2-D Photosynthesis Model

We model leaf photosynthesis using a two-dimensional porous medium approximation. The model is solved using a finite element method (FEM) using the `steady.2d()` function in the *R* package **rootSolve** version 1.8.2.4 (Soetaert and Herman 2009). Table S1 is a glossary model terms and symbols.

Leaf anatomy

We assume that the leaf is a homogenous 2-D medium. The mesophyll is T_{leaf} thick and the stomata are regularly spaced apart by distance U on both ab- and adaxial surfaces. In this scenario, we assume that the stomata on each surface are precisely offset from each other by distance $U/2$. This minimizes the average distance between any point in the mesophyll and its nearest stomate. Because of the regular spacing, we only need to model the region between a stomate on surface and the next stomate on the other surface (Fig. S1). The rest of the mesophyll will be the same because of symmetry.

Table S1: Glossary of model terms and mathematical symbols.

Name	Symbol	Value	Units	Notes
Whole-leaf light absorption	α	0.8	mol mol^{-1}	assumed
Chlorophyll spatial distribution coefficient	$b_{0,\mathrm{chl}}$	67.5	—	Borsuk and Brodersen (2019); $f_{z,\mathrm{chl}} = b_{0,\mathrm{chl}} + b_{1,\mathrm{chl}}z + b_{2,\mathrm{chl}}z^2$
Chlorophyll spatial distribution coefficient	$b_{1,\mathrm{chl}}$	41.5	—	Borsuk and Brodersen (2019); $f_{z,\mathrm{chl}} = b_{0,\mathrm{chl}} + b_{1,\mathrm{chl}}z + b_{2,\mathrm{chl}}z^2$
Chlorophyll spatial distribution coefficient	$b_{2,\mathrm{chl}}$	-29	—	Borsuk and Brodersen (2019); $f_{z,\mathrm{chl}} = b_{0,\mathrm{chl}} + b_{1,\mathrm{chl}}z + b_{2,\mathrm{chl}}z^2$
Fraction of light absorbed by PSII	β	0.5	mol mol^{-1}	assumed
[CO_2] in intercellular airspace	C_{ias}	—	mol m^{-3}	Equation S1 and Equation S10
[CO_2] in chloroplast stroma	C_{liq}	—	mol m^{-3}	Equation S1
[CO_2] in substomatal cavity	C_{stom}	1.50×10^{-2}	mol m^{-3} leaf	assumed
[CO_2] compensation point	Γ^*	1.35×10^{-3}	mol m^{-3} stroma	Caemmerer (2000)
Diffusivity of [CO_2] in intercellular airspace	D_{c}	1.54×10^{-5}	m^2 s^{-1}	assumed
Effective diffusivity of [CO_2] in intercellular airspace	D_{e}	—	m^2 s^{-1}	Equation S3
Fraction of palisade mesophyll	f_{pal}	0.6	1	$1 = f_{\mathrm{pal}} + f_{\mathrm{spg}}$
Fraction of spongy mesophyll	f_{spg}	0.4	1	$1 = f_{\mathrm{pal}} + f_{\mathrm{spg}}$
Chlorophyll fluoresence profile along leaf depth normalized by total fluoresence	$F_{\mathrm{z,chl}}$	—	1	Borsuk and Brodersen (2019); $f_{z,\mathrm{chl}} = b_{0,\mathrm{chl}} + b_{0,\mathrm{chl}}z + b_{2,\mathrm{chl}}z^2$
Conductance of cell wall, plasmalemma, cytosol, chloroplast envelope, and chloroplast stroma	g_{liq}	2.50×10^{-4}	m^3 m^{-2} stroma s^{-1}	Evans et al. (2009)
PPFD incident on the leaf surface	I_0	1.50×10^{-3}	mol m^{-2} s^{-1}	assumed
Potential photosynthetic e$^-$ transport rate on a leaf area basis	J_∞	—	mol m^{-2} leaf s^{-1}	Equation S9
Maximum photosynthetic e$^-$ transport rate on a leaf area basis	J_{max}	2.75×10^{-4}	mol m^{-2} leaf s^{-1}	assumed

