Supporting Information for Development of a multi-layer canopy model for E3SM Land Model with support for heterogeneous computing

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Text S1. Canopy profile

The leaf area density (LAD), $a(z)$ [m^2 m^{-3}], at height z are given by a beta distribution as

$$a(z) = \left(\frac{L}{h_c}\right)\left(\frac{(z/h_c)^{p-1}(1-(z/h_c)^{q-1})}{B(p,q)}\right) \quad (1)$$

where p and q are the shape function of the beta distribution, $B(p,q)$ is a normalization constant, h_c is the canopy height. The total leaf area index (LAI), L [m^2 m^{-2}] and the cumulative leaf area index, $L(z)$ [m^2 m^{-2}], from the top of the canopy is given as

$$L = \int_0^{h_c} a(z)dz \quad (2)$$

$$L(z) = \int_z^{h_c} a(z)dz \quad (3)$$

The stem area density (SAD) is also similarly modeled by a beta distribution. The plant area density (PAD) is the sum of LAD and SAD.

Text S2. Shortwave radiation model

The downwelling, $I_i^{\downarrow}$ [Wm^{-2}], and upwelling, $I_{i+1}^{\uparrow}$ [Wm^{-2}], scattered radiation fluxes at i-th and $(i+1)$-th level are given as

$$I_i^{\downarrow} = I_{i+1}^{\downarrow}\left[\tau_{d,i+1} + (1-\tau_{d,i+1})\tau_{\ell,i+1}\right] + I_i^{\uparrow}(1-\tau_{d,i+1})\rho_{\ell,i+1} + I_{sky,b}^{\downarrow}T_{b,i+1}(1-\tau_{b,i+1})\tau_{\ell,i+1} \quad (4a)$$

$$I_{i+1}^{\uparrow} = I_i^{\uparrow}\left[\tau_{d,i+1} + (1-\tau_{d,i+1})\tau_{\ell,i+1}\right] + I_{i+1}^{\downarrow}(1-\tau_{d,i+1})\rho_{\ell,i+1} + I_{sky,b}^{\downarrow}T_{b,i+1}(1-\tau_{b,i+1})\rho_{\ell,i+1} \quad (4b)$$

where $\tau_{d,i+1}$ [-] and $\tau_{b,i+1}$ [-] are the diffuse and direct beam transmittances through $(i+1)$-th layer, $\rho_{\ell,i+1}$ [-] is the leaf reflectance of $(i+1)$-th layer, $I_{sky,b}$ [Wm^{-2}] is the direct beam radiation incident on the top of the canopy, and $T_{b,i+1}$ [-] is the fraction of direct beam radiation that is not intercepted through the cumulative leaf area above the $(i+1)$-th layer.

Transmittance

The direct beam transmittance through the $(i+1)$-th layer with leaf area index ΔL_{i+1} is

$$\tau_{d,i+1} = 2\int_0^{\pi/2} \exp\left[-\frac{G(Z_i)\Omega}{\cos(Z_i)}\Delta L_{i+1}\right]\sin(Z_i)\cos(Z_i)dZ \quad (5)$$

where Z is the sky zenith angle and Ω is the leaf clumping factor. The Ross-Goudriann function, $G(Z)$, is given by

$$G(Z) = \phi_1 + \phi_2\cos(Z) \quad (6)$$

where $\phi_1 = 0.5 - 0.633\chi_\ell - 0.33\chi_\ell^2$ and $\phi_2 = 0.877(1 - 2\phi_1)$. The leaf departure angle from from spherical orientation, χ_ℓ, in restricted to $-0.4 \leq \chi_\ell \leq 0.6$. The equation 6 is numerically approximation for nine sky zones as

$$\tau_{d,i+1} = 2\sum_{i=1}^{9} \exp\left[-\frac{G(Z_i)\Omega}{\cos(Z_i)}\Delta L_{i+1}\right]\sin(Z_i)\cos(Z_i)\Delta Z_i \tag{7}$$

with $\Delta Z_i = \pi/18$.

The diffuse beam transmittance through the $(i+1)$-th layer is

$$\tau_{b,i+1} = \exp\left(-K_{b,i+1}\Omega\Delta L_{i+1}\right) \tag{8}$$

where $K_{b,i+1} = G(Z)/\cos(Z)$ is the extinction coefficient for the direct beam. The fraction of direct been that is not intercepted through the cumulative leaf area above the $(i+1)$-th layer is computed as

$$T_{b,i+1} = \prod_{j=i+1}^{N} \exp\left(-K_{b,j}\Omega_j\Delta L_j\right) \tag{9}$$

Linear system

The equation 4 can be written as a system of linear equations

$$-a_i I_i^{\uparrow} + I_i^{\downarrow} - b_i I_{i+1}^{\uparrow} = d_i \tag{10a}$$

$$-e_{i+1} I_i^{\downarrow} + I_{i+1}^{\uparrow} - f_{i+1} I_{i+1}^{\downarrow} = c_{i+1} \tag{10b}$$

where

$$a_i = f_{i+1} = (1 - \tau_{d,i+1})\rho_{\ell,i+1} - \frac{[\tau_{d,i+1} + (1 - \tau_{d,i+1})\tau_{\ell,i+1}]^2}{(1 - \tau_{d,i+1})/\rho_{\ell,i+1}} \tag{11a}$$

$$b_i = e_{i+1} = \frac{\tau_{d,i+1} + (1 - \tau_{d,i+1})\tau_{\ell,i+1}}{(1 - \tau_{d,i+1})\rho_{\ell,i+1}} \tag{11b}$$

$$c_i = I^{\downarrow}_{sky,b} T_{b,i} (1 - \tau_{b,i})(\rho_{\ell,i} - \tau_{\ell,i}.e_i) \tag{11c}$$

$$d_i = I^{\downarrow}_{sky,b} T_{b,i+1} (1 - \tau_{b,i+1})(\tau_{\ell,i+1} - \rho_{\ell,i+1} b_i) \tag{11d}$$

The boundary conditions for the downwelling radiation at the bottom layer, $i = 0$, and the upwelling radiation at the top layer, $i = N$, are given by

$$c_0 = \rho_{gb} I^{\downarrow}_{sky,b} T_{b,0} \tag{12a}$$

$$f_0 = \rho_{gd} \tag{12b}$$

$$d_N = I^{\downarrow}_{sky,d} \tag{12c}$$

where ρ_{gb} [-] is the surface albedo for beam radiation, ρ_{gd} [-] is the surface albedo for diffuse radiation, and $I_{sky,d}$ [Wm^{-2}] is the diffuse radiation incident on the top of the canopy.

The linear system of equations given in equation 10 can be written as

$$\begin{bmatrix} 1 & -\rho_{gd} & & & & & & \\ -a_0 & 1 & -b_0 & & & & & \\ & -e_1 & 1 & -f_1 & & & & \\ & & -a_1 & 1 & -b_1 & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & & \ddots & \ddots & \ddots & \\ & & & & & -e_N & 1 & -f_N \\ & & & & & & 0 & 1 \end{bmatrix} \begin{bmatrix} I^{\uparrow}_0 \\ I^{\downarrow}_0 \\ I^{\uparrow}_1 \\ I^{\downarrow}_1 \\ \vdots \\ \vdots \\ I^{\uparrow}_N \\ I^{\downarrow}_N \end{bmatrix} = \begin{bmatrix} c_0 \\ d_0 \\ c_1 \\ d_1 \\ \vdots \\ \vdots \\ c_N \\ d_N \end{bmatrix} \tag{13}$$

Absorbed radiative fluxes

The diffuse, $\overrightarrow{I}_{cd,i}$ [$\mathrm{Wm}^{-2}_{ground}$], and direct beam, $\overrightarrow{I}_{cb,i}$ [$\mathrm{Wm}^{-2}_{ground}$], radiation absorbed by the i-th canopy layer is

$$\overrightarrow{I}_{cd,i} = \left(I_i^{\downarrow} + I_{i-1}^{\uparrow}\right)(1 - \tau_{d,i})(1 - \omega_{\ell,i}) \tag{14a}$$

$$\overrightarrow{I}_{cb,i} = I^{\downarrow}_{sky,b} T_{b,i}(1 - \tau_{b,i})(1 - \omega_{\ell,i}) \tag{14b}$$

The radiation absorbed at the ground, $\overrightarrow{I}_g$ [$\mathrm{Wm}^{-2}_{ground}$], is

$$\overrightarrow{I}_g = \left(1 - \rho_{gd}\right) I_0^{\downarrow} + \left(1 - \rho_{gb}\right) I^{\downarrow}_{sky,b} T_{b,0} \tag{15}$$

