An Optimality Approach of the Leaf Stomatal Conductance

Team 11: Rui Gao[a], Sahil Desai[a], Murali Thimma Selvan Babu[b]

[a]*Robert Fredrick Smith School of Chemical and Biomolecular Engineering, Cornell University;*
[b]*The School of Operations Research and Information Engineering, Cornell University, Ithaca, New York 14850*

Abstract: To successfully model the water transport in plants, the stomatal conductance of leaves is a key parameter, which is directly related to water transpiration and carbon assimilation. Current approaches to explain the stomatal dynamics rely mainly on biophysical models that are mathematically complex with many assumptions on parameters and cannot demonstrate the full range of stomatal response accurately. In this work, we propose a novel way to perform optimization within a mechanistic framework. Our objective function integrates the carbon assimilation and water transpiration into one cost function. With the optimized parameters, we will perform a stability analysis to validate the transient mechanistic model. By combining the mechanistic and optimization approaches, we aim to bring a better understanding to the stomatal dynamics in response to environmental stimuli.

1. Introduction

Plants live gracefully and cleverly, with complex control system not yet accomplished by human technologies. They act as the interface connecting soil and atmosphere and rely on water to remain hydrated. This concept of water transport through a soil-plant-atmosphere continuum (SPAC)[1] can be traced back to 1948 by Van den Honert[2] and the central part of it, the cohesion-tension theory goes back to Boehm, Askenasy, Dixon and Joly from the 1890's[3]. Figure 1 exhibits one physiological model incorporating the SPAC concept that was previously devised by the Stroock group. The model utilizes a circuit analogy with evapotranspiration (ET) as the current source. Under stressed conditions, water flow is driven across successive compartments of the continuum such that it either evaporates from the soil or transpires through the leaves, where the stomatal conductance is one of the most important factors affecting the transpiration[4,5]. Understanding this drought response is central for improving water management, which has called urgent attention in recent years with the increasing frequency and severity of extreme weather conditions.

The survival of plants also depends on maintaining an adequate internal water status as this status defines their growth, yield, quality and susceptibility to disease[6,7]. Successful model predictions of the plant water status not only bring breakthrough to the studies of ecology and physiology but also help enhancing irrigation scheduling in agriculture which, as the single largest consumer of water, accounts for approximately 70% of all human uses[8].

The stomata are crucial in the physiological balance of higher land plants. In some perspectives, they are like valves but performing the task of opening and closing at a much higher frequency. The stomata need to allow sufficient carbon assimilation while preventing excessive water loss. They are regulated with both positive feedforward from the photosynthetic rate and negative feedback from the water potential in the leaf[3]. Despite of this crucial role, fundamental questions such as the mechanics of the guard cell motion still remain unknown. There is no unified answer to what a plant does to control its stomata and whether this control is optimal. Various mechanisms have been proposed in the past to rationalize the stomatal dynamics observed during experiments such as the temporal oscillations associated
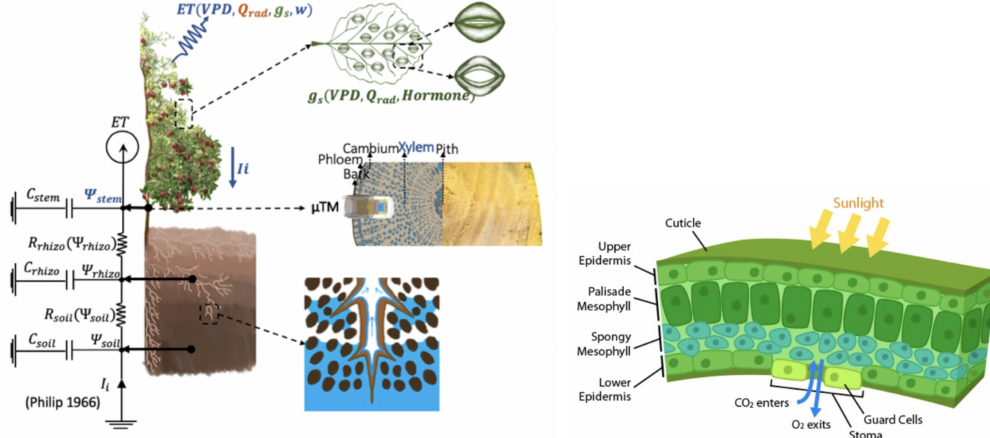
Figure 1: (a) Diagram of a three-compartment SPAC model (Courtesy of Siyu Zhu) where the soil, root (labeled as rhizo, the abbreviation of rhizosphere) and trunk (labeled as stem) are represented by capacitors and resistors. (b) Cross section of the stomatal system (Courtesy of Arizona State University), which controls the carbon dioxide (CO_2) influx from the atmosphere and the water vapor outflux from the leaf.