Name	Symbol	Value	Units	Notes
Effective photosynthetic e^- transport rate on a stroma volume basis	j_e	—	mol m^{-3} stroma s^{-1}	Equation S8
Potential photosynthetic e^- transport rate on a stroma volume basis	j_∞	—	mol m^{-3} stroma s^{-1}	see text
Maximum photosynthetic e^- transport rate on a stroma volume basis	j_{max}	—	mol m^{-3} stroma s^{-1}	see text
Catalytic rate of Rubisco	k_c	2.84	m^{-1}	Tholen and Zhu (2011)
Rubisco effective K_m	K_m	1.87×10^{-2}	mol m^{-3}	Caemmerer (2000)
Number of elements in x direction	n_x	100	—	$U = 2n_x t_{elem}$
Number of elements in z direction	n_z	200	—	$T_{leaf} = n_z t_{elem}$
Fraction of intercellular airspace (aka porosity), palisade	φ_{pal}	0.1	m^3 airspace m^{-3} leaf	assumed
Fraction of intercellular airspace (aka porosity), spongy	φ_{spg}	0.3	m^3 airspace m^{-3} leaf	assumed
Quantum yield of PSII e^- transport	ϕ_{PSII}	0.85	mol mol^{-1}	assumed
Volumetric rate of RuBP carboxylation	r_c	—	mol m^{-2} stroma s^{-1}	Equation S5
Volumetric respiration rate	r_d	6.60×10^{-2}	mol m^{-2} stroma s^{-1}	Earles et al. (2017); Tholen and Zhu (2011)
Volumetric rate of photorespiratory CO_2 release	r_p	—	mol m^{-2} stroma s^{-1}	Earles et al. (2017); Equation S4
Leaf surface area-to-mesophyll surface area ratio, palisiade	$S_{m,pal}$	20	m^2 mesophyll m^{-2} leaf	assumed
Leaf surface area-to-mesophyll surface area ratio spongy	$S_{m,spg}$	2	m^2 mesophyll m^{-2} leaf	assumed
Tortuosity of intercellular airspace	τ	1.55	m m^{-1}	Syvertsen et al. (1995)
Thickness of element in both x and z directions	t_{elem}	1.00×10^{-6}	m	$T_{leaf} = n_z t_{elem}$

Name	Symbol	Value	Units	Notes
Leaf thickness	T_{leaf}	—	m	$T_{\text{leaf}} = n_z t_{\text{elem}}$
Interstomatal distance	U	—	m	$U = n_x t_{\text{elem}}$
Stroma volume-to-mesophyll surface area ratio	V_{strom}	1.74×10^{-6}	m^3 stroma m^{-2} mesophyll	Earles et al. (2017); Tholen and Zhu (2011)
Rubisco-limited carboxylation rate	w_{c}	—	mol m^{-2} stroma s^{-1}	Equation S6
RuBP regeneration-limited carboxylation rate	w_{j}	—	mol m^{-2} stroma s^{-1}	Equation S7
Rubisco concentration in stroma	X_{c}	2.5	mol m^{-3} stroma	Tholen and Zhu (2011); Oguchi, Hikosaka, and Hirose (2003)

Solving within-leaf gradients in CO_2 assimilation and concentration

We extended the 1-D FEM of Earles et al. (2017) to solve a set of partial differential equations describing CO_2 diffusion, photosynthesis, and respiration throughout a 2-D leaf geometry. The diffusive flux of CO_2 through ab- and adaxial stoamta, intercellular airspace, and mesophyll cells in the x (length) and z (depth) dimensions is:

$$D_{\mathrm{e}}\nabla^2 C_{\mathrm{ias}} = D_{\mathrm{e}}\left(\frac{\partial^2 C_{\mathrm{ias}}}{\partial x^2} + \frac{\partial^2 C_{\mathrm{ias}}}{\partial z^2}\right) = -f_{\mathrm{liq}} \tag{S1}$$