It is assumed that the shaded leaves only absorb diffuse radiation, while sunlit leaves receive direct and diffuse radiations. The absorbed radiation fluxes by shaded, $\overrightarrow{I}_{\ell sha,i}$ [Wm^{-2}_{leaf}], and sunlit, $\overrightarrow{I}_{\ell sun,i}$ [Wm^{-2}_{leaf}], is given as

$$\overrightarrow{I}_{\ell sha,i} = \frac{I_{cd,i}}{\Delta L_i} \tag{16a}$$

$$\overrightarrow{I}_{\ell sun,i} = \overrightarrow{I}_{\ell sha,i} + \frac{\overrightarrow{I}_{cb,i}}{f_{sun,i}\Delta L_i} \tag{16b}$$

where f_{sun} [-] is the fraction of sunlit leaves at i-th layer. The absorbed canopy fluxes for shaded, $\overrightarrow{I}_{cSha}$ [$\mathrm{Wm}^{-2}_{ground}$], and sunlit, $\overrightarrow{I}_{cSun}$ [$\mathrm{Wm}^{-2}_{ground}$], are

$$\overrightarrow{I}_{cSha} = \sum_{i=1}^{N} \overrightarrow{I}_{\ell sha,i}(1 - f_{sun})\Delta L_i = \sum_{i=1}^{N} I_{cd,i}(1 - f_{sun}) \tag{17a}$$

$$\overrightarrow{I}_{cSun} = \sum_{i=1}^{N} \overrightarrow{I}_{\ell sun,i} f_{sun}\Delta L_i = \sum_{i=1}^{N} \left(\overrightarrow{I}_{cd,i} f_{sun} + \overrightarrow{I}_{cb,i}\right) \tag{17b}$$

Text S3. Longwave radiation model

The downwelling, $L_i^{\downarrow}$ [Wm^{-2}], and upwelling $L_{i+1}^{\uparrow}$ [Wm^{-2}], longwave radiation can be similarly described as the shortwave radiation model by replacing the direct beam scattering term (third term on RHS in equation 4) with a thermal radiation source term as

$$\begin{aligned} L_i^{\downarrow} &= L_{i+1}^{\downarrow}\left[\tau_{d,i+1} + (1-\tau_{d,i+1})\tau_{\ell,i+1}\right] + L_i^{\uparrow}(1-\tau_{d,i+1})\rho_{\ell,i+1} \\ &\quad + \varepsilon_\ell \sigma T_{\ell,i+1}^4 (1-\tau_{d,i+1}) \end{aligned} \tag{18a}$$

$$\begin{aligned} L_{i+1}^{\uparrow} &= L_i^{\uparrow}\left[\tau_{d,i+1} + (1-\tau_{d,i+1})\tau_{\ell,i+1}\right] + L_{i+1}^{\downarrow}(1-\tau_{d,i+1})\rho_{\ell,i+1} \\ &\quad + \varepsilon_\ell \sigma T_{\ell,i+1}^4 (1-\tau_{d,i+1}) \end{aligned} \tag{18b}$$

where ε_ℓ [-] is the leaf emissivity and T_ℓ [K] is the leaf temperature. If sunlit and shaded leaves are modeled explicitly, an effective leaf temperature is defined based on the sunlit and shaded leaf fraction.

Linear system

The linear system of equations for the longwave model can be written as

$$\begin{bmatrix} 1 & -(1-\varepsilon_g) & & & & & & & \\ -a_0 & 1 & -b_0 & & & & & & \\ & -e_1 & 1 & -f_1 & & & & & \\ & & -a_1 & 1 & -b_1 & & & & \\ & & & \ddots & \ddots & \ddots & & & \\ & & & & \ddots & \ddots & \ddots & & \\ & & & & & -e_N & 1 & -f_N \\ & & & & & & 0 & 1 \end{bmatrix} \begin{bmatrix} L_0^{\uparrow} \\ L_0^{\downarrow} \\ L_1^{\uparrow} \\ L_1^{\downarrow} \\ \vdots \\ \vdots \\ L_N^{\uparrow} \\ L_N^{\downarrow} \end{bmatrix} = \begin{bmatrix} c_0 \\ d_0 \\ c_1 \\ d_1 \\ \vdots \\ \vdots \\ c_N \\ d_N \end{bmatrix} \tag{19}$$

where

$$a_i = f_{i+1} = (1 - \tau_{d,i+1})\rho_{\ell,i+1} - \frac{[\tau_{d,i+1} + (1 - \tau_{d,i+1})\tau_{\ell,i+1}]^2}{(1 - \tau_{d,i+1})/\rho_{\ell,i+1}} \tag{20a}$$

$$b_i = e_{i+1} = \frac{\tau_{d,i+1} + (1 - \tau_{d,i+1})\tau_{\ell,i+1}}{(1 - \tau_{d,i+1})\rho_{\ell,i+1}} \tag{20b}$$

$$c_i = (1 - e_i)(1 - \tau_{d,i})\varepsilon_\ell \sigma T^4_{\ell,i} \tag{20c}$$

$$d_i = (1 - b_i)(1 - \tau_{d,i+1})\varepsilon_\ell \sigma T^4_{\ell,i+1} \tag{20d}$$

The boundary conditions for the downwelling radiation at the bottom layer, $i = 0$, and the upwelling radiation at the top layer, $i = N$, are given as

$$c_0 = \varepsilon_g \sigma T_g^4 \tag{21a}$$

$$d_N = L^{\downarrow}_{sky} \tag{21b}$$

where ε_g [-] is ground surface emissivity, T_g [K] is the ground surface temperature, and $L^{\downarrow}_{sky}$ [Wm^{-2}] is incident longwave radiation at the top of the canopy.

Absorbed fluxes

The net longwave flux absorbed per unit ground area, $\overrightarrow{L}_i$ [Wm^{-2}_{ground}], and per unit leaf area, $\overrightarrow{L}_{\ell,i}$ [Wm^{-2}_{leaf}], by the i-th layer are

$$\overrightarrow{L}_i = \varepsilon_\ell \left(L^{\downarrow}_i + L^{\uparrow}_{i-1}\right)(1 - \tau_{d,i}) - 2\varepsilon_\ell \sigma T^4_{\ell,i}(1 - \tau_{d,i}) \tag{22a}$$

$$\overrightarrow{L}_{\ell,i} = \frac{\overrightarrow{L}_i}{\Delta L_i} \tag{22b}$$

The radiation absorbed by the canopy, $\overrightarrow{L}_c$ [Wm^{-2}_{ground}], and the ground, $\overrightarrow{L}_g$ [Wm^{-2}_{ground}], is given by

$$\overrightarrow{L}_c = \sum_{i=1}^{N} \overrightarrow{L}_c \quad (23a)$$

$$\overrightarrow{L}_g = \varepsilon_g L_0^{\downarrow} - \varepsilon_g \sigma T_g^4 \quad (23b)$$

Text S4. Photosynthesis model: Biological demand

The net photosynthetic uptake of CO_2, A_n [μmol CO_2 m^{-2}s^{-1}], is given as

$$A_n = \min(A_c, A_j, A_p) - R_d$$
$$= A_g - R_d \tag{24}$$

where A_c [μmol CO_2 m^{-2}s^{-1}] is the Rubisco-limited CO_2 assimilation, A_j [μmol CO_2 m^{-2}s^{-1}] is the light-limited CO_2 assimilation, A_p [μmol CO_2 m^{-2}s^{-1}] is the PEP carboxylase-limited CO_2 assimilation, A_g [μmol CO_2 m^{-2}s^{-1}] is the co-limited gross CO_2 assimilation, and R_d [μmol CO_2 m^{-2}s^{-1}] is mitochondrial respiration. A_g is given as the smaller of two quadratic roots

$$0.98A_i^2 - (A_c + A_j) + A_c A_j = 0 \tag{25a}$$
$$0.98A_g^2 - (A_i + A_p) + A_i A_p = 0 \tag{25b}$$

The assimilation fluxes (A_c, A_j, and A_p) for C3 and C4 photosynthesis pathway are described next.

C3 Photosynthesis

The CO_2 assimilation fluxes for C3 photosynthesis are

$$A_c = \frac{V_{cmax}(c_i - \Gamma^*)}{c_i + K_c(1 - o_i/K_o)} \tag{26a}$$
$$A_j = \frac{J}{4}\left(\frac{c_i - \Gamma^*}{c_i + 2\Gamma^*}\right) \tag{26b}$$
$$A_p = 0 \tag{26c}$$

where V_{cmax} [μmol CO_2 m^{-2}s^{-1}] maximum rate of carboxylation, c_i [μmol CO_2 mol^{-1}] is the intercellular CO_2, o_i [μmol O_2 mol^{-1}] is the intercellular O_2, K_c [μmol CO_2 mol^{-1}] is the Michaelist-Mention constant for CO_2, K_o [μmol O_2 mol^{-1}] is the Michaelist-Mention constant for O_2, J [μmol CO_2 mol^{-1}] is the electron transport rate, and Γ^* [μmol CO_2 mol^{-1}] is the compensation point defined as the c_i at which no net CO_2 update occurs.

The rate of electron transport is related to photosynthetically active radiation and is given as the smaller root of the following quadratic equation.

$$\Theta_j J^2 - (I_{PSII} + J_{max}) + I_{PSII} J_{max} = 0 \tag{27}$$

where I_{PSII} [μmol CO_2 mol^{-1}] is the amount of light utilized in photosynthesis II, J_{max} [μmol CO_2 mol^{-1}] is the maximum transport rate, and $\Theta_j = 0.9$ is the curvature parameter. The amount of light utilized in photosynthesis II is

$$I_{PSII} = \frac{\Phi_{PSII}}{2} \alpha_\ell \overrightarrow{I}_{PAR} \tag{28}$$

where $\Phi_{PSII} = 0.7$ [mol mol^{-1}] is the quantum yield of photosystem II, $\alpha_\ell = 1$ is the leaf absorptance, $\overrightarrow{I}_{PAR}$ [μmol photon m^{-2} s^{-1}] is the absorbed photosynthetically active radiation.

