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) in the *R* package **deSolve** (Soetaert, Petzoldt, and Setzer 2010). Table 1 is a glossary model terms and symbols. Here we describe the model and associated *R* code.

## Leaf anatomy

We assume that the leaf is a homogenous 2-D medium. In the final version, we will incorporate differences in spongy and palisade porosity, gradients in light absorption, electron transport capacity, and Rubisco concentration. The mesophyll is thick and the stomata are regularly spaced apart by distance 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 . 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. 1). The rest of the mesophyll will be the same because of symmetry.

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

Table 1: glossary of model terms and mathematical symbols.

| Name | Symbol | Value | Units | Notes |
| --- | --- | --- | --- | --- |
| [CO] in intercellular airspace |  |  | mol m | equations [Equation 5](#eq-2d_pm_flux) and [Equation 6](#eq-fliq2) |
| [CO] in chloroplast stroma |  |  | mol m | equation [Equation 5](#eq-2d_pm_flux) |
| [CO] in substomatal cavity |  |  | mol m leaf | assumed |
| [CO] compensation point |  |  | mol m stroma | Caemmerer (2000) |
| Diffusivity of [CO] in intercellular airspace |  |  | m s | assumed |
| Effective diffusivity of [CO] in intercellular airspace |  |  | m s | equation [Equation 3](#eq-De) |
| Conductance of cell wall, plasmalemma, cytosol, chloroplast envelope, and chloroplast stroma |  |  | m m stroma s | Evans et al. (2009) |
| Maximum photosynthetic e transport rate on a leaf area basis |  |  | mol m leaf s | assumed |
| Maximum photosynthetic e transport rate on a stroma volume basis |  |  | mol m stroma s | equation not listed yet |
| Catalytic rate of Rubisco |  |  | m | Tholen and Zhu (2011) |
| Rubisco effective |  |  | mol m | Caemmerer (2000) |
| Number of elements in direction |  |  | NA |  |
| Number of elements in direction |  |  | NA |  |
| Fraction of intercellular airspace (aka porosity) |  |  | m airspace m leaf | assumed |
| Volumetric rate of RuBP carboxylation |  |  | mol m stroma s | equation not listed yet |
| Volumetric respiration rate |  |  | mol m stroma s | Earles et al. (2017); Tholen and Zhu (2011) |
| Volumetric rate of photorespiratory CO release |  |  | mol m stroma s | equation not listed yet |
| Leaf surface area-to-mesophyll surface area ratio |  |  | m mesophyll m leaf | assumed |
| Tortuosity of intercellular airspace |  |  | m m | Syvertsen et al. (1995) |
| Thickness of element in both and directions |  |  | m |  |
| Leaf thickness |  |  | m |  |
| Stroma volume-to-mesophyll surface area ratio |  |  | m stroma m mesophyll | Earles et al. (2017); Tholen and Zhu (2011) |
| Rubisco-limited carboxylation rate |  |  | mol m stroma s | equation not listed yet |
| RuBP regeneration-limited carboxylation rate |  |  | mol m stroma s | equation not listed yet |
| Rubisco concentration in stroma |  |  | mol m stroma | Tholen and Zhu (2011); Oguchi, Hikosaka, and Hirose (2003) |

## Solution

Below I have copied the section from Earles et al. (2017) (pg. 1094) on which I based my model. After that, I’ll explain my modification for 2-D. I also think Earles et al. (2017) made one error that I will describe below.

“We developed a FEM to solve a set of partial differential equations that describe CO diffusion, photosynthesis, and respiration throughout the 1-D leaf geometry. The partial differential equations were solved for steady state using the R library **deSolve** (Soetaert, Petzoldt, and Setzer 2010). Specifically, the diffusive flux of CO through the stomatal boundaries, intercellular airspace, and mesophyll cells was described by:

where

is the effective diffusivity of a porous medium composed of a porous intercellular airspace with a given porosity (; m m) and tortuosity (; m m), ] is the diffusion coefficient (m s) for CO in the intercellular airspace, is the [CO] (mol m) at a depth in the intercellular airspace, is the volumetric rate of CO diffusion from the intercellular airspace into the chloroplast stroma (mol m s), is the volumetric rate of ribulose 1,5-bisphosphate (RuBP) carboxylation (mol m s), is the volumetric respiration rate (mol m s), and is the volumetric photorespiration rate by Rubisco (mol m s).

