₂ concentration	C_i	μmol mol ⁻¹
internal vapor pressure	e_i	kPa
leaf water potential	Ψ_l	MPa
sensitivity function of stomata to Ψ_l	f_{sv}	-
total H ₂ O storage capacity of a canopy layer	S_t	mm
H ₂ O stored on a canopy layer	S_o	mm
incident H ₂ O on canopy	S	mm
incident H ₂ O on i 'th canopy layer	S_i	mm

Variable Description	Symbol	Units
<u>Plant & Canopy States</u>		
resistance to flow through the plant	R_p	MPa s m ⁻¹
root fraction	r_f	-
leaf area density	LAD	m ² m ⁻³
leaf area index	LAI	m ² m ⁻²
cumulative LAI from canopy top	ξ	m ² m ⁻²
leaf area index of i 'th layer	L_i	m ² m ⁻²
<u>Energy Balance</u>		
sensible heat flux	H	W m ⁻²
latent heat flux	LE	W m ⁻²
transpiration	T_r	mm s ⁻¹ LAI^{-1}
energy consumed in photosynthesis	M_e	J (μ mol CO ₂) ⁻¹
two-sided absorbed energy by leaf	R_{abs}	W m ⁻²
energy absorbed by soil	$R_{abs,s}$	W m ⁻²
soil sensible heat flux	H_s	W m ⁻²
soil latent heat flux	LE_s	W m ⁻²
soil sensible heat flux	H_s	W m ⁻²
heat conducted into soil	G	W m ⁻²
soil longwave emission	$LW_{out,s}$	W m ⁻²
soil surface exchange coefficients (heat,momentum)	$D_{w,h}$	m s ⁻¹
soil temperature	T_s	°C
<u>Canopy Microenvironment</u>		
eddy diffusivity	K_m	m ² s ⁻¹
mixing length	l_m	m
scalar quantity transported within canopy	c	variable dependent
scalar source strength	S_c	variable dependent
<u>Radiation</u>		
incident short-wave radiation	R_g	W m ⁻²
incident long-wave radiation from atmosphere	R_{lw}	W m ⁻²
incident photosynthetically active radiation	Q_p	μ mol m ⁻² s ⁻¹
incident near-infrared active radiation	Q_n	W m ⁻²
absorbed photosynthetically active radiation	$Q_{p,abs}$	μ mol m ⁻² s ⁻¹
absorbed near-infrared active radiation	$Q_{n,abs}$	μ mol m ⁻² s ⁻¹
absorbed shortwave radiation	$Q_{s,abs}$	W m ⁻²
absorbed longwave radiation	$Q_{l,abs}$	W m ⁻²
net long-wave radiation	LW_{net}	W m ⁻²
net radiation	R_n	W m ⁻²
beam extinction coefficient	K_b	-
sunlit leaf fraction	f_{sun}	-
shaded leaf fraction	f_{shade}	-
PAR reflection coefficient	ρ_p	-
NIR reflection coefficient	ρ_n	-
transmitted radiation fraction	τ	-
<u>Soil States & Fluxes</u>		
volumetric soil moisture	θ	m ³ m ⁻³
soil moisture at dryness	θ_d	m ³ m ⁻³
porosity	θ_s	m ³ m ⁻³
root pressure potential	Ψ_r	MPa
soil pressure potential	Ψ_s	MPa
root profile-weighted root pressure potential	$\Psi_{r,wgt}$	MPa
soil hydraulic conductivity	K_{sh}	mm s ⁻¹
soil thermal conductivity	K_T	W m ⁻¹ °C ⁻¹
root sink term	S_r	mm s ⁻¹
root fraction	r_f	-
root radial moisture conductivity	K_r	s ⁻¹
total root system radial conductivity	$K_{r,tot}$	s ⁻¹
soil CO ₂ flux	$F_{c,s}$	μ mol m ⁻² s ⁻¹
<u>Constants</u>		
number of soil layers	n_s	-
latent heat of vaporization	L_v	J mol ⁻¹
specific heat of dry air	c_p	J mol ⁻¹ °C ⁻¹
Stefan-Boltzmann constant	σ	W m ⁻² K ⁻⁴
von Karman constant	k_v	-