Optimizing Nitrogen Fertilizer Quantities in Cereal Crop Root Systems to Minimize Leaching

Keywords: fertilizer, absorption, nitrogen, cereal crop, leaching

BEE 4530/5530 Computer Aided Engineering

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1. EXECUTIVE SUMMARY

Loss of nitrogen due to leaching is one of the most pressing issues in agriculture as it leads to excessive crop production costs and pollution. N leaching contributes to atmospheric and aquatic pollution [1]. The production of nitrogen fertilizers accounts for 3% of worldwide natural gas consumption and contributes to 3% of global greenhouse gas emissions. Fertilizer leaching accounts for 23 trillion grams of nitrogen loss per year [2].

Understanding resource capture in cereal root systems provides yield and production data useful for environmental and economic efficiency. Thus, there is already considerable research on modeling water and N uptake by root systems. There are general models that describe uptake with root length density over the course of a season [3]. There are also a variety of existing models used to simulate mineral movement in soil systems that have been adapted to model N leaching in crop root systems, including DRAINMOD, DSSAT, N_ABLE, and EPIC [4]. We aim to model the consumption of nitrogen by cereal crop roots, as well as leaching under topsoil fertilizer placement in order to optimize the amount of fertilizer needed. An optimized amount of fertilizer will maximize plant uptake while minimizing the amount leached in the soil. It will save farmers money while minimizing ecological impact.

We will model the nitrogen distribution and absorption over a set amount of time. During this length of time, rainfall will occur at certain periods in order to mimic real environmental conditions. In order to accurately model the top-down system, we must first simulate the uptake of the fertilizer into the water during rainfall. We model our system as 2D axisymmetric. We will describe our system using mass transfer equations representing the convective flow, transient uptake and dispersion over time under known initial concentrations and dispersive constants. We then use fluid flow equations to model the traversal of water through the soil/root system. The absorption of the water and N by the plant is a function of the root density, for which the equations are known. Using this information in simulation, we will be able to model how much nitrogen is absorbed by the root system as well as how much is leached beyond the boundaries of the crop. We found that most root uptake of nitrogen occurs in the top-most region which was expected. N uptake also increases as root length density increases. We plotted total N flow and uptake against time and found that only 30.3% of initial nitrogen was absorbed by the plant over the course of 90 days.

Additionally, our water content and matric potential are validated using a study by Wu et. al. in which matric potential, h, and water content, θ, were measured 5 days after an irrigation event [5]. We modeled our precipitation to match their field conditions. We plotted our matric potential with respect to depth into the soil layer and our water content with respect to depth against the Wu et. al. results. The trend of our model matches that of the measured values with reasonable precision. Our matric potential with respect to depth plot rendered an R^2 value of 0.766 and our plot of water content with respect to depth achieved an R^2 of 0.937 (Fig. 12 & 13).

2. INTRODUCTION

Nitrogen is essential for plant function and growth. It is a key component of amino acids that form the building blocks of proteins and enzymes which make up structural materials and facilitate biochemical reactions within the plant. Nitrogen is also what allows for photosynthesis to take place in plants as it is a component of the chlorophyll molecule. It is also present in roots and functions to help regulate the uptake of water and other nutrients. In agriculture, nitrogen fertilizer is used to speed up crop growth and increase crop yields.

The natural nitrogen cycle is subject to multiple means of leakage due to leaching, volatilization, and denitrification. These losses lead to run off and the release of gasses that cause environmental issues like air pollution, soil acidification, ozone depletion, eutrophication and the creation of ocean dead zones, alkaline air, and more. Nitrogen fertilizer is also subject to these losses and contributes to agricultural inefficiency. In a book chapter published in 2019, it was noted that less than half of the 109 million tons of nitrogen fertilizer used to improve global food production were assimilated into the aboveground biomass of crops [6]. Our study focuses on the issue of nitrogen leaching, but developing a way to optimize nitrogen fertilizer quantities will reduce the potential for each type of nitrogen loss and the consequent pollution. It also had the potential to increase efficiency of farming.

Most crops besides N-fixing legumes rely on nitrogen in the soil. Cereal crops can be genetically engineered to incorporate bacterial *nif* genes into the plant that allow the plant to fix nitrogen from the atmosphere. The bacterial *nif* gene requires lots of ATP, and in prokaryotes, this is not a big problem. However in eukaryotes like plants, these genes must be inserted in the plant mitochondria or chloroplasts. Nitrogen fixing from the *nif* gene is not effective in the presence of oxygen which is created in these locations from the plant's light reactions. Therefore, the N-fixing can only occur during dark reactions or at night rather than constantly like in prokaryotes like E. Coli and yeast [7]. Adding the *nif* gene still has the potential to reduce nitrogen fertilizer amounts necessary to maximize plant growth and minimize issues such as excess cost, leaching, and consequent environmental harm. Our goal is to design a model that can incorporate the effects of the bacterial *nif* gene in order to determine how we can minimize leaching into the soil while still having healthy levels of nitrogen.

The Liu, J. study published in 2010 found that nearly two-fifths of nitrogen inputs are lost in ecosystems with their finding of a global average nitrogen recovery rate about 59% [2]. A study done by H.M. van Es, K. J. Czymmek, and Q.M. Ketterings between 1991 and 2000 found that timing and rate of nitrogen fertilizer additions and soil type influenced nitrogen leaching losses, and that the N leaching Index at that time could be improved by considering management practices [6].

In 2003, a study done by King, J. and his colleagues modeled cereal root systems for water and nitrogen capture. However, this study was done with the intent of evaluating the model economically and trying to optimize economic returns. While many equations are similar to the ones we use in our model, we are focused on the environmental impacts that an excess of nitrogen may have. Our model has the ability to calculate uptake of water and nitrogen in the plant as well as nitrogen leached into the soil.

2.1 PROBLEM STATEMENT AND SCHEMATIC

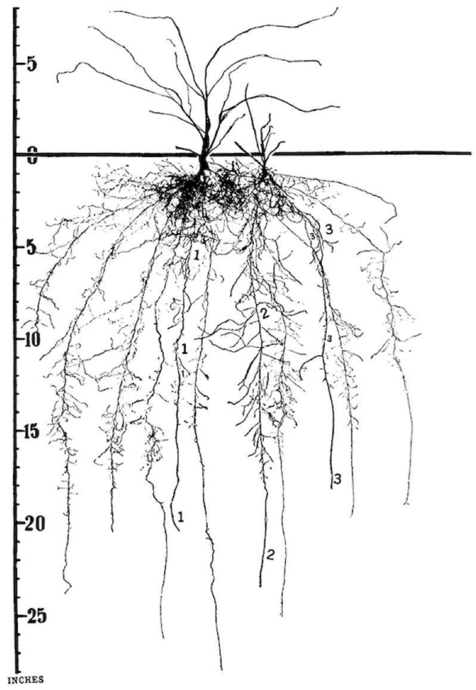


Fig 1. Typical wheat root system [8]. In nature, root systems for plants can be very complex. However, the overall densities and lengths of roots can be determined through data. Using this information can help create a model based on known plant root depths and densities.

Root systems have complex geometries that vary in density with depth. The 2D image of the wheat plant shown below provides a visual example of how plant roots typically grow (**Figure 1**). This geometry would be overly complicated to model in COMSOL. In our schematic and process diagram (**Figures 2 & 3**), we represent the root system with a triangle that points down into the Earth.

