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"3-d simulation of nutrient uptake"

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Comparison of nutrient uptake between 3-dimensional simulation and an averaged root system model

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Abstract. We present a new numerical approach describing nutrient uptake in three dimensions. Dynamic boundary conditions are considered at the individual root surfaces within a root system. As an example we compare the 3-dimensional simulation results of phosphate uptake by a young maize root system to the corresponding effective solution. We show that the two solutions are similar concerning phosphate uptake and the size of the depletion zones. The presented approach makes it possible to verify simplifications that are made in the development of effective models. Furthermore, it is possible to extend existing models by including spatial heterogeneities which will increase our understanding of rhizosphere processes.

Keywords: Mathematical modelling, phosphate depletion, nutrient uptake, Comsol Multiphysics, 3-dimensional simulation.

Understanding rhizosphere processes is fundamental for breeding nutrient efficient crops and for increasing plant resource efficiency. Nutrient uptake of a single root was described by Barber (1995) and Tinker and Nye (2000) using the convection diffusion equation. This classical model was developed further in numerous ways including more rhizosphere processes, such as exudation Kirk (1990) or the effect of root hairs Leitner et al. (2010b).

From these mechanistic single root models, sink terms were developed depending on root length densities, that can be used for models on plant scale and for 3-dimensional simulations. This approach was done for water uptake of transient root systems from soil by Clausnitzer and Hopmans (1994) and was extended for nutrient uptake by Somma et al. (1998) and Dunbabin et al. (2002). Furthermore, water uptake was coupled to water transport within the roots' xylems Doussan et al. (2006) Javaux et al. (2008). The development of such sink terms is one of the current challenges. Recently, mathematical methods like homogenisation and averaging are likely to offer improvements Roose and Schnepf (2008).

With increasing computer power it will soon be possible to solve the underlying mechanistic equations explicitly in three dimensions. In this work, we present first advances in directly solving these equations using the root surfaces as geometric boundaries in a finite element simulation. We describe phosphate uptake of a growing maize root and compare the results to the up-scaled effective model presented in Roose et al. (2001).

Material and methods

First we describe nutrient uptake and growth. Then the uptake by a growing root system is solved using two different approaches: firstly, by solving the 3-dimensional model numerically based on Schnepf and Leitner (2009); secondly, by using an effective model as by Roose et al. (2001).

Plant nutrient uptake and dynamic root growth

Water transport is neglected which is a frequently used assumption for sparingly soluble nutrients Roose and Kirk (2009). Therefore, we describe nutrient transport by the impeded diffusion equation Barber (1995); Tinker and Nye (2000) that takes into account soil diffusion, impedance and equilibrium binding of nutrients to the soil particle surfaces:

$$(\theta + b)\frac{\partial c}{\partial t} = \nabla \cdot (D_l f \theta \nabla c), \tag{1}$$

where c is the phosphate concentration in soil water, t the time, θ the constant volumetric water content, b the buffer power, D_l the diffusion coefficient in water and f the impedance factor of diffusion in a porous medium. At the root surface, active nutrient uptake is described by Michaelis Menten kinetics

$$D_l f \theta \nabla c \cdot \boldsymbol{n} = -\frac{F_m c}{K_m + c}, \tag{2}$$

where $\boldsymbol{n}$ is the unit normal pointing away from the root surface, F_m is the maximal influx into the root and K_m is the Michaelis Menten constant.

We assume a homogeneous initial concentration $c = c_0$ at time $t = 0$. We consider root growth for each topological root order i Roose et al. (2001). The length of each order i root, which has been created at time $t = 0$, is given by

$$\lambda_i(t) = k_i(1 - \exp(-\frac{r_i}{k_i}t)), \tag{3}$$

where k_i is the maximal root length and r_i is the initial growth rate for order i roots.

Explicit 3-dimensional model

By adding spatial information we derive a dynamic root growth model similar to that proposed by Pages et al. (1989). We create the root system geometry by using L-Systems Leitner et al. (2010a). This results in a number of cylindrical segments representing the roots at the final simulation time.

Furthermore, the creation time ct_i of each cylindrical segment i is determined. We use DistMesh Persson and Strang (2004) to create a 3-dimensional mesh of the soil domain around the final root system, where the root surfaces are represented by geometric boundaries, see Figure 2(c). The mesh is imported to Comsol Multiphysics 3.5 to solve the nutrient transport equation. The dynamic root growth is implemented by using a transient boundary condition at the root surface:

$$D_l f \theta \nabla c \cdot \boldsymbol{n} = \begin{cases} t > ct_i & : -\frac{F_m c}{K_m + c} \\ t \leq ct_i & : 0 \end{cases}, \tag{4}$$

where ct_i is the creation time of the cylindrical root segment surface i. Thus at simulation start ($t = 0$) all root surface boundary conditions are set to no-flux. The root system develops with increasing time and the boundary conditions of the corresponding root segments are set to Michaelis Menten influx. Root surface creation times are precomputed and passed to Comsol Multiphysics 3.5 as a 3-dimensional interpolated function.

