Mechanistic numerical modeling of solute uptake by plant roots

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Core ideas

- idea 1
- idea 2
- idea 3
- optional idea 4
- optional idea 5

Abstract

A modification in an existing water uptake and solute transport numerical model was implemented in order to allow the model to simulate solute uptake by the roots. The convection-dispersion equation (CDE) was solved numerically, using a complete implicit scheme, considering a transient state for water and solute fluxes and a soil solute concentration dependent boundary for the uptake at the root surface, based on the Michaelis-Menten (MM) equation. Additionally, a linear approximation was developed for the MM equation such that the CDE has a linear and a non-linear solution. A radial geometry was assumed, considering a single root with its surface acting as the uptake boundary and the outer boundary being the half distance between neighboring roots, a function of root density. The proposed solute transport model includes active and passive solute uptake and predicts solute concentration as a function of time and distance from the root surface. It also estimates the relative transpiration of the plant, on its turn directly affecting water and solute uptake and related to water and osmotic stress status of the plant. Performed simulations show that the linear and non-linear solutions result in significantly different solute uptake predictions when the soil solute concentration is below a limiting value (C_{lim}). This reduction in uptake at low concentrations may result in a further reduction in the relative transpiration. The contributions of active and passive uptake vary with parameters related to the ion species, the plant, the atmosphere and the soil hydraulic properties. The model showed a good agreement with an analytical model that uses a linear concentration dependent equation as boundary condition for uptake at the root surface. The advantage of the numerical model is it allows simulation of transient solute and water uptake and, therefore, can be used in a wider range of situations. Simulation with different scenarios and comparison with experimental results are needed to verify model performance and possibly suggest improvements.

Text

Crop growth is directly related to plant transpiration, and the closer the cumulative transpiration over a growing season is to its potential value, the higher will be the crop yield. Any stress occurring during crop development results in stomata closure and transpiration reduction, affecting productivity. Therefore, knowing how plants respond to abiotic stresses like those related to water and salt, and predicting and quantifying them, is important not only to improve the understanding of plant-soil interactions, but also to propose better crop management practices. The interpretation of experimental data to analyze the combined water and salt stress on transpiration and yield has been shown to be difficult due to the great range of possible interactions between the factors determining the behavior of the soil-plant-atmosphere (SPA) system. Modeling has been shown to be an elucidative manner to analyze the involved processes and mechanisms, providing insight in the interaction of water and salt stress.

Analytical models describing transport of nutrients in soil towards plant roots usually consider steady state conditions with respect to water flow to deal with the high non-linearity of soil hydraulic functions. Several simplifications (assumptions) are needed regarding the uptake of solutes by the roots, most of them also imposed by the non-linearity of the influx rate function. Consequently, although analytical models describe the processes involved in transport and uptake of solutes, they are only capable of simulating water and solute flow just for specific boundary conditions. Therefore, applying these models in situations that do not exactly correspond to their boundary condition may lead to a rough approximation but may also result in erroneous predictions. Many of the available analytical solutions include special math functions (Bessels, Airys or infinite series, for example) that need, at some point, numerical algorithms to compute results. For the case of the convection-diffusion equation, even the fully analytical solutions are restricted by numerical procedures, although with computationally efficient and reliable results.

As a substitute to analytical solutions, numerical modeling allows more flexibility when dealing with non-linear equations, being an alternative to better cope with diverse boundary conditions. The functions can be solved considering transient conditions for water and solute flow but with some pullbacks regarding numerical stability and more processing to perform calculations. In general, numerical models use empirical functions that relate osmotic stress to some electric conductivity of the soil solution. The parameters of these empirical models depend on soil, plant and atmospheric conditions in a range covered by the experiments used to generate data for model calibration. Using these models out of the measured range is not recommended and, in these cases, a new parameter calibration should be done. Physical/mechanistic models for the solute transport equations describe the involved processes in a wider range of situations since it is less dependent on experimental data, giving more reliable results.

