

# Root architecture modelling in heterogeneous soils - Describing root responses using a dynamic root architecture model

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## Zusammenfassung

Die Modellierung der Wurzelarchitektur ist wichtig um die Effizienz von Wurzelreaktionen in nährstoffarmen Szenarien zu untersuchen und Entscheidungen in der Pflanzenzucht sowie in der Bewirtschaftung zu leiten. Momentan werden Wurzelreaktionen empirisch beschrieben wobei die Wurzelarchitektur in Wasser- und Nährstofftransportmodellen eingeht. Unser Ziel eine genauere Beschreibung der Nährstoffaufnahme und der Wurzelreaktionen, was durch den Klimawandel und eine mögliche zukünftige Phosphatkrise an Bedeutung gewinnt.

In dieser Arbeit präsentieren wir eine Modellstudie, welche Konzepte der Wurzelreaktion auf heterogene Phosphatverteilung im Boden demonstriert. Wir verwenden dazu das dynamische Wurzelarchitekturmodell von LEITNER et al. (2010a). Das Wachstum des Wurzelsystems wird in einem virtuellen Topf simuliert und der Einfluss der Wurzeigenschaften auf die Gesamtaufnahme untersucht. Wurzeigenschaften sind dabei anatomische sowie morphologische Änderungen wie der Winkel zwischen Wurzeln, Gravitropismus, Chemotropismus, und die Ausbreitung der Wurzeln (z.B.: Anzahl der Seitenwurzeln, primäre Wachstumsrate). Die resultierende Phosphate (P) Konzentration wird untersucht und die kumulative Aufnahme des Wurzelsystems analysiert. Diese Daten werden mit gemessenen Werten und Literaturdaten verglichen.

Die Simulationen wurden in Matlab durchgeführt. Die partiellen Differentialgleichungen des Modells wurden in Comsol Multiphysics gelöst. Durch mathematische Modellierung hoffen wir, das Verständnis der zugrundeliegenden Prozesse zu fördern, und ein flexibles Tool für experimentelles Design zur Verfügung zu stellen.

## Introduction

Since the 1950s crops were improved by breeding for high-input agroecosystems. Extensive use of fertilizers lead to environmental problems and high production costs. Changed environmental conditions due to global warming as well as increased fertilizer costs threaten the global food supply. A further management intensification is not a sustainable option. LYNCH (2007) called for a 'Second Green Revolution' where crops are bred to improve the productivity

## Summary

Root architecture modelling is of prime importance to assess the efficiency of plant root responses under nutrient limited situations for crop growth and thereby guide breeding and management decisions. Currently, the representation of stress responses of root systems is largely empirical in macroscopic root models build into water and nutrient transport simulation tools. We aim for an accurate description of plant nutrient uptake and root system response, which is an important challenge in the light of upcoming shortages of mineral fertilizers and climate change.

In this work we will present a modelling study demonstrating concepts how plant response to heterogeneous phosphate distribution. We will use the dynamic root architecture model presented in LEITNER et al. (2010a). Root system growth is simulated in virtual pot and the impact of various root system traits to overall uptake is analysed. Root system traits will include anatomical and morphological changes such as changes in the angle between roots, gravitropism, chemotropism, and root proliferation (e.g. lateral root initiation frequency and elongation rate). The resulting phosphate (P) concentration will be investigated and the cumulative root system uptake over time will be analysed. The values are compared to measured data and literature values.

The simulations are performed using Matlab. The partial differential equations of the model are solved using Comsol Multiphysics. By mathematical modelling we hope to increase insight into underlying processes and to provide a flexible tool for experimental design.

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and sustainability of low-input agroecosystems. In such a breeding strategy the root architecture is crucial for the selection process. Architectural, morphological, anatomical and physiological root traits influence plant nutrient and water uptake (LYNCH 1995). However, it is difficult to quantify the effect of a specific root system trait, since plant nutrient and water uptake are influenced by complex rhizosphere processes. A deeper knowledge of the growing root system and its dynamic rhizosphere will enable us to determine suitable root system traits for management optimization.

