Proceedings of ALGORITMY 2012
pp. 105–112

MODELLING ROOT SYSTEM PHOSPHATE UPTAKE FROM A SOIL COLUMN AS AFFECTED BY ROOT EXUDATION

ANDREA SCHNEPF*, PETER SCHOLL†, GERNOT BODNER‡, AND DANIEL LEITNER§

Key words. convection-dispersion equation, soil, phosphate, root branching structure

AMS subject classifications. 92F05, 92B05, 65Z05

1. Introduction.

Phosphorus is commonly a limiting nutrient for plant growth in many soils around the world (McDowell & Stewart, 2006). Plants take up phosphorus in the form of phosphate from the soil solution and its availability to the roots is hence determined from the solubility of phosphate in the soil. Furthermore, there is a feedback between phosphate availability and root system architecture. In most soils, phosphate is strongly sorbed to the soil solid phase. Plant release of organic acid anions such as citrate that compete for the same sorption sites with phosphate can increase phosphate availability to plants.

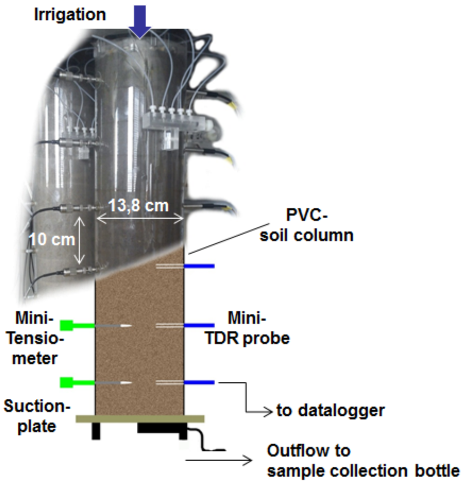


FIG. 1.1. *Experimental setup*

In this work, we present a mathematical model of phosphate and citrate competition in soil and its effect on plant phosphate uptake. The model considers two spatial scales: the scale of an individual root and the scale of the whole root system. The

---

*BOKU - University of Natural Resources and Life Sciences, Department of Water, Air and Environment, Institute of Hydraulics and Rural Water Management, Muthgasse 18, A-1190 Vienna, Austria (`andrea.schnepf@boku.ac.at`).

†BOKU - University of Natural Resources and Life Sciences, Division of Agronomy, Konrad Lorenz-Straße 24, A-3430 Tulln an der Donau, Austria.

‡BOKU - University of Natural Resources and Life Sciences, Division of Agronomy, Konrad Lorenz-Straße 24, A-3430 Tulln an der Donau, Austria.

§University of Vienna, Computational Science Center, Nordbergstraße 15, A-1090 Vienna, Austria.

mathematical model is described in Schnepf *et al.* (2012). Aim of this study was to provide a modelling tool to help interpret experimental results. We set up the three dimensional model domain for a specific experiment where three plants are grown in a column that is filled with soil and where the influence of plant root system on water and nutrient dynamics can be measured (see Fig. 1.1) (Scholl *et al.*, 2011).

Parameterisation of this specific experiment is ongoing. Here, we present a theoretical case study on this geometry that is parameterised with literature data for oilseed rape plants grown in a soil with low phosphate concentrations (Schnepf *et al.*, 2012). With this modelling work we hope to enhance the general understanding of root growth dynamics and its effect on plant mineral nutrition. The research question of this study is to quantify the effect of different exudation patterns on phosphate uptake from the soil column by the root systems of three oilseed rape plants. Root exudation of individual roots is difficult to measure. Most available data report exudation rates for whole plants grown in nutrient solution and in most models, constant exudation rates are used (Kirk, 1999). However, Hoffland *et al.* (1989) showed that organic anion efflux in phosphate-stressed oilseed rape is largely restricted to the root apices. In this study, we investigate the effects of these two different exudation patterns on root phosphate uptake. In the first scenario we assume that roots exude constantly along the whole root axis during the whole simulation time, in the second scenario we assume that roots only exude for one day, i.e. at the root tip. We assume that the overall amount of citrate exuded per unit root length is the same in both cases during the simulation time. Additionally, results are compared to a non-exudation scenario. The three cases are depicted in Fig. 1.2 and explained further in section 2.2.

