Transport in Porous Media **14**: 123–141, 1994.

K^+ Uptake by Root Systems Grown in Soil Under Salinity: II. Sensitivity Analysis

ALEX YAKIREVICH, SHAUL SOREK*, and MOSHE SILBERBUSH
J. Blaustein Institute for Desert Research, Ben-Gurion University of the Negev, Sede-Boker Campus 84990, Israel

(Received: 13 April 1992; in final form: 11 August 1993)

Abstract. A numerical algorithm for the solution of multicomponent transport of Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^- in soil and their uptake by plant roots has been developed. The model emphasizes adsorption-desorption due to cation exchange mechanism, dissolution-precipitation of $CaCO_3$, and pH changes at the root surface controlled by the anion-cation influx balance. A fully implicit finite difference scheme is used for numerical implementation. Sensitivity analysis was conducted to evaluate the effect of each parameter on nutrient uptake. Each parameter (independent of all others) was varied between 0.25 to 4 times its speculated 'average' level. Predicted K^+ uptake was found to be more sensitive to changes of root radius and the parameter indicating maximal influx of K^+. Effective diffusion coefficient and soil moisture are less influential. The influence of $CaCO_3$ dissolution and different kinds of boundary conditions were also considered.

Key words. Cation exchange, multicomponent transport, ion uptake, finite differences, dissolution and precipitation, soil moisture, sensitivity analysis, soil salinity, permeability of root surface.

Nomenclature

A, B, E	matrices of coefficients for finite difference scheme
b_i	coefficients of equation for H^+ concentration
C^I	concentration of the I-component in water
C_0^I	initial concentration of the I-component
$C_{r_0}^I$	concentration of the I-component at the inner side of the root surface
$C_{r_1}^I$	concentration of the I-component at the external boundary
C_{cr}^{Na}	critical concentration for Na^+ influx into root
CEC	cation exchange capacity
D^{*I}	effective diffusion coefficient of the I-component in soil
F^I	concentration of the I-component on the exchange complex
G	vector of coefficients in finite difference scheme
h	Hill's cooperativity index for K^+ influx
h^0	value of h when $C^{Na} = 0$
J^I	uptake of the I-component by a root length unit
$J_{r_0}^I$	influx at the root surface of the I-component
J_{max}	maximal influx of K^+

* Also affiliated with the Department of Mechanical Engineering, Ben-Gurion University of the Negev.

J^0_{max}	value of J_{max} when $C^{Na} = 0$
K_a	apparent Michaelis–Menten coefficient for K^+ influx
K^0_a	value of K_a when $C^{Na} = 0$
K_i	selectivity coefficient of the exchange reaction
P^I_m	permeability of root surface for the I-component
P_{CO_2}	partial pressure of CO_2
r	radial distance
r_0	root radius
r_l	half the distance between adjacent root (external boundary)
$R^{I\beta}$	retardation factor of the β-component in mass balance equation for the I-component
t	time
t_0	initial time
T	simulation time
v_0	water radial velocity at the root surface
x_i	coordinate of nodes of finite difference mesh

Greek

α	coefficient of linear change of K^+ influx
α'	coefficient of linear change of Na^+ influx
ρ_s	mass density of soil solid phase
ϕ	soil porosity
θ	volumetric content of liquid in soil
λ_i	coefficients in formulae for parameters of K^+ influx
ω	parameter of perturbation in finite difference scheme
γ^I	activity coefficient of the I-component
ϵ	accuracy of iteration convergence
τ	time step for finite difference scheme
Δ	steps of finite difference mesh

Special Symbols

$[\ldots]$	activity symbol

1. Introduction

Recent research has focused attention on investigation and modeling of nutrient interactions that occur at the soil-root interface (Baldwin *et al.*, 1973; Claassen and Barber, 1976; Cushman, 1979; Bouldin, 1989; Bar-Tal *et al.*, 1991). A sensitivity analysis, conducted in these and many other works (Silberbush and Barber, 1983; Rengel and Robinson, 1990; Van Rees *et al.*, 1990) gives us an improved understanding of the processes, being simulated by their models.

A multicomponent model of K^+ uptake by root systems in saline soils have been developed (Silberbush *et al.*, 1993). In this model roots are assumed to be lumped into a smooth cylinder, absorbing nutrients from the soil. The model takes into account simultaneous transport of Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^- in the soil solution, cation exchange reactions with the solid phase of the soil, dissolution/precipitation

of $CaCO_3$ and pH changes near the root surface. Most of these processes are nonlinear and the mathematical model is a good tool for their study by a series of speculative simulation exercises.

2. Brief Description of the Theoretical Model

Detailed description of the model is given in our previous paper (Silberbush *et al.*, 1993). Here we cite only some main features.

The following phases and components are being considered within the porous medium domain:

- Three phases: solid, liquid and gaseous.
- Five components: Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^- in the liquid.
- Four components: Ca^{2+}, Mg^{2+}, Na^+, K^+ on the solid.
- One component CO_2, in the gas.

The main assumptions are:

(1) The entire system is under isothermal conditions.
(2) The solid matrix remains undeformable and immobile.
(3) The gas phase is immobile.
(4) The cation exchange reaction undergoes instantaneous equilibrium
(5) The activity coefficients of the adsorbed components are approximately equal to unity.
(6) The Cl^- component does not undergo negative adsorption.
(7) Precipitation and dissolution of the ion species is negligible (except of that at the root surface, which will be treated separately).
(8) Roots are assumed to be lumped into a smooth cylinder, with a constant radius r_0.

We consider one dimensional problem of transport to the root by flow with a radial symmetry.