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The root system architecture is a fundamental aspect for crop productivity. In this work we will focus on P efficiency of *B. napus*. P uptake efficiency is a current challenge due to upcoming phosphate crisis (VANCE 2003). For studying plant water and nutrient uptake, various dynamic 3-dimensional root system models were developed by DIGGLE (1988) (RootMap) and PAGES et al. (1989), which are based on a herringbone topology. LYNCH et al. (1997) (SimRoot) and SPEK (1997) (ArtRoot) extended these root growth models with focus on visualisation. PAGES et al. (2004) presented a root system model allowing different types of roots which are not strictly related to a topological order (Root Typ). The existing dynamic root growth models are mostly based on generic software, therefore it is often not apparent what the underlying equations and assumptions are. In contrast LEITNER et al. (2010a) developed a dynamic root architecture model based on L-Systems and demonstrated its use for modelling various kinds of root tropisms. In this work this approach is used to calculate root growth effected by gravitropism and restricted by the rhizotron geometry.

Root architecture models determine nutrient uptake using sink terms, which estimate the soil status, i.e. P depletion in a representative elementary volume. Sink terms are frequently based on mass flow and diffusion around a single root (BARBER 1995, TINKER and NYE 2000). Depending on the exact single root model under consideration the sink term is either solved by static approximations (YANAI 1994), analytically (DE WILLIGEN and VAN NOORDWIJK 1994a, 1994b), by asymptotic approximation (ROOSE et al. 2001, ROOSE and KIRK 2009) or by numerical methods (LEITNER et al. 2010c). More recently, multi-scale analysis and homogenisation helped to develop new sink terms (LEITNER et al. 2010b). In this work we solve the single root model numerically using Comsol Multiphysics.

We present a simulation case study where a maize root system is grown in a virtual pot. Root growth and P uptake is calculated simultaneously and spatial P distribution within the pot can be investigated. With this approach simulation results can be easily compared to experimental studies. Our simulation environment can be used to develop quantified hypothesis and aids in experimental design.

## Methods

Root system architecture was simulated using the model of LEITNER et al. (2010a). In the simulation study we will compare the efficiency of gravitropism and chemotropism in a virtual pot. Dynamic root and soil interaction is described by applying two models in turns, one for root growth and one for plant P uptake. In the following we describe the relevant part of the root architecture model and the P uptake model under consideration.

### Root architecture modelling - Tropisms and foraging strategies

In this work we only present the way in which tropisms are described. A complete description of the dynamic root growth model is given in LEITNER et al. (2010a).

We describe tropisms by randomly picking  $N$  different root head rotations  $(\alpha, \beta)$ , where  $\alpha$  describes a pitching rotation and  $\beta$  a rolling rotation. The angle  $\alpha$  is a normally distributed random number with mean 0 and standard deviation  $\sigma_{dx}$  which is dependent of the spatial resolution  $dx$ . The angle  $\beta$  is uniformly distributed from  $-\pi$  to  $\pi$ . From the  $N$  choices we pick the optimal pair  $(\alpha, \beta)$  regarding a specific objective functions. Therefore, in the model tropisms are characterized by the two parameters  $N$  and  $\sigma_{dx}$ . This approach has two advantages: The effect of tropisms is not depend on the spatial resolution along the root axis and the objective function can be freely chosen. In this way, different tropisms can be realised.

Gravitropism can be achieved by the objective function  $f=h_z$ , where  $h_z$  is the vertical  $z$ -component of the vector  $h$  pointing in the direction of the root tip.

Chemotropism is achieved by  $f=-s(x+dx h)$ , where  $s$  is a scalar field which contains the nutrient concentration,  $x$  is the position of the root head, and  $dx h$  is the change in root tip position. Other tropisms could be described by setting  $s(x)$  to scalar fields of water content, pressure head or temperature. Objective functions can be freely combined (e.g. by linear combination). In this way, various types of tropisms can be realised.