The parameters K_c, K_o, Γ^*, V_{cmax}, J_{max}, and R_d vary from their values at 25^0C as function of leaf temperature, T_ℓ, that are given as

$$K_c = K_{c25} f(T_\ell) \tag{29a}$$

$$K_o = K_{o25} f(T_\ell) \tag{29b}$$

$$\Gamma^* = \Gamma^* f(T_\ell) \tag{29c}$$

$$V_{cmax} = V_{cmax25} f(T_\ell) f_H(T_\ell) \tag{29d}$$

$$J_{max} = J_{cmax25} f(T_\ell) f_H(T_\ell) \tag{29e}$$

$$R_d = R_{d25} f(T_\ell) f_H(T_\ell) \tag{29f}$$

where

$$f(T_\ell) = \exp\left[\frac{\Delta H_a}{298.15\mathcal{R}}\left(1 - \frac{298.15}{T_\ell}\right)\right] \tag{30a}$$

$$f_H(T_\ell) = \left[1 + \exp\left(\frac{298.15\Delta S - \Delta H_d}{298.15\mathcal{R}}\right)\right]\left[1 + \exp\left(\frac{\Delta S T_\ell - \Delta H_d}{\mathcal{R} T_\ell}\right)\right]^{-1} \tag{30b}$$

Lastly, the J_{max} and R_d at 25^0C are given as

$$J_{max25} = 1.67 V_{cmax25} \tag{31a}$$

$$R_{d25} = 0.015 V_{cmax25} \tag{31b}$$

C4 Photosynthesis

The CO_2 assimilation fluxes for C4 photosynthesis are

$$A_c = V_{cmax} \tag{32a}$$

$$A_j = \alpha_\ell \overrightarrow{I}_{PAR} E \tag{32b}$$

$$A_p = k_p c_i \tag{32c}$$

where $E = 0.05$ [mol mol^{-2}] is the quantum yield and k_p [mol m^{-2}s^{-1}] is the initial slope of the CO_2 response curve. The temperature dependence of V_{cmax}, R_d, and k_p are given as

$$V_{cmax} = V_{cmax25} Q_{10}^{(T_\ell - 298.16)/10} \left(1 + \exp[s_1(T_\ell - s_2)]\right)^{-1} \left(1 + \exp[s_3(s_4 - T_\ell)]\right)^{-1} \tag{33a}$$

$$R_d = R_{d25} Q_{10}^{(T_\ell - 298.16)/10} \left(1 + \exp[s_5(s_6 - T_\ell)]\right)^{-1} \tag{33b}$$

$$k_p = k_{p25} Q_{10}^{(T_\ell - 298.16)/10} \tag{33c}$$

where $Q_{10} = 2$, $s_1 = 0.3$ [K^{-1}], $s_2 = 313.15$ [K], $s_3 = 0.2$ [K^{-1}], $s_4 = 288.15$ [K], $s_5 = 1.3$ [K^{-1}], and $s_6 = 328.15$ [K]. The max R_d and k_p at 25^0C are given as

$$R_{d25} = 0.025 V_{cmax25} \tag{34a}$$

$$k_{p25} = 0.02 V_{cmax25} \tag{34b}$$

Text S5. Photosynthesis model: Diffusion

The net CO_2 assimilation due to biological demand (Equation 24) must match the diffusion of CO_2 from the surrounding air to the leaf surface and into the leaf, and is given by

$$A_n = g_{bc}(c_a - c_s) = g_{sc}(c_s - c_i) = g_{\ell c}(c_a - c_i) \tag{35}$$

where c_a [μmol CO_2 mol^{-1}] is the atmospheric CO_2, c_s [μmol CO_2 mol^{-1}] is the leaf surface CO_2, c_i [μmol CO_2 mol^{-1}] is the intercellular CO_2, g_{bc} [mol m^{-1}s^{-2}] is the boundary conductance of CO_2, g_{sc} [mol m^{-1}s^{-2}] is the stomatal conductance of CO_2, and $g_{\ell c}$ [mol m^{-1}s^{-2}] is the leaf conductance of CO_2.

Similarly, the transpiration of flux, E [mol H_2Om^{-2}s^{-1}], is given as

$$E = g_{bw}(q_a - q_s) = g_{sw}(q_s - q_i) = g_{\ell w}(q_a - q_i) \tag{36}$$

where q_a [μmol H_2O mol^{-1}] is the atmospheric H_2O, q_s [μmol H_2O mol^{-1}] is the leaf surface H_2O, q_i [μmol H_2O mol^{-1}] is the intercellular H_2O, g_{bc} [mol m^{-1}s^{-2}] is the boundary conductance of H_2O, g_{sc} [mol m^{-1}s^{-2}] is the stomatal conductance of H_2O, and $g_{\ell c}$ [mol m^{-1}s^{-2}] is the leaf conductance of H_2O. The leaf conductances can be written in terms of boundary and stomatal conductances as

$$g_{\ell c} = \frac{1}{g_{bc}^{-1} + g_{sc}^{-1}} \tag{37a}$$

$$g_{\ell w} = \frac{1}{g_{bw}^{-1} + g_{sw}^{-1}} \tag{37b}$$

It is assumed that $g_{sc} = g_{sw}/1.6$. Using equations 35 and 37a, c_i can be given as

$$c_i = c_a - \frac{A_n}{g_{\ell c}} \tag{38}$$

Text S6. Photosynthesis model: Stomatal conductance

The photosynthesis model has two equations (Equations 24 and 38) that involves three unknowns (c_i, A_n, and g_{sw}). Thus, an additional equation is needed for stomatal conductance to close the system of equations. In the literature, multiple stomatal conductance models (SCMs) have been developed that are based on empirical, semi-empirical, or optimization approach. Furthermore, SMCs can exclude or include plant hydraulics.

Semi-empirical models without accounting for plant hydraulics

1. **Ball-Berry model:** The semi-empirical Ball-Berry (BB) SCM (Ball et al., 1987) is given as

$$g_{sw} = g_0 + g_1 \frac{A_n}{c_s} h_s \tag{39}$$

where g_0 [mol $H_2O m^{-2} s^{-1}$] is the minimum stomatal conductance, g_1 [mol $H_2O m^{-2} s^{-1}$] is the slope of the relationship, and h_s [-] is the fractional humidity at the leaf surface. The fractional humidity at the leaf surface is $h_s = e_s/e_{sat}(T_\ell)$ where e_s and $e_{sat}(T_\ell)$ are the vapor pressure at the leaf surface and saturated vapor pressure at leaf temperature, T_ℓ, respectively. The vapor pressure at leaf surface can be given as

$$e_s = \frac{g_{bw} e_a + g_{sw} e_{sat}(T_\ell)}{g_{bw} + g_{sw}} \tag{40}$$

Substituting equation 40 in equation 39 leads the following quadratic equation in which g_{sw} is the larger root of the equation.

$$\alpha g_{sw}^2 + \beta g_{sw} + \gamma = 0 \tag{41}$$

where

$$\alpha = 1 \tag{42a}$$

$$\beta = g_{gw} - g_0 - \frac{g_1 A_n}{c_s} \tag{42b}$$

$$\gamma = -g_{bw}\left[g_0 + \frac{g_1 A_n e_a}{c_s e_{sat}(T_\ell)}\right] \tag{42c}$$

2. **Medlyn model:** The semi-empirical Medlyn SCM (Medlyn et al., 2011) is given as

$$g_{sw} = g_0 + 1.6\frac{A_n}{c_s}\left(1 + \frac{g_1}{\sqrt{D_s}}\right) \tag{43}$$

where g_0 [mol H_2Om^{-2} s^{-1}] is the minimum stomatal conductance, g_1 [mol H_2Om^{-2} s^{-1}] is the slope of the relationship, and $D_s = (e_{sat}(T_\ell) - e_s)$ [KPa] is the vapor pressure deficit. Similar to BB model, substituting equation 40 in equation 43 leads to following quadratic equations, whose larger root is g_{sw}.

$$\alpha g_{sw}^2 + \beta g_{sw} + \gamma = 0 \tag{44}$$

where

$$\alpha = 1 \tag{45a}$$

$$\beta = -2\left(g_0 - 1.6\frac{g_1 A_n}{c_s}\right) - \left(\frac{1.6 A_n g_1}{c_s}\right)^2 \frac{1}{g_{bw} D_\ell} \tag{45b}$$

$$\gamma = -\left[2g_0 + \frac{1.6A_n}{c_s}\left(1 - \frac{g_\ell^2}{D_\ell}\right)\right]\frac{1.6 A_n g_1}{c_s} \tag{45c}$$

with $D_\ell = e_{sat}(T_\ell) - e_a$.

