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Analysis and simulation of a model of phosphorus uptake by plant roots

Myriam Comte

Abstract

This aim of this paper is to simulate the movement of groundwater and its uptake by plant roots as well as nutrient transport and uptake by plant roots. We study mechanistic models of soil water movement and solute transport with root uptake that explicitly take into account the geometry of the root system. We are interested in the mathematical and numerical treatment of the equations arising from these models.

1 Introduction

Among mineral nutrients, nitrogen (N) and phosphorus (P) are key elements for plant growth. However, in heavily fertilized agriculture, these nutrients can be potentially pollutants for water resources and, in the case of P, its availability might be limited in the future, as a non-renewable resource. As an answer to these problems, low-input agriculture shall be devised by optimizing the use of fertilizers (or soil natural resources) and water by plant roots in the soil. The aim of this paper is to better understand the interactive effects between root system architecture (geometry, growth) and P / water uptake, in relation with the soil spatial variability of resources. This will be undertaken by numerical modeling and mathematical optimization with different levels of details in the description of the root system. This should result in a modeling coupling soil water/nutrient transfer and uptake by a root system architecture, including retro-actions between aerial and subterranean parts of the plant.

In this paper we :

- simulate water movement in soil and water uptake by plant roots, together with the transport and uptake of nutrients,

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- explicitly take into account the geometry of a root system,
- study how water and nutrient uptake is affected by the type and shape of root systems.

In part 2 we describe the mathematical analysis of a model of phosphorus uptake by plant roots. The evolution of the concentration of P in the soil solution is governed by a convection-diffusion equation with a nonlinear boundary condition at the root surface, which is included as a boundary of the soil domain. A shape optimization problem is formulated in order to find root shapes maximizing P uptake. In part 3, we use unstructured mesh adaptation and parallel computing to develop numerical models of soil water and solute movement with root water and nutrient uptake at the plant scale.

2 Nutrient uptake : problem statement

2.1 Soil solute transport

The Richards equation represents commonly the movement of water in unsaturated soils. Combining Darcy's law

$$\mathbf{q} = -K(h)\nabla(h+z),$$

with the continuity equation [15] gives the Richards equation :

$$\frac{\partial \theta(h)}{\partial t} = \nabla \cdot (K(h)\nabla(h+z)) + S$$

where

- h is the matric head,
- \mathbf{q} is the Darcy flux,
- $\theta(h)$ is the volumetric water content,
- $K(h)$ is the hydraulic conductivity,
- z is the elevation
- S represents sources or sinks.

The nonlinear relationships $\theta(h)$ and $K(h)$ are given by empirical models whose parameters depend on the soil physical properties.

Several models can be used, such as the Brooks-Corey model or the van Genuchten model.

The evolution of the concentration c of a nutrient in the soil solution is governed by the following mechanisms:

- diffusion of nutrient ions in the soil solution, (*dominant for phosphate*),
- transport of nutrients by mass flow, (*dominant for nitrate*)

- absorption of nutrient ions in the soil solid phase, (*strong for phosphate, negligible for nitrate*).

Active nutrient uptake and its ion-selectivity can be regarded as a kinetic process equivalent to that described by Michaelis-Menten type kinetics, used for the description of enzym-catalyzed reactions [20]. Here, the Michaelis-Menten model relates the uptake rate to the concentration in the soil solution. The uptake rate h is related to the concentration in the soil solution and is given by

$$h(c) = \frac{I_m c}{K_m + c}, \quad I_m > 0, \quad K_m > 0$$

where I_m is the maximum uptake rate. The Michaelis constant K_m is the concentration at which the uptake rate is half of I_m . The Michaelis-Menten parameters I_m and K_m are ion-specific and depend on several factors such as plant species and plant age.

