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Supporting Information for "A model of C_4 photosynthetic acclimation based on least-cost optimality theory suitable for Earth System Model incorporation"

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Introduction

Optimal χ_m Calculation

0.0.1. Linearization of Environmental Effects on the Ratio of Intercellular to Atmospheric CO$_2$ (χ_m)

The least cost hypothesis states that, optimally, plants will minimize the combined costs per unit of photosynthetic assimilation of maintaining capacities for carboxylation and transpiration (Wright et al., 2003). This was applied to the regulation of stomata by Prentice et al. (Prentice et al., 2014) for C_3 plants. Here, we derive an analogous stomatal model for C_4 plants that considers the unit costs of transpiration (E) and carboxylation in the mesophyll via PEPc (Main text equation 2). This results in a derived optimality criterion for χ_m:

$$a\frac{\delta(E/A_n)}{\delta\chi_m} + b\frac{\delta(V_{pmax}/A_n)}{\delta\chi_m} = 0 \tag{1}$$

where a and b are the dimensionless cost factors for E and V_{pmax}, respectively. This differs from the C_3 model as it takes into consideration the cost of carboxylation via PEPc rather than by RuBisCO.

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By using the coordination hypothesis assumption that $A_C = A_L = A_P$ We can define V_{pmax}/A_n by rearranging equation 11 in the main text.

By substituting these definitions into equation 1, and taking the derivatives, χ_{m0} satisfies the following:

$$1.6\frac{aD/c_a}{(1-\chi_m)^2} - b\frac{K_p}{\chi_m^2 c_a} = 0 \tag{4}$$

So that χ_{m0} can be expressed as:

$$\chi_{m0} = \frac{\xi}{\xi + \sqrt{D}}, \text{ where } \xi = \sqrt{\frac{bK_p}{1.6a}} \tag{5}$$

By taking the logit transformation of equation 4, the sensitivity of χ_{m0} to environmental variables can be expressed as:

$$\text{logit}(\chi_{m0}) = \ln\left[\frac{\chi_{m0}}{(1-\chi_{m0})}\right] = \frac{1}{2}\ln b - \frac{1}{2}\ln a + \frac{1}{2}\ln K_p - \frac{1}{2}\ln D - \frac{1}{2}\ln 1.6 \tag{6}$$

The cost factor for PEPc (b) reflects the ratio of mitochonidrial respiration to carboxylation capacity and is taken as a constant. Variables a, K_p, and D are each dependent on environmental conditions. This equation can be rewritten by replacing each of these dependent variables with a coefficient to a change in environmental conditions from standard values (temperature = 298 K, elevation = 0 m), and pooling all constants in a y-intercept term (C).

a reflects the ratio of stem respiration to transpiration capacity and is dependent on temperature through the viscosity of water. As such, it is rewritten as a coefficient that is dependent on temperature ($f_a(T)$). K_p is also dependent on temperature, denoted by the coefficient $f_{K_p}(T)$. $f_D(z)$ reflects the dependency of D elevation caused by decreasing vapor pressure with higher elevations, while the saturation vapor pressure remains constant, causing an increase in vapor pressure deficit.

Replacing equation 6 with these coefficients yields:

$$\text{logit}(\chi_{m0}) = \ln\left[\frac{\chi_{m0}}{(1-\chi_{m0})}\right] = -\frac{1}{2}\ln f_a(T) + \frac{1}{2}\ln f_{K_p}(T) - \frac{1}{2}\ln f_D(z) - \frac{1}{2}\ln D_0 + C \tag{7}$$

where:

$$C = \frac{1}{2}(\ln b_1 - \ln a + \ln K_{\text{p ref}} - \ln 1.6)$$
$$= \frac{1}{2}(\ln \beta + \ln K_{\text{p ref}} - \ln 1.6) \tag{8}$$

where $K_{p(25)}$ is the Michaelis-Menten constant for PEPc at 25 °C, and where:

$$\beta = \frac{b}{a} \tag{9}$$

β replaces the individual terms a and b in this equation for simplicity.