The volumetric rate of CO diffusion from the intercellular airspace into the chloroplast stroma, , is defined as:

where is the CO conductance from the intercellular airspace into the chloroplast stroma (m s), (mol m) is the [CO] in the stroma, and is the finite element length through which diffusion occurs (m).” (n.b.  is the same as in my Table 1)

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

As I worked through Earles et al. (2017) model, it did not seem like dividing by in equation [Equation 4](#eq-fliq1) made sense. The FEM is a discretization of a continuous model. Intuitively, it does make sense why a coarser grid (greater ) would lead to a larger [CO] drawdown for a given assimilation rate. Noting that is conductance per m of stroma, I think the correct way is to divide by , which gives the mesophyll surface area per stroma volume available for liquid-phase diffusion. Here I assume that the chloroplasts line the entire inner wall of the mesophyll, so 1 [m] mesophyll = 1 [m] stroma, but this could be modified to the correct value. My equation is therefore:

Here’s how I work out the units for equation [Equation 6](#eq-fliq2).

This still doesn’t seem quite right to me because it seems like the change in airspace concentration should be affected by the porosity since a smaller volume of air will experience a greater drop in concentration for the same amount of assimilation, but maybe I am thinking about this incorrectly.

Coincidentally, this had little effect on Earles et al. (2017) model because their element size was m, which is quantitatively similar to m. However, when you change the element size on their model, the solution is quite different; when you change the element size on my model, the solution is only slightly affected but the discretization is an approximation of the true solution.

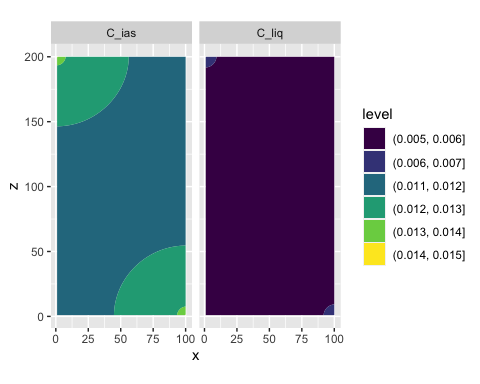
I calculated assimilation and respiration the same way as Earles et al. (2017) using the standard C$\_3$ biochemical model.

The boundary conditions are that the CO concentration in the substomatal cavity is constant at . 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.

library(dplyr)  
library(ggforce)  
library(ggplot2)  
library(magrittr)  
library(readr)  
library(rootSolve)  
library(tidyr)  
  
source("../r/photo\_2d\_pm.R")  
  
# Define function for 2D FEM  
photo\_2d\_pm = function(t, Y, parms) {  
  
 # Arguments:  
 # \* t, time step used by steady.2d() to find steady-state solution  
 # \* Y, vector of length 2 \* n\_x \* n\_z. The first half are the elements  
 # corresponding to C\_ias[i,j]; the second half are correspoding elements for  
 # C\_liq[i,j].  
 # \* parms, list of model parameters. Use `get\_2d\_pm\_default\_parms()` for  
 # default parameter values.  
  
 # Set up:  
 # The leaf is divided to an area n\_x elements wide, n\_z units deep  
 n = parms[["n\_z"]] \* parms[["n\_x"]]  
  
 # Create empty matrices for computation  
 C\_ias = matrix(nrow = parms[["n\_z"]], ncol = parms[["n\_x"]],  
 data = Y[1:n])  
 C\_liq = matrix(nrow = parms[["n\_z"]], ncol = parms[["n\_x"]],  
 data = Y[(n + 1):(2 \* n)])  
 dC\_ias = dC\_liq = numeric(length = n) # empty vectors  
  