2.2 Root nutrient uptake

Let us consider a shape modeling the root surface. The exterior domain around the root is the studied section of the soil. Let us denote by $\Omega \subset \mathbb{R}^d (d = 2, 3)$ the soil domain, delimited by the root surface and the domain boundaries. Let Γ_1 be the boundary representing the root surface and $\Gamma_2 = \partial\Omega \setminus \Gamma_1$.

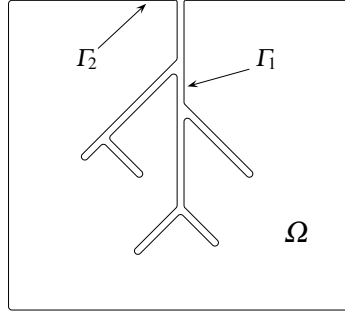


Fig. 1 Configuration of the domain

Let $T > 0$ be given and $I = [0, T]$. The concentration of P in the soil solution c is given by the following convection-diffusion equation :

$$\begin{cases} \partial_t(\theta c + \varphi(c)) = \nabla(A\nabla c - \mathbf{q}c) - R & \text{in } I \times \Omega, \\ \alpha h(c) = -(A\nabla c - \mathbf{q}c) \cdot \mathbf{n} & \text{on } I \times \Gamma_1 \\ 0 = (A\nabla c - \mathbf{q}c) \cdot \mathbf{n} & \text{on } I \times \Gamma_2 = I \times (\partial\Omega \setminus \Gamma_1), \\ c(0, x) = c^0(x) & \text{in } \Omega, \end{cases} \quad (1)$$

where

- \mathbf{n} is the unit outward normal to the boundary of the domain,
- c^0 is the initial P concentration,
- A is the diffusion coefficient of P in soil,
- θ is the volumetric water content,
- \mathbf{q} is the Darcy flux,
- R represent additional optional source or sink terms to the system; we will only consider source terms, such as fertilizer application,
- α is a parameter we introduce in order to obtain sufficient regularity of the boundary condition in the case $\Gamma_1 \cap \Gamma_2 \neq \emptyset$: $\alpha \in C^2(\partial\Omega)$ such that for $x \in \partial\Omega$

$$\begin{cases} 0 < \alpha(x) \leq 1 & \text{on } \Gamma_1 \\ \alpha(x) = 0 & \text{on } \Gamma_2, \end{cases}$$

- φ is an adsorption isotherm relating the amount of adsorbed P to the equilibrium concentration of P in solution ; an example is the Freundlich adsorption isotherm, defined by [17] :

$$\varphi(c) = \kappa \times c^b \text{ for } c \in [0, +\infty[, \kappa > 0 , b \in]0, 1[,$$

- h is a model of enzyme kinetics, relating in this case the root uptake rate of P to its concentration at the root surface ; an example has been given previously : the Michaelis-Menten model.

We don't restrict ourselves to considering explicit forms for φ or h : we only use general properties of these functions.

With J.-M. Coron, S. Guerrero, and P.-H. Tournier, we prove in [1] the following result :

Theorem 1 *Let $\beta \in (0, 1)$.*

Under suitable regularity conditions on the data and assuming $c^0 > 0$, problem (1) has a unique strictly positive solution in the space $C^{1+\beta/2, 2+\beta}(\overline{Q})$.

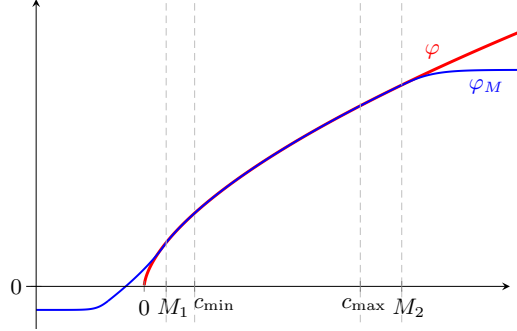
Proof. (some steps)