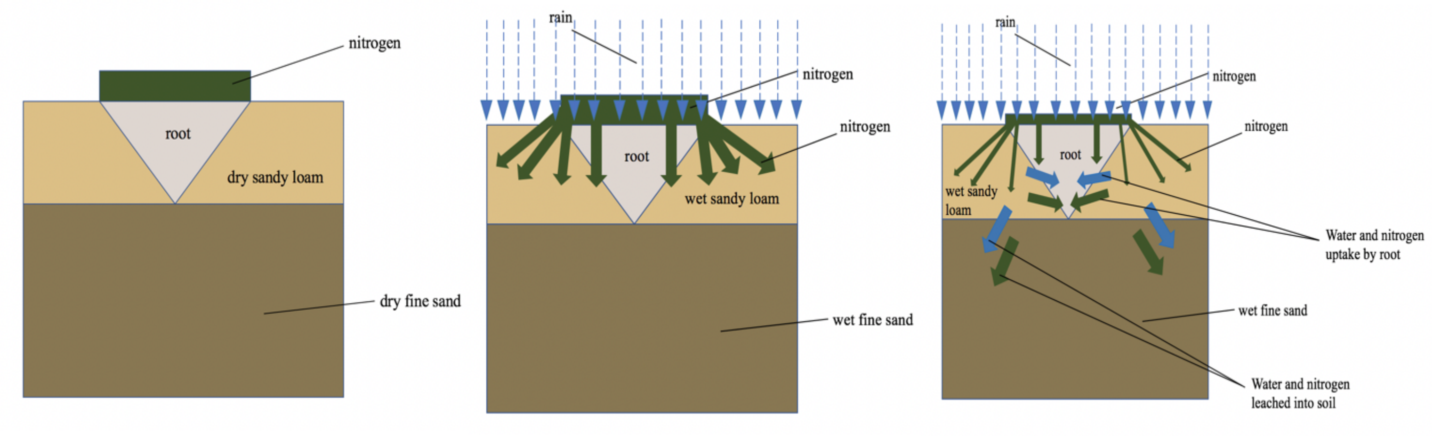


Fig 2. Rainfall and nitrogen absorption process. During rainfall, water is absorbed by both the plant and soil. The water from the rain also absorbs some nitrogen when passing through the fertilizer layer. The nitrogen travels with the water and is either absorbed by the plant, absorbed by the soil, or eventually goes into runoff.

Figure 2 depicts the physical process of rainfall and subsequent nitrogen absorption through our system domain in three stages. Initially, there is a nitrogen fertilizer layer directly above the root system. Assume the soil is unsaturated with respect to water. At t = 0.5 days, rainfall causes nitrogen to start to dissolve into water and move with the water into the soil (fluid flow). Finally, roots absorb water along with the nitrogen inside the water (mass transfer), but some water and nitrogen do not get taken up by the plant and leach into the soil.

We are aiming to develop a model that accurately represents the uptake of nitrogen by the cereal root system as well as nitrogen leaching. This will provide an understanding of how much nitrogen plants will require to grow efficiently. Our model will be a sufficient example of one cereal crop's uptake of nitrogen under semi-realistic soil conditions using paired mass transfer and fluid flow simulations. We will also be able to understand how various parameters influence how nitrogen flows within water throughout the soil, with root uptake. Our design will replicate the process that maximizes the nitrogen uptake by the root, while minimizing leaching. It will also take into account the criteria of compatibility, testability, and reliability.

2.2 DESIGN OBJECTIVES

We are attempting to simulate the nitrogen absorption process of cereal crop roots with topsoil fertilizer placement and to calculate the percentage of fertilizer that leaches. This constitutes:

a) Modeling the ammonia-carrying-fluid flow through the soil.
b) Modeling uptake of ammonia by roots.
c) Modeling leaching of unabsorbed fertilizer, where leaching is defined as all the nitrogen not absorbed by the plant.
d) Designing a way to maximize nitrogen uptake by the plant while minimizing leaching into the soil.

3. METHODS

3.1 SCHEMATIC

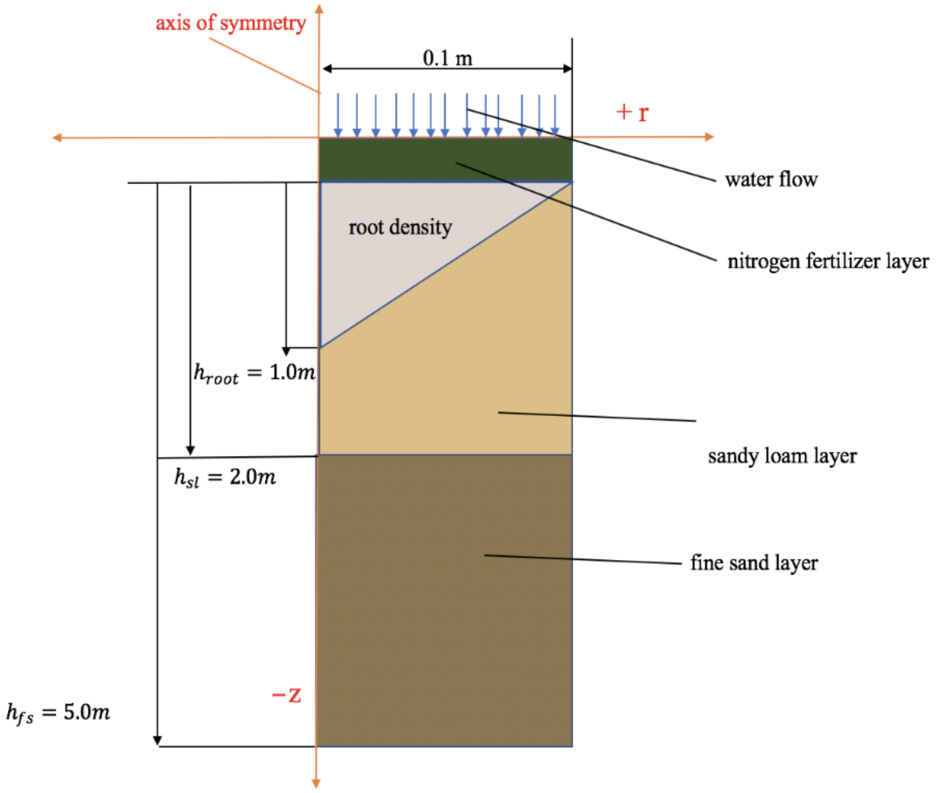


Fig 3. 2D axisymmetric domain. For our model, we decided to use a 2D axisymmetric geometry. This represents the general, cylindrical shape of a column of soil that includes the plant. The plant roots are modeled by a triangular section that represents the relative root density. We also have two different layers of soil to model real world soil more closely.

Our problem is 2D and axisymmetric. The schematic does not include the left half of the root density due to the axisymmetric property of our problem. For the topsoil placement of nitrogen fertilizer, we model a layer of fertilizer on top of a rectangular layer of soil. The root density function is currently being depicted by the triangle pointing in the negative Z direction (into the Earth), due to the general shape of root systems to be increasingly dense towards the top of the soil. We found that crop plant densities vary from 30-400 $\frac{plants}{m^2}$ with a root depth of 1.0-2.0 m [9]. Winter wheat has a lower density, so we chose a value of 30 $\frac{plants}{m^2}$, which dictated the z dimension of our domain for a single crop to be r = 0.1 m. Root length L_r = 1 m, and the total domain height is the distance from the soil surface to the water table, or 3.4 m.

3.2 ASSUMPTIONS

3.2.1 Geometric Assumptions

We assume our model is axisymmetric and that the nitrogen transport and fluid flow can be described in two dimensions: vertically along the z-axis and radially. In this simplified version of our model, the plant growth is modeled by an increase in root length density. Our soil model is made up of two different types of soil: sandy loam and fine sand. We are assuming there is a distinct horizontal boundary between the two layers with no overlap. Each layer has different parameters that are held constant throughout the respective layer.

3.2.2 Mass Transfer Assumptions

Due to our 2D geometric assumption, we can model our mass transfer using cylindrical coordinates, omitting the θ direction. We do not include a diffusion term because it can be assumed to be included in dispersion [10]. We assume that there is degradation due to the root uptake of water and nitrogen as well as diffusion into the soil. These are the only ways that nitrogen is removed from the system. There is a set amount of nitrogen placed as a fertilizer layer in the sandy loam which does not affect the properties of the soil at all. The initial amount of nitrogen set is fixed and there is no addition of nitrogen occurring in our model.

3.2.3 Fluid Flow Assumptions

In our fluid flow model, we are assuming that the periodic cycle of rainfall and the water table are the only ways that water is entering our system. We assume rainfall is evenly distributed across the layer of fertilizer. Additionally, at the water table, we are assuming the water content level is close enough to saturation that the matric potential can be assumed to be 0. We are including evapotranspiration from the plant in our sink term, but ignoring the loss of water due to evaporation. The plant we are modeling is assumed to be far enough away from other plants that there is no radial flux occurring along the rightmost boundary. In reality, matric potential values are either negative or 0. In this study, based on the papers we collected data from and how we defined our geometry, matric potential is simply negated from its original form so that all values are positive.