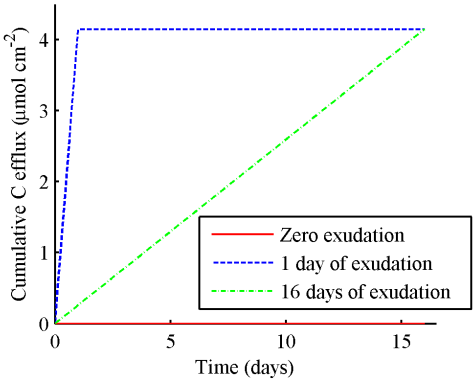


FIG. 1.2. *The three exudation scenarios*

2. Model description.

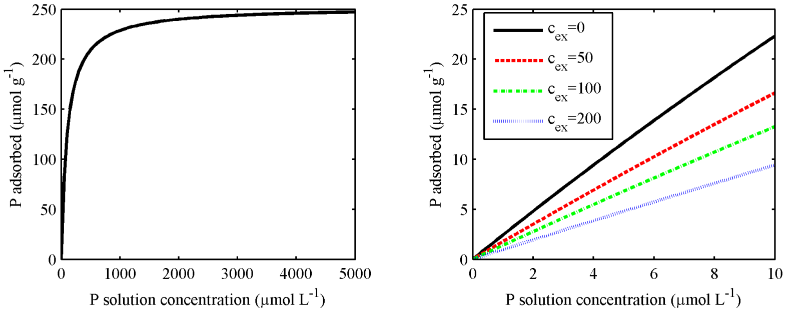
2.1. Competitive Langmuir isotherms. Phosphate and citrate are anions that compete for the same sorption sites in soil. Using the competitive Langmuir isotherm (Van De Weerd *et al.*, 1999), we describes a situation where the soil has a finite amount of sorption sites that can be occupied by both citrate and phosphate (see equations 2.1-2.2).

$$s_p = \frac{k_{L,p} s_{max,p} c_p}{1 + k_{L,ex} c_{ex} + k_{L,p} c_p} \tag{2.1}$$

$$s_{ex} = \frac{k_{L,ex} s_{max,ex} c_{ex}}{1 + k_{L,ex} c_{ex} + k_{L,p} c_p}, \tag{2.2}$$

where c_p and c_{ex} are the solution concentrations of phosphate and citrate, s_p and s_{ex} are the adsorbed concentrations of phosphate and citrate, $k_{L,p}$ and $k_{L,ex}$ are the affinity constants of phosphate and citrate, $s_{max,p}$ and $s_{max,ex}$ are the maximum sorption capacities for phosphate and citrate.

Fig. 2.1(a) shows that when the solution concentration is very large, the adsorbed concentration reaches the maximal sorption capacity for phosphate. However, at realistic solution concentrations of phosphate in low P soils (0.1 - 10 $\mu mol\ L^{-1}$) sorbed concentration is far away from the sorption maximum. Fig. 2.1(b) shows the competitive effect of different citrate concentrations in soil solution. The more citrate there is in solution, the lower is the concentration of phosphate in the adsorbed phase. Thus, at the same total (dissolved plus adsorbed) phosphate concentration, more phosphate becomes available in the soil solution when citrate is added to the soil.



