

### Steady-state conservation statements for a composite of cells and airspace

In steady state, conservation of molecules requires that the total flux into a representative volume of mesophyll is equal to the flux out – storage is zero. In a volume of mesophyll however, composed of both liquid gas phases, only the total flux, not the individual vapor or liquid fluxes, is conserved (i.e., molecules can jump from one phase to another). Thus, a local change in the liquid flux (due to evaporation or condensation) must be balanced by an equal and opposite change in the vapor flux,

$$0 = \frac{\partial J_{total}}{\partial z} \rightarrow \mathcal{A}_l \frac{\partial J_l}{\partial z} = -\mathcal{A}_v \frac{\partial J_v}{\partial z}. \quad (1.1)$$

Conservation of thermal energy balances conduction in the liquid and vapor phases ( $q_l, q_v$ ), enthalpy transport (i.e., the ‘heat content’ that moves with the molecules) in the liquid and vapor fluxes ( $\bar{H}_l J_l, \bar{H}_v J_v$ ), and the absorbed short wave radiation  $\dot{Q}$ . In steady state,

$$0 = -\mathcal{A}_l \frac{\partial q_l}{\partial z} - \mathcal{A}_v \frac{\partial q_v}{\partial z} - \mathcal{A}_l \bar{H}_l \frac{\partial J_l}{\partial z} - \mathcal{A}_v \bar{H}_v \frac{\partial J_v}{\partial z} + \dot{Q} \quad (1.2)$$

Combining energy conservation (1.2) and molecular conservation (1.1) leads to the introduction of the latent heat of vaporization as the difference in ‘heat content’ between the two phases,  $\bar{\lambda} = \bar{H}_v - \bar{H}_l$ ,

$$0 = -\mathcal{A}_l \frac{\partial q_l}{\partial z} - \mathcal{A}_v \frac{\partial q_v}{\partial z} + \mathcal{A}_l \bar{\lambda} \frac{\partial J_l}{\partial z} + \dot{Q} \quad (1.3)$$

This equation says that in the mesophyll, absorbed short wave radiation can be dissipated by an increase in heat conduction in either phase, or by the change of a liquid flux into the vapor phase. Here we have neglected the convection of enthalpy in the absence of a phase change that accompanies a flux of molecules through a temperature field, as the effect is small relative to conduction and latent transport (Supplemental Text S2).

### Non-dimensional parameters and forms of the governing equations

To gain insight into which process, heat conduction or latent heat transport, is more important, we rescale temperature and water potential in reference to their values at the vascular plane (subscript o) and normalize by their characteristic gradients. We do not yet know what the latter are; their particular form will be defined later to satisfy the

constraint that the derivatives are order one. For a domain of thickness  $L$  in  $z$ , the transformed variables are,

$$Z = \frac{z}{L}, \quad \Theta = \frac{T - T_o}{\Delta T_c}, \quad \Psi = \frac{\psi - \psi_o}{\Delta \psi_c}. \quad (1.4)$$

Normalizing the energy load by either the conductive or latent heat flux in (1.3), and using molecular conservation (1.1), leads to separate (but linked) governing equations for the potential and temperature fields (Supplemental Text S2). With the transformed variables, the water potential field is governed by,

$$0 = - \left( 1 + \frac{\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T}{\mathcal{A}_v \bar{\lambda} c D_v \chi_T} + \frac{\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T}{\mathcal{A}_l \bar{\lambda} k_l} \frac{\chi_\psi}{\chi_T} \right) \frac{\partial^2 \Psi}{\partial Z^2} + \frac{\dot{Q}L^2}{\mathcal{A}_l \bar{\lambda} k_l \Delta \psi_c}. \quad (1.5)$$

For convenience we label the term in brackets,

$$\Pi_\psi \equiv 1 + \frac{\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T}{\mathcal{A}_v \bar{\lambda} c D_v \chi_T} + \frac{\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T}{\mathcal{A}_l \bar{\lambda} k_l} \frac{\chi_\psi}{\chi_T} \quad (1.6)$$