with stomatal opening, first mentioned by Cowan[9] in 1972. However, none is capable of explaining the full range of observed behaviors while using biologically rational parameters.

In this project, we propose to incorporate constrained optimization into the traditional mechanistic approach of modelling stomatal conductance. With this bridge, we aim to further clarify the roles played by the components of the stomata. For instance, by computing the theoretically optimal pattern of the stomatal conductance, we can compare this pattern to observations and therefore validate the proposed mechanism. Although stomata are important in drought studies which involves a prolonged period, the stomata start to respond in less than 10 minutes. Hence, as a starting point, we will focus on the short-term dynamics and rationalize how stomata can instantaneously respond.

2. Background

As overviewed in *Introduction*, the carbon gain and water loss in a leaf are regulated by stomata. The diffusive rate of water vapor in air is greater than that of carbon dioxide in air. Hence, when the stomata open to assimilate carbon dioxide, the amount of water lost is much greater than the amount of carbon dioxide gained. This trade-off could be a matter of concern in plants that grow in a climate with limited water supply.

The opening and closing of stomata are regulated by a series of coupled processes which can be thought of as a control system. The positive feedforward response from photosynthesis triggers the stomata to open and the negative feedback from the leaf water potential triggers them to close. However, how this regulation occurs in a plant, is still elusive. The models for these phenomena have primarily been empirical or mechanistic.

Cowan and Farquhar[10] in 1977 first suggested that the plants try to maximize the carbon gain for a particular amount of water supplied over a period of time (further discussion under *Literature Review*). In the same year, Delwiche[11] developed a mechanistic model to analyze the hydraulic aspects of the stomatal system. Delwiche formulated the model in terms of coupled non-linear differential equations between hydrostatic pressure, water potential and osmotic potential of the cells as well as water fluxes and water vapor resistances. Even though Delwiches model is able to demonstrate certain dynamical response such as stomatal oscillation, it does not account for the effect of photosynthetically active radiation on stomatal conductance. As reviewed by Buckley[12], the optimality model proposed by Cowan and Farquhar was based on the understanding that marginal carbon revenue of water remaining constant. It explained the constant marginal revenue of water by considering diurnal variations in the stomatal conductance. However, when biophysical parameters are used for the estimation of the conductance, this optimization procedure becomes iterative and several assumptions need to be taken for the problem to be solvable.

Therefore, our project aims to bridge the mechanistic approach and constrained optimization. By examining whether the stomata are optimal within the Delwiche's mechanistic

4

framework, we bring a novel perspective into the function of the stomatal system.

The novelty of our work includes:

- We introduce a system of equations to the existing Delwiche model of stomatal dynamics to establish a coupling between the carbon assimilation and the transpiration.

- Using the optimized parameters, we will perform a stability analysis to validate this transient mechanistic model and a sensitivity analysis to study the effect of parameters on the stomatal conductance variation.

3. Literature Review

The last four decades have witnessed a significant growth in the modelling approaches of stomatal conductance in response to environmental stimuli. According to Buckley[13], these approaches can be generalized into three categories: the data-based empirical approach, the process-based mechanistic approach and the optimization-based economic approach. We will give an overview of exemplary models from each approach below with emphasis on the ones based on optimization.