- we derive a priori estimates for positive solutions in $C^{1,2}(\overline{Q})$ using a comparison principle:

$$0 < c_{\min} \leq c(t, x) \leq c_{\max}, \quad (t, x) \in Q,$$

- we prove uniqueness of solution in $C^{1,2}(\overline{Q})$,

- we define φ_M by extending φ beyond arbitrary bounds M_1, M_2 with $0 < M_1 < M_2$ such that $\varphi_M \in C^3(\mathbb{R})$, $\varphi'_M \geq 0$ and $\varphi'_M(c) = \varphi''_M(c) = \varphi'''_M(c) = 0$ for $|c| > M_2 + \varepsilon_M$,



- the new problem (Pb_M) has a unique solution c_M in the space

$$C^{1+\beta/2, 2+\beta}(\overline{Q}),$$

- c_M can be bounded independently of M_1, M_2 :

$$0 < c_{\min} \leq c_M(t, x) \leq c_{\max}, \quad (t, x) \in Q,$$

- we choose M_1, M_2 such that $M_1 < c_{\min}$ et $c_{\max} < M_2$. It follows that the unique solution c_M of problem (Pb_M) is also a solution of the original problem (1). Thus, using the fact that problem (1) has at most one solution in the space $C^{1,2}(\overline{Q})$, we can deduce that problem (1) has a unique solution in the space $C^{1+\beta/2, 2+\beta}(\overline{Q})$.

2.3 Shape optimization

Experiments have shown that the uptake of phosphorus especially for young plants whose growth depends strongly on the uptake capacity of phosphorus, is influenced by the structure and distribution of the root system : phosphorus uptake creates a depletion profile in the vicinity of the surface of the root, and due to the slow diffusion of phosphorus, a root system that explores a greater volume of soil is more effective. In order to study this phenomenon, we consider two caricature forms of root systems in dimension 2 of equal surface :

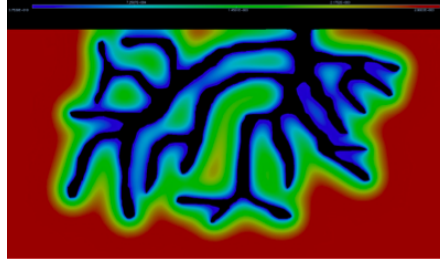


Fig. 2 Dense root, concentration profile after 6 days

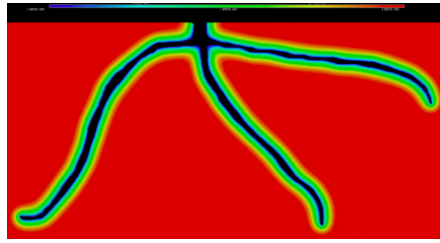


Fig. 3 Root explorer, concentration profile after 6 days

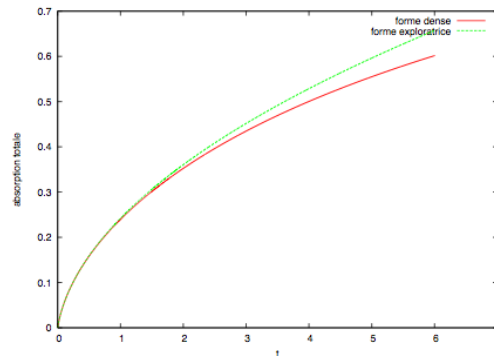


Fig. 4 Root explorer

We note that for short times, here $t < 6$ hours, the differences in local and global structures between the two forms do not influence the P uptake : the absorbed quantities are identical with equal surface. However, for longer times, the shape that

explores a larger useful volume is becoming more and more efficient, with a total gain of more than 8 percent after 6 days.

We will prove mathematically the results of this experiments. For this we use the tools of shape optimization presented in ([22], [8] and [10]) in order to find root shapes that increase the amount of absorbed P. More specifically, we want to deform Ω in order to maximize the shape functional

$$J(c) = \int_0^T \int_{\Gamma_1} \alpha h(c),$$

where $|\Omega| =$ is a given constant.