3.3 GOVERNING EQUATIONS

Our project utilizes two governing equations. One to model dispersion mass transfer of nitrogen through the soil and root system, and one to model the fluid flow of water through the domain. Both the soil and the root will uptake nitrogen and water.

3.3.1 Mass Transfer Governing Equation

Our mass transfer equation includes dispersion, since the flow of water due to gravity will cause dispersion. We do not include a diffusion term because it can be assumed to be included in dispersion.

$$\left(1 + \frac{\rho_s K^*}{\theta}\right)\frac{\partial c^*}{\partial t} + \frac{u}{\theta}\frac{\partial c^*}{\partial z} = E\frac{\partial^2 c^*}{\partial z^2} - S_n \quad (1)$$

In Equation (1), c* is the concentration of N absorbed by the water as a fraction of the total volume of water ρ_s is the density of topsoil, θ is the water content, u is the velocity of nitrogen, and k* is the. S_n is the sink term describing nitrogen uptake by the root. E is the dispersion coefficient of the soil, u is the velocity of water flow, and z is the depth at which all of this is occurring. We can relate c, the dissolved concentration of N per unit volume of soil, to c* with the equation

$$c = c^* \cdot \theta \quad (2)$$

where θ is the volumetric water content of the soil. Further, we can relate c^{ad} to c* with the equation:

$$c^{ad} = c^{*} \cdot k^{*} \cdot \rho_s \quad (3)$$

where k* is the distribution coefficient between the soil and the solute and ρ_s is the dry bulk density of the soil. The c^{ad} term represents the N absorbed into the soil with time, whereas the S term is a sink representing the absorption of N by the root. The only mechanism by which the roots absorb N is by mass flow water absorption, so we can approximate the term S_n as a linear proportion of the fluid flow sink term, representing the water uptaken by the root, multiplied by the concentration of N in the water in the root region. Thus

$$S_n = \alpha \cdot c^* \cdot S \quad (4)$$

In order to determine our proportionality constant, α, we refer to the initial N absorption of winter wheat and plug in the initial values for S and c in our root region to match the experimental S_n [11]. We then maintain this constant for the season. More information about the calculation of the water flow sink term, S, can be found in the fluid flow section below.

3.3.2 Fluid Flow Governing Equation

The flow through a porous medium is described by Darcy's Law. The analog of Darcy's Law is the water conservation equation, written using Darcy's law for an unsaturated soil, also known as Richard's Equation, is shown below.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial h}{\partial z} + 1\right)\right] - S \quad (5)$$

In Richard's Equation, the sink term (S) accounts for water uptake by plant roots. K is the hydraulic conductivity, h is the matric potential. Matric potential is the portion of the water potential that can be attributed to the attraction of the soil matrix for water due to capillary and absorptive forces due to the binding of water to soil particles (Elsevier, 2005). The depth from the surface is denoted as z, θ is the volumetric water content, and t is time.

In COMSOL, we solved our dependent variable for θ, and used the Stabilized Convection Diffusion equation,

$$d_a \frac{\partial \theta}{\partial t} + \nabla \cdot (-c\nabla\theta + \alpha\theta) + \beta \cdot \nabla\theta + a\theta = f \quad (6)$$

where $d_a = 1$, c = $-\ k\frac{\partial h}{\partial \theta}$, $\beta = -\ \frac{\partial k}{\partial \theta}$ in z, f = S in the root domain, and all other coefficients are zero. In order to determine $\frac{\partial h}{\partial \theta}$, we had to use the empirically deduced Van Genuchten relation,

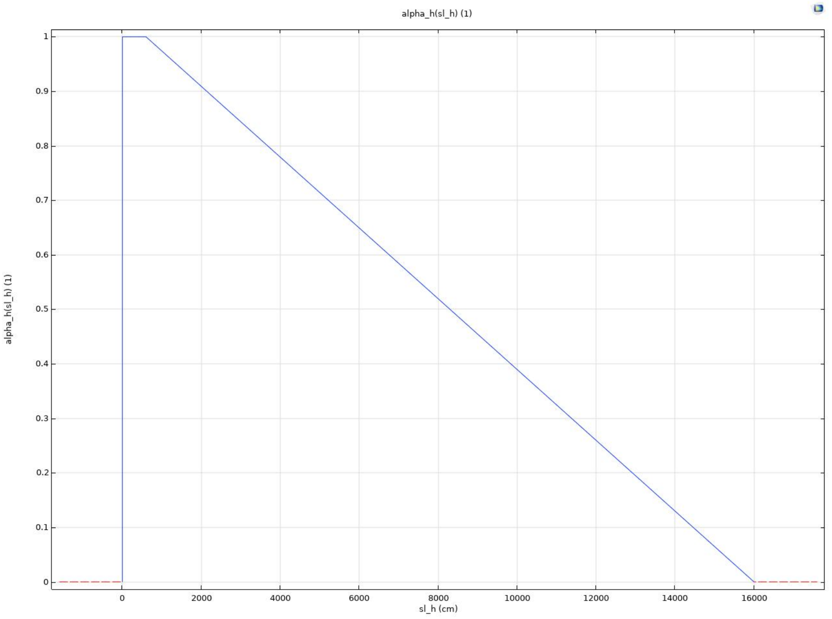
$$\theta\ = \theta_r + \frac{\theta_s - \theta_r}{[1+|\alpha h|^n]^m}$$

Where θ_r, θ_s, α, n, and m are functions of material properties, the values for which can be found in Appendix A.

The sink term S (represented by f in equation (6)) is shown below.

$$S\ =\ 2\alpha(h)\frac{T_p}{L_r}(1\ -\ z/L_r)\ \ (7)$$

In the sink equation above α(h) is the water response function dependent on soil matric potential, h, and plant species, T_P is the potential maximum transpiration rate and L_r is the rooting depth. In our model, we parameterized the rooting depth (L_r) and held potential max transpiration rate (T_p) to be constant. This way, the only parameters the sink term accounts for is the depth and water response function. The sink term changes throughout the depth of the root due to the change in z. Additionally, the function for α(h) was determined by interpolating α(h) graphs from literature [12]. **Figure 4** shows our interpolated α(h) graph.



$$\alpha(h) = \begin{cases} h & 0 < h < 1 \\ 1 & 1 < h < 600 \\ \left(-\frac{h}{15400}\right) + \left(1 + \frac{600}{15400}\right) & 600 < h < 16000 \end{cases}$$

(8)

Fig 4. Plot of water response function α(h) vs. h. In the top image, the water response function, α(h), is plotted against sandy loam matric potential, h. The piecewise function, Equation (8), is the interpolated equation for the graph [13].

We are able to use Richard’s equation to solve for our velocities in the r and z directions denoted as u_r and u_z respectively.

$$u_r = -K(\theta)\left(\frac{\partial h(\theta)}{\partial r} + 0\right) \quad (9)$$

$$u_z = -K(\theta)\left(\frac{\partial h(\theta)}{\partial z} + 1\right) \quad (10)$$

We used Darcy’s Law to calculate the superficial speed of water flow. We then paired the speed of waterflow with the convection term in the transport equation.

3.4 BOUNDARY EQUATIONS

3.4.1 Mass Transfer Boundary Conditions

$$-\frac{\partial c}{\partial z}\Big|_{z=0} = 0 \quad (11)$$

$$-\frac{\partial c}{\partial z}\Big|_{z=-3.4} = 0 \quad (12)$$

There is no nitrogen being transferred between the top layer and air, leading to a zero flux boundary condition at z=0. Additionally, nitrogen does not penetrate deep enough to get past the water table. This is the reason for a zero flux boundary condition at z=-3.4

$$\frac{\partial c}{\partial r}\Big|_{r=0} = 0 \quad (13)$$

$$\frac{\partial c}{\partial r}\Big|_{r=0.1} = 0 \quad (14)$$

There is no flux through the vertical boundaries of our systems that are both zero due to symmetry.