3.1. The Empirical Approach

The empirical approach focuses on the environmental regulation of stomatal opening. They are frequently employed in ecological and hydrological studies because they can be verified experimentally. This approach is useful for canopy-scale and whole field modelling as it is often easier to track numerically compared to the other approaches. By incorporating field data with the assumption that the stomatal conductance is a product of independent functions of each environmental parameter, Jarvis[4] in 1976 adopted a non-linear, least-square method to formulate the stomatal conductance. The Jarvis model emphasizes the impact of exogenous environmental variables such as photosynthetically active radiation (PAR) and vapor pressure deficit (VPD) on the stomatal conductance, as shown in eqn.(1) below:

$$g_s = g_{max}(1 - \alpha VPD)\frac{1}{(1 + \frac{\beta_g}{PAR})}(1 - e^{-\gamma_g(\psi_{stem} - \psi_m)}) \tag{1}$$

Where g_s is the stomatal conductance in cm/s; g_{max} corresponds to an empirical maximum g_s; α and β are also empirical parameters; ψ_{stem} is the stem water potential and ψ_m is the stem water potential when the stomata are closed ($g_s = 0$). This model was further simplified for the well-watered situation in 1980 by Thorpe[14], where the exponential term is removed as ψ_m is equivalent to ψ_{stem} when the stomata remain open. These empirical models provide reliable predictions of g_s when the parameters are finely tuned. Yet, with time independent g_s, they cannot provide insight into the governing controls underlying the gas exchange.

3.2. The Mechanistic Approach

The mechanistic approach rationalizes the dynamics behind stomatal opening. It is a tool to better investigate the dynamics of the stomatal system and must converge to the empirical approach at some scale to validate the proposed mechanism. This approach is useful in exploring the cellular processes involved in environmental sensing, signal transduction, and ion movement[13]. The time-dependent, mechanistic model by Delwiche[11] will be the main focus in this context and further illustrated under *Problem Statement*. The Delwiche model transforms the water relations and hydraulic properties of the stomatal system (guard cell, subsidiary cells and mesophyll) into coupled, nonlinear ordinary differential equations and therefore provides a promising framework to further untangle the stomatal mechanism. Yet, the system is mathematically complex with a multitude of parameters not sure which the stomatal conductance is most sensitive to.

3.3. The Optimization Approach

First proposed by Cowen and Farquhar (abbreviated as CF below)[10] in 1977, the optimization approach opens another perspective to study the stomatal function by focusing on the economy of the plant. This approach is derived from an empirical perspective by assuming the conservation of certain emergent properties of stomatal conductance[13]. By introducing the optimal control theory[15] which aims to find a control law for a dynamical system to the stomatal complex, the stomatal optimization theory'examines its regulatory role. This

optimization statement focuses on the trade-off between the photosynthetic carbon gain (assimilation) and the transpiration water loss with stomatal opening and relates the Lagrange multiplier defined by the optimal control theory to the instantaneous marginal water use efficiency[16]. Therefore, this approach addresses the intrinsic relationship between carbon assimilation and water transpiration without assuming a functional response of stomatal conductance to environmental factors such as VPD. Katul[16] in 2009 utilized the Pontryagins maximum principle to CFs theory, suggesting the maximization of the cumulative carbon gain over an arbitrary time interval is equivalent to maximizing it at each instant in time, thereby releasing the integral on the objective function. The optimization approach generally deals with short-time dynamics. However, as stated by Chapin[17], the carbon-water economy of plants is also affected by processes occurring at longer time scales and at the whole-plant level. Therefore, a way to more closely relate the optimization to mechanistic approach that can explain the day-to-day variation will be necessary and beneficial.

4. Problem Statement

Optimization as a tool will be used to investigate the stomatal mechanism proposed by Delwiche[11]. Our proposed model couples non-linear hydraulic and biochemical equations, which is non-linear programming (NLP). We aim to formulate the model into multiple discretized time intervals ($\Delta t = 1\ hr$) over a total time period of one diurnal ($12hrs$). Hence, we propose a multi-period NLP model subject to the steady state of the Delwiche mechanisitic model for transpiration ($E(g_s)$) and the Farquhar photosynthesis model for carbon assimilation ($A(g_s)$), where g_s is the stomatal conductance.