(a) Maximal sorption capacity

(b) Low P soil solution range

FIG. 2.1. *Competitive Langmuir isotherms*

2.2. Solute movement in the soil near one individual root. We describe solute movement near one individual root in 1-dimensional axisymmetric geometry. We assume that each individual root grows into a soil with initially homogeneous phosphate concentration. The root takes up phosphate and excretes citrate, and both solutes move in the soil solution by diffusion. Conservation of mass leads to the system of coupled partial differential equations given by equations (2.3)-(2.9). We solved this model with Comsol Multiphysics 42a. For more efficient handling and coupling with the root growth model, the Comsol model was converted into a Matlab function so that all simulations are performed within Matlab.

$$\begin{aligned}&\left[\theta+\rho\frac{k_{L,p}k_{L,ex}s_{max,p}c_{ex}+k_{L,p}s_{max,p}}{(1+k_{L,p}c_p+k_{L,ex}c_{ex})^2}\right]\frac{\partial c_p}{\partial t}-\rho\frac{k_{L,p}k_{L,ex}s_{max,p}c_p}{(1+k_{L,p}c_p+k_{L,ex}c_{ex})^2}\frac{\partial c_{ex}}{\partial t}=\\&=\frac{1}{r}\frac{\partial}{\partial r}r\left(D_{lp}\theta f\frac{\partial c_p}{\partial r}\right),\end{aligned}\tag{2.3}$$

$$\begin{aligned}&\left[\theta+\rho\frac{k_{L,p}k_{L,ex}s_{max,ex}c_p+k_{L,ex}s_{max,ex}}{(1+k_{L,p}c_p+k_{L,ex}c_{ex})^2}\right]\frac{\partial c_{ex}}{\partial t}-\rho\frac{k_{L,p}k_{L,ex}s_{max,ex}c_{ex}}{(1+k_{L,p}c_p+k_{L,ex}c_{ex})^2}\frac{\partial c_p}{\partial t}=\\&=\frac{1}{r}\frac{\partial}{\partial r}r\left(D_{lex}\theta f\frac{\partial c_{ex}}{\partial r}\right)-k_{dec}\theta c_{ex},\end{aligned}\tag{2.4}$$

$$D_{lp}\theta f\frac{\partial c_p}{\partial r}=\frac{F_m c_p}{K_m+c_p}+ac_p \quad \text{at} \quad r=a_0,\tag{2.5}$$

$$D_{lex}\theta f\frac{\partial c_{ex}}{\partial r}=-F_{ex}(t) \quad \text{at} \quad r=a_0,\tag{2.6}$$

$$D_{lp}\theta f\frac{\partial c_p}{\partial r}=0 \quad \text{at} \quad r=L,\tag{2.7}$$

$$D_{lex}\theta f\frac{\partial c_{ex}}{\partial r}=0 \quad \text{at} \quad r=L,\tag{2.8}$$

$$c_p=c_{p,0},c_{ex}=0 \quad \text{at} \quad t=0,\tag{2.9}$$

where t is the time, r is the radial distance from the root axis, a_0 is the root radius, L is the mean half distance between neighbouring roots, D_{lp} and D_{lex} are the diffusion coefficients of phosphate and citrate in water, θ is the volumetric water content, ρ is the soil bulk density, f is the impedance factor, k_{dec} is the decomposition rate constant of citrate, F_m and K_m are the Michaelis Menten parameters, a is the coefficient of the linear uptake term, $c_{p,0}$ is the initial phosphate concentration in soil solution, $F_{ex}(t)$ is the exudation rate of citrate.

We investigate the impact on phosphate availability and uptake when citrate is continually exuded at a constant rate and when all the citrate is exuded initially within one day. In the first case,

$$F_{ex}=F_{ex,c},$$

where $F_{ex,c}$ is a constant exudation rate. In the second case,

$$F_{ex}(t)=\left\{\begin{array}{lll}TF_{ex,c} & \text{when} & t\leq 1,\\ 0 & \text{when} & t>1\end{array}\right\},$$

where T is the simulation time. Thus, in both cases, each root exudes the same amount during the simulation time, but the dynamics of exudation are different (see Fig. 1.2).

2.3. Phosphate uptake and citrate exudation by the whole root system.

2.3.1. Root system growth model. We aim to simulate the growth of the root systems of three initial seeds of oilseed rape plants in the confined geometry of the soil column. The model is based on L-Systems and it is described in Leitner *et al.* (2010). Briefly, the algorithm computes elongation and branching of the roots according to the initial growth speed, lengths of apical and basal zones as well as internodal distances, the maximal number of branches and the branching angles. Growth direction can follow user defined tropisms. In this study, roots follow gravitropism, i.e. the tendency to grow vertically downwards, as well as thigmotropism, the tendency to grow along a barrier. The latter is necessary for root system growth in a confined geometry. The model has a stochastic component in that all parameters can be given with mean and standard deviation. The algorithm is written in Matlab R2010a and provided online at www.boku.ac.at/marhizo.