In this study, we develop a mechanistic based numerical scheme to solve the convection-dispersion equation for radial root solute extraction. The model uses the water uptake scheme from De Jong van Lier et al. (2006). Assuming a boundary condition at root surface of concentration dependent solute uptake, the solution for the CDE considers transient flow of water and solute, as well as root competition. The model allows prediction of active and passive contributions to the solute uptake, which can be used to separate ionic and osmotic stresses by considering solute concentration inside the plant.

MATERIAL AND METHODS

Hydraulic Properties and Soil

Solute uptake was analyzed using hydraulic data for three topsoils from the Dutch Staring series (Wösten et al., 2001) as listed in Table 1. The Van Genuchten (1980) equation system was used to describe K–θ–h relations for these soils:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^{1-(1/n)}} \tag{1}$$

$$K(\theta) = K_s \Theta^{\lambda} [1 - (1 - \Theta^{n/(n-1)})^{(1-(1/n))}]^2 \tag{2}$$

where θ (m^3 m^{-3}) is the water content, K (m s^{-1}) and K_s (m s^{-1}) are respectively the hydraulic conductivity and the saturated hydraulic conductivity, h is the pressure head (m), Θ (–) is the effective saturation defined by $\frac{(\theta-\theta_r)}{(\theta_s-\theta_r)}$; θ_s (m^3 m^{-3}) and θ_r (m^3 m^{-3}) are the saturated and residual water contents, respectively; and α (m^{-1}), λ (–) and n (–) are empirical parameters.

Table 1: Soil hydraulic parameters used in simulations

Staring soil ID	**Textural class**	**Reference in this paper**	$\boldsymbol{\theta_r}$	$\boldsymbol{\theta_s}$	$\boldsymbol{\alpha}$	$\boldsymbol{\lambda}$	**n**	$\boldsymbol{K_s}$
			m^3 m^{-3}		m^{-1}	–	–	m d^{-1}
B3	Loamy sand	Sand	0.02	0.46	1.44	-0.215	1.534	0.1542
B11	Heavy clay	Clay	0.01	0.59	1.95	-5.901	1.109	0.0453
B13	Sandy loam	Loam	0.01	0.42	0.84	-1.497	1.441	0.1298

Model Description

The geometry of the soil-root system considers an uniformly distributed parallel cylindrical root of radius r_0 and length z. To each root, a concentric cylinder of radius r_m and length z can be assigned to represent its extraction volume (Figure **??**).

The discretization needed for the numerical solution was performed at the single root scale. As the extraction properties of the root are considered uniform along its length, and assuming no vertical differences in root density and fluxes, the cylinder can be represented by its cross-section, a circle. The area of this circle, representing the extraction region, was subdivided into n circular segments of variable size Δr (m), small near the root and increasing with distance, according to the equation De Jong van Lier et al. (2009):

$$\Delta r = \Delta r_{min} + (\Delta r_{max} - \Delta r_{min}) \left(\frac{r - r_0}{r_m - r_0} \right)^S \tag{3}$$

where the subscripts in Δr indicate the minimum and maximum segment sizes defined by the user, and S gives the rate at which the segment size increases. The parameter r_0 (m) represents the root radius, and r_m (m) is the radius of the root extraction zone, equal to the half-distance between roots, which relates to the root density R (m m^{-3}) according to Equation **??**. This variable size discretization has the advantage to result in smaller segments in regions that need more detail in the calculations (near the root soil interface) due to the greater variation of expected fluxes. Figure **??** shows a schematic representation of the discretization as projected by Equation .