4.1. Model Formulation

4.1.1. Objective Function

The objective function in our model is of the form of a cost function, described in Eqn.(2). This general form is first mentioned by CF[10], where λ is the conversion to ensure that the carbon gain and water loss are in the same cost unit. λ is also known as the marginal water use efficiency[16]. The precise equations for A and E are given in 4.1.2 *Constraints*. We will also discuss the parameters to be optimized in the following section.

$$max \int (A(g_s) - \lambda E(g_s))dt \tag{2}$$

4.1.2. Constraints

We will adopt a modified version[16] of the Farquhar's model for the assimilation of CO_2, given in Eqn.(3) – (5). All the relevant parameters will be accessed through literature and are bounded by physical rationale, for e.g., the carbon dioxide fixation can not be infinite.

$$A(g_s) = \frac{1}{2}\Bigg(a_1 + (a_2 + c_{ta})g_s -$$
$$\sqrt{[a_1 + g_s(a_2 - c_{at})]^2 + 4g_s[a_1(36.9 + 1.18(T - 25) + 0.036(T - 25)^2) + a_2 c_{ta} g_s]}\Bigg) \tag{3}$$

$$a_1 = V_{cmax,25}\frac{e^{0.088(T-25)}}{1 + e^{0.29(T-41)}} \tag{4}$$

$$a_2 = K_{c,25}e^{0.074(T-25)}\left(1 + \frac{C_{o,at}}{K_{o,25}e^{0.015(T-25)}}\right) \tag{5}$$

To formulate the E part, we will obtain a steady state response of the transient dynamics given in the Delwiche model. The time rate of changes in the hydrostatic pressures of the guard cells ($\frac{dP_g}{dt} = \frac{\epsilon_g}{V_g^\circ}J_2$), of the subsidiary cells ($\frac{dP_s}{dt} = \frac{\epsilon_s}{V_s^\circ}(-J_2 + J_3)$) and of the mesophyll cells ($\frac{dP_m}{dt} = \frac{\epsilon_m}{V_m^\circ}J_4$) will be set zero to obtain the steady-state J_2, J_3 and J_4. By substituting these values in Eqn.(6) – (8), we will obtain the steady-state hydrostatic pressures P_g, P_s, P_m, which will then be used in Eqn.(11) to solve for the stomatal aperture (A_{st}) in Eqn.(10). The steady-state stomatal resistance, the inverse of g_s, is then obtained using Eqn.(9) and the transpirational flux J_1, which is E in the model is obtained via Eqn.(12). The b_0, b_g, b_m in Eqn.(11) are parameters of the multilinear approximation of A_{st} and are the outcome of our optimization. They are defined by the genotype of the plants and are invariant over time. Therefore, we propose these b parameters may not be optimal within each time interval, but they may be optimal over a period of time.

$$J_2 = \frac{1}{2}LA_2\left[P_s - P_g - \pi_s^\circ(1 - \frac{P_s}{\epsilon_s}) + \pi_g^\circ(1 - \frac{P_g}{\epsilon_g}) + \widetilde{\pi}_g\right] \tag{6}$$

$$J_3 = LA_3\left[\psi_r - (J_1 + \frac{J_3}{A_5} + \frac{J_4}{A_5})R_p - P_s + \pi_s^\circ(1 - \frac{P_s}{\epsilon_s})\right] \tag{7}$$

$$J_4 = LA_4\left[\psi_r - (J_1 + \frac{J_3}{A_5} + \frac{J_4}{A_5})R_p - P_m + \pi_m^\circ(1 - \frac{P_m}{\epsilon_m}) + \widetilde{\pi}_m\right] \tag{8}$$

$$R_t = \frac{1}{g_s} = \frac{1}{D}\left[\delta_{dias} + \frac{d+r}{nA_{st}} + \zeta\sqrt{\frac{l}{v}}\right] \tag{9}$$

$$A_{st} = \pi ab \tag{10}$$

$$a = \begin{cases} b_0 + b_g P_g + b_s P_s, & \text{if } b_0 + b_g P_g + b_s P_s \geq 0 \\ 0, & \text{if } b_0 + b_g P_g + b_s P_s < 0. \end{cases} \tag{11}$$

$$J_1 = \frac{c_m - c_{ta}}{R_t} \tag{12}$$

4.2. Outcome Interpretation

Our steady-state model will give optimal plant parameters such as rigidity modulus and stomata aperture parameters. We will back substitute these optimal parameters in the original transient Delwiche model for stability analysis. We will then conduct sensitivity analysis on this transient model to identify which parameters really matter. Based on the optimized parameter values, we can draw conclusions such as: for unrealistic plant parameter values, we can deduce that the plant life may not be optimized for the fitness function and can have implicit dependency on more hidden parameters.