Optimization-based models

Optimization-based SCMs maximize carbon update, A_n, while minimizing the cost associated with carbon update, Θ, related a measure of stomatal opening, χ (Wang et al., 2020). Such models can be formulated as

$$\max_{\chi} \quad (A_n - \Theta) \tag{46}$$

and the solution of equation 46 is obtained by finding χ that satisfies the following equation

$$\frac{\partial A_n}{\partial \chi} - \frac{\partial \Theta}{\partial \chi} = 0 \tag{47}$$

1. **Marginal water-use efficiency (WUE) model without accounting for plant hydraulics:** In this model, $\chi = E$ and $\Theta = \xi E$, where ξ is a constant model parameter. Thus, equation 47 reduces to

$$\frac{\partial A_n}{\partial E} = \xi \tag{48}$$

Buckley, Sack, and Farquhar (2017) derived the LHS term of equation 48 as

$$\frac{\partial A_n}{\partial E} = \left(\frac{c_a - c_i}{w_l}\right)\left(\frac{\partial A_n/\partial c_i}{\partial A_n/\partial c_i + g_{lc}}\right)1.6\frac{g_{lc}^2}{g_{\ell w}^2} \tag{49}$$

where $w_\ell = \left[e_{sat}(T_\ell) - e_a\right]/P_{ref}$ [mol mol^{-1}] is the vapor pressure deficit.

2. **Intrinsic WUE (iWUE) model without accounting for plant hydraulics:** In this model, $\chi = g_{sw}$ and the cost function is similar to that of the WUE model (i.e. $\Theta = \xi E$). The equation 47 then reduces to

$$\begin{aligned}\frac{\partial A_n}{\partial g_{sw}} &= \xi \frac{\partial E}{\partial g_{sw}} \\ &= \xi \frac{\partial}{\partial g_{sw}} \left(\frac{(e_{sat}(T_\ell) - e_s) g_{sw}}{P_{ref}} \right) \\ &\approx \xi w_s\end{aligned} \tag{50}$$

where $w_s (= [e_{sat}(T_\ell) - e_s]/P_{ref})$ [mol mol^{-1}] is the water vapor deficit at the leaf surface. In equation 50, the term $\partial e_s/\partial g_{sw}$ is neglected.

3. **Water-use efficiency model including plant hydraulics:** Manzoni et al. (2011) modified the marginal WUE model to account for loss of xylem conductivity by including dependence of ξ in equation 48 on leaf water potential as

$$\xi(\psi_\ell) = \exp(\beta \psi_\ell) \tag{51}$$

where β is a model parameter.

4. **Co-optimization model of Bonan, Williams, Fisher, and Oleson (2014):** Bonan et al. (2014) developed a SCM that maximizes g_{sw} while satisfying two constraints: (1) WUE or iWUE is greater than a threshold (i.e. $\partial A_n/\partial E \geq \xi$ or $(\partial A_n/\partial g_{sw})/w_s \geq \xi$, and (2) leaf water potential is greater than a threshold (i.e. $\psi_\ell \geq \psi_{\ell,min}$). The plant hydraulics model assumes leaves (sunlit or shaded) at any height are directly connected to multiple soil layers via a root system. The leaf water storage is given by

$$\frac{d\psi_\ell}{dt} = \frac{K_L(\psi_s - \psi_\ell - \rho_w g h) - 10^3 \times E}{C_p} \tag{52}$$

where ψ_ℓ [MPa] is the leaf water potential, ψ_s [MPa] is the soil water potential, $\rho_w g h$ [MPa] is the gravitational head, C_p [μmol H_2O m_ℓ^{-2} MPa^{-1}] is the leaf capacitance, and K_L [μmol H_2O m_ℓ^{-2} s^{-1} MPa^{-1}] is the whole plant hydraulic conductance, and E [mmol

H_2O m_ℓ^{-2} s^{-1}] is the transpiration flux. The K_L is independent of ψ_l and thus integrating equation 52 provides an analytical expression for the change of leaf water potential, $\Delta\psi_\ell^{t+\Delta t}$, for time step, Δt, as

$$\Delta\psi_\ell^{t+\Delta t} = \left[\psi_s - \psi_\ell^t - \rho_w g h - \frac{10^3 \times E}{K_L}\right]\left(1 - e^{-K_L \Delta t / C_p}\right) \tag{53}$$

The second constraint of the co-optimization approach leads to

$$\psi_\ell^t + \Delta\psi_\ell^{t+\Delta t} \geq \psi_{\ell,min} \tag{54}$$

The whole plant hydraulic conductance depends on soil-to-stem conductance, $K_{L,s2s}$ [μmol H_2O m_ℓ^{-2} s^{-1} MPa^{-1}], and stem-to-leave conductance, $K_{L,s2\ell}$ [μmol H_2O m_ℓ^{-2} s^{-1} MPa^{-1}] as

$$\frac{1}{K_L} = \frac{1}{K_{L,s2s}} + \frac{1}{K_{L,s2\ell}} \tag{55}$$

5. **Modified Bonan et al. (2014) model:** In this study, we propose a modified plant hydraulic model of Bonan et al. (2014) by including dependence of leaf water potential on stem-to-soil conductance, which is modeled by a Weibull function as

$$K_{L,s2\ell}(\psi_\ell) = \psi_{L,s2\ell}^{max} \exp\left[\left(\frac{-\psi_\ell}{b}\right)^c\right] \tag{56}$$

where b [MPa] and c [-] are parameters. The modified equation 52 is solved using the forward Euler time-integration scheme.

6. **Wang et al. (2020) model:** In this model, $\chi = E$ and the cost function is given as

$$\Theta = A_n \frac{E_\ell}{E_{critical}} \tag{57}$$

where $E_{critical}$ is the critical transpiration for hydraulic failure.

Semi-empirical model with downregulation due to plant hydraulics

Empirical models have been proposed for reducing g_{sw} to account for loss of xylem hydraulic conductivity with water potential. Example of such empirical stomatal down-regulation models include Christoffersen et al. (2016) (equation 58a) and Bohrer et al. (2005) (equation 58b).

$$g_{sw} = g_{sw,max}\left[1 + \left(\frac{-\psi_\ell}{\psi_{50}}\right)^a\right]^{-1} \tag{58a}$$

$$g_{sw} = g_{sw,max}\exp\left[-\left(\frac{\psi_\ell}{\psi_{50}}\right)^a\right] \tag{58b}$$

where a [-] and ψ_{50} [KPa] are model parameters. In these empirical stomatal downregulation models, $g_{sw,max}$ is obtained from equation 39 or 43 or 48 or 50.

Text S7. Photosynthesis model: Numerical solution

The set of nonlinear equations for photosynthesis model include: (1) biological demand (equation 35), (2) diffusion (equation 24), and (3) stomatal conductance model (equations given in section 1). The set of nonlinear equations are numerically solved when the residual equation, $R(x)$, where x is the unknown variable. The solution, x^*, of the nonlinear is obtained when $R(x^*) = 0$. The residual equation for photosynthesis model with various SCMs is provided below.

1. **BB and Medlyn model:** The unknown variable is c_i and the residual equation is

$$R(c_i) \equiv A_n - g_{\ell c}(c_a - c_i) = 0 \tag{59}$$

2. **Marginal WUE:** The unknown variable is g_ℓ and with the residual equation for model without plant hydraulics (i.e. ξ is independent of ψ_ℓ) is

$$R(g_\ell) \equiv \frac{\partial A_n}{\partial g_{sw}} - \xi = 0 \tag{60}$$

For models that include plant hydraulics, equation 60 is modified by making ξ depend on ψ_ℓ.

3. **iWUE:** The unknown variable is g_ℓ and with the residual equation for model without plant hydraulics (i.e. ξ is independent of ψ_ℓ) is

$$R(g_\ell) \equiv \frac{\partial A_n}{\partial g_{sw}} - \xi w_s = 0 \tag{61}$$

For models that include plant hydraulics, equation 61 is modified by make ξ depend on ψ_ℓ.

4. **SCM with stomatal dowregulation:** Depending on the choice of $g_{sw,max}$ in 58, the residual equation is given by equation 59 or 60 or 61.

5. **Original and modified Bonan et al. (2014) co-optimization model:** The unknown variable is g_ℓ and the residual equation for the first constraint is given by equation 60 or 61. The residual equation for the second constraint is given as

$$R(g_\ell) \equiv \psi_\ell^t + \Delta\psi_\ell^{t+\Delta t} - \psi_{\ell,min} = 0 \tag{62}$$

6. **Wang et al. (2020):** The unknown variable is g_ℓ and the residual equation is

$$R(g_\ell) \equiv \left(1 - \frac{E_\ell}{E_{critical}}\right)\frac{\partial\Theta}{\partial E} - \frac{A_n}{E_{critical}}\frac{\partial E_\ell}{E} = 0 \tag{63}$$

Text S8. Leaf boundary layer model

The boundary conductance controls the transfer of heat and mass (both, H_2O and CO_2) from the leaf surface to the surrounding air. The Nusslet number, *Nu* [-], is the ratio of convective to conductive heat transfer, while the Sherwood number, *Sh* [-], is the ratio of convective to conductive mass transfer that are given by

$$\mathrm{Nu} = \frac{g_{bh} d_\ell}{\rho_m D_h} \tag{64a}$$

$$\mathrm{Sh}_w = \frac{g_{bw} d_\ell}{\rho_m D_w} \tag{64b}$$

$$\mathrm{Sh}_c = \frac{g_{bc} d_\ell}{\rho_m D_c} \tag{64c}$$

where g_{bh} [mol m^{-2}_{leaf} s^{-1}] is boundary conductance for heat , g_{bv} [mol m^{-2}_{leaf} s^{-1}] is boundary conductance for H_2O, g_{bc} [mol m^{-2}_{leaf} s^{-1}] is boundary conductance for CO_2, D_h [m^2 s^{-1}] is the molecular diffusivity for heat, D_w [m^2 s^{-1}] is the molecular diffusivity for H_2O, D_c [m^2 s^{-1}] is the molecular diffusivity for CO_2, ρ_m [mol m^{-3}] is molar density, d_ℓ [m] is the representative leaf dimension, and Sh_w and Sh_c are Sherwood number for water vapor and CO_2, respectively.

