Accounting for Solution Composition in a Plant Roots Active Nutrient Uptake Model

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Abstract

The objective of this study was to include the nutrient uptake deficiency stress in the generic multicomponent transport model, HP1 (the geochemical code PHREEQC coupled to the transient water and solute transport model HYDRUS-1D). The first step was the incorporation of a combined passive-active root nutrient uptake model in HP1 (Jacques et al., 2006). The nutrient uptake model is based on the model of Silberbush et al. (2005). For example, Ca is taken up by passive and active processes, in which the parameters of the Michaelis-Menten active uptake model depend on the solution chemistry. Simulations were compared with experimental data from four irrigation treatments with different Na(-Cl) concentrations. The results are a preliminary attempt to predict uptake of different ions under varying conditions of salinity. Results for Na and K are promising.

1. Introduction

Plant nutrient uptake is controlled by both the plant and soil system (Feddes and Raats, 2004). Under saline conditions, plants are stressed through different processes, including reduced osmotic potential of the soil solution, specific ion toxicity, and ion competition (Taiz and Zeiger, 2002). Models can take into account the effects of general salinity characterized by electrical conductivity (*EC*) by decreasing water uptake as a result of a lower osmotic potential. In addition, models that calculate specific active uptake of solutes can decrease the uptake as a function of the concentration of specific toxic ions (Hopmans and Bristow, 2002). Generally, models that focus on water movement and solute transport in the soil will use the first approach, and plant based models will use the second approach. However, real field conditions are complex and their modeling demands integration of principles of soil and plant science (Hopmans and Bristow, 2002).

In this framework of coupling various soil and plant factors, Šimůnek and Hopmans (2009) presented an improvement to the classic macroscopic scale approach. In the classic approach (e.g., HYDRUS can serve as an example of the model for water movement and solute transport in unsaturated conditions), nutrient uptake is represented by a passive sink term based on root water uptake. The improved model includes active as well as passive nutrient uptake and uptake reduction due to salinity, in an attempt to connect soil modeling with root uptake modeling. A main limitation of this model is that uptake of a solute is independent of concentrations, activities, or speciation of the other solutes in the soil solution (Šimůnek and Hopmans, 2009).

Silberbush et al. (2005) proposed a root nutrient uptake model in which active uptake is specific for each solute according to Michaelis-Menten kinetics and takes into account salinity conditions (as a function of Na^+ and Cl^- concentrations) as well as passive nutrient uptake with water. This model is applied to a soilless culture of known hydraulic properties and follows a Darcy type flow.

The objective of the current study was to describe a model that combines the generic multi-component solute transport model, HP1 (geochemical code PHREEQC coupled to the transient water movement and solute transport model HYDRUS-1D), with a multi-component passive and active root solute uptake model (with parts taken from Silberbush et al. (2005)). The model integrates the strengths of both plant and soil approaches and will help explain and understand the root nutrient uptake deficiency stress under different salinity conditions. In addition, the model will help to separate the passive nutrient uptake reduction due to osmotic stress and the specific nutrient uptake reduction due to specific ion toxicity (Na-Cl, in this case).

2. HP1 Implementation of the Nutrient Uptake Model

The three subparts of the Silberbush et al. (2005) uptake model (passive uptake for Na, active uptake for K, and combined passive and active uptake for Ca) were implemented in HP1 (Jacques and Simůnek, 2005).

2.1. Passive Na root water uptake with maximum uptake flux controlled by solution chemistry

The generic passive uptake model is defined by Eq (1):

$$\begin{aligned} p_a(x,t) = \min[&s_w(x,t)\min\left[c(x,t), c_{\max}\right], \\ &A_{root}(x,t)\,J_{p,\max}\left(\omega(x,t)\right), \\ &p_p(x,t)] \qquad \text{if } c(x,t) > c_r \\ = 0 \qquad &\text{otherwise} \end{aligned} \tag{1}$$