References

[1] Omar, G.T.; lvaro, L.B.; Luca, T.; Francisco, J.V. A soil-plant-atmosphere-continuum (SPAC) model for simulating tree transpiration with a soil multi-compartment solution. *Plant and Soil.* 2017. doi: 10.1007/s11104-016-3049-0

[2] Van den Honert, T.H. Water transport in plants as a catenary process. *Discuss. Faraday Soc.* 1948. doi: 10.1039/DF9480300146

[3] Stroock, A.D.; Pagay, V.; Zwieniecki, M.A.; Michele Holbrook, N. The physicochemical hydrodynamics of vascular plants. *Annual Review of Fluid Mechanics.* 2014. doi: 10.1103/PhysRevLett.113.134501

[4] Jarvis, P.G.; McNaughton, K.G. Stomatal control of transpiration: scaling up from leaf to region. *Advances in Ecological Research.* 1986. doi: 10.1016/S0065-2504(08)60119-1

[5] Buckley, T.N. Modeling stomatal conductance. *Plant Physiology.* 1986. doi: 10.1104/pp.16.01772

[6] Stroock, A.D. Optimizing irrigation for sustainable production of almonds, apples and grapes. *SCRI Proposal.* 2018.

[7] Chalmers, D.J.; Mitchell, P.D.; Vanheek, L. Control of peach tree growth and productivity by regulated water supply, tree density and summer pruning. *Journal of the American Society of Horticultural Science.* 1981.

[8] Fereres, E.; Soriano, M.A. Deficit irrigation for reducing agricultural water use. *Journal of Experimental Botany.* 2007. doi: 10.1093/jxb/erl165

[9] Cowan, I.R. An electrical analogue of evaporation from, and flow of water in plants. *Planta.* 1972. doi: 106(3):221-226

[10] Cowan, I.R.; Farquhar, G.D. Stomatal function in relation to leaf metabolism and environment. *Symposia of Society for Experimental Biology.* 1977. doi: 31:471-505

[11] Delwiche, M.; Cooke, J.R. An analytical model of the hydraulic aspects of stomatal dynamics. *Journal of Theoretical Biology.* 1977. doi: 69, 113-141

[12] Buckley, T.N.; Sack, L.; Farquhar, G.D. Optimal plant water economy. *Plant Cell Environ .* 2017. doi: 10.1111/pce.12823

[13] Buckley, T.N.; Mott, K.A. Modelling stomatal conductance in response to environmental factors. *Plant, Cell Environment.* 2013. doi: 10.1111/pce.12140

[14] Thorpe, M.; Warrit, B.; Landsberg. Responses of apple leaf stomata: a model for single leaves and a whole tree. *Plant, Cell and Environment.* 1980. doi: 10.1111/1365-3040.ep11580508

[15] Luenberger; David G. Optimal control: introduction to dynamic systems. *New York: John Wiley Sons..* 1979.

[16] Katul, G.; Manzoni, S.; Palmroth, S.; Oren, R. A stomatal optimization theory to describe the effects of atmospheric CO_2 on leaf photosynthesis and transpiration. *Annals of Botany.* 2009. doi: 10.1093/aob/mcp292

[17] Chapin, F. Integrated responses of plants to stress. *BioScience.* 1991. doi: 10.2307/1311538.2307/1311538

[18] Farquhar, G.D.; von Caemmerer, S.; Berry, J.A. A biochemical model of photosynthetic CO_2 assimilation in leaves of C_3 species. *Planta.* 1980. doi: 10.1007/BF00386231