Empirical studies have developed relationship for Nu, Sh_w, and Sh_c for laminar flow:

$$\mathrm{Nu}^{Laminar} = b_1 0.66 \mathrm{Pr}^{0.33} Re^{0.5} \tag{65a}$$

$$\mathrm{Sh}_w^{Laminar} = b_1 0.66 \mathrm{Sc}_w^{0.33} Re^{0.5} \tag{65b}$$

$$\mathrm{Sh}_c^{Laminar} = b_1 0.66 \mathrm{Sc}_c^{0.33} Re^{0.5} \tag{65c}$$

and turbulent flow:

$$\mathrm{Nu}^{Turbulent} = b_1 0.036 \mathrm{Pr}^{0.33} Re^{0.8} \tag{66a}$$

$$\mathrm{Sh}_w^{Turbulent} = b_1 0.036 \mathrm{Sc}_w^{0.33} Re^{0.8} \tag{66b}$$

$$\mathrm{Sh}_c^{Turbulent} = b_1 0.036 \mathrm{Sc}_c^{0.33} Re^{0.8} \tag{66c}$$

where Re [-] is the Reynolds number that is a ratio of inertial forces to viscous forces, Pr [-] is the Prandtl number that is a ratio of diffusivity of momentum to diffusivity of heat in fluid, Sc_w [-] and Sc_c [-] are the Schmidt numbers that are ratio of diffusivity of momentum to diffusivity of mass for H_2O and CO_2) in fluid, respectively, and $b_1 = 1.5$ is a typical value that converts the empirical relationship developed for a flat rectangular plate to for leaves. The Prandtl, Reynolds, and Schmidt numbers are

$$\mathrm{Re} = \frac{u d_\ell}{\nu} \tag{67a}$$

$$\mathrm{Pr} = \frac{\nu}{D_h} \tag{67b}$$

$$\mathrm{Sc}_w = \frac{\nu}{D_w} \tag{67c}$$

$$\mathrm{Sc}_c = \frac{\nu}{D_c} \tag{67d}$$

where ν [m^2 s^{-1}] is the kinematic viscosity. The forced flow due to laminar and turbulent flow is given as

$$\mathrm{Nu}^{forced} = \max(\mathrm{Nu}^{Laminar}, \mathrm{Nu}^{Turbulen}) \tag{68a}$$

$$\mathrm{Sh}_w^{forced} = \max(Shv^{Laminar}, \mathrm{Sh}_w^{Turbulent}) \tag{68b}$$

$$\mathrm{Sh}_c^{forced} = \max(Shc^{Laminar}, \mathrm{Sh}_c^{Turbulent}) \tag{68c}$$

In free convection, The Nusselt and Scherwood number are described in terms of Grashof number, Gr [-], as

$$\mathrm{Nu}^{Free} = 0.54\mathrm{Pr}^{0.25}\mathrm{Gr}^{0.25} \tag{69a}$$

$$\mathrm{Sh}_w^{Free} = 0.54\mathrm{Sc}_c^{0.25}\mathrm{Gr}^{0.25} \tag{69b}$$

$$\mathrm{Sh}_c^{Free} = 0.54\mathrm{Sc}_c^{0.25}\mathrm{Gr}^{0.25} \tag{69c}$$

$$\tag{69d}$$

The Grashof number is given as

$$\mathrm{Gr} = \frac{g d_\ell^3 (T_\ell - T_a)}{\nu^2 T_a} \tag{70}$$

where g [m s^{-2}] is the gravitational acceleration, T_ℓ [K] is the leaf temperature, and T_a [K] is the air temperature. Lastly, the combined Nusselt and Scherwood number for forced and free flow are given as

$$\mathrm{Nu} = \mathrm{Nu}^{Forced} + \mathrm{Nu}^{free} \tag{71a}$$

$$\mathrm{Sh}_w = \mathrm{Sh}_w^{Forced} + \mathrm{Sh}_w^{free} \tag{71b}$$

$$\mathrm{Sh}_c = \mathrm{Sh}_c^{Forced} + \mathrm{Sh}_c^{free} \tag{71c}$$

250 The leaf boundary conductances for heat, H_2O, and CO_2 are given by combining
251 equations 64 and 71

$$g_{bh} = \frac{D_h \times \mathrm{Nu}}{d_\ell}\rho_m \tag{72a}$$

$$g_{bw} = \frac{D_w \times Sh_v}{d_\ell}\rho_m \tag{72b}$$

$$g_{bc} = \frac{D_c \times Sh_c}{d_\ell}\rho_m \tag{72c}$$

252 The kinematic viscosity and molecular diffusivities are adjusted to account for air
253 temperature and air pressure, P_a [Pa], as

$$\nu = f \times \nu_0 \tag{73a}$$

$$D_h = f \times Dh_0 \tag{73b}$$

$$D_w = f \times Dv_0 \tag{73c}$$

$$D_c = f \times Dc_0 \tag{73d}$$

$$f = \frac{10325}{P_a} \times \left(\frac{T_a}{272.15}\right)^{1.81} \tag{73e}$$

254 where ν_0 is kinematic viscosity at 0^0 C, and Dh_0, Dv_0, Dc_0 are molecular diffusivity for
255 heat, H_2O, and CO_2 at 0^0 C.

Text S9. Roughness sublayer model

Wind profile above canopy

The wind profile, u, above canopy the is given as

$$\frac{\kappa(z-d)}{u_*}\frac{\partial u}{\partial z} = \Phi_m(z) \tag{74}$$

where Φ_m [-] is an effective similarity function that is given by

$$\Phi_m(z) = \phi_m\left(\frac{z-d}{L_{MO}}\right)\hat{\phi}_m\left(\frac{z-d}{l_m/\beta}\right) \tag{75}$$

$$u(z) = \frac{u_*}{\kappa}\left[\ln\left(\frac{z-d}{z_{0m}}\right) - \psi_m\left(\frac{z-d}{L_{MO}}\right) + \psi_m\left(\frac{z_{0m}}{L_{MO}}\right) + \hat{\psi}_m(z)\right] \tag{76}$$

where

$$\hat{\psi}_m = \int_z^\infty \phi_m\left(\frac{z'-d}{L_{MO}}\right)\left[1 - \hat{\phi}_m\left(\frac{z'-d}{l_m/\beta}\right)\right]\frac{dz'}{z'-d} \tag{77}$$

Given equation 77, the wind at canopy height is given by

$$u_{hc} = \frac{u_*}{\beta} \tag{78}$$

$$u(z) = \frac{u_*}{\kappa}\left[\ln\left(\frac{z-d}{h_c-d}\right) - \psi_m\left(\frac{z-d}{L_{MO}}\right) + \psi_m\left(\frac{h_c-d}{L_{MO}}\right) + \hat{\psi}_m(z) - \hat{\psi}_m(h_c) + \frac{\kappa}{\beta}\right] \tag{79}$$

Wind profile within canopy

HF-2007 assumed an exponential wind profile within the canopy that is given as

$$u(z) = u(h_c)\exp\left(\frac{z-h_c}{l_m/\beta}\right) \tag{80}$$

and the derivative of the wind profile is

$$\begin{aligned}\frac{\partial u(z)}{\partial z} &= \frac{u(h_c)}{l_m/\beta} \exp\left(\frac{z-h_c}{l_m/\beta}\right) \\ &= \frac{u(z)}{l_m/\beta} \qquad (81a)\end{aligned}$$

$$h_c - d = \frac{l_m}{2\beta} = \beta^2 L_c \qquad (82)$$

Enforcing the continuity of derivative of wind at canopy height (h_c) from equation 74 and 80 leads to

$$\begin{aligned}\frac{u_*}{\kappa(h_c-d)}\Phi_m(h_c) &= \frac{u(h_c)}{l_m/\beta} \\ \Phi_m(h_c) &= \frac{u(h_c)}{u_*} \times \frac{\kappa(h_c-d)}{l_m/\beta} \\ \Phi_m(h_c) &= \frac{1}{\beta} \times \frac{\kappa l_m/(2\beta)}{l_m/\beta} \\ \Phi_m(h_c) &= \frac{\kappa l_m}{2\beta} \qquad (83a)\end{aligned}$$

Wind similarity function

For the above canopy wind profile, HF-2007 assumed the similarity function for momentum to be

$$\hat{\phi}_m\left(\frac{z-d}{l_m/\beta}\right) = 1 - c_1 \exp\left[-c_2\left(\frac{z-d}{l_m/\beta}\right)\right] \qquad (84)$$

where c_1 and $c_2(= 0.5)$ are parameters. The parameter c_1 is found by evaluating $\hat{\phi}_m$ at $z = h_c$ that gives

$$\begin{aligned}
\hat{\phi}_m\left(\frac{h_c - d}{l_m/\beta}\right) &= 1 - c_1 \exp\left[-c_2\left(\frac{h_c - d}{l_m/\beta}\right)\right] \\
&= 1 - c_1 \exp\left[-c_2\left(\frac{l_m/(2\beta)}{l_m/\beta}\right)\right] \\
&= 1 - c_1 \exp\left(-0.5c_2\right) \\
c_1 &= \left[1 - \hat{\phi}_m\left(\frac{h_c - d}{l_m/\beta}\right)\right]\exp(0.5c_2) \qquad (85a)
\end{aligned}$$