Equation (1.5) says that for a radiation load  $\dot{Q}L$  in mesophyll tissue to be consumed by local evaporation  $\mathcal{A}_l \bar{\lambda} k_l \Delta \psi_c / L$ ,  $\Pi_\psi$  must be equal to one, as the derivative term is order one by construction. The ratios that appear in  $\Pi_\psi$  represent heat conduction over particular forms of latent heat transport, and are analogous to Bowen ratios in ecophysiological (i.e., zero thickness) leaf energy balances (Lambers et al., 1998).  $\Pi_\psi$  can be thought of as describing the tendency of internal leaf tissue toward dissipating a thermal load by internal heat conduction (dominant when  $\Pi_\psi$  is large) versus internal latent heat transport (dominant when it  $\Pi_\psi$  is close to one).  $\Pi_\psi$  is not itself sufficient to determine where evaporation occurs within a leaf, boundary conditions at the leaf surfaces matter, but it plays an important role.

The equation governing the temperature field follows as,

$$0 = \left( 1 + \frac{\mathcal{A}_l \bar{\lambda} k_l}{\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T} \frac{\chi_T}{\chi_\psi} \frac{\mathcal{A}_v c D_v \chi_\psi}{\mathcal{A}_l k_l + \mathcal{A}_v c D_v \chi_\psi} \right) \frac{\partial^2 \Theta}{\partial Z^2} + \frac{\dot{Q}L^2}{(\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T) \Delta T_c}. \quad (1.7)$$

We again define,

$$\Pi_T \equiv 1 + \frac{\mathcal{A}_l \bar{\lambda} k_l}{\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T} \frac{\chi_T}{\chi_\psi} \frac{\mathcal{A}_v c D_v \chi_\psi}{\mathcal{A}_l k_l + \mathcal{A}_v c D_v \chi_\psi}. \quad (1.8)$$

To the extent that the energy load is balanced by thermal conduction,  $\Pi_T$  must be one. However, there is no new information in  $\Pi_T$  regarding the balance of heat conduction versus latent heat transport, as it can be shown that  $\Pi_T^{-1} + \Pi_\psi^{-1} = 1$ . The definitions for the characteristic gradients that make the derivative terms order one can now be found as,

$$\Delta T_c = \frac{\dot{Q}L^2}{\Pi_T(\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T)}, \quad \Delta \psi_c = \frac{\dot{Q}L^2}{\Pi_\psi \mathcal{A}_l \bar{\lambda} k_l}. \quad (1.9)$$

Combining (1.7) through (1.9) reduces the governing equations to,

$$0 = -\frac{\partial^2 \Psi}{\partial Z^2} + 1 \quad (1.10)$$

for the potential field, and similarly

$$0 = \frac{\partial^2 \Theta}{\partial Z^2} + 1 \quad (1.11)$$

for the temperature field.

### Boundary conditions and solutions for a non-transpiring epidermis

For a non-transpiring surface, molecular conservation says that the sum of the vapor and liquid fluxes arriving at the epidermis is equal to zero (modeling leaf temperatures below the ambient dew point, as for example occur during foliar uptake of water from fog, would require modifying this boundary condition). Formally, this condition is stated,

$$(\mathcal{A}_l J_l + \mathcal{A}_v J_v)|_{z=L} = 0. \quad (1.12)$$

Thermal energy conservation requires that the sum of net long wave radiative transfer and conduction across the boundary layer to the environment balance internal conduction and the transport of enthalpy  $\bar{H}$  with the molecular flux from the mesophyll,

$$(\mathcal{A}_l q_l + \mathcal{A}_v q_v + \mathcal{A}_l J_l \bar{H}_l + \mathcal{A}_v J_v \bar{H}_v)|_{z=L} = (q_c + q_r)|_{z=L}. \quad (1.13)$$