We also assume that A and \mathbf{q} are constants and we take $R = 0$.

Introducing a deformation field \mathbf{V} and considering $\Omega_s = (Id + s\mathbf{V})(\Omega)$, $s < 1$, we prove in [1] that the shape derivative of J at Ω in the direction \mathbf{V} is

$$dJ(c, \mathbf{V}) = \int_{\Gamma_1 \cup \Gamma_2} j(\mathbf{V} \cdot \mathbf{n}),$$

where j does not depend on \mathbf{V} .

The shape gradient

$$dJ(c, \mathbf{V}) = \int_{\Gamma_1 \cup \Gamma_2} j(\mathbf{V} \cdot \mathbf{n})$$

provides a natural ascent direction $\mathbf{V} = j\mathbf{n}$. This yields

$$dJ(c, \mathbf{V}) = \int_{\Gamma_1 \cup \Gamma_2} j^2 > 0,$$

which ensures that J increases as the domain is iteratively deformed.

Numerical resolution of the state and adjoint equations in two spatial dimensions is carried out using the free finite element software `FreeFEM++`[9], and we obtain in [1]



Fig. 5 Snapshots of the domain and P concentration at different steps of the shape optimization process

3 Coupling soil and root water flow

In this part we will describe the model used in [24]. With F. Hecht and P.-H. Tournier, we describe an adaptive finite element model of soil water and nutrient transport with root uptake. The model aims at including local processes in the rhizosphere at the whole root system scale by taking advantage of unstructured mesh adaptation. The model is comparable to [3], where the root system is represented as a tree-like network composed of cylindrical root segments and radial and axial water flows are defined for each segment. Soil and root water flows are coupled via a sink term in Richards equation and the two problems are solved iteratively until convergence at each time step. The sink terms representing root water and nutrient uptake are built from a characteristic function of the root system, representative of its geometry. This characteristic function is used to drive the mesh adaptation procedure, so that the adapted mesh can accurately resolve the complex geometry of the root system as well as small-scale phenomena in the vicinity of the roots. Since such an approach can be computationally intensive, a parallelization technique based on a scalable two-level Schwarz domain decomposition method is used to solve linear systems arising from the discretization of the soil problems. Some numerical experiments are conducted to illustrate the capabilities of the model.



3.1 *Water flow within the root system*

We consider that the root system is composed of cylindrical root segments. The geometry of the root system can then be represented as a series of interconnected nodes forming a network of root segments Σ , each segment with its own parameters (radius, conductivity, ...).

Such a representation can be generated by RootBox [14] which implements a root growth model using L-Systems.

For a cylindrical root segment of radius r and length l and according to the Ohm's law analogy, the volumetric radial water flow between the soil-root interface and the root xylem can be written as

$$J_r = L_r s_r (h_s - h_r), \quad (2)$$

where

- L_r is the radial conductivity of the root,
- $s_r = 2\pi r l$ is the root-soil interface area,
- h_s is the soil water potential at the root surface,
- h_r is the water potential in the xylem.

Water moves through the root system due to the transpiration-cohesion-tension mechanism. The longitudinal water flow in the xylem is defined as

$$J_x = -K_r \frac{dh_r}{dl}, \quad (3)$$

where K_r is the xylem conductance.

The radial and longitudinal flow equations

$$J_r = L_r s_r (h_s - h_r), \quad J_x = -K_x \frac{d(h_r + z)}{dl}$$

can be used to define the following water mass balance for a given root node i of parent node p in the tree-like structure:

$$\begin{aligned} -K_{r,i} \frac{h_{r,p} - h_{r,i}}{l_i} = & - \sum_{j \in \text{childs}(i)} \left(K_{r,j} \frac{h_{r,i} - h_{r,j}}{l_j} \right) \\ & + L_{r,i} 2\pi r_i l_i \frac{(h_{s,i} - h_{r,i}) + (h_{s,p} - h_{r,p})}{2}. \end{aligned}$$

Here $K_{r,i}$, $L_{r,i}$, r_i and l_i refer to the root segment (p, i) while $K_{r,j}$ and l_j relate to the root segment (i, j) . $h_{s,i}$ and $h_{r,i}$ are the soil water potential at root node i and the xylem water potential at root node i respectively. We approximate the potentials h_s and h_r for segment (i, p) by averaging their value at the two nodes i and p . Parameters L_r and K_r are given for each segment and can depend on various data such as root type and age.