The mass balance equation for an individual I-component reads

$$\frac{\partial(\theta C^I)}{\partial t} + \rho_s(1-\phi)\frac{\partial F^I}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\theta D^{*I}\frac{\partial C^I}{\partial r} + \theta v_0 r_0 C^I\right] \tag{1.1}$$

for $I \equiv$ Ca, Mg, Na, K, and

$$\frac{\partial(\theta C^I)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\theta D^{*I}\frac{\partial C^I}{\partial r} + \theta v_0 r_0 C^I\right] \tag{1.2}$$

for $I \equiv$ Cl, where C^I and F^I denote concentration of the I-component in the liquid and on the exchange complex, respectively, r_0 and r denote root radius and radial distance from root center, respectively, ρ_s denotes mass density of solid phase, θ and ϕ denote volumetric content of liquid in soil and soil porosity, respectively, v_0

denotes water radial velocity at the root surface, D^{*I} denotes the effective diffusion coefficient of the I-component and t denotes time.

We assume that cation exchange reactions are subject to Gapon's isotherm, i.e.

$$\left(\frac{\gamma^{\mathrm{Ca}}C^{\mathrm{Ca}}}{\gamma^{\mathrm{Mg}}C^{\mathrm{Mg}}}\right)^{0.5}\frac{F^{1/2\mathrm{Mg}}}{F^{1/2\mathrm{Ca}}} = K_1, \tag{2.1}$$

$$\frac{\gamma^{\mathrm{Na}}C^{\mathrm{Na}}}{(\gamma^{\mathrm{Ca}}C^{\mathrm{Ca}})^{0.5}}\frac{F^{1/2\mathrm{Ca}}}{F^{\mathrm{Na}}} = K_2, \tag{2.2}$$

$$\frac{\gamma^{\mathrm{K}}C^{\mathrm{K}}}{(\gamma^{\mathrm{Ca}}C^{\mathrm{Ca}})^{0.5}}\frac{F^{1/2\mathrm{Ca}}}{F^{\mathrm{K}}} = K_3 \tag{2.3}$$

where γ^I denotes the activity coefficient of the I-component which is calculated according to the Debye–Huckel relation, K_i denotes the selectivity coefficient.

To the set (1) and (2.1) to (2.3) we add the balance relation

$$\mathrm{CEC} = F^{1/2\mathrm{Ca}} + F^{1/2\mathrm{Mg}} + F^{\mathrm{Na}} + F^{\mathrm{K}} \tag{2.4}$$

where CEC (assumed to be constant) denotes the cation exchange capacity.

(9) In addition we now assume that water content (θ) being constant in space and time.

Therefore in view of (2) we rewrite (1) in the form (Silberbush *et al.*, 1993)

$$\sum_{\beta=1}^{5} R^{I\beta}\frac{\partial C^{\beta}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD^{*I}\frac{\partial C^{I}}{\partial r} + v_0 r_0 C^{I}\right], \quad I \equiv 1, \ldots, 5, \tag{3}$$

where $R^{I\beta}$ denotes a retardation term, given by

$$R^{I\beta} = \begin{cases} -\frac{1-\phi}{\theta}\rho_s \frac{1}{a_I a_\beta}\frac{F^I F^\beta}{C^\beta(\mathrm{CEC})}, & \text{if } I \neq \beta, \\ 1 + \frac{1-\phi}{\theta}\rho_s \frac{1}{a_I^2}\frac{F^I}{C^I}\left(1 - \frac{F^I}{\mathrm{CEC}}\right), & \text{if } I = \beta, \end{cases} \tag{4.1}$$

for $I, \beta = 1, 2, 3, 4$,

$$R^{55} = 1, \qquad R^{5\beta} = R^{I5} = 0, \qquad I, \beta \equiv 1, 2, 3, 4, \tag{4.2}$$

where $a_1 = a_2 = 2$, $a_3 = a_4 = 1$ and indices $I, \beta \equiv 1, 2, 3, 4, 5$ correspond to Ca, Mg, Na, K, Cl, respectively.

Thus we have a 5×5 matrix of retardation terms. In each mass balance equation (3) for the I-component there are five $R^{I\beta}$ factors, characterizing the cross-interactions between the components I and β.

By virtue of (2), the cations on the exchange complex are governed by

$$F^{1/2\mathrm{Ca}} = \frac{(C^{\mathrm{Ca}})^{0.5}}{d}(\mathrm{CEC}), \tag{5.1}$$

$$F^{1/2\mathrm{Mg}} = K_1^* \frac{(C^{\mathrm{Mg}})^{0.5}}{d}(\mathrm{CEC}), \tag{5.2}$$

$$F^{\mathrm{Na}} = \frac{1}{K_2^*}\frac{C^{\mathrm{Na}}}{d}(\mathrm{CEC}), \tag{5.3}$$

$$F^{\mathrm{K}} = \frac{1}{K_3^*}\frac{C^{\mathrm{K}}}{d}(\mathrm{CEC}), \tag{5.4}$$

where

$$d \equiv (C^{\mathrm{Ca}})^{0.5} + K_1^*(C^{\mathrm{Mg}})^{0.5} + \frac{C^{\mathrm{Na}}}{K_2^*} + \frac{C^{\mathrm{K}}}{K_3^*},$$

$$K_1^* \equiv K_1\left(\frac{\gamma^{\mathrm{Mg}}}{\gamma^{\mathrm{Ca}}}\right)^{0.5}, \quad K_2^* \equiv K_2\frac{(\gamma^{\mathrm{Ca}})^{0.5}}{\gamma^{\mathrm{Na}}} \quad K_3^* \equiv K_3\frac{(\gamma^{\mathrm{Ca}})^{0.5}}{\gamma\mathrm{K}}.$$