Insertion of the expressions for the molecular fluxes (1.2) and (1.5) and re-arrangement of (1.12) and (1.13) yield the required two conditions on potential and temperature at the non-transpiring surface. At the vascular plane boundary, we label the water potential and temperature that exist there ( $z=0$ ) as,

$$\psi(z=0) = \psi_o, \quad T(z=0) = T_o, \quad (1.14)$$

with the understanding that these are among the unknowns to be solved for. For water potential, the non-dimensionalized boundary conditions are then,

$$\frac{\partial \Psi}{\partial Z} \Big|_{z=1} = \frac{(q_c + q_r)}{\dot{Q}L}, \quad \Psi(Z=0) = 0, \quad (1.15)$$

for temperature,

$$\frac{\partial \Theta}{\partial Z} \Big|_{z=1} = -\frac{(q_c + q_r)}{\dot{Q}L}, \quad \Theta(Z=0) = 0. \quad (1.16)$$

The solutions to (1.10) and (1.11) for a domain bounded by the vascular plane and a non-transpiring surface follows from integration and the application of the boundary conditions (1.15) and (1.16). The potential profile is given by,

$$\psi(z) = \psi_o + \frac{\dot{Q}L^2}{\Pi_\psi \bar{\lambda} \mathcal{A}_l k_l} \left[ \frac{z^2}{2L^2} - \frac{z}{L} \right] + \frac{L(q_c + q_r)}{\Pi_\psi \bar{\lambda} \mathcal{A}_l k_l} \frac{z}{L}, \quad (1.17)$$

and the temperature profile follows as,

$$T(z) = T_o - \frac{\dot{Q}L^2}{\Pi_T (\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T)} \left[ \frac{z^2}{2L^2} - \frac{z}{L} \right] - \frac{L(q_c + q_r)}{\Pi_T (\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T)} \frac{z}{L}. \quad (1.18)$$

### Boundary conditions and solutions for a transpiring epidermis

For a domain bounded by a transpiring surface, molecular conservation balances internal transport and transpiration  $E$  at the surface,

$$(\mathcal{A}_l J_l + \mathcal{A}_v J_v) \Big|_{z=L} = E \Big|_{z=L}. \quad (1.19)$$

Conservation of thermal energy similarly has the addition, compared to (1.13), of the flux of enthalpy accompanying transpiration,

$$(\mathcal{A}_l q_l + \mathcal{A}_v q_v + \mathcal{A}_l J_l \bar{H}_l + \mathcal{A}_v J_v \bar{H}_v) \Big|_{z=L} = (E \bar{H}_v + q_c + q_r) \Big|_{z=L}. \quad (1.20)$$

Unlike a standard ecophysiological leaf energy balance analysis (Lambers et al., 1998), a latent heat term does not appear directly as a term in the energy balance at the transpiring surface; rather, it enters as a difference in the enthalpy between the vapor and liquid phases. The non-dimensionalized boundary conditions are found as,

$$\frac{\partial \Psi}{\partial Z} \Big|_{z=1} = \frac{(q_c + q_r)}{\dot{Q}L} - \frac{\bar{\lambda} E (\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T)}{\dot{Q}L \bar{\lambda} \mathcal{A}_v c D_v \chi_T}, \quad \Psi(Z=0) = 0, \quad (1.21)$$

for the potential profile, and for temperature,

$$\frac{\partial \Theta}{\partial Z} \Big|_{z=1} = -\frac{(q_c + q_r)}{\dot{Q}L} - \frac{\bar{\lambda} E \mathcal{A}_l k_l}{\dot{Q}L (\mathcal{A}_l k_l + \mathcal{A}_v c D_v \chi_\psi)}, \quad \Theta(Z=0) = 0. \quad (1.22)$$