2.3.2. Overall P uptake and exudation by the root system. Overall P uptake and exudation by the root system is calculated by summing the uptake over all root segments, i.e.

$$F_{p,\text{root system}}(t) = \sum_{s=1}^{s=N(t)} 2a_0\pi l_s \frac{F_m c_p(t-t_b)|_{r=a_0}}{K_m + c_p(t-t_b)|_{r=a_0}} + a c_p(t-t_b)|_{r=a_0}, \tag{2.10}$$

$$F_{ex,\text{root system}}(t) = \sum_{s=1}^{s=N(t)} 2a_0\pi l_s F_{ex}(t-t_b), \tag{2.11}$$

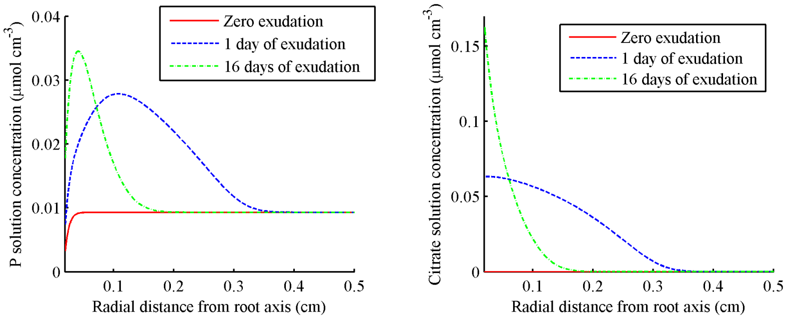
where $N(t)$ is the number of root segments at time t, t_b is the birth time of the root segment and l_s is the length of the root segment. Thus, phosphate uptake and citrate exudation by the root system are dependent on the age of each root segment, the radius and length of each root segment as well as the mean half distance between neighbouring roots. The solution concentration at the root surface at time $t - t_b$ is computed with the model given by equations (2.3)-(2.9). Thereby, we account for the dynamic development of the phosphate and citrate concentration profiles around each root segment.

In order to calculate P and C concentration in the whole soil domain, we use the same model as given by equations (2.3)-(2.9) on a 3-dimensional domain with no-flux boundary conditions and include volumetric sink and source terms for root phosphate uptake and citrate exudation in predefined representative elementary volumes ($F_{P,REV}$, $F_{ex,REV}$).

3. Results and Discussion.

3.1. Single root scale. Figs. 3.1(a)-3.1(b) show the concentrations profiles of phosphate and citrate after 16 days with respect to distance from the root axis. When there is no exudation, there is a depletion zone of phosphate near the root surface due to concentration dependent uptake. When the root exudes along the whole root axis for 16 days, there is a peak of phosphate near the root surface that coincides with the region of increased citrate concentration. Thus, citrate did mobilise phosphate and increase solution concentration by up to a factor of three. When the roots exude only for one day (but with exudation rate 16 times larger), citrate diffuses further away from the root surface, inducing an accordant peak of phosphate in this region. The initially larger exudation rate in the 1 day scenario causes a small advantage in P uptake during the first five days. After that, cumulative phosphate uptake is largest in the case where root exudes constantly along the whole root axis for 16 days (Fig. 3.2).

3.2. Root system scale. Fig. 3.3 shows total (dissolved plus adsorbed) phosphate concentrations in a vertical slice through the soil column. The slice only cuts through one of the three root systems where we can see concentration changes in the soil. 3-dimensional root systems are added to the plot for comparison with the phosphate concentrations. In this front view, on root system is hidden behind one of the other root systems. Depletion zones stay close to the roots in all cases. As expected, depletion is larger in the two exudation scenarios. Fig. 3.4 shows that total citrate concentrations in the soil are different for the two exudation scenarios. In the case when roots exudate only for one day, citrate concentration is largest near the root tips of the root system.