where $p_a(x,t)$ is the actual passive nutrient uptake rate [$ML^{-3}T^{-1}$] for a given depth x [L] and time t [T], $s_w(x,t)$ is the root water uptake rate [$L^3L^{-3}T^{-1}$], $c(x,t)$ is concentration [ML^{-3}], $c_{\max}$ is the maximum allowed concentration for root uptake [ML^{-3}], $A_{root}(x,t)$ is the root surface area [L^2L^{-3}], $J_{p,\max}$ is the maximum allowed passive nutrient uptake rate [$ML^{-2}T^{-1}$], $\omega(x,t)$ is the geochemical condition at x and t, p_p is the potential passive nutrient uptake rate [$ML^{-3}T^{-1}$], and c_r is the critical concentration below which passive root uptake is zero [ML^{-3}]. This expression is generic as it limits uptake by (i) a maximum allowable concentration for uptake ($\min[c(.),c_{\max}]$), (ii) a maximum nutrient uptake flux ($\min[s_w(.)\min[c(.),c_{\max}]$, $A_{root}(.)J_{p,\max}(.)]$, and (iii) a maximum potential root uptake. Uptake below a critical value, c_r, equals zero.

Passive uptake of Na is controlled by the root water uptake rate (s_w) or by the coefficient of passive Na influx, P_m^{Na} (as in Silberbush et al. (2005)).

Three possible variants of this general equation are defined (in all variants, uptake is not limited by a potential uptake, i.e., p_p = 4 mol m^{-3} s^{-1} in Eq. (1)):

- *Variant 1*: Passive Na uptake is not limited (i.e., c_{max} = 4 mol m^{-3}, $J_{p,max}$ = 4 m^{-2} s^{-1}, and c_r = 0 mol m^{-3} in Eq. (1)). The charge balance in the soil solution is controlled by an exudation of protons, which results in pH changes in the soil solution.
- *Variant 2*: Na uptake is only limited by a maximum Na concentration (i.e., $J_{p,max}$ = 4 m^{-2} s^{-1} and c_r = 0 mol/m³ in Eq. (1)). The charge balance in the soil solution is controlled by an exudation of protons.
- *Variant 3*: Na uptake is only limited by a maximum allowable Na uptake flux and is zero below c_r (i.e., c_{max} = 4 mol m^{-3} in Eq. (1)). $J_{p,max}$ depends on the soil solution chemistry as shown in Eq. (2). In Silberbush et al. (2005), the Ca concentration will affect the active Na uptake. In this implementation to HP1, the uptake of Na is only passive, so this factor is included in the passive uptake according to Eqs. (1) and (2).

$$J_{p,\max} = 2.5\times10^{-11} c^{\mathrm{Na}} \left(c^{\mathrm{Ca}}\right)^{-0.24} \tag{2}$$

Note also that passive uptake is zero when c_{max} = 0 mol m^{-3}. In Eq. (2), c^{Na} and c^{Ca} are concentrations of Na and Ca, respectively.

2.2. Active K uptake with Michaelis-Menten kinetic rate parameters dependent on solution chemistry

Active nutrient uptake is described by the Michaelis-Menten rate equation:

$$a_a\left(x,t\right) = A_{root}\left(x,t\right) J_{a,\max}\left(\omega\left(x,t\right)\right) \frac{c(x,t)-c_{\min}}{K_m(\omega(x,t)+(c(x,t)-c_{\min})} \tag{3}$$

where $a_a(x,t)$ is the actual active nutrient uptake [$ML^{-3}T^{-1}$], $J_{a,max}$ is the maximum allowed active uptake [$ML^{-2}T^{-1}$], K_m is the Michaelis-Menten constant [ML^{-3}], and c_{min} is the minimum concentration below which active uptake is zero [ML^{-3}].