3.4.2 Mass Transfer Initial Conditions

The initial mass of nitrogen in the upper layer of the model is 0.000563 kg. For our model, we need to convert this mass into a concentration. To do this, we divided the initial mass by the volume and initial water content.

$$c(z,t)\big|_{0<z<-0.1} = 0.779\frac{kg}{m^3} \quad (15)$$

$$c(z,t)\big|_{-0.1<z<-3.4} = 0 \quad (16)$$

The initial value of the concentration of nitrogen in the top layer is calculated to be 0.779 kg/m^3. The initial value of nitrogen everywhere else is 0.

3.4.3 Fluid Flow Boundary Conditions

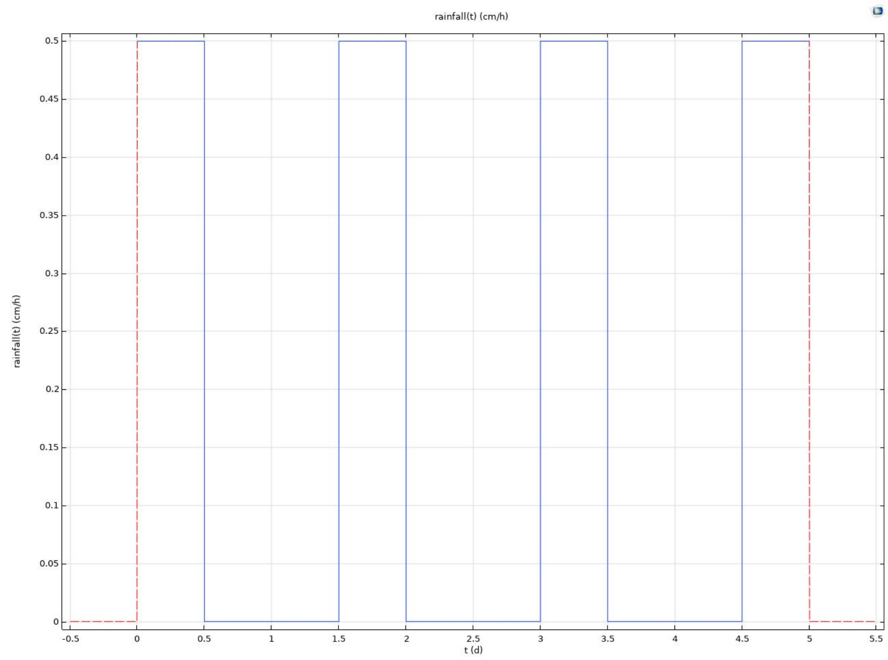


Fig 5. Fluid flow boundary condition for top layer. We modeled the rainfall as a piecewise function that is cyclical. A rainfall of 0.5 cm/hr occurs for 0.5 days and then stops for 1 day. This data comes from the average rainfall in Scotland[14].

Our boundary condition at the surface of the soil follows the function of **Figure 7**. In order to simplify our model, we are assuming a rainfall of 0.5 $\frac{cm}{hr}$ occurs over half a day and then stops for one day [14]. This repeats for 5 days.

The boundary at the bottom of the model is a water table. This means that at that boundary, the soil is completely saturated with water. The complete saturation of soil at this boundary has a θ value of 0.3524.

$$\theta(z,t)\big|_{z=-3.4} = 0.3524 \quad (17)$$

3.4.4 Fluid Flow Initial Conditions

$$\theta(z,t)\big|_{0<z<-2.1,\, t=0} = 0.23 \quad (18)$$

$$\theta(z,t)|_{-2.1<z<-3.4,\, t=0} = 0.15 \quad (19)$$

The initial volumetric water content in the two soil types is known [12]. In the sandy loam (from a z value of 0 down to -2.1), the water content starts at 0.23. In the fine sand (from a z value of -2.1 to -3.4), the water content starts at 0.15.

4. RESULTS

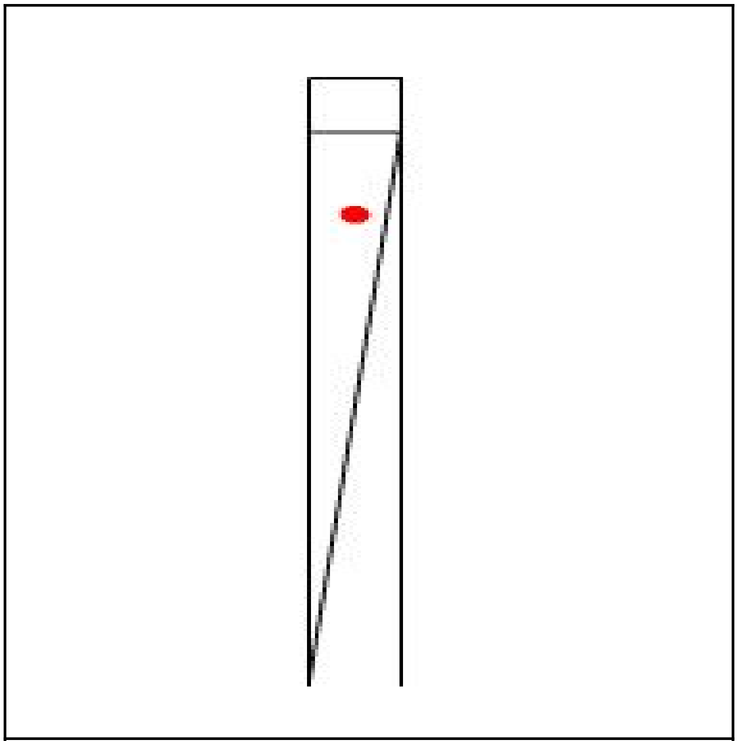


Fig 6. Point of data collection in the root system. This point (0.05m, -0.25m) was picked as the point in which we would collect water data, nitrogen concentration data, and perform a mesh convergence. This point was picked because it is located in the transit area for both water and nitrogen.

All of the following data in graphs will be located at the point shown in Figure 6. In order to be consistent, we found data for how rainfall behaves, how the concentration of nitrogen behaves, and our mesh convergences all at this point. This point was chosen because it is located in the transit area inside the root that will be able to observe the change of nitrogen and water flow. Because of this, it is a good point to see the changes occurring in the model.

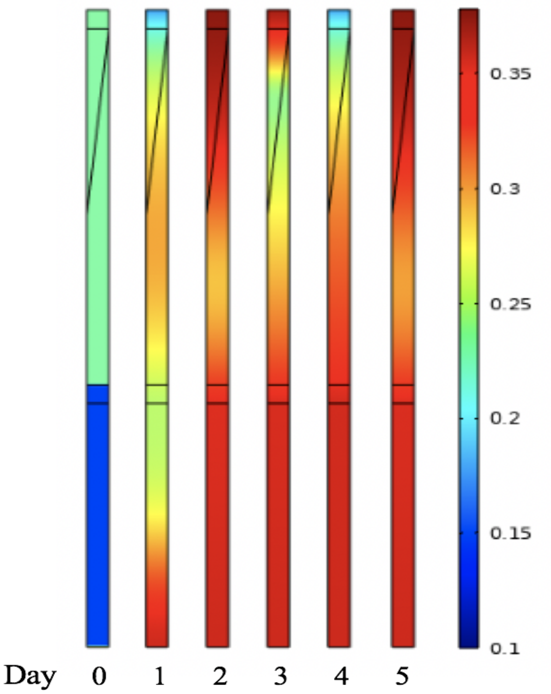


Fig 7. The 2D schematics of θ across the entire domain from day 0 to day 5 (left to right respectively). The initial water content distribution at day 0 is shown at the leftmost plot. The water content distribution at the end of each day from day 1 to day 5 respectively.

As seen in **Figure 6**, the increase in θ at the top is due to rainfall (**Figure 5**) and the increase at the bottom is due to the rising water table. The root absorbed water throughout the duration of the model, but the uptake is not significant enough to be seen in the schematic during this time period. However, we can see how water goes downwards through θ. For example at **Figure 6(b)** when the rain stops for half a day we still can see a region where θ is around 0.29 in the middle. It will keep moving down under the effect of gravity.

