

# Master's Thesis Proposal: Modeling Carbon Dynamics Using FACE Data from Duke Forest

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## Introduction

The recent increase in atmospheric carbon dioxide ( $\text{CO}_2$ ) has impacted various processes and functions in several ecosystems around the globe. However, the exact effects are debated and still somewhat unknown. Recent studies have focused on the concentration of carbon in soil as a predictor of the long-term impacts of climate change. However, a large portion of this carbon is first transmitted through plants and subsequently released into the soil. Thus, plant life is a key player in global carbon exchange. Understanding carbon dynamics, specifically in tree roots, will be vital to understanding the long-term influence of increased  $\text{CO}_2$  concentrations in the atmosphere.

In collaboration with Allan Strand and Seth Pritchard from the biology department, we will begin by studying data taken from roots of pine trees to investigate carbon dynamics. The data set originates from an intriguing experiment conducted by a team of researchers from Duke University. The experiment is referred to as free-air  $\text{CO}_2$  enrichment (FACE). The team released highly concentrated levels of  $\text{CO}_2$  into a test site within Duke Forest. Most of the research has focused on analyzing the test site soil thus far. We believe we can gain additional insight by shifting our attention to the data collected from the roots. To gain such insight, we will first construct a mathematical model of carbon transport throughout a root system. Next, we aim to fit the parameters present in the model to the FACE data. This process will yield relevant results corresponding to specific situations in Duke Forest.

## Part I: Mathematical Modeling

During the FACE experiment, the test site was fumigated with high levels of artificially engineered carbon dioxide. Artificial  $\text{CO}_2$  has a different carbon isotope than that which is naturally present in the atmosphere. In particular, there is less of the stable isotope C13. By comparing fumigated roots to a control group, researchers were able to measure the ratio of artificial and natural carbon. This may provide insight into how long trees are retaining C through photosynthesis. Such insight is significant since the potential for soil, roots, and trees to sequester carbon is not fully understood. Ecologists assert that the understanding of this potential is an important tool in combating climate change.

To gain more understanding as to how trees may segregate and store carbon, we will construct a mathematical model of carbon transport in pine tree roots. One possibility is to define the model as a reaction-diffusion system. The study of systems of this type is a rich area in research. Equations in a reaction-diffusion system in one dimension have the canonical form

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} + R(t, x, u)$$

where the state variable  $u(t, x)$  is a function of time and space (e.g., carbon concentration along a root),  $D$  is the diffusion coefficient, and  $R(t, x, u)$  defines local reactions. Reaction-diffusion systems can be applied to study several different types of dynamical systems including propagation of action potentials, neuronal networks, predator/prey movement, and many more.

One possibility for the construction of a relevant reaction-diffusion system is to extend the Introductory Carbon Balance Model (ICBM)

$$\begin{aligned} \frac{dY}{dt} &= i - k_1 r Y \\ \frac{dO}{dt} &= h k_1 r Y - k_2 r O \end{aligned}$$

to include diffusion of the carbon concentration. In the ICBM,  $Y$  and  $O$  are defined as young and old carbon respectively,  $k_1$  and  $k_2$  describe rates at which young and old carbon are lost to the atmosphere,  $r$  describes carbon decomposition,  $h$  is the fraction of carbon flowing from  $Y$  to  $O$ , and  $i$  is the mean annual input of carbon into  $Y$  (1). The ICBM will share similarities with its spatial extension, however, certain differences will exist as well. For example, in the spatial extension, it is likely that we will label carbon pools by isotopes (C12, C13, etc.) rather than age. Another distinction is that we will acknowledge more parameters and perhaps more than two dependent variables (resulting in additional equations).

The ICBM is convenient in that the equations are linear and they can be solved analytically (expressions for exact solutions exist). A spatial extension of the ICBM that incorporates diffusion will also be linear. Thus, we expect exact solutions to exist, which are convenient for analysis. However, the full model may necessarily contain nonlinear terms, so we will rely on numerical methods for approximations. To obtain numerical approximations for solutions to a reaction-diffusion system, we can discretize using the method of finite differences to simplify the system of partial differential equations down to a system of ordinary differential equations. Subsequently, it becomes possible to implement a numerical method, such as the Crank-Nicolson method, in Python to obtain the desired results. These results will be plotted and explained clearly in the paper we write.

## Part II: Data Analysis

Once we have constructed a reasonable mathematical model, we can begin to take data from the FACE experiment to fit the model. We seek both simple and sophisticated options for approaches. Parameters in the ICBM were fit using the REG (linear) and NLIN (nonlinear) regression procedures in SAS. In turn, Andrén and Kätterer succeeded in fitting their model to clay soil data originating from an experiment that took place over the course of 30 years in Sweden. One of the authors' goals in using regression was to determine certain values for the parameters  $(k_1, k_2, i, r, h)$  to reflect specific environmental circumstances. For example, choosing a high carbon decomposition rate of  $r = 5.36$  corresponds to a hot and humid climate while  $r = 1$  corresponds to a colder climate (1). Since we have experience in SAS, the regression procedures mentioned above can potentially be applied to certain portions of the data from Duke Forest as well. However, as we can see, Andrén and Kätterer fit a fairly simple system of ordinary differential equations to their data. Their methods provide inspiration for a somewhat simplistic approach to be expanded upon.

Another option, time permitting, is to use multi-objective optimization. This strategy involves fitting a large number of parameters to objectives which are typically taken from the physical constraints of the system or the data. For example, it is hypothesized (2) that naturally occurring carbon is stored within reservoirs in trees. Parameters associated with a reservoir, such as the rate carbon is stored, may not be directly measurable. Multi-objective optimization can be accomplished in SAS using the Local Search Optimization

(LSO) solver. It seems that both Python and SAS could be useful during our research. However, it is important to note that, comparatively, we wish to spend more time in Python. Our goal is to investigate carbon dynamics mainly from a mathematical approach rather than statistical. We believe the mathematical model will provide invaluable insight into the effects of climate change within tree systems.

## Timeline

- Summer 2021: Complete a literature review to better understand the current knowledge of carbon dynamics in soil and plant life. Search for relevant mathematical models.
- Fall 2021: Officially begin the first semester of MATH 700. Begin the first draft of the paper. Gather enough research to present at the 3MT competition. Begin implementation of the chosen mathematical model in Python. Begin parameter fitting and debugging (time permitting).
- Spring 2022: Officially begin the second semester of MATH 700. Revise the paper multiple times and complete the final draft. Present at the graduate research poster session. Finish parameter fitting and debugging. Defend the thesis in April.

## Committee

- Alex Kasman (math department)
- Daniel Poll (math department)
- Allan Strand (biology department)

## References

1. Andrén, Olof, and Thomas Kätterer. “ICBM: The Introductory Carbon Balance Model for Exploration of Soil Carbon Balances.” The Ecological Society of America, John Wiley & Sons, Ltd, 1 Nov. 1997.
2. Sala, Anna, et al. “Carbon Dynamics in Trees: Feast or Famine?” OUP Academic, Oxford University Press, 1 Feb. 2012.