Both $J_{a,max}$ (mol m^{-2} s^{-1}) and K_m (mol m^{-3}) parameters depend on Na concentrations as described in Silberbush et al. (2005) (Eqs. (4) and (5), respectively).

$$J_{a,\max} = 5.12\times10^{-8} \exp(-0.023 c^{\mathrm{Na}}) \tag{4}$$

$$K_m = 0.0127 + 2.34\times10^{-4} c^{\mathrm{Na}} \tag{5}$$

2.3. Simultaneous passive and active Ca uptake with Michaelis-Menten parameters dependent on solution chemistry

In Šimůnek and Hopmans (2009), passive uptake is calculated first, and if it cannot supply the potential demand, active uptake is activated. In our HP1 implementation, passive and active uptake are calculated simultaneously as:

$$
\begin{aligned}
r_a(x,t) &= p_a + a_a \\
&= \beta s_w(x,t) c(x,t) + \\
&\quad + A_{root}(x,t) J_{a,\max}\left(\omega(x,t)\right) \frac{c(x,t) - c_{\min}}{K_m(\omega(x,t) + (c(x,t) - c_{\min})}
\end{aligned} \tag{6}
$$

where $r_a(x,t)$ is the actual root uptake [$ML^{-3}T^{-1}$], and β is he fraction of root water uptake active in Ca uptake [-]. $J_{a,\max}$ varies with Na concentrations as described in Silberbush et al. (2005) (Eq. (7) in mol cm^{-2} d^{-1}). K_m and β are constants.

$$
J_{a,\max} = 8.64 \times 8.90 \times 10^{-9} \left(1 - 2.56 \times 10^{-4} c^{\mathrm{Na}}\right) \tag{7}
$$

3. Numerical Example and Experimental Data

The nutrient uptake model was implemented in a generic problem described as:

- 1 m deep loamy soil. Soil hydraulic characteristics are described using the van Genuchten-Mualem model (van Genuchten, 1980).
- The bottom of the soil profile has a constant pressure head of 0 cm. The initial condition at the top is -10 cm with a linear decrease in pressure heads from the top to the bottom.
- A constant potential evaporation and transpiration of 0.01 and 0.15 cm day^{-1}, respectively. Between days 20 and 23, and between days 60 and 63, there is irrigation of 1 cm day^{-1}.
- The plant has a uniform root distribution down to a depth of 30 cm. The water stress reduction function of Feddes et al. (1978) is taken with values: P_0 = -10 cm, P_{Opt} = -25 cm, P_{2H} = -200 cm, P_{2L} = -800 cm, P_3 = -8000 cm, r_{2H} = 0.5 cm day^{-1}, r_{2L} = 0.1 cm day^{-1}. For simplicity, the area of the root surface is taken to be 1 $cm^2 dm^{-3}$ soil.
- The same four irrigation treatments used in the laboratory experiment are simulated (Table 1). Initial solution chemistry in the soil corresponds to the solution of Treatment 1.

Table 1. Solution composition for different treatments, concentrations in ppm.

	Treatment 1 (0 mM NaCl)	Treatment 3 (5 mM NaCl)	Treatment 5 (10 mM NaCl)	Treatment 7 (20 mM NaCl)
pH	5.7	5.7	5.7	5.8
Na	3.5	100.4	201.5	415.9
Cl	10.6	185.1	371.6	760.4
NH_4	6.6	6.6	6	5.9
NO_3	79.7	79.6	80.7	83.6
P	16.5	16.7	17.4	19
K	65.3	65	67.1	71.5
Ca	78.8	79.4	81.9	85.9
Mg	19.7	19.4	19.9	20.2

The dataset used to validate this model was from a laboratory experiment with sweet basil (Ocimum basilicum) grown in lysimeters. The controlled upper boundary conditions consisted of

different salinity treatments (Table 1). The bottom boundary conditions were measured to account for a complete water and macro-nutrient balance. Transpiration, growth, and nutrient uptake of sweet basil as a function of irrigation water amount, nutrient concentration, and salinity were measured over time, and compared with calculated data of K, Ca, and Na.

4. Numerical Results

As a first illustration, three different variants of passive uptake for the first subpart are shown in Figure 1. Because uptake is limited by a maximum concentration, cumulative uptake is smaller in variant 2 compared to variant 1, and also the differences between the treatments with higher Na concentrations is smaller compared to variant 1. Limiting the Na uptake by a maximum uptake flux has a large impact on the cumulative uptake (at least with the current parameter setting).