In the following paragraphs we derive each coefficient in equation 7.

Temperature Dependence of a: The viscosity of water (η) varies with temperature, affecting the value of a, as η determines the rate of the cost of E. The temperature dependency of η is approximated by the Vogel equation:

$$\eta = 10^{-3} \exp \left[A + \frac{B}{C + T} \right] \tag{10}$$

Where A, B, and C are -3.719, 580, and -138, respectively, and T is the temperature of interest (Kelvin). By taking the partial derivative of this expression with respect to temperature, the sensitivity of η to temperature is given as:

$$\left(\frac{1}{\eta} \right) \frac{\delta \eta}{\delta T} = \frac{\delta \ln \eta}{\delta T} = \frac{-B}{(C + T)^2} \tag{11}$$

η at T can be determined by the the derivative given in equation 11 and a reference value of η at 25°C (η_{ref}):

$$\eta \approx \eta_{\text{ref}} \exp \left[\frac{-B}{(C + T)^2} \Delta T \right] \tag{12}$$
$$\text{Where, } \Delta T = T - 298$$

Therefore:

$$f_a(T) = \exp \left[\frac{-B}{(C + T)^2} \Delta T \right] \tag{13}$$
$$= \exp[-0.0227\Delta T]$$

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Temperature Dependence of K_p: An Arrhenius relationship can be used to describe the response of any biochemical rate parameter (x) to temperature, given an experimentally derived value for the activation energy (ΔH)

$$\frac{\delta \ln x}{\delta T} = \frac{\Delta H}{R} \frac{1}{T^2} \tag{14}$$

The sensitivity of the PEPc Michealis-Menten constant (K_p) to temperature can be expressed as:

$$f_{K_p}(T) = \exp\left[\frac{\Delta H_p}{R} \frac{1}{T^2} \Delta T\right] \tag{15}$$

where ΔH_p is the activation energy of K_p (36.3 kJ mol^{-1}) (Boyd et al., 2015), yielding the following at T = 298 K:

$$f_{K_p}(T) = \exp[0.0492\Delta T] \tag{16}$$

Elevation Dependency of D: The vapor pressure deficit is calculated as a function of elevation as seen below.

$$D = e_s - e_{a0} \exp[-0.114z] \tag{17}$$

where e_s is the saturation vapor pressure, and e_{a0} is the actual vapor pressure at sea level. From this, the dependency of D on elevation is:

$$\frac{\delta \ln D}{\delta z} = \frac{0.114e_{a0} \exp[-0.114z]}{e_s - e_{a0} \exp[-0.114z]} \tag{18}$$

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In the relevant range of elevations for this study, $\exp[-0.114z]$ can be approximated as being equal to 1, so that the dependency of D on elevation can be simplified to the following:

$$\frac{\delta \ln D}{\delta z} = \frac{0.114 e_{a0}}{D_0}$$
$$= 0.114 \frac{R_0}{1 - R_0} \tag{19}$$

where D_0 is the humidity of air with the same water content at sea level, and R_0 is relative humidity $(= \frac{e_{a0}}{e_s})$. This yields:

$$f_D(z) = \exp\left[0.114 \frac{R_0}{1 - R_0} z\right] \tag{20}$$

When this is evaluated at the standard, $R_0 = 50\%$ it yields the following for the response coefficient:

$$f_D(z) = \exp[0.114z] \tag{21}$$

Linearized Expression for χ_{m0} in Terms of Environmental Conditions: With the derived coefficients, equation 7 can be rewritten as:

$$\begin{aligned} \text{logit}(\chi_0) = \ln\left[\frac{\chi_0}{(1 - \chi_0)}\right] &= -\frac{1}{2}\ln \exp[-0.0227\Delta T] \\ &+ \frac{1}{2}\ln \exp[0.0492\Delta T] - \frac{1}{2}\ln \exp[0.114z] - \frac{1}{2}\ln D_0 \\ &\qquad\qquad + \gamma \end{aligned} \tag{22}$$