The xylem water potential vector $(h_{r,i})_i$ is then solution of a linear system, with the right-hand side containing the soil factors $h_{s,i}$.

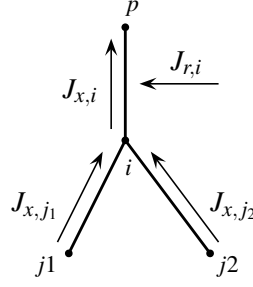


Fig. 6 Water mass balance for root node i

3.2 Coupling soil and root water flow

Root water uptake is taken into account in the soil model by defining a sink term S in the Richards equation.

The usual approach ([5], [11]) is to compute the sink term by summing contributions of root segments to water uptake in each soil voxel.

Our approach aims at

- defining an accurate sink term whose shape matches the geometry of the root system,
- resolving small-scale phenomena at the individual root level.

For this we build a characteristic function of the root system f_c representative of its geometry and use it to define the sink term as well as to guide the mesh adaptation procedure. The function f_c is constructed as follows:

- For a point x of the domain Ω the distance d from x to the root is computed:

$$d(x) = \min_{s \in \Sigma} d_s(x), \quad (4)$$

with Σ the set of root segments in the tree-like network. For each root segment s , the distance $d_s(x)$ from the point x to the segment s is easily computed using distance from line and point routines.

- The distance function d is then used to compute the characteristic function. There is a variety of admissible transformations that we can use, and we choose the following:

$$f_c(x) = f_d(d(x)) = 1 - \tanh\left(\frac{6d(x)}{\varepsilon}\right). \quad (5)$$

We can take ε equal to the radius of the root.

- Consider the case of a single cylindrical root segment (i,j):

$$J_r = L_r s_r \frac{(h_{s,i} - h_{r,i}) + (h_{s,j} - h_{r,j})}{2}.$$

We build the corresponding sink term $S = -\lambda f_c h_l$, where h_l linearly interpolates $h_s - h_r$ along the segment and with $\lambda > 0$ such that

$$\int_{\Omega} S = -J_r.$$

3.3 Numerical experiment

The algorithm we use in [24] is the following. The coupling between the root and soil models consists in iteratively solving the two problems until convergence. Let h_s^i be the soil water potential distribution at time t_i , h_s^k and h_r^k the soil and xylem water potentials at inner iteration k and time t_{i+1} .

1. $h_s^0 = h_s^i$.
2. Solve the linear system arising from the problem defined on the tree-like root network with soil factors h_s^k , obtain h_r^k .
3. Compute the sink term S using h_s^k and h_r^k .
4. Solve the linearized problem corresponding to one Newton step of Richards equation, obtain h_s .
5. $h_s^{k+1} = h_s^k + \alpha_k(h_s - h_s^k)$, where $0 < \alpha_k \leq 1$ is a damping parameter that ensures convergence of the system.
6. If $\|h_s - h_s^k\| > \varepsilon$, go to 2 with $k := k + 1$.

We then use an unstructured volume mesh adaptation (see[2]). Unstructured volume mesh adaptation is a flexible and powerful tool in the case of complex geometries. In our case, the tetrahedral mesh is adapted to the variations of the characteristic function f_c so as to resolve the geometry accurately and capture high gradients and small scale phenomena expected near the roots (local conductivity drop). To summarize the mesh adaptation procedure is an iterative algorithm which consists in

- computing the characteristic function f_c on the current mesh.
- defining a nodal-based anisotropic metric tensor field based on the interpolation error using the reconstructed Hessian of f_c (*mshmet*, P. Frey).
- building a unit mesh for which all edges are of unit length in the prescribed metric, using local mesh modifications and anisotropic Delaunay kernel (*mmg3d*, ([4], [2])).