Initial conditions:

$$C^I(r, t_0) = C_0^I(r), \quad I \equiv \mathrm{Ca},\ \mathrm{Mg},\ \mathrm{Na},\ \mathrm{K},\ \mathrm{Cl}. \tag{6}$$

Boundary conditions at the root surface, $r = r_0$:

$$\theta D^{*I}\frac{\partial C^I}{\partial r} + \theta v_0 C^I = J_{r_0}^I; \quad I \equiv \mathrm{Na},\ \mathrm{K}, \tag{7}$$

where

$$J_{r_0}^K = J_{\max}\frac{(C^{\mathrm{K}})^h}{(K_a)^h + (C^{\mathrm{K}})^h} + \alpha C^{\mathrm{K}}, \tag{8}$$

where $J_{\max}$ denotes maximum flux uptake, K_a denotes the apparent Michaelis–Menten coefficient, h denotes the cooperativity (Hill) power index, and α denotes the linear change of influx with respect to relatively high (above 0.2 mM) concentration.

$$J_{r_0}^{\mathrm{Na}} = \begin{cases} 0, & C^{\mathrm{Na}} \le C_{\mathrm{cr}}^{\mathrm{Na}} \\ \alpha'\theta C^{\mathrm{Na}}, & C^{\mathrm{Na}} > C_{\mathrm{cr}}^{\mathrm{Na}} \end{cases} \tag{9}$$

where $C_{\mathrm{cr}}^{\mathrm{Na}}$ denotes a critical Na^+ concentration and α' denotes the linear change of influx associated with C^{Na}.

In case of $I = \mathrm{Ca}, \mathrm{Mg}, \mathrm{Cl}$, we check two feasible boundary conditions:

(A) Considering passive uptake as diffusion through root surface,

$$D^{*I}\frac{\partial C^I}{\partial r} + v_0 C^I = -P_m^I(C_{r_0}^I - C^I), \quad I \equiv \text{Ca, Mg, Cl} \tag{10.1}$$

(B) Considering passive uptake with advective flow

$$\frac{\partial C^I}{\partial r} = 0, \quad I \equiv \text{Ca, Mg, Cl} \tag{10.2}$$

Boundary condition at $r = r_1$.

Again at this boundary we consider two possibilities:

(A) Continuous supply of ions

$$C^I(r_1, t) = C_{r_1}^I, \quad I \equiv \text{Ca, Mg, Na, K, Cl} \tag{11.1}$$

(B) No supply of ions

$$D^{*I}\frac{\partial C^I}{\partial r} + \frac{v_0 r_0}{r_1} C^I = 0, \quad I \equiv \text{Ca, Mg, Na, K, Cl.} \tag{11.2}$$

At the root surface we take into account dissolution and precipitation of $CaCO_3$ and pH change as a result of cation-anion influx balance. By virtue of the following thermodynamic relations (Garrels and Christ, 1965)

$$[H_2CO_3] = 10^{-1.46} P_{CO_2} \tag{12.1}$$

$$[HCO_3^-] = 10^{-6.36}\frac{[H_2CO_3]}{[H^+]} \tag{12.2}$$

$$[CO_3^{2-}] = 10^{-10.33}\frac{[HCO_3^-]}{[H^+]} \tag{12.3}$$

$$[Ca^{2+}] = 10^{-8.31}\frac{1}{[CO_3^{2-}]} \tag{12.4}$$

combined with the equation of electroneutrality, we obtain the algebraic equation of 4th order for H^+ concentration (C^H)

$$\sum_{n=0}^{4} b_n (C^H)^n = 0, \tag{13}$$

where

$$b_0 = -\frac{2 \times 10^{-18.16} P_{CO_2}}{\gamma^{CO_3}(\gamma^H)^2}, \qquad b_1 = -\frac{10^{-7.82} P_{CO_2}}{\gamma^H \gamma^{HCO_3}},$$

$$b_2 = 2C^{Mg} + C^{Na} + C^K - C^{Cl}, \qquad b_3 = 0, \qquad b_4 = \frac{2 \times 10^{9.85}(\gamma^H)^2}{\gamma^{Ca} P_{CO_2}},$$

where P_{CO_2} denotes partial pressure of CO_2.

For known values of C^{Mg}, C^{Na}, C^K, C^{Cl} and P_{CO_2}, and by solving (13) we obtain C^H. From (12.2)–(12.3), we calculate concentrations of HCO_3^- and CO_3^{2-}. The concentration of Ca^{2+} is corrected by relation (12.4).

3. Numerical Algorithm

The set of Equations (3) to (13) is nonlinear and it is extremely difficult to solve it analytically. Instead we rely on a numerical algorithm based on fully implicit finite difference scheme.

Consider a nonuniform grid applied at the inter-root distance

$$\{x_1, x_2, \ldots, x_n\}, \quad x_1 = r_0, \quad x_n = r_1, \tag{14}$$

where x_i denotes the spatial coordinate of node i, and n denotes number of nodes. Steps of the coordinate mesh are defined by

$$\Delta_i = x_i - x_{i-1}, \quad i = 2, 3, \ldots, n-1, \ \Delta_1 = 0, \ \Delta_{n+1} = 0, \tag{15.1}$$

while intermediate steps are given by

$$\Delta_{i+0.5} = (\Delta_{i+1} + \Delta_i)/2, \quad i = 1, 2, \ldots, n. \tag{15.2}$$

The finite difference scheme for Equation (3), following Samarskii (1977), is

$$\begin{aligned}
&\sum_{\beta=1}^{5} (R^{I\beta})_i^j \frac{C_i^{\beta,j+1} - C_i^{\beta,j}}{\tau^j} \\
&\quad = \frac{\omega_i}{\Delta_{i+0.5} x_i} \left(x_{i+0.5} D_{i+0.5}^{*I} \frac{C_{i+1}^{I,j+1} - C_i^{I,j+1}}{\Delta_{i+1}} \right. \\
&\quad \left. - x_{i-0.5} D_{i-0.5}^{*I} \frac{C_i^{I,j+1} - C_{i-1}^{I,j+1}}{\Delta_i} \right) \\
&\quad + \frac{r_0 v_0}{x_i^2 D_i^{*I}} x_{i+0.5} D_{i+0.5}^{*I} \frac{C_{i+1}^{I,j+1} - C_i^{I,j+1}}{\Delta_{i+1}}, \quad i = 2, 3, \ldots, n-1,
\end{aligned} \tag{16}$$

in which j denotes a time index and τ^j denotes the length of time step.