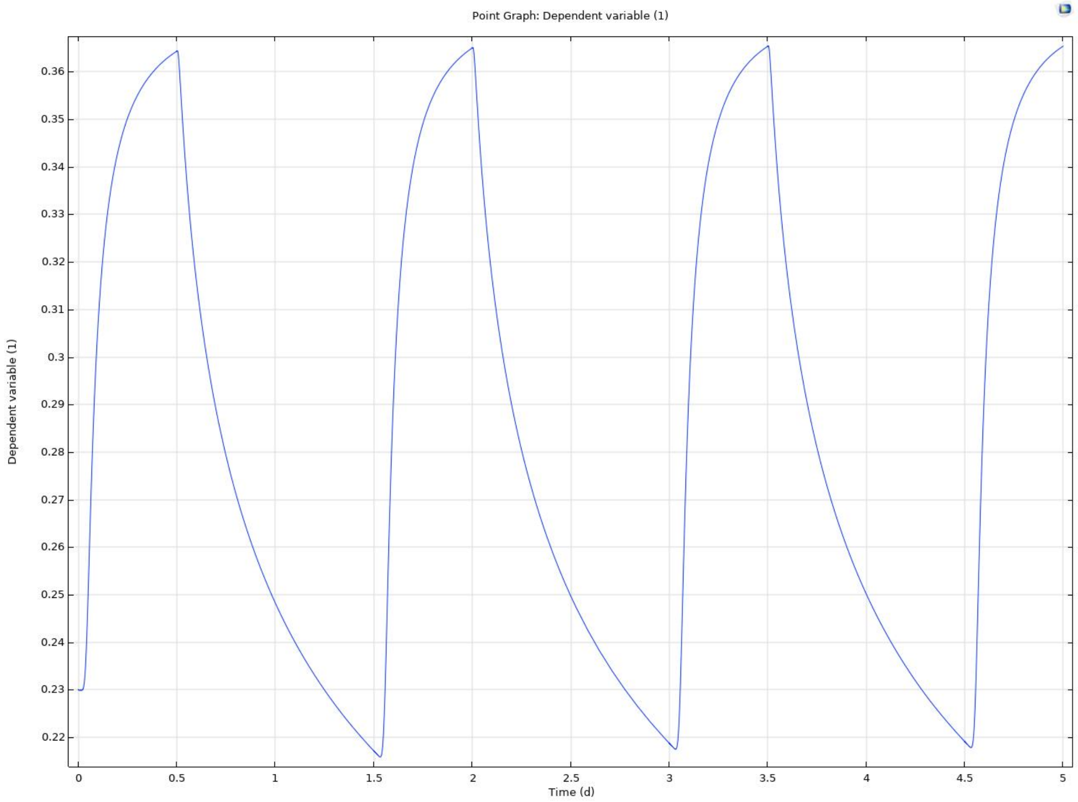


Fig 8. The change in θ at (0.05, -0.5) over the course of 5 days. This point is in the root domain and is affected by the sink term which includes the root uptake and transpiration.

The water content changes according to our periodic rainfall that starts half day and stops for one day. It initially starts at $\theta = 0.23$ and as rainfall keeps adding in water, it rises to around 0.365 at the time rain stops. Then it will keep dropping until 0.215 as rain stops because water keeps moving down due to gravity and matric potential.

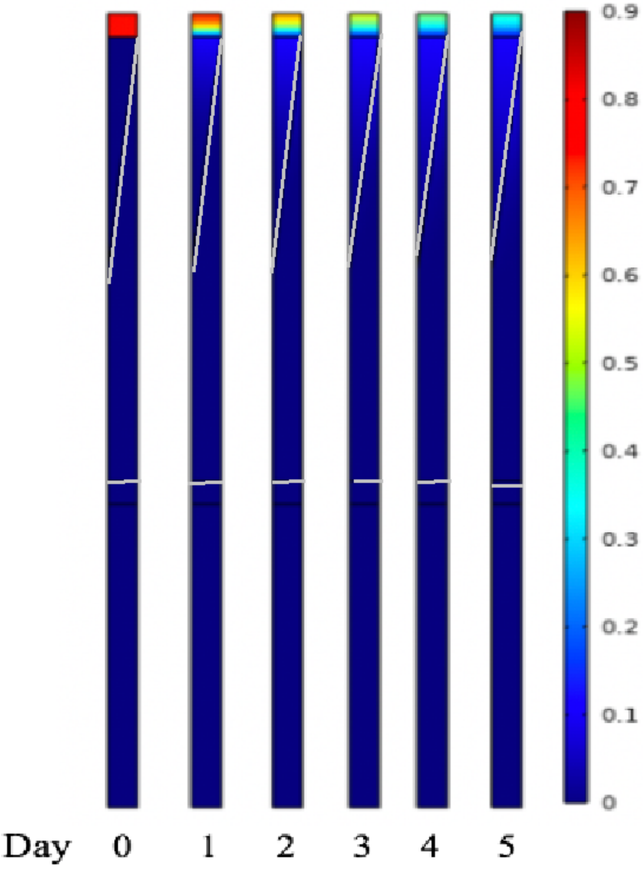


Fig 9. The 2D schematics of the concentration of nitrogen across the entire domain from day 0 to day 5 (left to right respectively). The initial concentration of nitrogen distribution at day 0 (leftmost plot). The nitrogen concentration distribution at the end of each day from day 1 to day 5 respectively.

Nitrogen disperses throughout the soil due to the movement of water in the model. It moves faster when rain is occurring and slower when there is no rainfall. The concentration of nitrogen slowly diffuses throughout the soil. However, the mass of nitrogen diffused is minimal over the short time frame used for water flow validation.

4.1 MESH CONVERGENCE

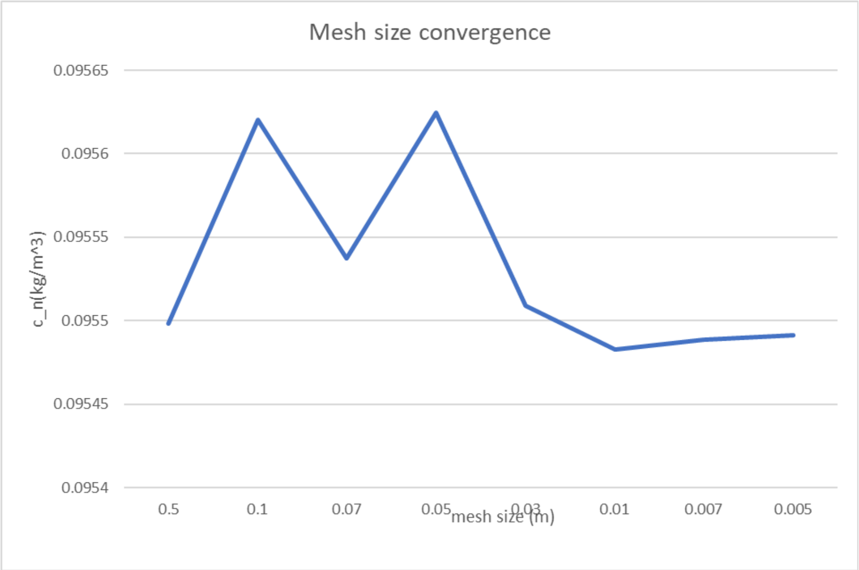


Fig 10. Element size mesh convergence. We started a mesh convergence at the point of data collection with a mesh size of 0.5. Reducing the mesh size showed that at 0.01, the mesh started to converge.

We performed a mesh convergence test on the concentration of nitrogen on day 5 at the point of the upper half of the root (Figure 7) with a starting mesh size of 0.5. The mesh begins to converge at a concentration of approximately 0.0955 $\frac{kg}{m^3}$, so we decided to use the corresponding mesh size of 0.01.

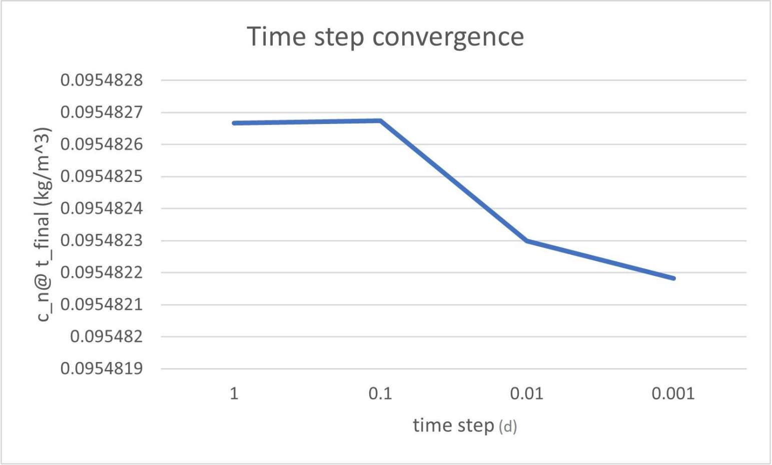


Fig 11. Time step convergence starting at step size of 1 day. Nitrogen concentration at final time was graphed against time step size to depict time step convergence. In this figure, it can be seen that the concentration values start to converge at a time step of around 1 day. This indicates 1 day will be our maximum time step size.