In many experiments like pot or rhizobox experiments, root growth is spatially bounded (DOUSSAN et al. 2006). We can bound our root growth simulations by an arbitrary geometry which is given implicitly by a signed distance function. The signed distance function determines how close a given point is to a boundary and returns a negative value if the point is outside the boundary (following PERSSON and STRANG 2004). Additionally, this provides a way to include obstacles in our model.

The following algorithm takes the spatial boundaries into account. In a first step, the rotation angles  $\alpha$  and  $\beta$  are chosen as described before. If the new root tip position does not lie within the geometric boundaries, then a new pair  $(\alpha, \beta)$  is chosen as follows: First, only  $\beta$  is chosen uniformly random between  $-\pi$  and  $\pi$  while  $\alpha$  is left unchanged. If, after a maximal number of trials  $n_\beta$ , no new valid pair  $\alpha$  and  $\beta$  has been found,  $\alpha$  is increased for a small fixed angle  $d\alpha$  and the procedure for finding an angle  $\beta$  is started again. This simple approach leads to a realistic root behaviour at the boundaries, where thigmotropism can be observed.

### Nutrient uptake model

We describe P uptake using Michaelis Menten kinetics. P transport around a single root is described by the axisymmetric impeded diffusion equation (BARBER 1995, TINKER and NYE 2000):

$$(\theta + b) \frac{\partial c}{\partial t} = \nabla \cdot (D_l f \theta \nabla c)$$

where  $c$  is the phosphate concentration in soil solution,  $t$  the time,  $\theta$  the constant volumetric water content,  $b$  the buffer power,  $D_l$  the diffusion coefficient in soil solution and  $f$  the impedance factor of diffusion in a porous medium. At the

root surface ( $r=a$ ), active nutrient uptake is described by Michaelis Menten kinetics

$$D_l f \theta \nabla c \cdot \mathbf{n} = -\frac{v_{max} c}{K_m + c},$$

where  $\mathbf{n}$  is the unit normal pointing away from the root surface,  $v_{max}$  is the maximal influx into the root and  $K_m$  is the Michaelis Menten constant. For P passive uptake due to water uptake can be neglected (ROOSE and KIRK 2009). At the outer boundary at the half mean inter-root distance ( $r=L/2$ ) we imply a no flux boundary condition

$$D_l f \theta \nabla c \cdot \mathbf{n} = 0.$$

Initially, we assume heterogeneous initial concentration,  $c=c_{L0}$  at the left half of the pot and  $c=c_{R0}$  at the right half at time  $t=0$ .

The partial differential equations are solved using Comsol Multiphysics. We calculate root uptake for each time ( $t$ ) and mean inter-root distance ( $L$ ) obtaining a two dimensional look up table for each class of root radii ( $a$ ).

## Results

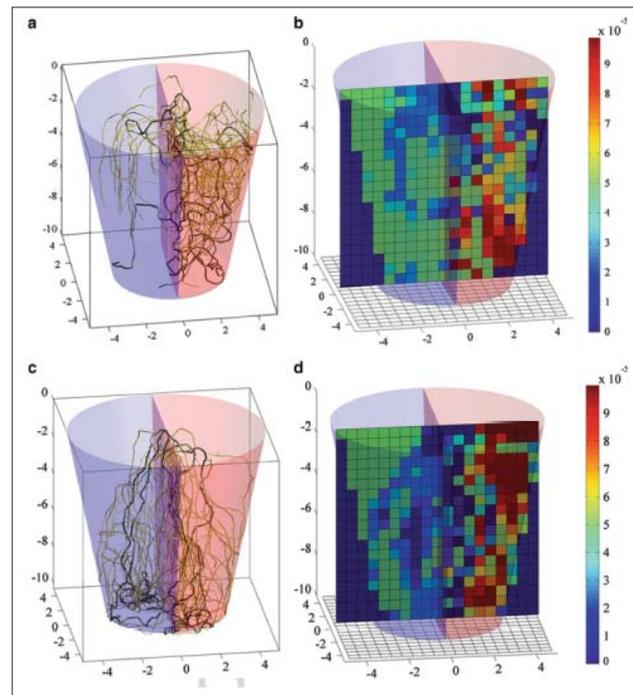
In the simulation case study we simulated two root system in virtual pots with a simulation time of 20 days. We compared the effect of gravitropism on P depletion. *Figure 1a* shows root system development due to chemotropism, while *Figure 1c* shows the development under gravitropism only. We can observe that using chemotropism the root system is much more dense in the right pot part and generally more evenly distributed. *Figure 1b,d* represents the corresponding P concentration in the virtual pots. We see that the right part of the pot with high initial P concentration is stronger depleted in the case using chemotropism (*Figure 1b*). This leads to a higher P uptake of the root system using chemotropism.