The parameter of perturbation, ω_i, which gives an approximation of order $O(\Delta^2)$ in spite of the first-order approximation of the advective term, is given by

$$\omega_i = \left(1 + \frac{0.5 \Delta_i v_0 r_0}{D_i^{*I} x_i} \right)^{-1}. \tag{17}$$

When applying (16) near the boundary (say, at $r = r_0$, i.e. $i = 1$ and $\Delta_1 \Rightarrow 0$), we exchange the second term on the r.h.s. by the its exact expression at the boundary. Hence, if for example we refer to (7) we will obtain (in view of (7) and (16))

$$\Delta_{1+0.5} r_0 \sum_{\beta=1}^{5} (R^{I\beta})_1^j \frac{C_1^{\beta,j+1} - C_1^{\beta,j}}{\tau_j}$$

$$= x_{1+0.5} D^{*I}_{1+0.5} \frac{C_2^{I,j+1} - C_1^{I,j+1}}{\Delta_2} \left(\omega_1 + \frac{r_0 v_0}{x_1 D_1^{*I}} \Delta_{1+0.5} \right) - \tag{18}$$

$$- \omega_1 r_0 (J_{r_0}^{I,j+1} - v_0 C_1^{I,j+1}).$$

Similarly, we obtain the finite difference schemes for boundary conditions (10.1), (10.2), (11.2).

Applying the finite difference approximation to (3) and (7) to (11) yields a matrix form for each node, i,

$$-\mathbf{A}_i \mathbf{C}_{i-1} + \mathbf{B}_i \mathbf{C}_i - \mathbf{E}_i \mathbf{C}_{i+1} = \mathbf{G}_i, \quad i = 2, 3, \ldots, n-1, \tag{19.1}$$

$$\mathbf{B}_1 \mathbf{C}_1 = \mathbf{E}_1 \mathbf{C}_2 + \mathbf{G}_1, \tag{19.2}$$

$$-\mathbf{A}_n \mathbf{C}_{n-1} = -\mathbf{B}_n \mathbf{C}_n + \mathbf{G}_n, \tag{19.3}$$

where $\mathbf{C}_i = \{C_i^{I,j+1}\}$ denotes the vector of concentrations at node i at time level $(j+1)$,

$$\mathbf{A}_i \equiv \{a_i^{I\beta}\}, \qquad \mathbf{B}_i \equiv \{b_i^{I\beta}\}, \qquad \mathbf{E}_i \equiv \{e_i^{I\beta,j}\}$$

are square (5×5) matrices and $\mathbf{G}_i \equiv \{g_i^{I,j}\}$ denotes the vector of coefficients.

For example, for $i = 2, 3, \ldots, n-1$ we have

$$a_i^{I\beta} = \begin{cases} 0, & I \neq \beta, \\ x_{i-0.5} D^{*I}_{i-0.5} \omega_i / \Delta_i, & I = \beta, \end{cases} \tag{20.1}$$

$$b_i^{I\beta} = \begin{cases} 0, & I \neq \beta, \\ x_{i+0.5} D^{*I}_{i+0.5} \left(\omega_i + \frac{\Delta_{i+0.5} r_0 v_0}{x_i D_i^{*I}} \right) / \Delta_{i+1}, & I = \beta, \end{cases} \tag{20.2}$$

$$e_i^{i\beta,j} = \begin{cases} -R^{I\beta,j} \frac{\Delta_{i+0.5} x_i}{\tau_j}, & I \neq \beta, \\ -R^{I\beta,j} \frac{\Delta_{i+0.5} x_i}{\tau_j} - a_i^{I\beta} - b_i^{I\beta}, & I = \beta, \end{cases} \tag{20.3}$$

$$g_i^{I,j} = -\sum_{\beta=1}^{5} R^{I\beta,j} \frac{\Delta_{i+0.5} x_i}{\tau_j} C_i^{\beta,j} \tag{20.4}$$

The coefficient matrices, in (19), are functions of system state variables. We use an iterative procedure to solve the nonlinear algebraic set of equations. At each iteration we solve (19), find new values of C_i^I, which are then introduced into F_i^I in (5). Using Equation (13) and relations (12), we determine concentrations of H^+, Ca^{2+}, HCO_3^-, CO_3^{2-} at $r = r_0$. We then update the coefficient matrices of (19) to yield a new iteration. The procedure is repeated until a desired degree of convergence is obtained, namely

$$\max_i \left| \overset{s+1}{\mathbf{C}}_i - \overset{s}{\mathbf{C}}_i \right| < \epsilon, \tag{21}$$

where s denotes the number of iteration ($s = 0$ corresponds to the j time level), ϵ is a predetermined accuracy.

Detailed representations of the numerical behavior of the algorithm is beyond the scope of the present report. However, the performance of the numerical scheme was investigated in terms of its ability to conserve mass of each component, its consistency and convergency as well as stability. The scheme was found robust and mass was conserved in deviation of one percent.