$$f_{\mathrm{liq}} = r_{\mathrm{d}} + r_{\mathrm{p}} - r_{\mathrm{c}} \tag{S2}$$

where

$$D_{\mathrm{e}} = \frac{\varphi}{\tau} D_{\mathrm{c}} \tag{S3}$$

is the effective diffusivity of CO_2 though a porous medium composed of an intercellular airspace with a porosity (φ; $\mathrm{m^3}$ airspace $\mathrm{m^{-3}}$ leaf) and tortuosity (τ; m $\mathrm{m^{-1}}$). D_{c} is the diffusion coefficient (m $\mathrm{s^{-1}}$) for CO_2 in the intercellular airspace, C_{ias} is the [CO_2] (mol $\mathrm{m^{-3}}$) at horizontal positions x and depth z in the intercellular airspace, f_{liq} is the volumetric rate of CO_2 diffusion from the intercellular airspace into the chloroplast stroma (mol $\mathrm{m^{-3}}$ $\mathrm{s^{-1}}$), r_{c} is the volumetric rate of ribulose 1,5-bisphosphate (RuBP) carboxylation (mol $\mathrm{m^{-3}}$ $\mathrm{s^{-1}}$), r_{d} is the volumetric respiration rate (mol $\mathrm{m^{-3}}$ $\mathrm{s^{-1}}$), and r_{p} is the volumetric photorespiration rate by Rubisco (mol $\mathrm{m^{-3}}$ $\mathrm{s^{-1}}$). Following Earles et al. (2017), r_{d} is assumed constant per stroma surface area (Table S1) and r_{p} is a function of carboxylation (r_{c}) and C_{liq}:

$$r_{\mathrm{p}} = r_{\mathrm{c}}\frac{\Gamma^*}{C_{\mathrm{liq}}} \tag{S4}$$

Carboxylation rate is the minimum of the Rubisco-limited (w_{c}) or RuBP-regeneration limited (w_{j}) carboxylation rate:

$$r_{\mathrm{c}} = \min(w_{\mathrm{c}}, w_{\mathrm{j}}) \tag{S5}$$

where

$$w_{\mathrm{c}} = \frac{k_{\mathrm{c}} X_{\mathrm{c}} C_{\mathrm{liq}}}{K_{\mathrm{m}} + C_{\mathrm{liq}}},\ \text{and} \tag{S6}$$

$$w_{\mathrm{j}} = \frac{C_{\mathrm{liq}} j_{\mathrm{e}}}{4C_{\mathrm{liq}} + 8\Gamma^*}. \tag{S7}$$

k_c is the catalytic rate of Rubisco (m^{-1}) and K_m is effective Michaelis-Menten constant for Rubisco (mol m^{-3}). Following Earles et al. (2017), we assumed the relative concentration of Rubisco follows that of Nishio, Sun, and Vogelmann (1993), but scaled such that the bulk leaf Rubisco concentration integrates to X_c described in Table S1. We estimated a continuous function describing the relative Rubisco profile as a function of leaf depth using a generalized additive model with the `gam()` function in *R* package **mgcv** version 1.9.0 (Wood 2017).

The effective photosynthetic e^- transport rate (j_e) is the minimum of the maximum (j_{max}) and potential (j_∞) photosynthetic e^- transport rates at each position within the mesophyll:

$$j_e = \min(j_{max}, j_\infty) \tag{S8}$$

The local j_{max} follows the same profile as Rubisco as a function of leaf depth and is scaled so that it integrates to J_{max} on a leaf-area basis (Earles et al. 2017). Potential e^- transport is assumed proportional to the local chloroplast concentration so that it integrates to J_∞ on a leaf-area basis (Earles et al. 2017), where:

$$J_\infty = I_0 \alpha \beta \phi_{PSII}. \tag{S9}$$

Potential e^- transport is a product of PPFD incident on the leaf surface (I_0, mol m^{-2} s^{-1}), whole-leaf light absorption (α, mol mol^{-1}), the fraction of light absorbed by PSII (β, mol mol^{-1}), and the quantum yield of PSII e^- transport (ϕ_{PSII}, mol mol^{-1}).

