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 1: Table 1: glossary of model terms and mathematical symbols.

Name	Symbol	Value	Units	Notes
Whole-leaf light absorption	α	0.8	mol mol^{-1}$|assumed||Chlorophyllspatialdistributioncoefficie$	67.5
Chlorophyll spatial distribution coefficient	$b_{1,chl}$	41.5	NA	Borsuk and Brodersen (2019); $f_{z,\text{chl}} = b_{0,chl} + b_{0,chl}z + b_{2,chl}z^2$
Chlorophyll spatial distribution coefficient	$b_{2,chl}$	-29	NA	Borsuk and Brodersen (2019); $f_{z,\text{chl}} = b_{0,chl} + b_{0,chl}z + b_{2,chl}z^2$
Fraction of light absorbed by PSII	β	0.5	mol mol^{-1}$|assumed||[CO2]inintercellularairspace|Cias	NA
[CO_2] in chloroplast stroma	C_{liq}	NA	mol m^{-3}	equation Equation 5
[CO_2] in substomatal cavity	C_{stom}	1.50×10^{-2}	mol m^{-3} leaf	assumed

Name	Symbol	Value	Units	Notes
$[CO_2]$ 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	NA	m^2 s^{-1}	equation Equation 3
Fraction of palisade mesophyll	f_{pal}	0.6	1	$1 = f_{pal} + f_{spg}$
Fraction of spongy mesophyll	f_{spg}	0.4	1	$1 = f_{pal} + f_{spg}$
Chlorophyll fluoresence profile along leaf depth normalized by total fluoresence	$F_{z,chl}$	NA	1	Borsuk and Brodersen (2019); $f_{z,chl} = b_{0,chl} + b_{0,chl}z + b_{2,chl}z^2 \| \| Conductance of cell wall, plasmalemm$
PPFD incident on the leaf surface	I_0	1.50×10^{-3}	mol m^{-2} s^{-1}	assumed
Maximum photosynthetic e^- transport rate on a leaf area basis	J_{max}	2.75×10^{-4}	mol m^{-2} leaf s^{-1}	assumed
Maximum photosynthetic e^- transport rate on a stroma volume basis	j_{max}	NA	mol m^{-3} stroma s^{-1}	equation not listed yet
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	NA	$U = 2n_x t_{elem}$
Number of elements in z direction	n_z	200	NA	$T_{leaf} = n_z t_{elem}$
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 electron transport	φ_{PSII}	0.85	mol mol^{-1}	assumed
Volumetric rate of RuBP carboxylation	r_c	NA	mol m^{-2} stroma s^{-1}	equation not listed yet
Volumetric respiration rate	r_d	6.60×10^{-2}	mol m^{-2} stroma s^{-1}	Earles et al. (2017); Tholen and Zhu (2011)

Name	Symbol	Value	Units	Notes
Volumetric rate of photorespiratory CO_2 release	r_{p}	NA	mol m^{-2} stroma s^{-1}	equation not listed yet
Leaf surface area-to-mesophyll surface area ratio, palisiade	$S_{\mathrm{m,pal}}$	20	m^2 mesophyll m^{-2} leaf	assumed
Leaf surface area-to-mesophyll surface area ratio spongy	$S_{\mathrm{m,spg}}$	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	$T_{\mathrm{leaf}} = n_z t_{\mathrm{elem}}$
Leaf thickness	T_{leaf}	NA	m	$T_{\mathrm{leaf}} = n_z t_{\mathrm{elem}}$
Interstomatal distance	U	NA	m	$U = n_x t_{\mathrm{elem}}$
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}	NA	mol m^{-2} stroma s^{-1}	equation not listed yet
RuBP regeneration-limited carboxylation rate	w_{j}	NA	mol m^{-2} stroma s^{-1}	equation not listed yet
Rubisco concentration in stroma	X_{c}	2.5	mol m^{-3} stroma	Tholen and Zhu (2011); Oguchi, Hikosaka, and Hirose (2003)