Following the mesh convergence test, we explored how time steps affect our concentration of nitrogen at the final time. As seen in **Figure 10**, the result changes as we vary the maximum time step from 1 to 0.001 days. However, the variation is two orders of magnitude smaller than the variation with the element size. This indicates that the time step size will not have a significant impact on our model.

4.2 VALIDATION

The model was validated using a study by Wu et. al. [5]. The authors measured matric potential, h, and water content, θ, with respect to the depth below the soil surface for 5 days after an irrigation event. We modeled our precipitation to match their field conditions by taking a per-5 day average of the $66\frac{cm}{year}$ measured rainfall.

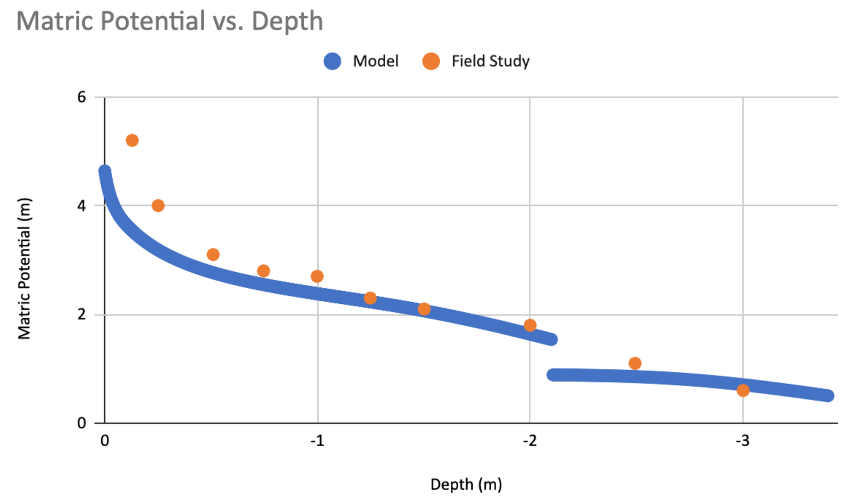


Fig 12. Matric potential with respect to depth. The blue line is our model's calculation of h, and the orange dots are data points collected from experimentation. The discontinuity occurs at the interface between sandy loam and fine sand. $R^2 = 0.766$.

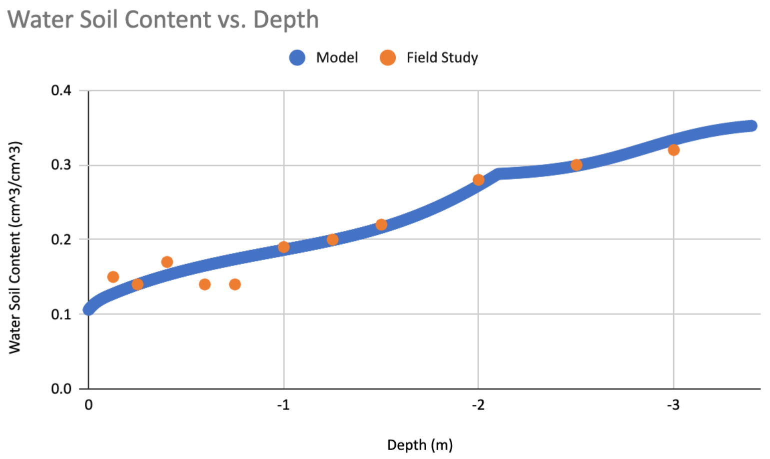


Fig 13. Water content with respect to depth. The blue line is our model's calculation of θ, and the orange dots are data points collected from experimentation [5]. The spike occurs at the interface between sandy loam and fine sand. $R^2 = 0.937$.

In the figures above, the orange points depict the experimentally yielded matric potential, h, and water content, θ, respectively. The computational results yielded by our model are represented by the blue line. The trend of our model matches that of the measured values with reasonable precision. The discontinuity in **Figure 13** is caused by the change in soil type, which switches at 2.0m from sandy loam to fine sand. The R^2 value of the simulation versus the experimental data is 0.766 for matric potential and 0.937 for water soil content.

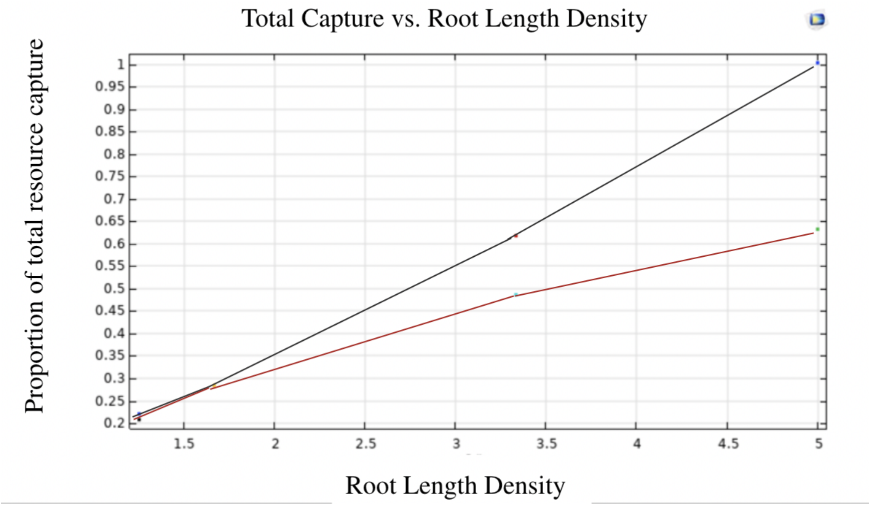


Fig 14. The change in how much of the total resources were captured by the root against the root length density. The black line represents the amount of nitrogen uptaken by the plant in our model, while the red line represents the theoretical value from a paper [15]. Under both assumptions, the total resource capture increases with an increasing root length density.

4.3 SENSITIVITY ANALYSIS

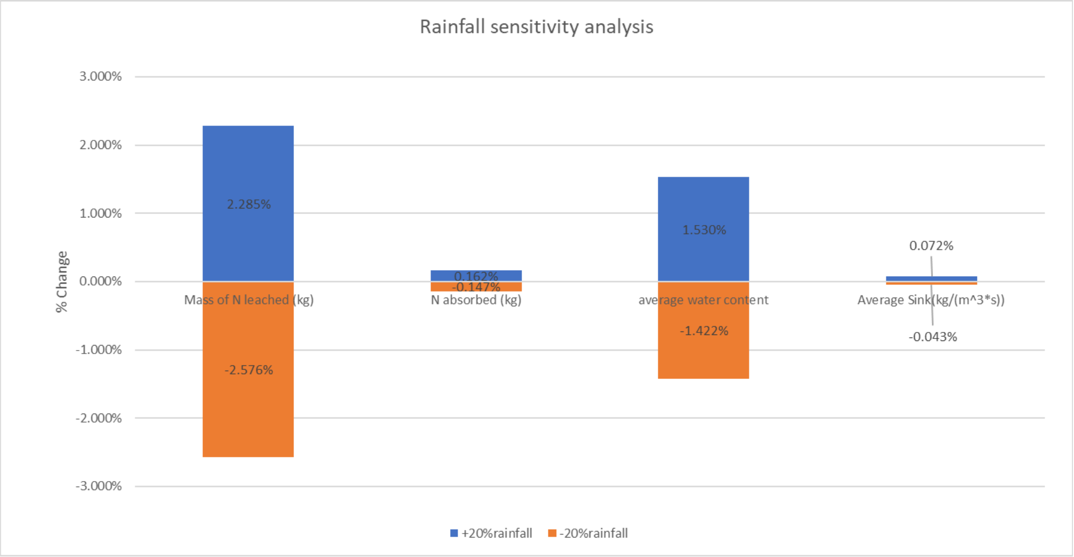


Fig 15. Sensitivity analysis for a 20% variation in rainfall over 7 days. The changes in mass of nitrogen, nitrogen absorbed by the plant, average water content, and average absorption are plotted. The mass of nitrogen leached has the most significant change over the period followed by average water content.