4. Sensitivity Analysis

The sensitivity of the model output was assessed in terms of ion uptake by roots, defined by

$$J^I = 2\pi r_0 \int_0^T J_{r_0}^I(t)\, \mathrm{d}t, \tag{22}$$

where J^I denotes the total mass uptake of the I-component per unit length of a root, and T denotes the simulation time period. We evaluated $J_{r_0}^I$ by using (8) and (9) concerning K^+ or Na^+ uptake, respectively. Since the ions Ca^{2+}, Mg^{2+}, Cl^- are assumed to be taken up passively, the appropriate influx, $J_{r_0}^I$, with respect to (10.1) is given by

$$J_{r_0}^I = -P_m^I \theta [C_{r_0}^I - C^I(r_0, t)], \quad I = \mathrm{Ca},\ \mathrm{Mg},\ \mathrm{Cl}. \tag{23}$$

However, when regarding condition (10.2), we use

$$J_{r_0}^I = \theta v_0 C^I(r_0, t), \quad I = \mathrm{Ca},\ \mathrm{Mg},\ \mathrm{Cl}. \tag{24}$$

In order to take into account the influence of Na^+ concentration on K^+ uptake, we used the following relations for parameters in the Michaelis–Menten isotherm (Silberbush and Ben Asher, 1987, 1989)

$$J_{\max} = J_{\max}^0 - \lambda_1 C_{r_0}^{\mathrm{Na}} \tag{25}$$

$$K_a = K_a^0 + \lambda_2 C_{r_0}^{\mathrm{Na}}, \tag{26}$$

$$h = h^0 + \lambda_3 C_{r_0}^{\mathrm{Na}}, \tag{27}$$

where $C_{r_0}^{\mathrm{Na}}$ denotes Na^+ concentration at the root surface ($r = r_0$) and $J_{\max}^0$, K_a^0, h^0, λ_1, λ_2, λ_3 are empirical coefficients.

Sensitivity analyses were conducted to assess the effect of parameters (actually, as ratios in relation to an assumed average) on the simulated nutrient uptake. Their individual values (see Table I) were changed between 0.25 and 4 times the assumed 'average' levels. The values of parameters θ, v_0 and D^{*I} were taken from Silberbush and Barber (1983), the concentrations $C_{r_0}^{\mathrm{Ca}}$ and $C_{r_0}^{\mathrm{Mg}}$ were taken from Bouldin *et al.* (1992), the values of parameter ρ_s, ϕ and $C_{r_0}^{\mathrm{Cl}}$ were set at a feasible level. A representative value of P_{CO_2} commonly used in soil models, is 0.01 Bar (Jurinak, 1984). All other parameters, mentioned in Table I, as well as initial values of concentrations were obtained experimentally with sorghum plants grown in soil, which was treated with different concentrations of NaCl (Silberbush, unpublished data).

The values of F_0^I ($I \equiv$ Ca, Mg, Na, K) presented in Table I were calculated according to (5). The charge balance between cations and CL^- is compensated by carbonates. Initial concentrations of HCO_3^-, CO_3^{2-} and pH were calculated by (12) and (13). Their values were found to be equal to 4.31 and 0.016 mmol L^{-1} and 7.37, respectively.

The parameters ρ_s, ϕ, $C_{\mathrm{cr}}^{\mathrm{Na}}$ and C_0^I were not changed. The parameters P_{CO_2} and θ were changed in the range from 0.5 to 2 times their listed (Table I) values. Parameter D^{*I} was changed only in the case of $I = K^+$. The sensitivity analysis was conducted for boundary conditions (7), (10.1) at $r = r_0$ and (11.2) at $r = r_1$. The simulations were carried out for conditions of relatively high initial concentration of NaCl in the soil solution in order to appreciate the influence of the soil salinity on K^+ uptake.

Predicted ion uptake as a function of the most influential parameters are described in Figures 1 to 5. Those figures demonstrate that increasing volumetric moisture content (θ) will raise the uptake of all ions. This can be explained by the effect of the increase of total amount of water being taken up by the roots. Varying the water radial velocity at the root surface (v_0) had qualitatively the same influence as θ on uptake of Ca^{2+}, Mg^{2+}, Na^+ and Cl^- (Figures 2 to 5). The increase of v_0 induces a rise of the concentration near the root surface and the increase of uptake of these ions by the roots. Such result was obtained since we assumed that the parameters α' and P_m^I ($I \equiv$ Ca, Mg, Cl) are constant. In the case of K^+, uptake the parameter of the maximum K^+ influx, $J_{\max}^{\mathrm{K}}$, decreases when the concentration of Na^+ increases near the root surface (see formula (25)). As a result we observe the drop of potassium uptake (Figure 1b) following the increase of v_0.

Predicted uptake of ions was most sensitive to changes in root radius, r_0. An increase in r_0 increased predicted ion uptake. This may be explained in view of linear relationship between root surface area and r_0. Note that uptake was calculated with no consideration to root growth. In real life conditions, a specific root area

TABLE I. Soil and root parameters for sensitivity analysis.