Effective model

In the second approach we assume that there is no inter root competition. Therefore, influx into each root can be calculated independently. For one root, we consider a 1-dimensional axial symmetric problem. Nutrient transport is described by the axial symmetric impeded diffusion equation, corresponding to Eqn (1), given by

$$(\theta + b)\frac{\partial c}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}(r D_l f \theta \frac{\partial}{\partial r} c), \tag{5}$$

where r is the distance to the root axis. At the root surface we assume Michaelis Menten uptake, see Eqn (2). At the outer boundary we assume a far field concentration which equals the initial concentration $c_{far} = c_0$. We solve the transient equation in Comsol Multiphysics 3.5. In this way we obtain the root surface influx $f_{as}(t, a_i)$, where t is time and a_i is the root radius of the topological order i. The overall root system uptake is calculated by integrating over the root length at time t.

The nutrient uptake rate $F_{ij}(t)$ of each root j of order i at time t is calculated by

$$F_{ij}(t) = 2\pi \int_0^{\lambda(t - t^*_{ij})} a_i f_{as}(t - t^*_{ij} - \tau_i(z), a_i) dz, \tag{6}$$

where a_i is the root radius, t^*_{ij} is the creation time of the root j, thus $t - t_{ij}$ is the age of the base, and τ_i is the inverse function of λ_i, thus $t - t^*_{ij} - \tau_i(z)$ is the age at length z. The integral is

numerically evaluated using adaptive Simpson quadrature.

Model parameters

In this example, we consider the uptake of phosphate by a young maize root. Typical parameter values appropriate for phosphate uptake of maize were taken from literature Tinker and Nye (2000); Föhse et al. (1991): buffer power $b = 239$, volumetric water content $\theta = 0.3$, impedance factor $f = 0.3$ and initial concentration $c_0 = 5 \cdot 10^{-4}$ μmol cm^{-3}; The diffusion coefficient $D_l = 10^{-5}$ cm^2 s^{-1}; Michaelis Menten parameter are maximal influx $F_m = 2.2 \cdot 10^{-7}$ μmol cm^{-2} s^{-1} and Michaelis Menten constant $K_m = 2.3 \cdot 10^{-3}$ μmol cm^{-3}. Root system parameters for the L-System root growth model Leitner et al. (2010a) were taken from Roose et al. (2001): initial growth rate $r_0 = 2$, $r_1 = 6.4$ cm day^{-1}, maximal root length $k_0 = 51.4$ cm, $k_1 = 7.6$ cm, length of basal zone $l_{b0} = 0.7$ cm, apical zone $l_a = 15.7$ cm, and inter branch distance $l_{0n} = 0.7$ cm; The root radius was assumed to be $a_0 = 0.08$ cm, $a_1 = 0.04$ cm. Numerical parameters of the 3-dimensional simulation are the spatial resolution along the root axis of 0.1 cm and the temporal resolution of 1 hour. The finite element mesh consists of 12681 nodes and 48876 tetrahedrons. The tetrahedron size grows linearly with increasing distance from the root surface, ranging from to 0.042 cm^3 to 4.634 cm^3, see Figure 2(c).

Results

We calculate the uptake of the growing maize root system with both methods, (a) explicit 3-dimensional simulation and (b) effective simulation of Roose et al. (2001). Simulation time of the 3-dimensional model was about 1 hour on a dual core computer with 2.2 GHz. Uptake and cumulative uptake over the first 12 days is given in Figure 1(a) and 1(b). The differences in the solutions have several reasons. Firstly, there are assumptions that will decrease the influx in the 3-dimensional model compared to the effect model: temporal and spatial resolution of the growing root system, the effect of inter-root competition and applying a no-flux condition at the container boundaries in the 3-dimensional model. Secondly, there are numerical errors that are expected to increase the influx: the root system's surfaces are less smooth due to triangulation, see Figure 2(b), and numerical dispersion could increase the effective diffusion. The size of the depletion zone at the base of the 0^{th} order root is 0.25 cm in 3-dimensional model and exactly equals the one of the effective model.