A fully implicit numerical treatment was given to the water and solute balance equations **??** and **??**. The Richards equation **??** for one-dimensional axis-symmetric flow can be written as

$$\frac{\partial \theta}{\partial t} = \frac{\partial \theta}{\partial H}\frac{\partial H}{\partial t} = C_w(H)\frac{\partial H}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rK(h)\frac{\partial H}{\partial r}\right) \tag{4}$$

where the total hydraulic head (H) is the sum of pressure (h) and osmotic (h_π) heads and C_w (m^{-1}) is the differential water capacity $\dfrac{\partial H}{\partial \theta}$. Relations between K, θ and h are described by the Van Genuchten (1980) equation system (Equations and). Analogous to Van Dam and Feddes (2000), Equation can be solved using an implicit scheme of finite differences with the Picard iterative process:

$$\begin{aligned} &{C_w}_i^{j+1,p-1}(H_i^{j+1,p} - H_i^{j+1,p-1}) + \theta_i^{j+1,p-1} - \theta_i^j = \frac{t^{j+1} - t^j}{r_i \Delta r_i} \times \\ &\left[r_{i-1/2}K_{i-1/2}^j \frac{H_{i-1}^{j+1,p} - H_i^{j+1,p}}{r_i - r_{i-1}} - r_{i+1/2}K_{i+1/2}^j \frac{H_i^{j+1,p} - H_{i+1}^{j+1,p}}{r_{i+1} - r_i} \right] \end{aligned} \tag{5}$$

where i ($1 \leq i \leq n$) refers to the segment number, j is the time step and p the iteration level. The Picard's method is used to reduce inaccuracies in the implicit numerical solution for the h-based Equation Celia et al. (1990).

The solution for Equation results in prediction of pressure head in soil as a function of time and distance from the root surface. The boundary conditions considered relate the flux density entering the root to the transpiration rate for the inner segment; and considers zero flux for the outer segment:

$$K(h)\frac{\partial h}{\partial r} = q = 0\,, \qquad r = r_m \tag{6}$$

$$K(h)\frac{\partial h}{\partial r} = q_0 = \frac{T_p}{2\pi r_0 R z}\,, \qquad r = r_0 \tag{7}$$

The computer algorithm that solves the Equation and applies boundary conditions 6 and 7 can be found in Appendix **??**.

The convection-dispersion equation **??** for one-dimensional axis-symmetric flow can be written as

$$r\frac{\partial(\theta C)}{\partial t} = -\frac{\partial}{\partial r}\left(rqC\right) + \frac{\partial}{\partial r}\left(rD\frac{\partial C}{\partial r}\right). \tag{8}$$

with initial condition corresponding to constant solute concentration (C_{ini}) in all segments:

$$C = C_{ini}\,, \quad t = 0,\ r = r_i,\ 1 \leq i \leq n. \tag{9}$$

Both boundary conditions are of the flux type, according to Equation **??**. From the assumed geometry (Figure **??**) it follows that the boundary condition at the outer segment corresponds to zero solute flux (q_s):

$$D(\theta)\frac{\partial C}{\partial r} - qC = q_s = 0 \,, \qquad\qquad r = r_m. \tag{10}$$

The boundary condition for solute transport at the root surface represents the concentration dependent solute uptake, described by the MM equation ??, with the following assumptions:

- Solute uptake by mass flow of water is only controlled by the transpiration flow, a convective flow that is considered to be passive;
- Plant regulated active uptake corresponds to diffusion;
- Plant demand is equal to the I_m parameter from the MM equation;
- At a soil solution concentration value C_{lim}, the solute flux limits the uptake.