Rainfall amounts will have a bigger influence on the fluid flow equation which is water content therefore bringing more or less nitrogen down to the soil and root system (Figure 15). However, it will not have too much influence on mass transfer although it changed the root absorption rate by around 0.15% therefore changed the amount of nitrogen absorbed over 7 days.

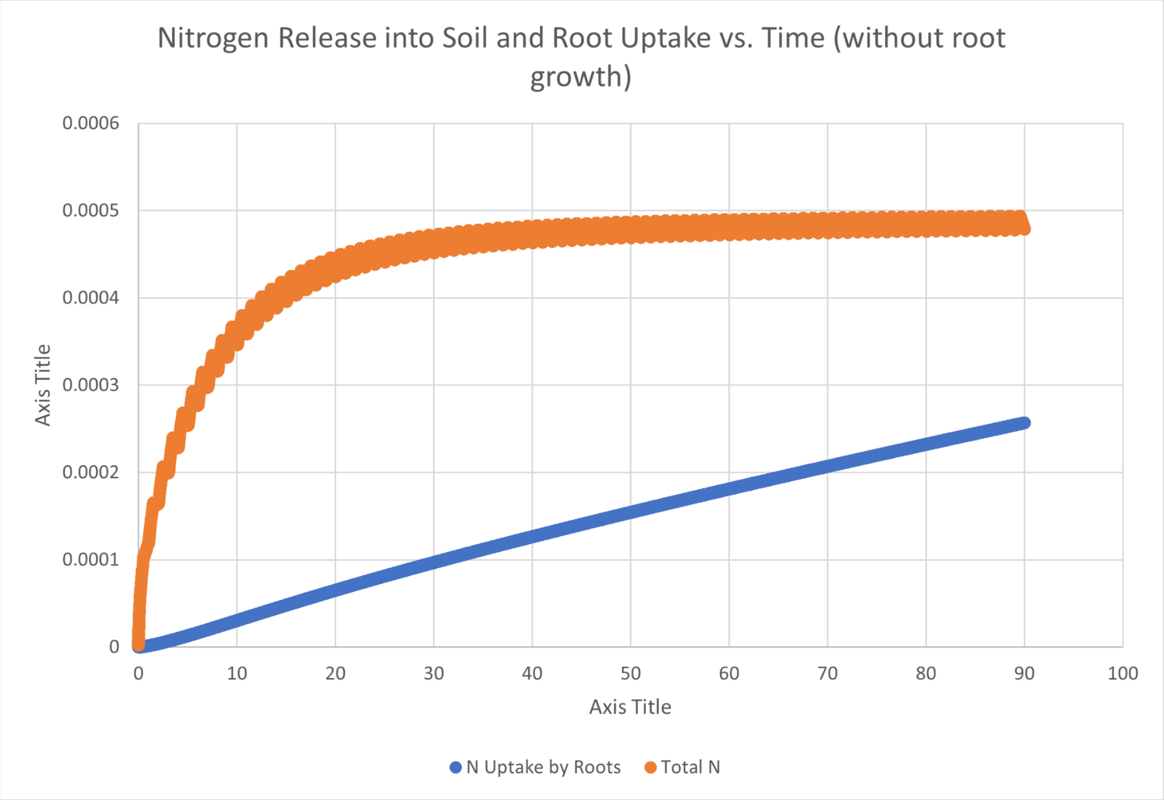


Figure 16. Amount of nitrogen flowed down into the soil over 90 days without root growth. 0.49 grams out of a total of 0.563 grams of nitrogen was released. 0.25 grams of the released nitrogen was absorbed by the plant roots.

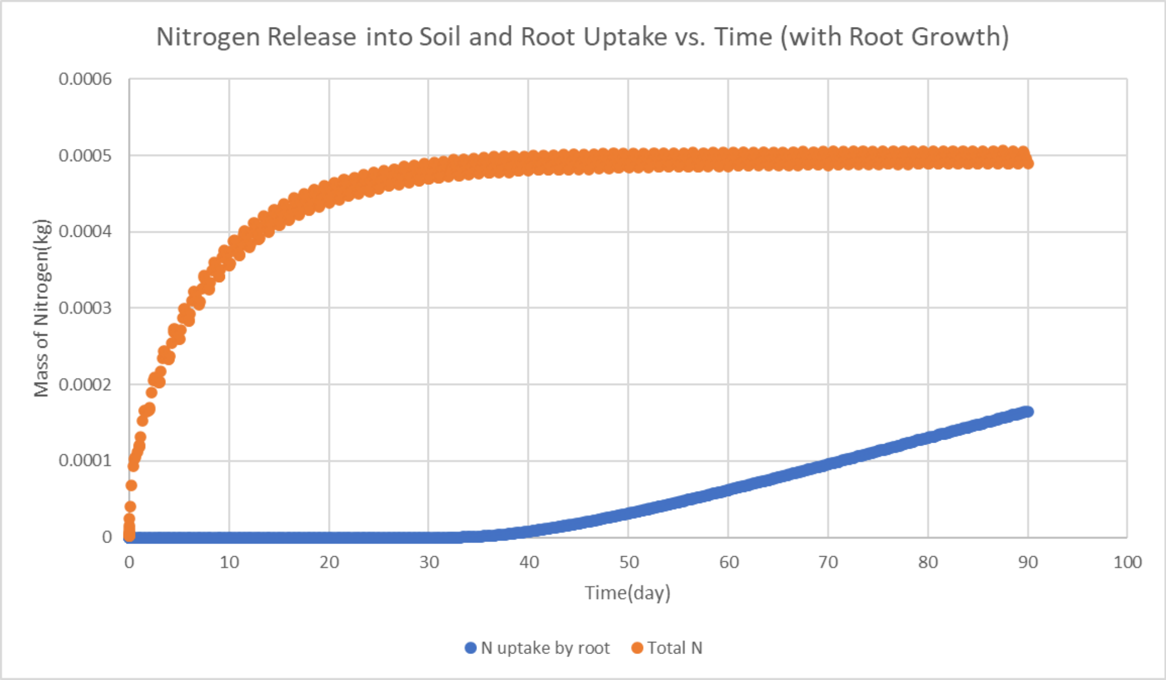


Figure 17. Amount of nitrogen flowed down into the soil over 90 days with root growth. 0.49 grams out of a total of 0.563 grams of nitrogen was released. 0.17 grams of the released nitrogen was absorbed by the plant roots.

The uptake and flow of nitrogen was modeled with root growth. Based on appendix C, our root length will start from 0 and reach around 0.95m over 90 days. In this case, only 30.3% of nitrogen was taken by the roots.

5. DISCUSSION AND CONCLUSION

The results of our model demonstrate that over half of the N placed in the fertilizer is unabsorbed by the roots. This necessitates some serious modifications to the root system in order to uptake more N. This includes the possible introduction of *nif* gene edited plants, or an N fixing microbial. The majority of uptake occurs in the upper third of the root domain, which is constant with time. This indicates that an optimal microbial will fix to the upper root domain, won't be susceptible to fluid driven convection, and may have more of an affinity for loamy soil such that it is not easily displaced from the major source of sink in the root system. By the same token, any gene modification to the crop root system should disproportionately affect the top roots.

5.1 DESIGN RECOMMENDATIONS

As seen in our model, with excess nitrogen, the plant takes up about 0.17 grams of nitrogen from the soil. This is about 30.3% of the amount of nitrogen in the fertilizer that was initially placed at the top. The addition of *nif* genes into plants would decrease the plant uptake term during night time cycles. Our design recommendation is for the plants to have enough active *nif* gene expression to have a production rate of 0.17 grams of nitrogen per week. Although the current rate and efficiency of *nif* expression is not known, following the recommendation will eliminate the need for additional nitrogen fertilizers and prevent leaching.

7. APPENDICES

7.1 APPENDIX A

Table 1: Soil parameters.