In order to compute c_1 from the above equation, an expression of $\hat{\phi}_m$ at $z = h_c$ is needed, which is obtained using equation 75 at $z = h_c$ and equation 83a as

$$\hat{\phi}_m\left(\frac{h_c - d}{l_m/\beta}\right) = \frac{\kappa}{2\beta}\phi_m^{-1}\left(\frac{h_c - d}{L_{MO}}\right) \qquad (86)$$

Wind beta term

The critical unknown in the roughness sublayer parameterization is β. HF-2007 derived an expression for β as

$$\beta\phi_m\left(\frac{h_c - d}{L_{MO}}\right) = \beta_N \qquad (87)$$

or

$$\beta\phi_m\left(\frac{\beta^3 L_c}{L_{MO}}\right) = \beta_N \qquad (88)$$

The solution of equation 88 depends on if ϕ is evaluated for unstable or stable condition and leads to following equations

$$(\beta^2)^2 + 16\frac{L_c}{L_{MO}}\beta^4\beta^2 - \beta_N^4 = 0 \qquad L_{MO} < 0 \qquad (89a)$$

$$5\frac{L_c}{L_{MO}}\beta^3 + \beta - \beta_N = 0 \qquad L_{MO} \geq 0 \qquad (89b)$$

The correct solution is the larger root for the sable condition, while the unstable case has only one real root.

Temperature profile

Similar to the equations for wind profiles, the equations describing profiles of heat (or scalar) above and within the canopy are given below.

$$\frac{\kappa(z-d)}{\theta_*}\frac{\partial\theta}{\partial z} = \Phi_c\,(z) \tag{90a}$$

$$\Phi_c(z) = \phi_c\left(\frac{z-d}{L_{MO}}\right)\hat{\phi}_c\left(\frac{z-d}{l_m/\beta}\right) \tag{90b}$$

$$\theta(z) - \theta_s = \frac{\theta_*}{\kappa}\left[\ln\left(\frac{z-d}{z_{0c}}\right) - \psi_m\left(\frac{z-d}{L_{MO}}\right) + \psi_m\left(\frac{z_{0c}}{L_{MO}}\right) + \hat{\psi}_c(z)\right] \tag{90c}$$

where

$$\hat{\psi}_c = \int_z^\infty \phi_c\left(\frac{z'-d}{L_{MO}}\right)\left[1 - \hat{\phi}_c\left(\frac{z'-d}{l_m/\beta}\right)\right]\frac{dz'}{z'-d} \tag{91}$$

An exponential profile of air temperature is assumed within the canopy that is given by

$$\theta(z) - \theta_s = (\theta(h_c) - \theta_s)\exp\left[\frac{f(z-h_c)}{l_m/\beta}\right] \tag{92}$$

where parameter f relates the length scale of heat (scalar) to that of momentum and is given by

$$f = \frac{1}{2}(1 + 4r_c\mathrm{Pr})^{1/2} - \frac{1}{2} \tag{93}$$

and

$$\mathrm{Pr} = 0.5 + 0.3\tanh(2L_c/L_{MO}) \tag{94}$$

The derivatives of the profile within the canopy is

$$\frac{\partial \theta(z)}{\partial z} = \frac{(\theta(h_c) - \theta_s) f}{l_m/\beta} \exp\left[\frac{f(z - h_c)}{l_m/\beta}\right] \tag{95}$$

Enforcing continuity of derivative at $z = h_c$ using equation 90a and 95

$$\left.\frac{\partial \theta}{\partial z}\right|_{z=h_c} = \frac{\theta_*}{\kappa(h_c - d)} \Phi_c(h_c) = \frac{f[\theta(h_c) - \theta_s]}{l_m/\beta} \tag{96}$$

so that

$$\frac{\theta(h_c) - \theta_s}{\theta_*} = \frac{\mathrm{Pr}}{f\beta} \tag{97}$$

An equation similar to equation 79 can be written for θ

$$\theta(z) - \theta_s = \frac{\theta_*}{\kappa}\left[\ln\left(\frac{z-d}{h_c-d}\right) - \psi_c\left(\frac{z-d}{L_{MO}}\right) + \psi_c\left(\frac{h_c-d}{L_{MO}}\right) + \hat{\psi}_c(z) - \hat{\psi}_c(h_c) + \frac{\kappa \mathrm{Pr}}{f\beta}\right] \tag{98}$$

For the above canopy wind profile, HF-2007 assumed the similarity function for momentum to be

$$\hat{\phi}_c\left(\frac{z-d}{l_m/\beta}\right) = 1 - c_1 \exp\left[-c_2\left(\frac{z-d}{l_m/\beta}\right)\right] \tag{99}$$

$$c_1 = \left[1 - \hat{\phi}_c\left(\frac{h_c-d}{l_m/\beta}\right)\right] \exp(0.5 c_2) \tag{100a}$$

$$\hat{\phi}_c\left(\frac{z-d}{l_m/\beta}\right) = \frac{\kappa \mathrm{Pr}}{2\beta} \phi_c^{-1}\left(\frac{z-d}{L_{MO}}\right) \tag{100b}$$

Aerodynamic conductance

The aerodynamic conductances for scalar, g_{ac}, is given as

$$\frac{1}{g_{ac}} = \int_{z_1}^{z_2} \frac{dz}{\rho_m K_c} \tag{101}$$

where K_c is the eddy diffusivity for scalar based on K-theory. The aerodynamic conductance above canopy is

$$g_{am,i+1/2} = \rho_m \kappa^2 u_* \left[\ln\left(\frac{z_{i+1} - d}{z_i - d}\right) + \psi_{i+1} - \psi_i\right]^{-1} \tag{102}$$

where

$$\psi_i = -\psi_c\left(\frac{z_i - d}{L_{MO}}\right) + \psi_c\left(\frac{h_c - d}{L_{MO}}\right) + \hat{\psi}_c(z_i) - \hat{\psi}_c(h_c) \tag{103}$$

The aerodynamic conductance within canopy is

$$g_{ac,i+1/2} = \frac{\rho\beta u_*}{\mathrm{Pr}}\left[\exp\left(\frac{-(z_{i+1} - h_c)}{l_m/\beta}\right) - \left(\frac{-(z_i - h_c)}{l_m/\beta}\right)\right]^{-1} \tag{104}$$

Text S10. Multi-layer canopy air space and canopy model

The equations for the time evolution of air temperature, θ, and water vapor, q, sunlit leaf temperature, $T_{\ell sun}$, and shaded leaf temperature, $T_{\ell shd}$, in a MLCM is given by

$$\rho_m c_p \left(\frac{\partial \theta}{\partial t}\right) = c_p \nabla \cdot (g_a \nabla \theta) + \frac{Q_{\theta sun,i} \Delta L_{sun,i}}{\Delta z_i} + \frac{Q_{\theta shd,i} \Delta L_{shd,i}}{\Delta z_i} + S_\theta \tag{105a}$$

$$\rho_m \left(\frac{\partial q}{\partial t}\right) = \nabla \cdot (g_a \nabla q) + \frac{Q_{qsun,i} \Delta L_{sun,i}}{\Delta z_i} + \frac{Q_{qshd,i} \Delta L_{shd,i}}{\Delta z_i} + S_q \tag{105b}$$

$$c_\ell \left(\frac{\partial T_{\ell sun}}{\partial t}\right) = \mathrm{R}_{n,sun} - Q_{\theta sun} - \lambda Q_{qsun} + S_{\ell sun} \tag{105c}$$

$$c_\ell \left(\frac{\partial T_{\ell shd}}{\partial t}\right) = \mathrm{R}_{n,shd} - Q_{\theta shd} - \lambda Q_{qshd} + S_{\ell shd} \tag{105d}$$

where ρ_m is density of air, λ is latent heat of vaporization for water, c_p is specific heat capacity of air, c_ℓ is specific heat capacity of leaf, g_a is atmospheric conductance, ΔL_{sun} is the leaf area index of the sunlit leaf, ΔL_{shd} is the leaf area index of the shaded leaf, $Q_{\theta sun}$ is the heat source from the sunlit leaf to the canopy air, $Q_{\theta shd}$ is the heat source from the shaded leaf to the canopy air, Q_{qsun} is the water vapor source from the sunlit leaf the canopy air, Q_{qsun} is the water vapor source from the shaded leaf the canopy air, Rn_{sun} is the net shortwave and longwave radiation absorbed by the sunlit leaf, and Rn_{shd} is the net shortwave and longwave radiation absorbed by the shaded leaf.