Symbol	Parameter	Initial value
ρ_s	mass density of solid phase	$2650\ \mathrm{kg\,m^{-3}}$
ϕ	porosity	$0.50\ \mathrm{m^{-3}m^{-3}}$
θ	volumetric content of liquid in soil	$0.25\ \mathrm{m^{-3}m^{-3}}$
v_0	water radial velocity at the root surface	$5 \times 10^{-9}\ \mathrm{m\,sec^{-1}}$
r_0	root radius	2×10^{-5} m
r_1	half distance between root	5×10^{-4} m
D^{*I}	the effective diffusion coefficient of I ion in soil (identical for all ions)	$3.45 \times 10^{-12}\ \mathrm{m^2\,sec^{-1}}$
P_{CO_2}	partial pressure of CO_2	0.01 bar
CEC	cation exchange capacity	$100\ \mathrm{meq\,kg^{-1}}$
K_1	selectivity coefficient of isotherm Ca⇔Mg	0.5
K_2	selectivity coefficient of isotherm Ca⇔Na	$100\ \mathrm{mmol^{0.5}}L^{-0.5}$
K_3	selectivity coefficient of isotherm Ca⇔K	$15\ \mathrm{mmol^{0.5}}L^{-0.5}$
J^0_{max}	maximal influx of K^+ when $C^{Na}_{r_0} = 0$	$6 \times 10^{-6}\ \mathrm{mmol\,m^{-2}\,sec^{-1}}$
K^0_α	apparent Michaelis–Menten constant for K^+ influx when $C^{Na}_{r_0} = 0$	$1.48 \times 10^{-2}\ \mathrm{mmol\,L^{-1}}$
h^0	cooperativity (Hill) index when $C^{Na}_{r_0} = 0$	1.49
λ_1	coefficient of linear change of J^0_{max}	$4 \times 10^{-8}\ \mathrm{L\,m^{-2}\,sec^{-1}}$
λ_2	coefficient of linear change of K_α	0.75×10^{-3}
λ_3	coefficient of linear change of h	$0.014\ \mathrm{mmol^{-1}L}$
α	coefficient of linear change of K^+ influx	$5 \times 10^{-10}\ \mathrm{m\,sec^{-1}}$
α'	coefficient of linear change of Na^+ influx	$2.5 \times 10^{-11}\ \mathrm{m\,sec^{-1}}$
C^{Na}_{cr}	critical concentration for Na^+ influx	$0.1\ \mathrm{mmol\,L^{-1}}$
P^{Ca}_m	permeability of root surface for Ca^{2+}	$10^{-6}\ \mathrm{m\,sec^{-1}}$
P^{Mg}_m	permeability of root surface for Mg^{2+}	$5 \times 10^{-7}\ \mathrm{m\,sec^{-1}}$
P^{Cl}_m	permeability of root surface for Cl^-	$2.5 \times 10^{-8}\ \mathrm{m\,sec^{-1}}$
$C^{Ca}_{r_0}$	concentration of Ca^{2+} at the inner side of the root surface	$0.25\ \mathrm{mmol\,L^{-1}}$
$C^{Mg}_{r_0}$	concentration of Mg^{2+} at the inner side of the root surface	$0.25\ \mathrm{mmol\,L^{-1}}$
$C^{Cl}_{r_0}$	concentration of Cl^- at the inner side of the root surface	$0.3\ \mathrm{mmol\,L^{-1}}$
C^{Ca}_0	initial concentration of Ca^{2+} in the soil solution	$2.42\ \mathrm{mmol\,L^{-1}}$
C^{Mg}_0	initial concentration of Mg^{2+} in the soil solution	$1\ \mathrm{mmol\,L^{-1}}$
C^{Na}_0	initial concentration of Na^+ in the soil solution	$30\ \mathrm{mmol\,L^{-1}}$
C^{K}_0	initial concentration of K^+ in the soil solution	$0.5\ \mathrm{mmol\,L^{-1}}$
C^{Cl}_0	initial concentration of Cl^- in the soil solution	$33\ \mathrm{mmol\,L^{-1}}$
$F^{1/2Ca}_0$	initial concentration of Ca^{2+} on the exchange complex	$63.3\ \mathrm{meq\,kg^{-1}}$
$F^{1/2Mg}_0$	initial concentration of Mg^{2+} on the exchange complex	$20.9\ \mathrm{meq\,kg^{-1}}$
F^{Na}_0	initial concentration of Na^+ on the exchange complex	$14.2\ \mathrm{meq\,kg^{-1}}$
F^{K}_0	initial concentration of K^+ on the exchange complex	$1.6\ \mathrm{meq\,kg^{-1}}$