The solutions to (1.10) and (1.11) can then be found in dimensional form as,

$$\psi(z) = \psi_o + \frac{\dot{Q}L^2}{\Pi_\psi \bar{\lambda} \mathcal{A}_l k_l} \left[ \frac{z^2}{2L^2} - \frac{z}{L} \right] + \left[ \frac{L(q_c + q_r)}{\Pi_\psi \bar{\lambda} \mathcal{A}_l k_l} - \frac{LE}{\Pi_\psi \bar{\lambda} \mathcal{A}_l k_l} \frac{(\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T)}{\mathcal{A}_v c D_v \chi_T} \right] \frac{z}{L}, \quad (1.23)$$

for the potential profile, and for the temperature profile,

$$T(z) = T_o - \frac{\dot{Q}L^2}{\Pi_T (\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T)} \left[ \frac{z^2}{2L^2} - \frac{z}{L} \right] - \left[ \frac{L(q_c + q_r)}{\Pi_T (\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T)} + \frac{L\bar{\lambda}E}{\Pi_T (\mathcal{A}_l k_l^T + \mathcal{A}_v k_v^T)} \frac{\mathcal{A}_l k_l}{(\mathcal{A}_l k_l + \mathcal{A}_v c D_v \chi_\psi)} \right] \frac{z}{L}. \quad (1.24)$$

For both transpiring and non-transpiring surfaces it will be noted that the solutions contain the surface energy fluxes as measured variables. These fluxes, as well as  $E$ , can also be expressed in terms of their dependence on surface and ambient temperatures, and combined with the solution forms above, to be solved as a system of simultaneous equations.

### Description of surface fluxes

With the subscript  $L$  denoting a quantity evaluated at the surface, the net radiative long wave flux  $q_r$  from a lower leaf surface to its surroundings (assumed to be at uniform temperature  $T_{sur}$ ), depends on their respective emissivities and the temperature difference in a highly non-linear fashion;

$$q_r = \epsilon_{IR} \sigma T_L^4 - a_{IR} \epsilon_{sur} \sigma T_{sur}^4. \quad (1.25)$$

Here the absorptance of the leaf is assumed to be equal to its emissivity as well as the emissivity of the surroundings,  $a_{IR} = \epsilon_{IR} = \epsilon_{sur}$ , and  $\sigma$  is Stephan-Boltzmann constant. For a leaf surface facing the sky, the relevant ambient temperature is that of the well-mixed air near the leaf,

$$q_r = \epsilon_{IR} \sigma T_L^4 - a_{IR} \epsilon_{atm} \sigma T_{air}^4. \quad (1.26)$$

The effective emissivity  $\epsilon_{atm}$  of the sky is defined by an empirical function that depends on the vapor pressure and temperature near the earth's surface, and the fraction of cloud cover  $f_c$  (0 to 1) (Campbell & Norman 1998),

$$\epsilon_{atm} = 0.84 f_c + (1 - 0.84 f_c) 1.72 \left( \frac{p_{atm} \chi_{air}}{10^3 T_{air}} \right)^{1/7}. \quad (1.27)$$

Conduction across the leaf's boundary layer to the well-mixed air, at  $T=T_{air}$ , is described by,

$$q_c = \frac{k_v^T}{\delta} (T_L - T_{air}), \quad (1.28)$$

with the boundary layer thickness  $\delta$  given by an empirical dependence on leaf size and wind speed according to (Nobel 2005),

$$\delta = 4 \times 10^{-3} \sqrt{\frac{\ell_c}{u_w}}. \quad (1.29)$$

Finally, transpiration can be expressed in terms of the temperature and potential at the surface, and the ambient air temperature, as

$$E = \left( \frac{1}{g_s} + \frac{1}{g_{bl}} \right)^{-1} (\chi_L - \chi_{air}), \quad (1.30)$$

with the boundary layer conductance  $g_{bl}$  in series with stomatal conductance  $g_s$  given by,

$$g_{bl} = \frac{c(T_{air})D_v(T_{air})}{\delta}. \quad (1.31)$$

### **Distribution of short wave radiation absorption in the body**

While the exchange of long wave thermal radiation with the environment occurs on the upper and lower epidermal surfaces, we regard the absorption of solar radiation as a process distributed through the body of a leaf (Pieruschka et al. 2010). Our reasoning is as follows. The high absorbance of leaves across the visible range of wavelengths (0.4 to 0.7  $\mu\text{m}$ ) is due to photosynthetic and protective pigments distributed through the thickness. In the range of 0.7 to 1.3  $\mu\text{m}$ , characterized by very low absorbance, the small amount of absorption is likely distributed through the thickness due to scattering. Beyond 1.3  $\mu\text{m}$ , the absorption spectrum of leaves is similar to an equivalent thickness of water, again suggesting a process distributed through the leaf thickness (Knipling 1970).