(a) Phosphate (b) Citrate

FIG. 3.1. *Concentration in soil solution around a single root*

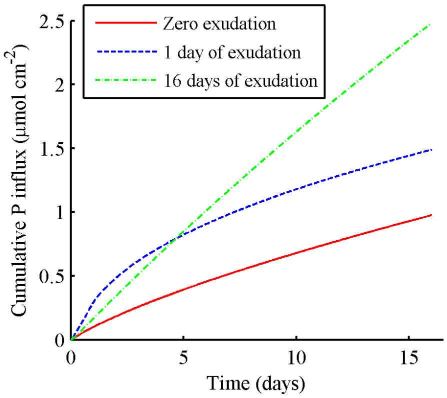
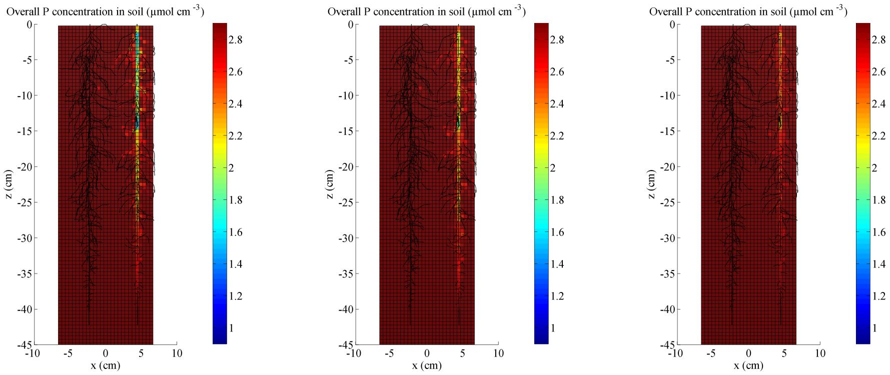


FIG. 3.2. *P influx into a single root in the three exudation scenarios*

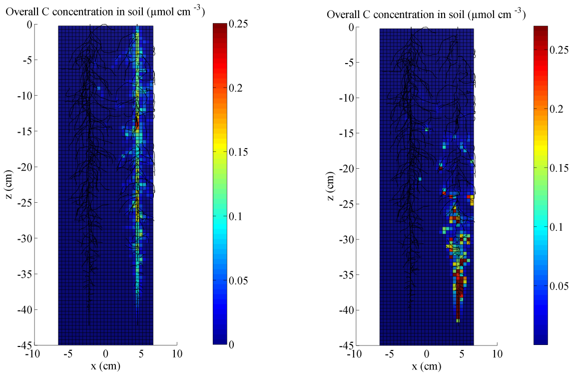
As expected, cumulative phosphate uptake is larger when the roots exudate citrate due to mobilisation of additional phosphate from the solid phase. The overall amount exuded by the root system is dependent on the age distribution of the root segments. A root system commonly exists mainly of young parts. In this simulation, more than half of all the root length is younger than six days. Therefore, the overall exudation of the whole root system is much larger when the roots exude everything at the beginning of their life time (Fig. 3.5(b)). However, for the plant and soil parameters used in this study, the additional mobilisation due to the higher citrate concentrations near the tips do not result in more P uptake (Fig. 3.5(a)) at the root system scale. Thus, the carbon costs per mol of additional phosphate taken up are much larger in the case where roots exude for one day only but with a larger exudation rate.