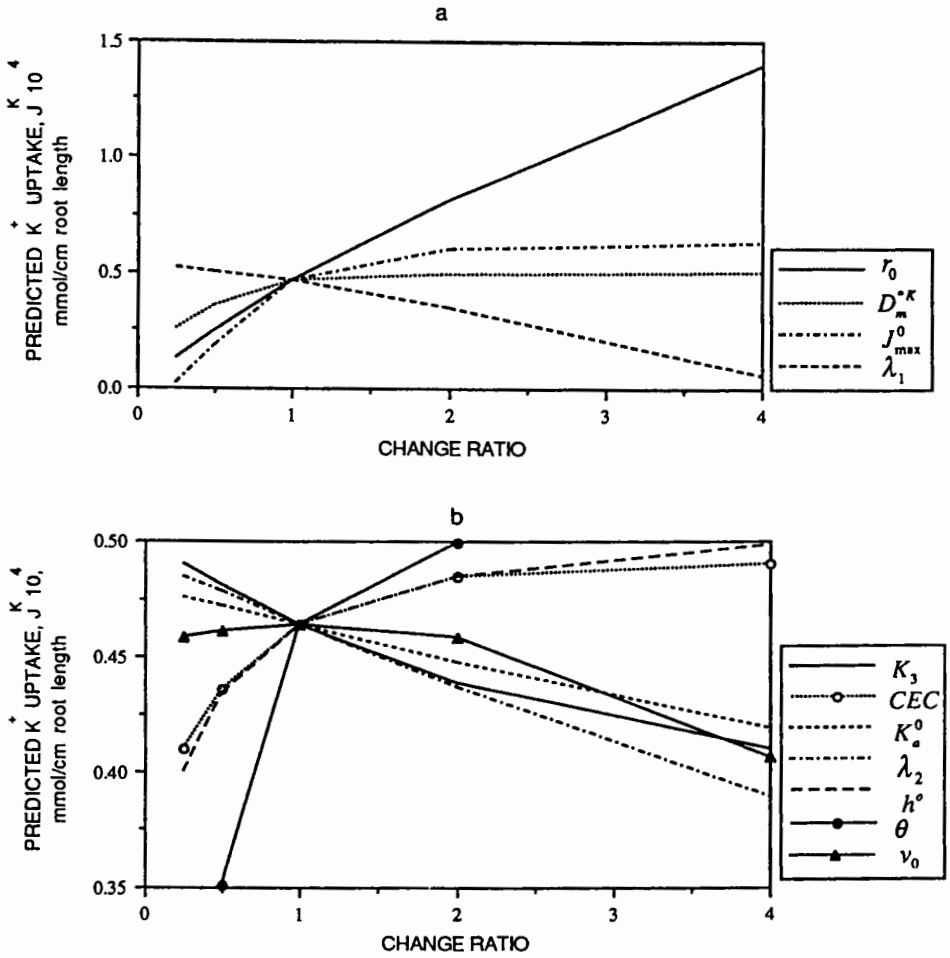

Fig. 1. Effect of varying parameters on predicted K uptake for 10 days.

is an important factor of nutrients uptake by plants. Yet, our simulation may be considered as a first approximation in order to study this effect.

Concerning boundary conditions at $r = r_1$, we found that in the case of (11.1), i.e. when continuous supply of ions occurs at the external boundary, the value of r_1 has no effect on ion uptake. When applying boundary condition (11.2), i.e. there is no supply of ion at the external boundary, a decrease of r_1 caused a small reduction of the ion uptake. However, it was reported (Silberbush and Barber, 1983) that the decrease of the ion uptake in this case may be considerable because of a reduction in the amount of soil supplying components to the root by advection and diffusion. Still there is no contradiction between their and our results, because of the difference in the initial amount of ions in the soil: initial concentration of K^+ in our simulation was almost twice as much as in the above mentioned report.

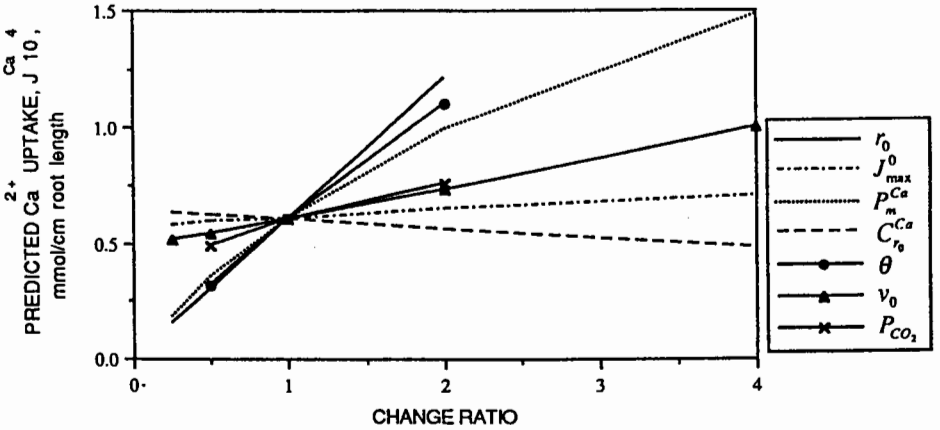

Fig. 2. Effect of varying parameters on predicted Ca uptake for 10 days.

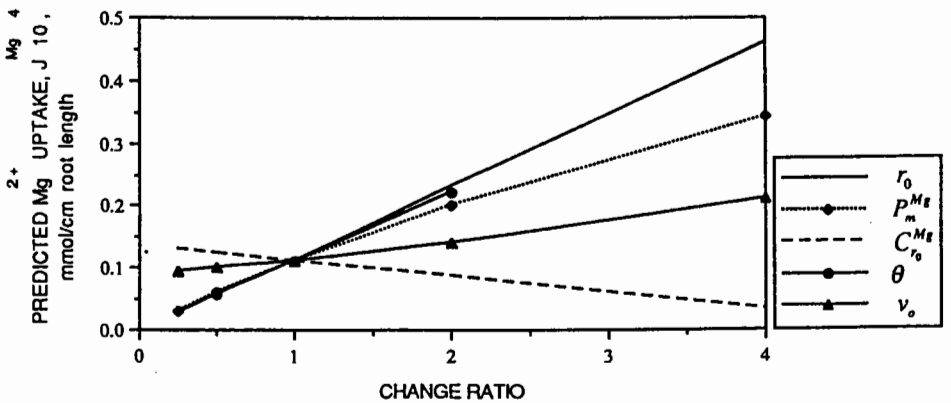

Fig. 3. Effect of varying parameters on predicted Mg uptake for 10 days.