The source of heat and water vapor for sunlit and shaded leaves at the i-th layer are given by

$$Q_{\theta sun} = 2c_p(T_{\ell sun} - \theta_i)g_{bh} \tag{106a}$$

$$Q_{\theta shd} = 2c_p(T_{\ell shd} - \theta_i)g_{bh} \tag{106b}$$

$$Q_{qsun} = (q_{sat}(T_{\ell sun}) - q_i)g_{\ell sun} \tag{106c}$$

$$Q_{qshd} = (q_{sat}(T_{\ell shd}) - q_i)g_{\ell shd} \tag{106d}$$

307 where $g_{bh,i}$ is the boundary layer conductance for heat, $g_{bw,i}$ is the boundary layer
308 conductance for water vapor, $g_{\ell sun,i}$ is the total leaf conductance for the sunlit leaf, and
309 $g_{\ell shd,i}$ is the total leaf conductance for the shaded leaf. The leaf conductances are given
310 as

$$g_{\ell sun} = \left(\frac{1}{g_{bw}^{-1} + g_{sw,sun}^{-1}}\right) f_{dry} + g_{bw} f_{wet} \tag{107a}$$

$$g_{\ell shd} = \left(\frac{1}{g_{bw}^{-1} + g_{sw,shd}^{-1}}\right) f_{dry} + g_{bw} f_{wet} \tag{107b}$$

311 where $g_{sw,sun}$ is the stomatal conductance for the sunlit leaf, and $g_{sw,shd}$ is the stomatal
312 conductance for the shaded leaf. The net radiation absorbed by sunlit and shaded leaf
313 are given by

$$\mathrm{Rn}_{sun} = \vec{I}^{d}_{sun} + \vec{I}^{b}_{sun} + \vec{L}_{sun} \tag{108a}$$

$$\mathrm{Rn}_{shd} = \vec{I}^{d}_{shd} + \vec{L}_{shd} \tag{108b}$$

314 where $\vec{I}^{d}$ is absorbed diffuse radiation, $\vec{I}^{b}$ is absorbed beam radiation, and $\vec{L}$ is ab-
315 sorbed longwave radiation. The finite volume and implicit time discretization of equa-
316 tion 105 leads to the following equations for the i-th layer can be written as

$$
\begin{bmatrix}
\alpha_{1,1} & \alpha_{1,2} & \alpha_{1,3} & \alpha_{1,4} & \alpha_{1,5} & \alpha_{0,6} & \alpha_{1,7} & \alpha_{1,8} \\
0 & 0 & 0 & \alpha_{2,4} & \alpha_{2,5} & \alpha_{2,6} & \alpha_{2,7} & \alpha_{2,8} \\
0 & \alpha_{3,2} & 0 & 0 & \alpha_{3,5} & 0 & \alpha_{3,7} & 0 \\
0 & \alpha_{4,2} & 0 & 0 & \alpha_{4,5} & 0 & 0 & \alpha_{4,8}
\end{bmatrix}
\begin{bmatrix}
\theta_{i-1}^{t+1} \\ \theta_{i}^{t+1} \\ \theta_{i+1}^{t+1} \\ q_{i-1}^{t+1} \\ q_{i}^{t+1} \\ q_{i+1}^{t+1} \\ T_{lsun,i}^{t+1} \\ T_{lshd,i}^{t+1}
\end{bmatrix}
=
\begin{bmatrix}
\beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4
\end{bmatrix}
\tag{109}
$$

317 **Air temperature equation**

318 The discretized equation 105a at an internal vertical layer (i.e. $0 < i < N$)

$$
\begin{aligned}
\frac{\rho_m}{\Delta t}\left(\theta_i^{t+1} - \theta_i^t\right) = &+ g_{a,i+\frac{1}{2}}\left(\frac{\theta_{i+1}^{t+1} - \theta_i^{t+1}}{z_{i+1}^c - z_i^c}\right) - g_{a,i-\frac{1}{2}}\left(\frac{\theta_i^{t+1} - \theta_{i-1}^{t+1}}{z_i^c - z_{i-1}^c}\right) \\
&+ 2\left(T_{\ell sun,i}^{t+1} - \theta_i^{t+1}\right)\left(\frac{g_{bh,i}\Delta L_{sun,i}}{\Delta z_i}\right) \\
&+ 2\left(T_{\ell shd,i}^{t+1} - \theta_i^{t+1}\right)\left(\frac{g_{bh,i}\Delta L_{shd,i}}{\Delta z_i}\right)
\end{aligned}
\tag{110}
$$

319 The non-zero coefficients $\alpha_{i=1,*}$ of equation 109 for $0 < i < N$ are thus given as

$$\alpha_{1,1} = -\left(\frac{g_{a,i-\frac{1}{2}}^{t+1}}{\Delta z_{i,i-1}^c}\right) \tag{111a}$$

$$\alpha_{1,2} = \left(\frac{\rho_m}{\Delta t}\right) + \left(\frac{g_{a,i+\frac{1}{2}}^{t+1}}{\Delta z_{i+1,i}^c}\right) + \left(\frac{g_{a,i+\frac{1}{2}}^{t+1}}{\Delta z_{i+1,i}^c}\right) + \frac{2g_{bh,i}^{t+1}\left(\Delta L_{sun,i} + \Delta L_{shd,i}\right)}{\Delta z_i} \tag{111b}$$

$$\alpha_{1,3} = -\left(\frac{g_{a,i+\frac{1}{2}}^{t+1}}{\Delta z_{i+1,i}^c}\right) \tag{111c}$$

$$\alpha_{1,7} = -\frac{2g_{bh,i}^{t+1}\Delta L_{sun,i}}{\Delta z_i} \tag{111d}$$

$$\alpha_{1,8} = -\frac{2g_{bh,i}^{t+1}\Delta L_{shd,i}}{\Delta z_i} \tag{111e}$$

$$\beta_1 = \left(\frac{\rho_m}{\Delta t}\right)\theta_i^{t+1} \tag{111f}$$

For the top vertical layer $i = N$, the coefficients $\alpha_{i=1,*}$ remain same as terms in equation 111 same except

$$\alpha_{1,3} = 0 \tag{112a}$$

$$\beta_1 = \left(\frac{\rho_m}{\Delta t}\right)\theta_i^{t+1} + \left(\frac{g^{t+1}_{a,i+\frac{1}{2}}}{\Delta z^c_{i+1,i}}\right)\theta^{t+1}_{ref} \tag{112b}$$

where θ^{n+1}_{ref} is prescribed atmospheric temperature.

For $i = 0$, the energy balance for the soil surface, Rn_0, is given by

$$\begin{aligned} Rn_0 &= c_p(T_0^{n+1} - \theta_1^{n+1})g_{a,0} + \lambda\left\{h_{s0}q_{sat}(T_0^{n+1}) - q_1^{n+1}\right\}g_{s0} + \frac{\kappa_1}{\Delta z_{1/2}}\left(T_0^{n+1} - T_{-1}^n\right) \\ &= c_p(T_0^{n+1} - \theta_1^{n+1})g_{a,0} + \lambda\left\{h_{s0}\left[q_{sat}(T_0^n) + s_0\left(T_0^{n+1} - T_0^n\right)\right] - q_1^{n+1}\right\}g_{s0} \\ &+ \frac{\kappa_1}{\Delta z_{1/2}}\left(T_0^{n+1} - T_{-1}^n\right) \end{aligned} \tag{113}$$

where $\theta_0^{n+1} = T_0^{n+1}$ is the soil surface temperature, T^n_{-1} is the soil temperature of the first soil layer, and $z_{1/2}$ is the distance between the soil surface and centroid of first soil layer. The non-zero coefficients $\alpha_{1,*}$ for $i = 0$ are thus given as

$$\alpha_{1,2} = \left(c_p g_{a,0} + \lambda h_{s0} g_{s0} s_0 + \frac{\kappa_1}{\Delta z_{1/2}}\right) \tag{114a}$$

$$\alpha_{1,3} = -c_p g_{a,0} \tag{114b}$$

$$\alpha_{1,6} = -\lambda g_{s,0} \tag{114c}$$

$$\beta_1 = Rn_0 - \lambda h_{s0}\left[q_{sat}(T_0^n) - s_0 T_0^n\right]g_{s0} + \frac{\kappa_1}{\Delta z_{1/2}}T^n_{-1} \tag{114d}$$

Air vapor pressure equation

The discretized equation 105b at an internal vertical layer (i.e. $0 < i < N$)

$$
\begin{aligned}
\frac{\rho_m}{\Delta t}\left(q_i^{t+1} - q_i^t\right) = &+g_{a,i+\frac{1}{2}}\left(\frac{q_{i+1}^{t+1} - q_i^{t+1}}{z_{i+1}^c - z_i^c}\right) - g_{a,i-\frac{1}{2}}\left(\frac{q_i^{t+1} - q_{i-1}^{t+1}}{z_i^c - z_{i+1}^c}\right)\\
&+ \left[q_{sat,\ell sun,i}^{t+1} - q_i^{t+1}\right]\left(\frac{g_{\ell sun,i}\Delta L_{sun,i}}{\Delta z_i}\right)\\
&+ \left[q_{sat,\ell sha,i}^{t+1} - q_i^{t+1}\right]\left(\frac{g_{\ell sun,i}\Delta L_{sun,i}}{\Delta z_i}\right)\\
&= +g_{a,i+\frac{1}{2}}\left(\frac{q_{i+1}^{t+1} - q_i^{t+1}}{z_{i+1}^c - z_i^c}\right) - g_{a,i-\frac{1}{2}}\left(\frac{q_i^{t+1} - q_{i-1}^{t+1}}{z_i^c - z_{i+1}^c}\right)\\
&+ \left[q_{sat,\ell sun,i}^{t} + s_{sun,i}\left(T_{\ell,sun}^{n+1} - T_{\ell,sun}^{n}\right) - q_i^{t+1}\right]\left(\frac{g_{\ell sun,i}\Delta L_{sun,i}}{\Delta z_i}\right)\\
&+ \left[q_{sat,\ell sha,i}^{t} + s_{sha,i}\left(T_{\ell,sha}^{n+1} - T_{\ell,sha}^{n}\right) - q_i^{t+1}\right]\left(\frac{g_{\ell sun,i}\Delta L_{sun,i}}{\Delta z_i}\right)
\end{aligned}
\tag{115}
$$