4. Conclusions and Outlook. Together with the paper of Schnepf *et al.* (2012) we are the first to show the root age dependency of citrate exudation on the root system scale and its effect on root phosphate uptake. Schnepf *et al.* (2012) simulated phosphate uptake by oilseed rape from a rhizotron, but in this case the exudation rate was always the same, no matter whether the roots exuded at the tips only or along the whole root axis. In that case, the amount of citrate exuded by the whole root system is of course less when roots exude only for one day. However, they also



(a) Roots exude all along the root (b) Roots exude only at the tip (c) No exudation

Fig. 3.3. *Overall phosphate concentration in the column after 16 days.*



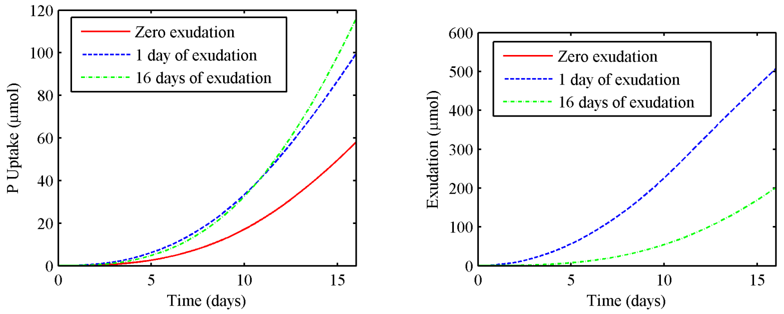
(a) Roots exude all along the root (b) Roots exude only at the tip

Fig. 3.4. *Overall citrate concentration in the column after 16 days.*

showed that overall phosphate uptake by the root system is largely dependent on the early dynamics of the single root model because the root system mainly consists of young roots.

Work on parameterisation and validation of this model is ongoing in close cooperation with experimentalists. Furthermore, we aim to advance the formulation of the sink and source terms in the 3-dimensional model such that the average macroscopic concentration fields feed back into the single root scale model.

With our mathematical modelling studies we hope to help interpret experimental results as we can adapt the geometry to any required shape of rhizotron, pot or column. Results are relevant for finding root traits that enhance plant phosphate efficiency. They will be beneficial for plant nutrition management as well as breeding programs. In particular, they will encourages the use of root architecture traits in future crop improvement efforts.



(a) Phosphate uptake (b) Citrate exudation

FIG. 3.5. *Whole root system dynamics*

Acknowledgments. This work was supported by Austrian Science Fund FWF (Grant Nos.: V 220-N13, P21836). Andrea Schnepf is an Elise-Richter research fellow. Daniel Leitner is recipient of an APART-fellowship of the Austrian Academy of Sciences at the Computational Science Center, University of Vienna.

References.

Hoffland E, **Findenegg G**, **Nelemans J**. **1989**. Solubilization of rock phosphate by rape. II. Local root exudation of organic acids as a response to P-starvation. *Plant and Soil* **113**: 161–165.

Kirk G. **1999**. A model of phosphate solubilization by organic anion excretion from plant roots. *European Journal of Soil Science* **50**: 369–378.

Leitner D, **Klepsch S**, **Bodner G**, **Schnepf A**. **2010**. A dynamic root system growth model based on l-systems. *Plant and Soil* **332**: 177–192.

McDowell R, **Stewart I**. **2006**. The phosphorus composition of contrasting soils in pastoral, native and forest management in otago, new zealand: Sequential extraction and 31p nmr. *Geoderma* **130**: 176 – 189.

Schnepf A, **Leitner D**, **Klepsch S**. **2012**. Modelling p uptake by a growing and exuding root system. *Vadose Zone Journal* **accepted**.

Scholl P, **Kammerer G**, **Schwen A**, **Kaul H**, **Loiskandl W**. **2011**. Methoden zur Bestimmung der Retentionseigenschaften des Bodens im Säulenvergleich. In: **Arbeitsgemeinschaft für Lebensmittel-, Veterinär- und Agrarwesen (ALVA)**, ed., *Landwirtschaft, Lebensmittel und Veterinärmedizin - Zukunft der Forschung in Österreich, 66. ALVA-Jahrestagung, Tagungsbericht 2011*, pp. 285 – 287.

Van De Weerd H, **Van Riemsdikj W**, **Leijnse A**. **1999**. Modeling the dynamic adsorption/desorption of a NOM mixture: Effects of physical and chemical heterogeneity. *Environmental Science and Technology* **33**: 1675 – 1681.