We obtain the following result :

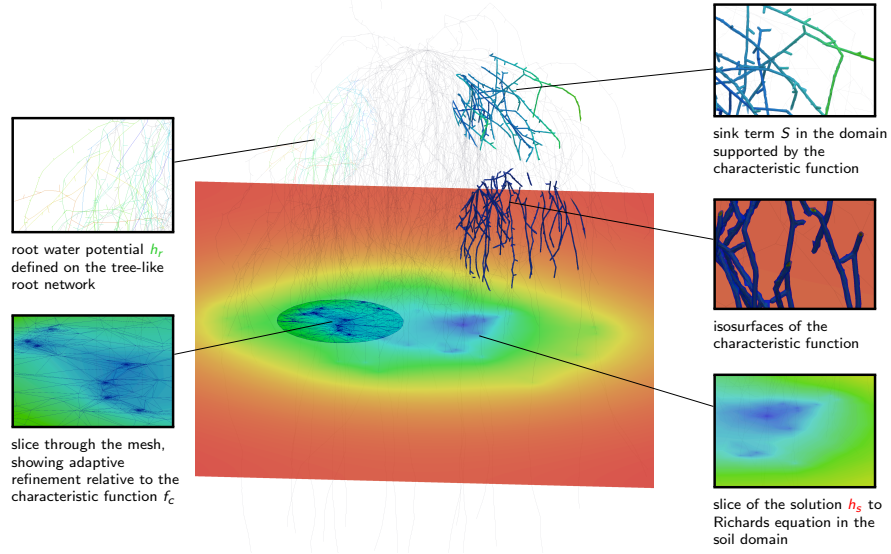


Fig. 7 Overview of the water model

4 Conclusion

In this work, we only considered homogeneous soils, and the model should be extended to heterogeneous soils. Root water uptake and soil heterogeneity have not often been considered simultaneously, although the variability of soil hydraulic properties significantly affects flow processes and root uptake patterns as stressed out in [12]. In addition, a number of soil processes affecting solute movement and availability are simplified or neglected. In most plant nutrition models, chemical interactions between dissolved elements and the soil are reduced to a buffer power or simplified by using the Freundlich adsorption isotherm, as is the case in this work. The Freundlich equation is an empirical relation between the solute concentration in the liquid phase and the amount adsorbed to soil particles and fails to account for changes of nutrient availability arising from the range of biogeochemical and biochemical processes that occur in the rhizosphere ([7], [21]). The model also makes a number of simplifications regarding root structure and function. Osmotic gradients were neglected, although they can significantly affect root water uptake, especially when considering salt accumulation at the root-soil interface caused by salt transport towards the roots by mass flow through the soil. This salinity buildup in the rhizosphere can lead to large osmotic gradients across the roots, effectively reducing root water uptake. In the simulations, we also used a simplified representation of the hydraulic architecture of the root system by considering constant radial and axial conductivities. In reality, root conductivity is a function of root type and age and varies along root axes. The radial conductivity is affected by the development

of apoplastic barriers [23] and by the activity of aquaporins [18], while the axial conductivity depends on the development stage of the xylem. On a similar note, we used a simple Michaelis-Menten model assuming that the nutrient uptake capacity is evenly distributed over the whole root system, while there is experimental evidence that nutrient uptake is not uniform along root axes [6].

Future root uptake models should be coupled with mechanistic surface complexation models using thermodynamic and kinetic relationships in order to include soil processes affecting sorbing surfaces ([19],[16]). In particular, biogeochemical interactions and microbial activity in the rhizosphere can have major effects on soil properties and ultimately impact the acquisition of nutrients by plants.

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