Soil Parameters			Soil Type	
	Symbol	**Units**	Sandy Loam	Fine Sand
Depth Below Surface	z	(-m)	0-2.0	2.0-3.5
Dispersion Coefficient	E	(cm^2/hr)	0.78	0.152
Saturated Hydraulic Conductivity	K_s	(cm/d)	73.5	384.7
Saturated Water Content	θ_s	(cm^3/cm^3)	0.445	0.356
Residual Water Content	θ_r	(cm^3/cm^3)	0.076	0.010
Van Genuchten Coefficients	α	(1/cm)	0.0070	0.0091
	n	dimensionless	3.12	5.59
Maximum Water Content	θ_f	(cm^3/cm^3)	0.42	0.36
Transpiration Rate	T	(mm/day)	4	N/A
Density of topsoil	ρ_s	$(\frac{kg}{m^3})$	1650	1750

Distribution Coefficient	K_d	dimensionless	0.24	0.76
Table 1 contains soil properties used in fluid flow and mass transfer calculations used in this model.				

Parameters in Table 1 sourced from [7, 9, 12, 18, 21, 22]

7.2 APPENDIX B

CPU time taken: 50 mins
Physical memory: 2.0 GB
Virtual memory: 2.2 GB

7.2.1 Solver

The Coefficient PDE and Stabilized Convection-Diffusion Equation in COMSOL were used to solve our mass transfer and fluid flow equations, respectively. The Coefficient PDE was altered to fit the mass transfer equation seen in eq(1). We neglect absorption coefficient, mass coefficient and the conservative flux term. The Stabilized Convection-Diffusion Equation was used to solve eq(5), the water flow equation. We can exclude the conservative flux convection coefficient and the absorption coefficient..

7.2.2 Time Stepping

Max Timestep: 0.1 day

7.2.3 Tolerance

Absolute tolerance: 0.01

Table 2: absolute error vs. concentration of nitrogen

ABS tol	C_N
0.1	0.095482674
0.01	0.095482674
0.001	0.095482674

We chose an absolute tolerance of 0.01 after a sweep over lower orders of magnitude proved to be inconsequential on the concentration of Nitrogen, as seen in the table above.

7.2.4 Solution Convergence and Mesh Refinement

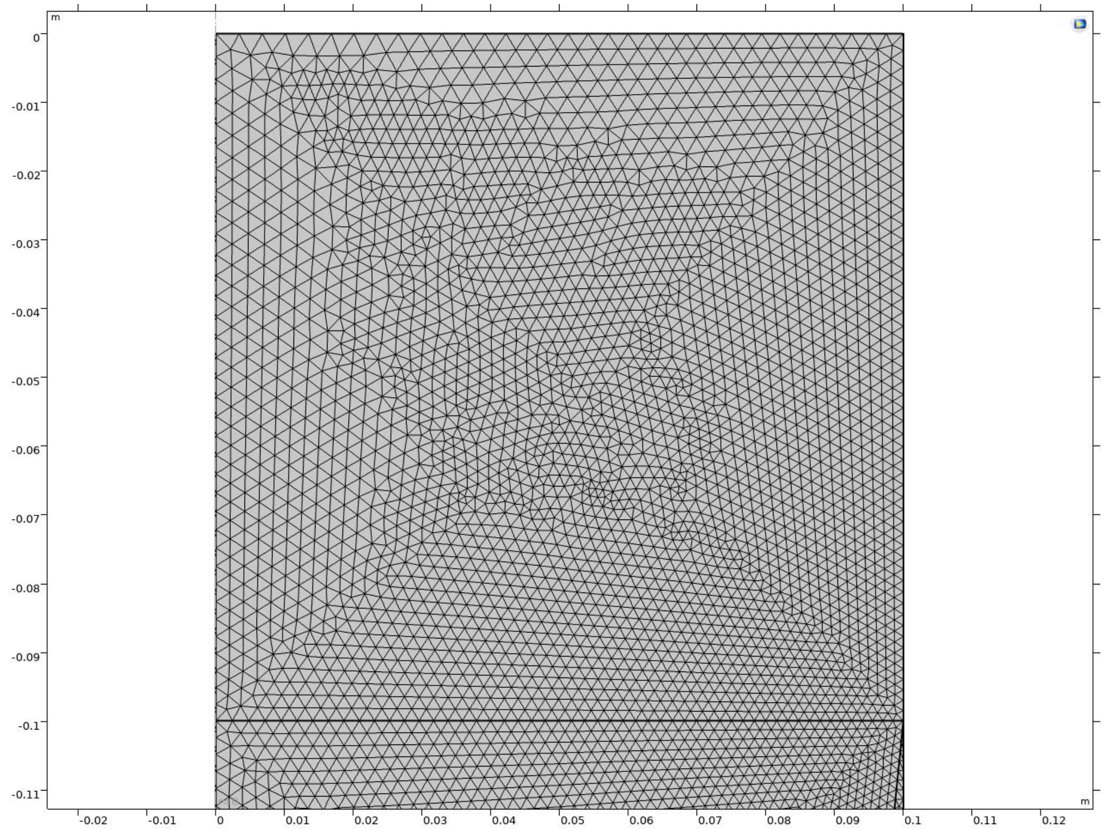


Fig 18. Plot of mesh size of 0.01m. A triangular mesh with a size of 0.01 is used in the model. This sizing was chosen due to a mesh convergence.

Figure 17 shows a close up of our mesh that was used to simulate soil. As seen in Figure 10, making the mesh smaller has no effect on the concentration of nitrogen (c_n). C_N converges to 0.0955kg/m^3 at our final time at the point shown in Figure 9. We chose to use a mesh size of 0.01, which corresponded to the value at which CN converged to in Figure 9.

7.3 APPENDIX C

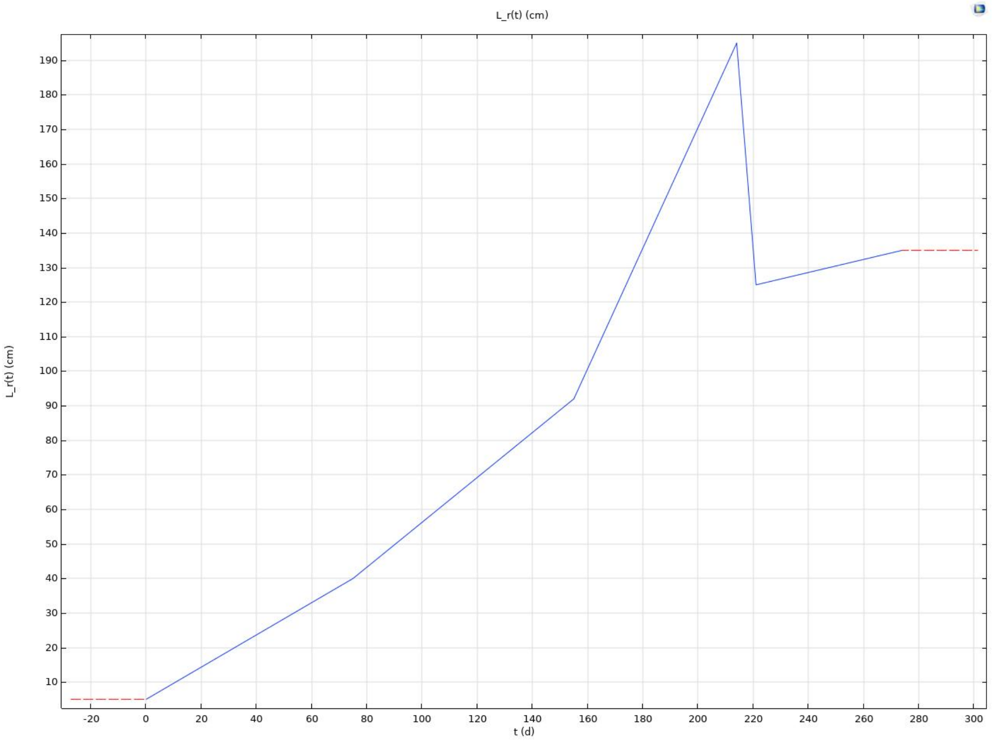


Fig 19. Plot of root length(L_r) over time. Over the course of 90 days, the model of how deep the roots grew into the soil follows the plot. This was the model used in the simulation for a full season.

7.4 APPENDIX D

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