The local chlorophyll concentration (SYMBOL) is a function of leaf depth following Equation XX from Borsuk and Brodersen (2019):

The volumetric rate of CO_2 diffusion from the intercellular airspace into the chloroplast stroma, f_{liq}, is:

$$f_{liq} = \frac{g_{liq}(C_{liq} - C_{ias})}{T_{leaf}/S_m} \tag{S10}$$

where g_{liq} is the CO_2 conductance from the intercellular airspace into the chloroplast stroma (m s^{-1}), C_{liq} (mol m^{-3}) is the [CO_2] in the stroma, and S_m is leaf surface area-to-mesophyll surface area ratio. Noting that g_{liq} is conductance per m^2 of stroma, this means the length scale to divide by should be the inverse of stroma area per unit bulk leaf volume, i.e. $1/[S_c(1/T_{leaf})] = T_{leaf}/S_c$. For simplicity, we assume that the entire mesophyll surface area is lined with chloroplasts, hence $S_m = S_c$.

I calculated assimilation and respiration the same way as Earles et al. (2017) using the standard C$_3$ biochemical model.

The boundary conditions are that the CO_2 concentration in the substomatal cavity is constant at C_{stom}. The fluxes on the left and right sides are 0 because of symmetry.

extra words

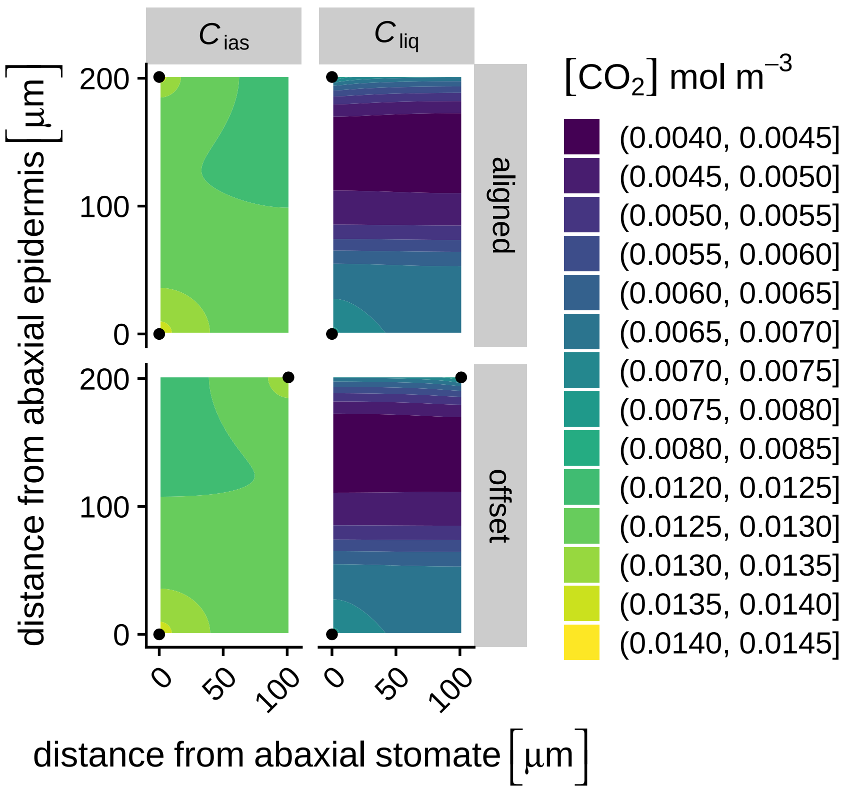

Figure S1: Example profiles of volumetric CO_2 concentrations within otherwise identical amphistomatous leaves that have stomatal positions offset (top row) or aligned (bottom row) based on the 2-D porous medium model. Stomatal positions are indicated by black points at the top and bottom of panels. When stomata are aligned, both ab- and adaxial stomata are position 0 along the x-axis; when stomata are offset, the adaxial stomate is positioned $U/2$ distance away. In this example, variables are set as: $I_0 = 1000$ μmol m^{-2} s^{-1}; $\varphi_{\text{pal}} = 0.2$ m^3 airspace m^{-3} leaf; $T_{\text{leaf}} = 200$ μm; $U = 200$ μm. All other parameter values are described in Table S1. C_{ias} = [CO_2] in intercellular airspace; C_{liq} = [CO_2] in chloroplast stroma; I_0 = PPFD incident on the leaf surface; φ_{pal} = Fraction of intercellular airspace (aka porosity), palisade; T_{leaf} = Leaf thickness; U = Interstomatal distance.

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