We assume that the plant demand for solute is constant in time. The uptake, however, can be higher or lower than the demand, depending on the concentration in the soil solution at the root surface (Figure ??). If the concentration is bellow a certain limiting value (C_{lim}), the uptake is limited by the solute flux, *i.e.* solute flux can not attend plant demand even with potential values of active uptake. Additionally, solute uptake by mass flow of water can be higher than the plant demand in situations of high transpiration rate and/or for high soil water content. In these cases, we assume that active uptake is zero and all uptake occurs by the passive process. A concentration C_2 (mol) for this situation is calculated. When the concentration is between C_{lim} and C_2, the uptake is equal to the plant demand as a result of the sum of active and passive contributions to the uptake. Assumption 1 states that passive uptake is not controlled by any physiological plant mechanisms and, in order to optimize the use of metabolic energy, active uptake is regulated in such way that it works as a complementary mechanism of extraction to achieve plant demand (Assumption 2). This results in a lower active uptake contribution than that of its potential value. However, the effect of the solute concentration inside the plant on solute uptake and plant demand is not considered in the model. Consequently, a scenario for which the demand is reduced due to an excess of solute concentration in the plant is not considered. This might, in certain situations, lead to an overestimated prediction of uptake.

A piecewise non-linear uptake function that considers these explicit boundary conditions was formulated as:

$$F = \begin{cases} \dfrac{I_m C_0}{K_m + C_0} + q_0 C_0, & \text{if } C_0 < C_{lim} \quad (11) \\ I_m, & \text{if } C_{lim} \leq C_0 \leq C_2 \quad (12) \\ q_0 C_0, & \text{if } C_0 > C_2 \quad (13) \end{cases}$$

with C_{lim} determined by the positive root of

$$C_{lim} = -\frac{K_m \pm \left({K_m}^2 + 4 I_m K_m / q_0\right)^{1/2}}{2}, \tag{14}$$

and C_2 by

$$C_2 = \frac{I_m}{q_0}. \tag{15}$$

The non-linear part of the uptake function resides in Equation 11. As implicit numerical implementations of non-linear functions may result in solutions with stability issues, a linearization of Equation 11 was made, resulting in:

$$F = (\alpha + q_0)\, C_0, \quad \text{if } C_0 < C_{lim} \tag{16}$$

where α (m s^{-1}) and q_0 (m s^{-1}) are the active and passive contributions for the solute uptake slope (α+q_0). This linearization is very similar to the one proposed by Tinker and Nye (2000), but does not consider the solute concentration inside the plant. The derivation of Equations to 16 is shown in Appendix **??**.

Finally, the boundary condition at the inner segment refers to the concentration dependent solute flux at the root surface (F, mol m^{-2} d^{-1}) in agreement to Equation and 16 for the non-linear and linear case, respectively. The uptake of each root equals $-F/R$ (mol d^{-1}, the negative sign indicating solute depletion), thus, the condition at the root surface is described by:

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Figures

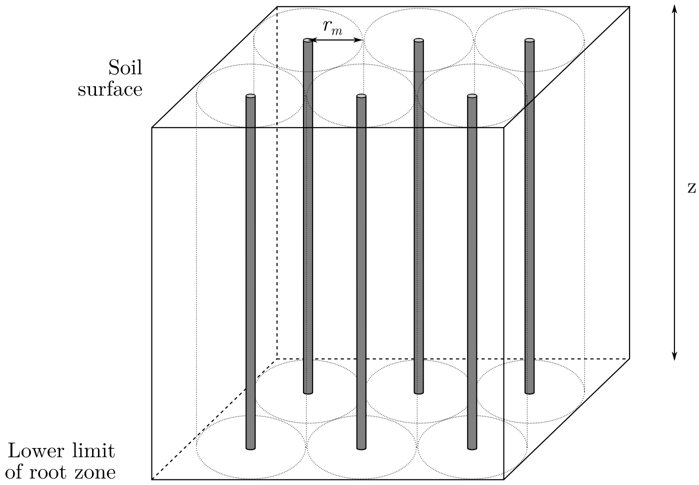

Figure 1: Schematic representation of the spatial distribution of roots in the root zone