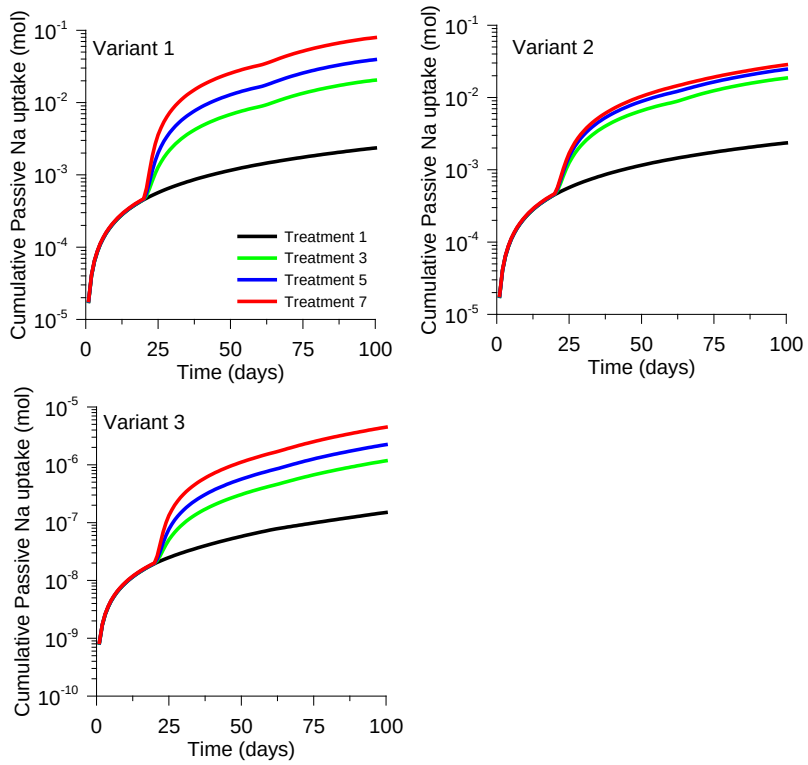

Figure 1. Cumulative passive Na for four salinity treatments simulated with three variants.

Numerical results from the combined implementation of the three subparts of the model of Silberbush et al. (2005) (with variant 3 for passive Na uptake) are shown in Figure 2, in which cumulative uptake of three specific ions under four different salinity treatments (Table 1) are shown. As salinity in irrigation water increases, Na uptake increases, K uptake decreases, and Ca uptake slightly increases.