Nevertheless, the distribution of light absorption within leaves is complex, first increasing with depth in the palisade (as chlorophyll concentrations increase) before decaying exponentially through the rest of the thickness, such that about 80% of the energy absorption occurs in the palisade, and 20% in the spongy mesophyll in spinach leaves (Vogelmann 2002). For the sake of simplicity, we approximate energy absorption

as constant through the thickness within either the palisade or spongy, with the distribution of the total solar radiation  $SR$  absorbed by a leaf following that of spinach,

$$\text{Palisade} \rightarrow \dot{Q}_d L_d = 0.8 SR, \quad (1.32)$$

$$\text{Spongy} \rightarrow \dot{Q}_b L_b = 0.2 SR. \quad (1.33)$$

Here the subscripts  $b, d$  refer to the domains below (abaxial) and above (adaxial) the vascular plane of the leaf. With  $a_{SR}$  the absorptance of a leaf for short wave solar radiation (i.e., PAR and NIR), and  $r$  the albedo or reflectance of the surroundings, net absorbed solar radiation  $SR$  can be estimated from light meter readings of photosynthetic flux density  $PPFD$  by,

$$SR = a_{SR} \left( \frac{PPFD}{0.45} 2.35 \times 10^5 \text{ J mol}^{-1} \right) (1+r) - A_e - F_e, \quad (1.34)$$

where 0.45 represents the fraction of incident solar energy in PAR, and  $2.35 \times 10^5$  is the energy per mole of PAR (Nobel 2005, Campbell 1998). As we are interested in the energy load to be dissipated as heat, we define  $SR$  to be net the energy stored in chemical bonds by photosynthesis  $A_e$  or re-emitted by fluorescence  $F_e$ . The former can be estimated from the assimilation rate [ $\text{mol m}^{-2} \text{s}^{-1}$ ] times the energy stored in chemical bonds per mole of assimilated  $\text{CO}_2$ ,  $479 \text{ kJ mol}^{-1}$  (Nobel 2005), while the latter is typically only  $\sim 1\%$  of absorbed solar energy.

### Global conservation statements and closure

Having defined absorption in the body in terms of  $PPFD$ , and the surface fluxes in terms of  $T_L$  and  $\psi_L$ , for a leaf composed of an abaxial (b) and an adaxial (d) domain we have four equations for the solutions to the temperature and potential profiles, and six unknowns:  $T_{Ld}, \psi_{Ld}, T_o, \psi_o, T_{Lb}, \psi_{Lb}$ . To close the system we turn to two global conservation statements for thermal energy and number of molecules.

First, the total amount of absorbed short solar radiation must equal the sum of the thermal fluxes from both surfaces, or

$$SR = q_{cb} + q_{cd} + q_{rb} + q_{rd} + \bar{\lambda} E_b + \bar{\lambda} E_d. \quad (1.35)$$

Second, the total number of water molecules leaving the leaf as vapor must balance the total number entering as liquid, or

$$E_b + E_d = J_x \equiv \varsigma h_A (\psi_o - \psi_r). \quad (1.36)$$

The transfer coefficient  $h_A$  is the hydraulic conductance of the leaf vasculature, normalized to the leaf area, as estimated from vein cutting experiments, and  $\varsigma$  is a correction factor accounting for the effect of vein spacing on the average potential at the vascular plane (Rockwell et al. 2014b). The reservoir potential  $\psi_r$  represents a known source, such as the parent stem potential, as estimated by a bagged (non-transpiring) leaf. With the environmental variables  $SR, T_{air}, T_{sur}, \psi_r, \chi_{air}$  known, the temperature, potential, and water vapor concentration profiles through the leaf thickness can be solved for as a system of six simultaneous equations with six unknowns.