After the 10^{th} day uptake increases strongly in both simulations. This is due to the emergence of first order roots, which grow expeditiously into undepleted soil. The cumulative uptake after

12 days is 2.8% higher in the 3-dimensional simulation. The 3-dimensional model can be used to visualise the processes under consideration. We use horizontal slices to show the phosphate concentration in the soil volume, see Figure 2(a) and 2(b). In the close up we can see how the depletion zones around the single roots look like. In the case of phosphate the depletion zone is narrow and overlapping depletion zones emerge only directly at the branching points. The colour at the root surface indicates the phosphate concentration at the boundary. We can see that the nutrient concentration is higher at the root tips since the depletion zone is only starting to emerge. This will result in higher influx into the root tips, see Eqn (2). In Figure 2(c) we show the mesh size, which is small near the root surface in order to resolve the steep concentration gradient.

Discussion

In this work, we present a numerical simulation of nutrient uptake in three dimensions. Though using root surfaces as geometric boundaries with a transient boundary condition is a simple and direct approach, it has never been implemented before. The main reasons for this are probably the huge memory requirements as well as the difficulties in implementation. The recent increase of computer power and the improvement of numerical software made it possible to partly overcome these problems. In our simulation we use this approach for the first time. However, at present it is limited to very small root systems because it is not possible to import more complex meshes into Comsol Multiphysics 3.5 due to parametrization errors of the boundary surfaces. We are looking for ways to solve this software problem. Currently, the mesh in the simulation is coarse leading to numerical errors and problems accurately representing the root system geometry.

The presented approach has two main applications. Firstly, comparing effective models to full 3-dimensional models provides a powerful tool in model development. If we can compute the underlying model in three dimensions we are able to verify simplifications that are made in the up-scaling process. Secondly, it is possible to extend existing models by including spatial heterogeneities. The proposed method can access inter-root competition, root dynamics, as well as differences in root function along the root axis. Especially the latter is promising for accurately describing the effect of exudation, since it occurs mainly at the root tips. By careful investigation of spatial heterogeneities we hope to be able to increase our understanding of important rhizosphere processes.

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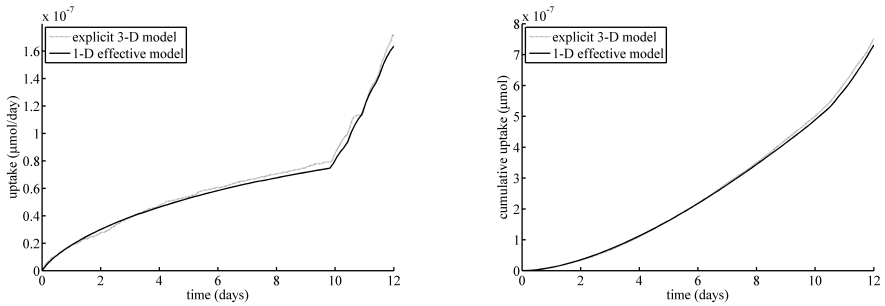
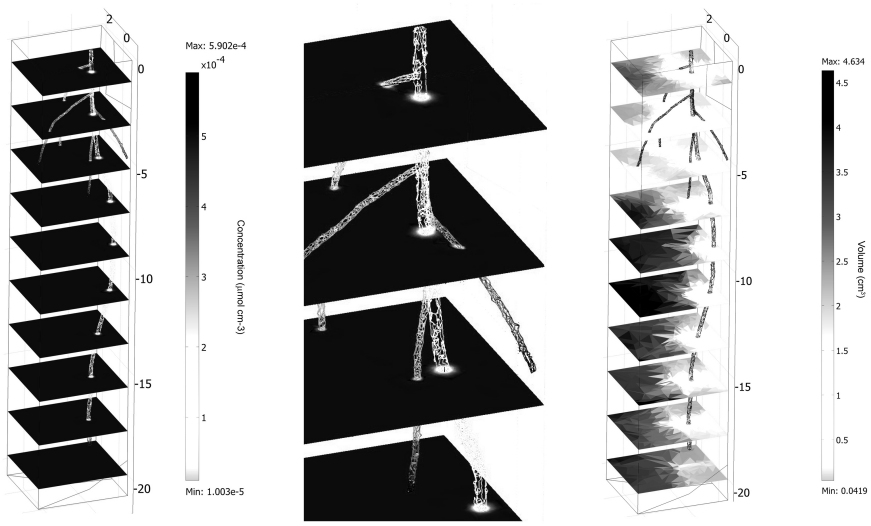


(a) Uptake (b) Cumulative uptake

Figure 1: Phosphate uptake of a maize root over 12 days since germination.



(a) Phosphate concentration (b) Close up of (a) (c) Mesh tetrahedron sizes

Figure 2: 3-dimensional simulation of a 12 days old maize root system for phosphate uptake.

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