Solving within 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 was described by:

$$D_{\mathrm{e}} \frac{\partial^2 C_{\mathrm{ias}}}{\partial x^2} = -f_{\mathrm{liq}} \tag{1}$$

$$f_{\mathrm{liq}} = r_{\mathrm{d}} + r_{\mathrm{d}} - r_{\mathrm{c}} \tag{2}$$

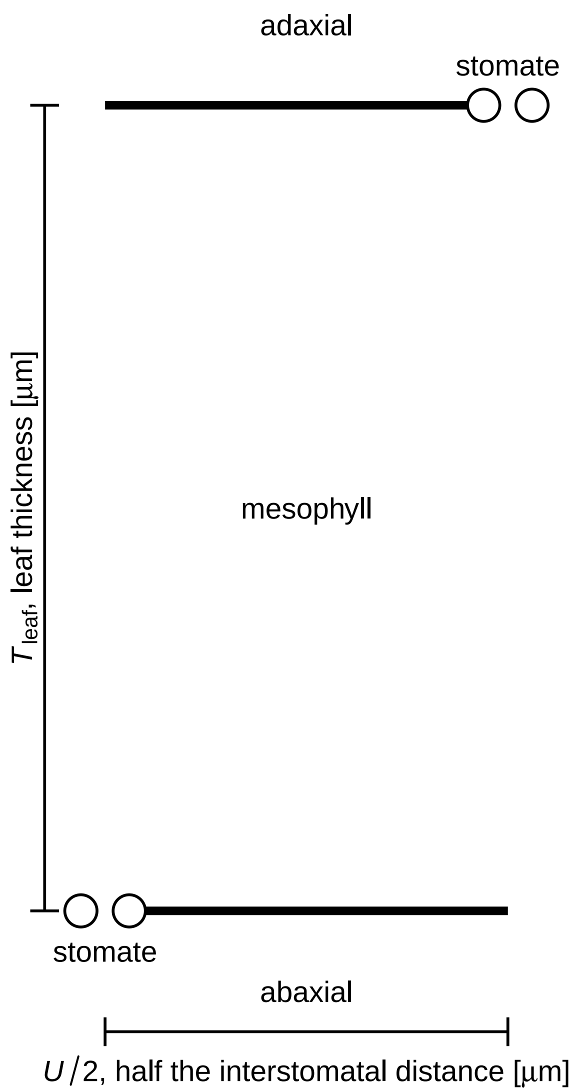

Figure 1: Example leaf anatomy analyzed by the 2-D FEM.

where

$$D_{\mathrm{e}} = \frac{\phi}{\tau} D_{\mathrm{c}} \tag{3}$$

is the effective diffusivity of CO_2 though a porous medium composed of an intercellular airspace with a porosity (ϕ; m^3 m^{-3}) and tortuosity (τ; m m^{-1}). D_{c} is the diffusion coefficient (m s^{-1}) for CO_2 in the intercellular airspace, C_{ias} is the [CO_2] (mol m^{-3}) at 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 m^{-3} s^{-1}), r_{c} is the volumetric rate of ribulose 1,5-bisphosphate (RuBP) carboxylation (mol m^{-3} s^{-1}), r_{d} is the volumetric respiration rate (mol m^{-3} s^{-1}), and r_{p} is the volumetric photorespiration rate by Rubisco (mol m^{-3} s^{-1}).

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

$$f_{\mathrm{liq}} = \frac{g_{\mathrm{liq}}(C_{\mathrm{liq}} - C_{\mathrm{ias}})}{l_z} \tag{4}$$

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 l_z is the finite element length through which diffusion occurs (m)." (n.b. l_z is the same as t_{elem} in my Table 1)

In the 2-D model, we extend the flux equation to x (length) and z (depth) dimensions:

$$D_{\mathrm{e}} \nabla^2 C_{\mathrm{ias}} = D_{\mathrm{e}} \left(\frac{\partial^2 C_{\mathrm{ias}}}{\partial x^2} + \frac{\partial^2 C_{\mathrm{ias}}}{\partial z^2} \right) = -f_{\mathrm{liq}} \tag{5}$$

As I worked through Earles et al. (2017) model, it did not seem like dividing g_{liq} by l_z in equation Equation 4 made sense. The FEM is a discretization of a continuous model. Intuitively, it does make sense why a coarser grid (greater l_z) would lead to a larger [CO_2] drawdown for a given assimilation rate. Noting that g_{liq} is conductance per m^2 of stroma, this means the length scale to divide by should be 1/(stroma area per unit bulk leaf volume). This is equivalent to 1/[(stroma area per leaf area)x(leaf area per bulk leaf volume)] = 1/[Sc x (1/Tleaf)] = Tleaf/Sc (for now I am assuming Sm = Sc, but we can correct this later). Our equation is therefore:

$$f_{\mathrm{liq}} = \frac{g_{\mathrm{liq}}(C_{\mathrm{liq}} - C_{\mathrm{ias}})}{T_{\mathrm{leaf}}/S_{\mathrm{m}}} \tag{6}$$

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.