Which can be simplified to:

$$\ln\left[\frac{\chi_0}{(1 - \chi_0)}\right] =$$
$$\frac{1}{2}(0.0227 + 0.0492)\Delta T - \frac{1}{2}0.114z - 0.5\ln D_0 + \gamma \tag{23}$$

And further to:

$$\ln\left[\frac{\chi_0}{(1 - \chi_0)}\right] = \frac{1}{2}0.0719\Delta T - \frac{1}{2}0.114z - 0.5\ln D_0 + \gamma \tag{24}$$

Estimating C from Stable Carbon Isotope Data: It is known that plants discriminate between ^{13}C and ^{12}C during assimilation through photosynthesis so that the plant

is depleted in ^{13}C relative to the atmosphere (Lloyd & Farquhar, 1994; G. Farquhar et al., 1989). Total discrimination against $^{13}CO_2$ during assimilation (Δ) is a sum of the discrimination associated with diffusion in the atmosphere and by the PEPc and Rubisco in C$_4$ plants (Lloyd & Farquhar, 1994). A standard equation can be used to calculate χ_m from isotopic discrimination values.

$$\chi = \frac{\Delta - a'}{b' - a'} \tag{25}$$

where a' has a standard value of 4.4 ‰, representing the fractionation against $^{13}CO_2$ in the free air. The same value for a' has been used for C$_3$ plants, as it is not dependent on photosynthetic pathway. Photosynthetic pathway will, however, affect the b' value, as it represents the discrimination by both PEPc and RuBisCO. b' for C$_4$ plants can be taken as (G. D. Farquhar et al., 1989):

$$b' = b_4 + b_3\psi \tag{26}$$

where b_4 is the discrimination by PEPc and is equal to -5.6 ‰ at 25°C (Lloyd & Farquhar, 1994; G. D. Farquhar et al., 1989; Kromdijk et al., 2008), and b_3 is the discrimination by RuBisCO and is equal to 30 ‰ (G. D. Farquhar et al., 1989). ψ is a measure of leakiness and is given as the ratio of CO_2 leakage from the bundle sheath to the rate of V_{pmax}. Here, we assumed a constant value of 0.2 (Kromdijk et al., 2008). The C$_4$ b' value is numerically much smaller than the same term for C$_3$ plants because the effective discrimination from PEPc is much less than that of RuBisCO (G. D. Farquhar et al., 1989).

Using this approach, we calculated χ_m from a worldwide data set of 140 Δ values (Cornwell et al., 2018), yielding stomatal conductance values across a range of environmental conditions. By fitting a linear regression model between the environmental predictors and the

logit transformation of the stomatal conductance values, we obtained a value of approximately 0.254 for the constant C

This yields an updated equation 24:

$$\ln\left[\frac{\chi_0}{(1-\chi_0)}\right] = \frac{1}{2}0.0719\Delta T - \frac{1}{2}0.114z - 0.5\ln(D_0) + 0.254 \qquad (27)$$

Full Expressions for the Optimal Leaf Internal Partial Pressure of CO$_2$: At standard conditions, equation 27 predicts the χ_{m0} as 0.56, which is substantially lower then the χ_0 derived for C$_3$ plants, which has a typical value of 0.77. This indicates that C$_4$ plants are able to achieve the same levels of photosynthesis while keeping the stomata more closed, thereby indicating a greater water use efficiency of C$_4$ plants in comparison to C$_3$ plants. From equation 8, the C value can be used to estimate β as ≈ 166 under standard conditions (Mean Growing Season Temperature = 25 °C, elevation = 0 m, R$_0$ = 50%). Therefore the optimal leaf internal partial pressure of CO$_2$ can be derived from equation 5. as:

$$\chi_m = \frac{\xi}{\xi + \sqrt{D}}, \text{ where } \xi = \sqrt{\frac{\beta K_p}{1.6\eta^*}} \qquad (28)$$

where η^* is the viscosity of water relative to its value at 25 °C ($\eta^* = \eta/\eta_{ref}$), representing the effect of changing viscosity on the value of a.

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