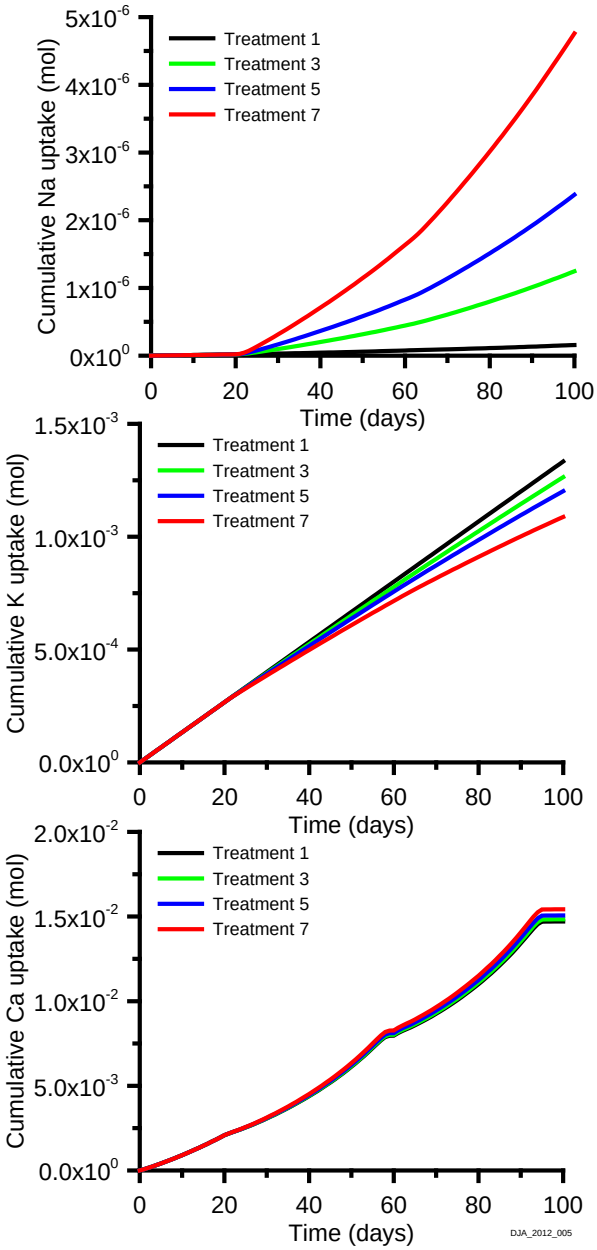

Figure 2. Cumulative Na, K, and Ca uptake for four salinity treatments.

The last result shows a comparison between the model and experimental data from basil grown in lysimeters (Figure 3). Relative uptake of Na, K, and Ca is plotted against four different *EC* values of irrigation water (differences in *EC* are due to different levels of NaCl added). Modeled values of Na and K are close to measured data. Ca shows disparities between measurements and model at high salinity values, indicating that not all parameters for simulations are accurate.

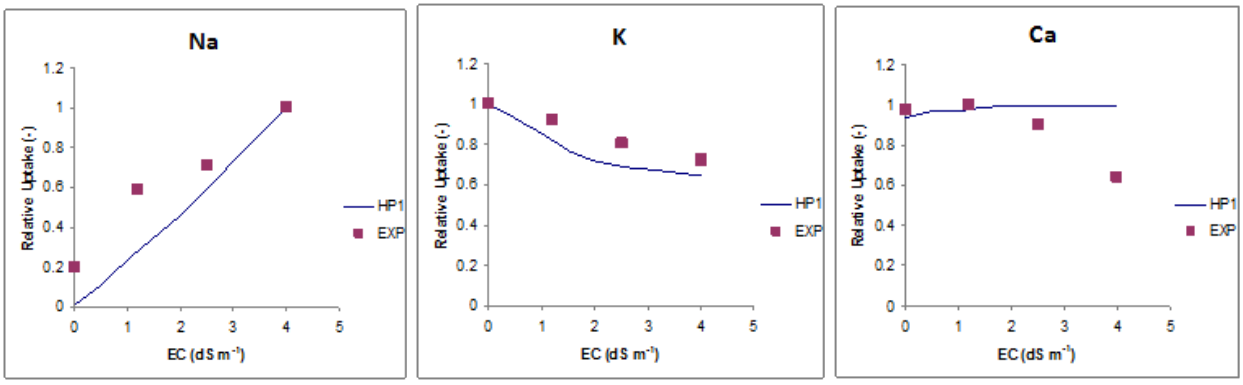

Figure 3. Relative uptake of Na, K, and Ca under various salinities. Comparison between the HP1 model simulations (lines) and experimental data (points) from basil plants grown in lysimeters.

5. Discussion and Conclusions

We have coupled a soil-focused model with a plant-focused model and have demonstrated the potential of linking the Silberbush et al. (2005) nutrient uptake model with HP1 (Jacques et al., 2006). Passive Na, active K, and passive and active Ca uptake with solution-dependent parameters were all integrated in a water movement and solute transport numerical model, as illustrated in the numerical experiment with HP1. Preliminary results are promising though parameters still need to be calibrated for different soils, climates, and crops.

What is ground-breaking in this model is the separation of the nutrient deficiency stress due to certain ions (e.g., Na or Cl) from the osmotic stress they pose. This will allow the functions describing water uptake reduction due to salinity (Maas and Hoffman, 1977; van Genuchten and Hoffman, 1984) to be strictly used to model osmotic stress (Ben-Gal et al., 2009), so that the additional stress due to the reduction in nutrient uptake and specific ion toxicity may then be quantified separately.

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