To quantify the difference between the two root system development strategies we calculated the cumulative root system P uptake over time (see *Figure 2*). After 20 days the root system with chemotropism showed an 1.5-fold increase of P-uptake.

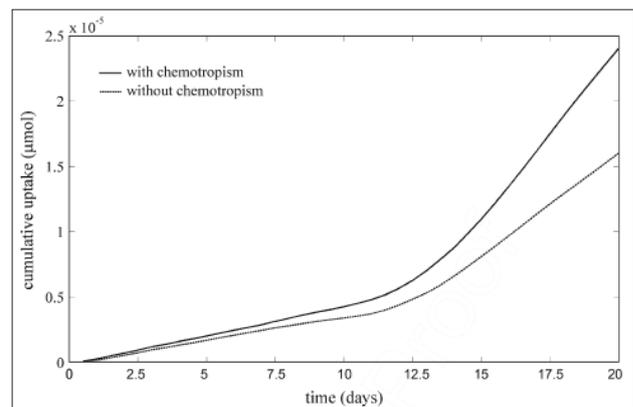
## Discussion

We presented a modelling approach to calculate P uptake of a growing root system in a virtual pot. The model is based on a simple mechanistic single root model (BARBER 1995) which is coupled to a growing root system. Because of the mechanistic nature of the model most parameters can be derived by direct measurements. The model takes the developing root system, emerging depletion zones as well as inter-root competition into account. By accurately describing these processes that hinder P uptake the model acts as lower bound for describing plant P uptake, i.e. modelled P uptake had the right magnitude but was clearly underestimated.

The reason for this is that important processes that enhance P uptake have not been included. On single root scale P



**Figure 1: Root architecture and P concentration after 20 days. The initial P concentration was  $1e-4 \mu\text{mol cm}^{-3}$  on the right half and  $5e-5 \mu\text{mol cm}^{-3}$  on the left half of the pot. (a) root system growth using chemotropism (b) soil depletion due to root system (a) (c) root system growth using gravitropism only (d) P depletion due to root system (c) (reproduced from SCHNEPF et al. 2010).**



**Figure 2: Cumulative P uptake by growing root systems, with and without chemotropism (reproduced from SCHNEPF et al. 2010).**

uptake is enhance by (a) root hairs (LEITNER et al. 2010b) (b) solubilisation due to organic acid anions (OBURGER 2011) (c) mycorrhizae and soil bacteria ALLEN (2007). The model approach can help to analyse complex biophysical systems by adding mechanisms step by step. Aim is to increase the fundamental understanding of plant nutrient uptake and root response. Analysis of root architecture traits will enable better plant breeding strategies.

In this work we presented a simulation case study where we compared different root foraging strategies (gravitropism and chemotropism). We showed that even in this simple

model settings cumulative uptake of the root systems were significantly different. In future work we plan a model validation using P rich patches in plant pots and analyse root systems in vitro using x-ray computer tomographic imaging (following TRACY et al. 2010).

The presented approach offers a framework for developing new quantified hypothesis and aids experimental design. By adding certain mechanisms we can quantify the influence of a specific root system trait on P uptake. Such a clear mechanistic description will facilitate experimental design for validation of the hypothesis.

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