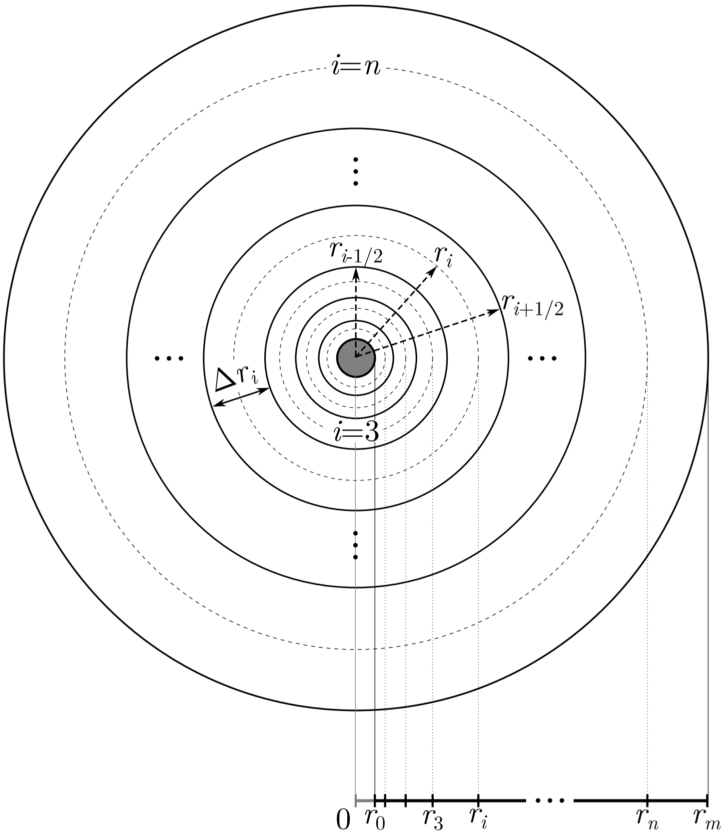

Figure 2: Schematic representation of the discretized domain considered in the model. Δr is the variable segment size, increasing with the distance from the root surface (r_0) to the half-distance between roots (r_m), and n is the number of segments

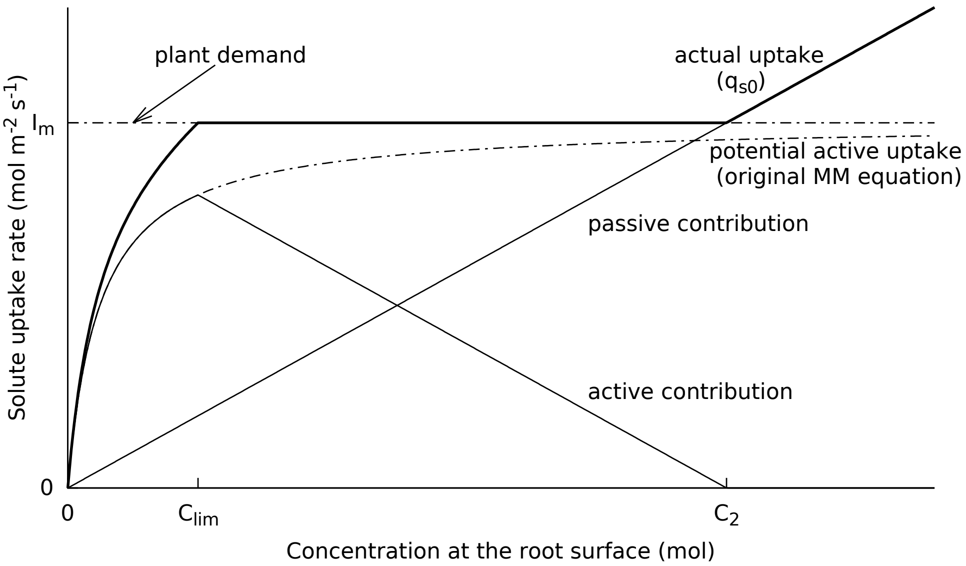

Figure 3: Solute uptake piecewise equation from MM equation **??** with boundary conditions. The bold line represents the actual uptake, thin lines represent active and passive contributions to the actual uptake, and dotted lines represent the plant demand and the potential active uptake