 # FLUX ----  
 D\_e = parms[["D\_c"]] \* parms[["phi"]] / parms[["tau"]]  
  
 # Boundary conditions  
 bound\_bottom = C\_ias[1,]  
 bound\_top = C\_ias[parms[["n\_z"]],]  
 bound\_left = C\_ias[,1]  
 bound\_right = C\_ias[, parms[["n\_x"]]]  
 bound\_top[1] = parms[["C\_stom"]]  
 bound\_bottom[parms[["n\_x"]]] = parms[["C\_stom"]]  
 # bound\_bottom[1] = parms[["C\_stom"]]  
  
 # diffusion in Z-direction; boundaries=imposed concentration  
 Flux = -D\_e / parms[["t\_elem"]] \* rbind(  
 C\_ias[1, ] - bound\_bottom,  
 (C\_ias[2:parms[["n\_z"]], ] - C\_ias[1:(parms[["n\_z"]] - 1), ]),  
 bound\_top - C\_ias[parms[["n\_z"]], ]  
 )  
 dC\_ias = dC\_ias -  
 (Flux[2:(parms[["n\_z"]] + 1), ] - Flux[1:parms[["n\_z"]], ]) / parms[["t\_elem"]]  
  
 # diffusion in X-direction  
 Flux = -D\_e / parms[["t\_elem"]] \* cbind(  
 C\_ias[, 1] - bound\_left,  
 (C\_ias[, 2:parms[["n\_x"]]] - C\_ias[, 1:(parms[["n\_x"]] - 1)]),  
 bound\_right - C\_ias[, parms[["n\_x"]]]  
 )  
 dC\_ias = dC\_ias -  
 (Flux[, 2:(parms[["n\_x"]] + 1)] - Flux[, 1:parms[["n\_x"]]]) /  
 parms[["t\_elem"]]  
  
 dC\_ias = dC\_ias + parms[["g\_liq"]] \* (C\_liq - C\_ias) /  
 (parms[["T\_leaf"]] / parms[["S\_m"]])  
  
 # CARBOXYLATION AND RESPIRATION ----  
 # Calculate volumetric j\_max from area-based J\_max. Here, I assume a single  
 # j\_max for every part of the leaf, but in the final model I will have a  
 # gradient of j\_max following Earles et al. (2017).  
 j\_max = parms[["J\_max"]] / (parms[["S\_m"]] \* parms[["V\_strom"]])  
  
 # Carboxylation (n.b. Rubisco concentration is assumed constant throughout  
 # the leaf, but in the final model I will have a garudent of X\_c following  
 # Earles et al. (2017))  
 w\_c = (parms[["k\_c"]] \* parms[["X\_c"]] \* C\_liq) / (parms[["K\_m"]] + C\_liq)  
 w\_j = C\_liq \* j\_max / (4 \* C\_liq + 8 \* parms[["gamma\_star"]])  
 r\_c = pmin(w\_c, w\_j)  
 r\_d = parms[["r\_d"]]  
 r\_p = r\_c \* parms[["gamma\_star"]] / C\_liq  
  
 dC\_liq = dC\_liq +  
 parms[["g\_liq"]] \* (C\_ias - C\_liq) / (parms[["T\_leaf"]] / parms[["S\_m"]]) +  
 (-r\_c + r\_p + r\_d) \* (parms[["S\_m"]] / parms[["T\_leaf"]]) \* parms[["V\_strom"]]  
  
 return(list(c(dC\_ias, dC\_liq)))  
  
}  
  
# Model parameters  
parms = get\_2d\_pm\_default\_parms() |>  
 derive\_2d\_pm\_parms()  
  
# Initial values  
C\_ias\_mat = matrix(nrow = parms[["n\_z"]], ncol = parms[["n\_x"]], parms[["C\_stom"]])  
C\_liq\_mat = matrix(nrow = parms[["n\_z"]], ncol = parms[["n\_x"]], parms[["C\_stom"]])  
  