R code

I've copied the *R* code to set up the model and solve it if you want to copy and paste on your own machine. I annotated the *R* code you would need to run the model and include an example result.

```r
# Variables
vars1 = read_rds("objects/model_var.rds") |>
  left_join(rename(parms, Variable = symbol), by = join_by(Variable))

vars2 = ph2d_offset$parms[pull(vars1, r)] |>
  as_tibble() |>
  pivot_longer(everything(), names_to = "r") |>
  full_join(vars1, by = join_by(r)) |>
  mutate(
    # convert from model unit to print unit
    value1 = case_when(
      r == "I_0" ~ value * 1e6,
      r == "phi_pal" ~ value,
      r == "T_leaf" ~ value * 1e6 - 1,
      r == "U" ~ 2 * (value * 1e6 - 1)
    )
  )

vars3 = vars2 |>
  transmute(
    s = glue("{var} = {value1}$ {Units}", var = str_remove(Variable, "\\$$"))
  ) |>
  pull(s) |>
  str_c(collapse = "; ")

# Guide to symbols
symbols = parms |>
  filter(r %in% c("C_ias", "C_liq", "I_0", "phi_pal", "T_leaf", "U")) |>
  transmute(s = glue("{symbol} = {name}")) |>
  pull(s) |>
  str_c(collapse = "; ")
```

extra words

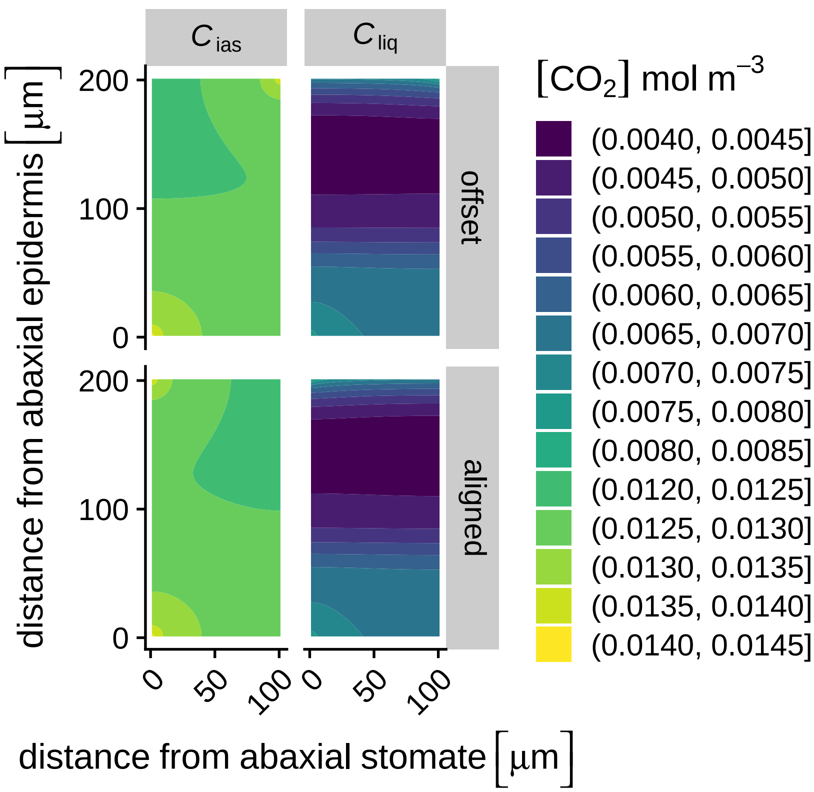

Figure 2: Example profiles of volumetric CO_2 concentrations within otherwise identical amphistomatous leaves that have stomatal positions offset (top row) or aligned (bottom row) based on the 2-D porous medium model. When stomata are aligned, both ab- and adaxial stomata are position 0 along the x-axis; 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}; $\varphi_{pal} = 0.2$ m^3 airspace m^{-3} leaf; $T_{leaf} = 200$ 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.

References

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