328 The non-zero coefficients $\alpha_{i=2,*}$ of equation 109 for $0 < i < N$ are thus given as

$$
\alpha_{2,4} = -\left(\frac{g_{a,i-\frac{1}{2}}^{t+1}}{\Delta z_{i,i-1}^c}\right) \tag{116a}
$$

$$
\alpha_{2,5} = \left(\frac{\rho_m}{\Delta t}\right) + \left(\frac{g_{a,i-\frac{1}{2}}^{t+1}}{\Delta z_{i,i-1}^c}\right) + \left(\frac{g_{a,i+\frac{1}{2}}^{t+1}}{\Delta z_{i+1,i}^c}\right) + \frac{g_{lsun,i}^{t+1}\Delta L_{sun,i} + g_{lshd,i}^{t+1}\Delta L_{shd,i}}{\Delta z_i} \tag{116b}
$$

$$
\alpha_{2,6} = -\left(\frac{g_{a,i+\frac{1}{2}}^{t+1}}{\Delta z_{i+1,i}^c}\right) \tag{116c}
$$

$$
\alpha_{2,7} = -\frac{s_{sun,i}g_{lsun,i}^{t+1}\Delta L_{sun,i}}{\Delta z_i} \tag{116d}
$$

$$
\alpha_{2,8} = -\frac{s_{shd,i}g_{lshd,i}^{t+1}\Delta L_{shd,i}}{\Delta z_i} \tag{116e}
$$

$$
\begin{aligned}
\beta_2 = &\left(\frac{\rho_m}{\Delta t}\right)q_i^{t+1}\\
&+ \frac{\left(q_{sat}\left(T_{lsun,i}^{t+1}\right) - s_{sun,i}T_{lsun}^{t+1}\right)g_{lsun,i}^{t+1}\Delta L_{sun,i}}{\Delta z_i}\\
&+ \frac{\left(q_{sat}\left(T_{lshd,i}^{t+1}\right) - s_{shd,i}T_{lshd}^{t+1}\right)g_{lshd,i}^{t+1}\Delta L_{shd,i}}{\Delta z_i}
\end{aligned}
\tag{116f}
$$

329 For the top vertical layer $i = N$, the coefficients $\alpha_{i=2,*}$ remain same as terms in equa-
330 tion 119 same except

$$\alpha_{2,6} = 0 \tag{117a}$$

$$\begin{aligned}\beta_2 &= \left(\frac{\rho_m}{\Delta t}\right) q_i^{t+1} \\ &+ \frac{\left(q_{sat}(T_{lsun,i}^{t+1}) - s_i T_{lsun}^{t+1}\right) g_{lsun,i}^{t+1} \Delta L_{sun,i}}{\Delta z_i} \\ &+ \frac{\left(q_{sat}(T_{lshd,i}^{t+1}) - s_i T_{lshd}^{t+1}\right) g_{lshd,i}^{t+1} \Delta L_{shd,i}}{\Delta z_i} \\ &+ \left(\frac{g_{a,i+\frac{1}{2}}^{t+1}}{\Delta z_{i+1,i}}\right) q_{ref}^{n+1}\end{aligned} \tag{117b}$$

where q_{ref}^{n+1} is prescribed atmospheric water vapor pressure.

For soil surface layer $i = 0$, the water vapor balance is given by

$$\begin{aligned} q_0^{n+1} &= h_{s0}\left[q_{sat}(T_0^n) + s_0\left(T_0^{n+1} - T_0^n\right)\right] \\ -h_{s0}s_0T_0^{n+1} + q_0^{n+1} &= h_{s0}\left[q_{sat}(T_0^n) - s_0T_0^n\right] \end{aligned} \tag{118}$$

The non-zero coefficients $\alpha_{1,*}$ for $i = 0$ are thus given as

$$\alpha_{2,2} = -h_{s0}s_0 \tag{119a}$$

$$\alpha_{2,5} = 1 \tag{119b}$$

$$\beta_2 = h_{s0}\left[q_{sat}(T_0^n) - s_0T_0^n\right] \tag{119c}$$

Sunlit leave temperature

The discretized equation 105c at an internal vertical layer (i.e. $0 < i < N$) is given by

$$
\begin{aligned}
\frac{c_{\ell,i}}{\Delta t}\left(T^{t+1}_{\ell sun,i} - T^{t}_{\ell sun,i}\right) &= \mathrm{Rn}_{sun} - 2\left(T^{t+1}_{\ell sun,i} - \theta^{t+1}_{i}\right) g_{bh,i} - \lambda\left[q^{t+1}_{sat,\ell sun,i} - q^{t+1}_{i}\right] g_{\ell sun,i} \\
&= \mathrm{Rn}_{sun} - 2\left(T^{t+1}_{\ell sun,i} - \theta^{t+1}_{i}\right) g_{bh,i} \\
&\quad - \lambda\left[q^{t}_{sat,\ell sun,i} + s_{sun,i}\left(T^{n+1}_{\ell,sun} - T^{n}_{\ell,sun}\right) - q^{t+1}_{i}\right] g_{\ell sun,i}
\end{aligned} \tag{120}
$$

336 The non-zero coefficients $\alpha_{i=3,*}$ of equation 109 for $0 < i < N$ are thus given as

$$\alpha_{3,1} = 0 \tag{121a}$$

$$\alpha_{3,2} = -2c_p g^{t+1}_{bh,i} \tag{121b}$$

$$\alpha_{3,3} = 0 \tag{121c}$$

$$\alpha_{3,4} = 0 \tag{121d}$$

$$\alpha_{3,5} = -\lambda g^{t+1}_{lsun,i} \tag{121e}$$

$$\alpha_{3,6} = 0 \tag{121f}$$

$$\alpha_{3,7} = \left(\frac{c_{L,i}}{\Delta t}\right) + 2c_p g^{t+1}_{bh,i} + \lambda s_i g^{t+1}_{lsun,i} \tag{121g}$$

$$\alpha_{3,8} = 0 \tag{121h}$$

$$\beta_3 = Rn^{t+1,0}_{sun} + \left(\frac{c_{L,i}}{\Delta t}\right) T^{t+1}_{lsun,i} - \lambda\left(q_{sat}(T^{t+1}_{lsun,i}) - s_i T^{t+1}_{lsun}\right) g^{t+1}_{lsun,i} \tag{121i}$$

337 **Shaded leave temperature**

338 The discretized equation 105d at an internal vertical layer (i.e. $0 < i < N$) is given by

$$
\begin{aligned}
\frac{c_{\ell,i}}{\Delta t}\left(T^{t+1}_{\ell shd,i} - T^{t}_{\ell shd,i}\right) &= \mathrm{Rn}_{shd} - 2\left(T^{t+1}_{\ell shd,i} - \theta^{t+1}_{i}\right) g_{bh,i} - \lambda\left[q^{t+1}_{sat,\ell shd,i} - q^{t+1}_{i}\right] g_{\ell shd,i} \\
&= \mathrm{Rn}_{shd} - 2\left(T^{t+1}_{\ell shd,i} - \theta^{t+1}_{i}\right) g_{bh,i} \\
&\quad - \lambda\left[q^{t}_{sat,\ell shd,i} + s_{shd,i}\left(T^{n+1}_{\ell,shd} - T^{n}_{\ell,shd}\right) - q^{t+1}_{i}\right] g_{\ell shd,i}
\end{aligned} \tag{122}
$$

339 The non-zero coefficients $\alpha_{i=4,*}$ of equation 109 for $0 < i < N$ are thus given as

$$\alpha_{4,1} = 0 \tag{123a}$$

$$\alpha_{4,2} = -2c_p g_{bh,i}^{t+1} \tag{123b}$$

$$\alpha_{4,3} = 0 \tag{123c}$$

$$\alpha_{4,4} = 0 \tag{123d}$$

$$\alpha_{4,5} = -\lambda g_{lshd,i}^{t+1} \tag{123e}$$

$$\alpha_{4,6} = 0 \tag{123f}$$

$$\alpha_{4,7} = 0 \tag{123g}$$

$$\alpha_{4,8} = \left(\frac{c_{L,i}}{\Delta t}\right) + 2c_p g_{bh,i}^{t+1} + \lambda s_i g_{lshd,i}^{t+1} \tag{123h}$$

$$\beta_4 = Rn_{shd}^{t+1,0} + \left(\frac{c_{L,i}}{\Delta t}\right) T_{lshd,i}^{t+1} - \lambda \left(q_{sat}(T_{lshd,i}^{t+1}) - s_i T_{lshd}^{t+1}\right) g_{lshd,i}^{t+1} \tag{123i}$$

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