# Solve for C\_ias and C\_liq  
soln = steady.2D(c(C\_ias\_mat, C\_liq\_mat), func = photo\_2d\_pm, parms = parms,  
 pos = FALSE, dimens = c(parms[["n\_z"]], parms[["n\_x"]]),  
 nspec = 2, lrw = 1e8, atol = 1e-10, rtol = 1e-10, ctol = 1e-10)  
  
# Plot results  
df\_C = expand.grid(  
 z = seq\_len(parms[["n\_z"]]),  
 x = seq\_len(parms[["n\_x"]]),  
 name = c("C\_ias", "C\_liq")  
) |>  
 mutate(value = soln$y)  
  
ggplot(df\_C, aes(x, z, z = value)) +  
 facet\_grid(~ name) +  
 geom\_contour\_filled() +  
 coord\_equal()



# Calculate area-based net photosynthesis  
C\_liq = df\_C |>  
 filter(name == "C\_liq") |>  
 pull(value)  
  
j\_max = parms[["J\_max"]] / (parms[["S\_m"]] \* parms[["V\_strom"]])  
  
w\_c = (parms[["k\_c"]] \* parms[["X\_c"]] \* C\_liq) / (parms[["K\_m"]] + C\_liq)  
w\_j = C\_liq \* j\_max / (4 \* C\_liq + 8 \* parms[["gamma\_star"]])  
r\_c = pmin(w\_c, w\_j)  
r\_d = parms[["r\_d"]]  
r\_p = r\_c \* parms[["gamma\_star"]] / C\_liq  
  
T\_leaf = parms[["n\_z"]] \* parms[["t\_elem"]]  
a\_n = (r\_c - r\_p - r\_d) \* (parms[["S\_m"]] \* 1 / T\_leaf) \* parms[["V\_strom"]]  
  
# 1 m^2 of 200 um thick leaf is 2e-04 m^3  
mean(a\_n) \* T\_leaf \* 1e6

[1] 32.38424

## References

Caemmerer, Susanne von. 2000. *Biochemical Models of Leaf Photosynthesis*. Techniques in Plant Science 2. Collingwood: CSIRO.

Earles, J. Mason, Guillaume Théroux-Rancourt, Matthew E. Gilbert, Andrew J. McElrone, and Craig R. Brodersen. 2017. “Excess Diffuse Light Absorption in Upper Mesophyll Limits CO Drawdown and Depresses Photosynthesis.” *Plant Physiology* 174 (2): 1082–96. <https://doi.org/10.1104/pp.17.00223>.

Evans, J. R., R. Kaldenhoff, B. Genty, and I. Terashima. 2009. “Resistances Along the CO Diffusion Pathway Inside Leaves.” *Journal of Experimental Botany* 60 (8): 2235–48. <https://doi.org/10.1093/jxb/erp117>.

Oguchi, R., K. Hikosaka, and T. Hirose. 2003. “Does the Photosynthetic Light-Acclimation Need Change in Leaf Anatomy?: Chloroplast Volume Change in Photosynthetic Light-Acclimation.” *Plant, Cell & Environment* 26 (4): 505–12. <https://doi.org/10.1046/j.1365-3040.2003.00981.x>.

Soetaert, Karline, Thomas Petzoldt, and R. Woodrow Setzer. 2010. “Solving Differential Equations in *r* : Package **deSolve**.” *Journal of Statistical Software* 33 (9). <https://doi.org/10.18637/jss.v033.i09>.

Syvertsen, J. P., J. Lloyd, C. McConchie, P. E. Kriedemann, and G. D. Farquhar. 1995. “On the Relationship Between Leaf Anatomy and CO2 Diffusion Through the Mesophyll of Hypostomatous Leaves.” *Plant, Cell and Environment* 18 (2): 149–57. <https://doi.org/10.1111/j.1365-3040.1995.tb00348.x>.

Tholen, D., and X.-G. Zhu. 2011. “The Mechanistic Basis of Internal Conductance: A Theoretical Analysis of Mesophyll Cell Photosynthesis and CO Diffusion.” *Plant Physiology* 156 (1): 90–105. <https://doi.org/10.1104/pp.111.172346>.