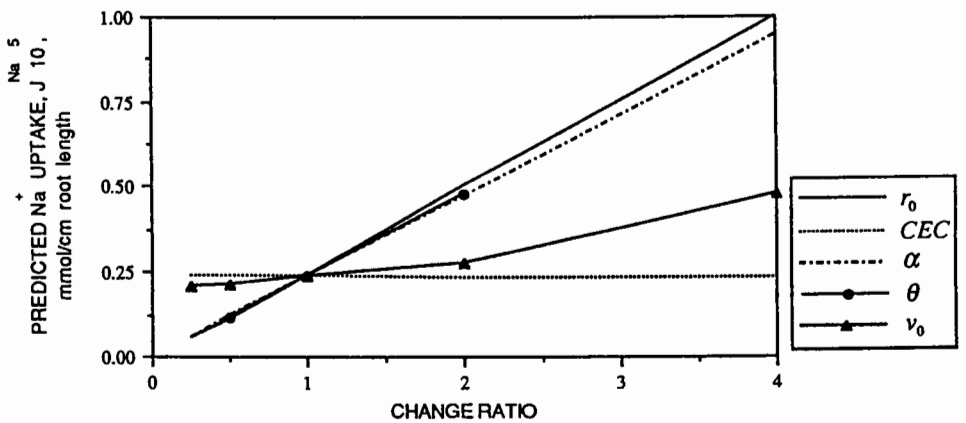

Fig. 4. Effect of varying parameters on predicted Na uptake for 10 days.

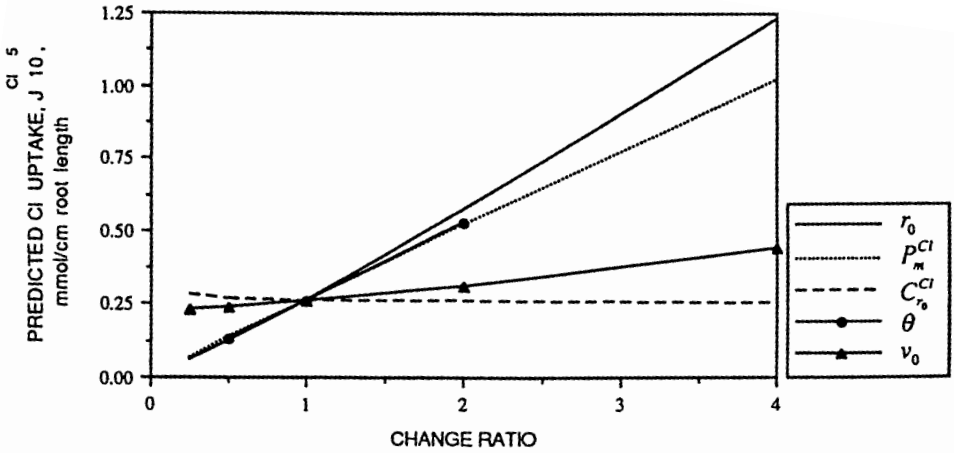

Fig. 5. Effect of varying parameters on predicted Cl uptake for 10 days.

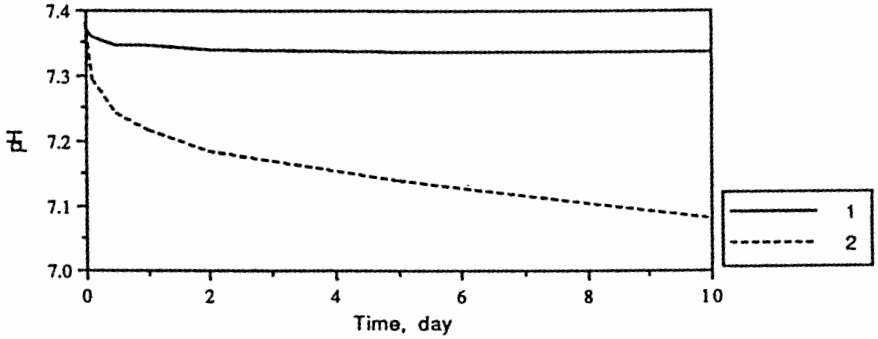

Fig. 6. pH change during the time at $r = r_0$: 1-with $CaCO_3$ dissolution, 2-without $CaCO_3$ dissolution.

Predicted K^+ uptake was rather sensitive to changes of effective diffusion coefficient, especially at low diffusion values. We found that, a decrease in D^{*K}, lowered K^+ (Figure 1a) uptake but somewhat increased Ca^{2+} uptake. This may be explained by the fact that when D^{*K} decreases, the concentration of K^+ at $r = r_0$ also decreases. This, in return, will lead to an increase of $CaCO_3$ solubility yielding an increase of Ca^{2+} uptake by roots.

It was found that Ca^{2+} uptake was the only one which was sensitive to changes in the partial pressure of carbon dioxide (Figure 2). An increase of P_{CO_2}, significantly raised solubility the of $CaCO_3$ and Ca^{2+} uptake by root. At the same time, this increase of P_{CO_2} caused pH decrease near the root. Although our model does not relate P_{CO_2} to the K^+ uptake, still via exchange reactions we found very little effect on the predicted value of J^K.

Uptake of K^+ was more sensitive to changes in cation exchange capacity (CEC)

(Figure 1). The reason may be as follows. As time evolves, a depletion zone of K^+ is intensively formed near the root (Figure 7). Hence, the concentration of this component considerably decreases in comparison to other cation concentrations. As a result, part of the ions Ca^{2+}, Mg^{2+}, Na^+ from the soil solution substitutes K^+ on the exchange complex, which causes additional K^+ uptake by the root. As we have higher CEC values, this may be considered as a greater pool for K^+ in soil which, in return, will yield more intensive potassium uptake.

The influence of the selectivity coefficients K_1 and K_2 (isotherms of $Ca^{2+} \Leftrightarrow Mg^{2+}$ and $Ca^{2+} \Leftrightarrow Na^+$, respectively) is rather negligible for all components and therefore this effect was not described graphically. However, our numerical sensitivity analysis demonstrates that increase of K_1 constitutes the decrease of soil selectivity to Ca^{2+} which in return reduces its participation in the exchange reactions. This results in greater amounts of Ca^{2+} in the soil solution which can be taken up by the roots. On the other hand, in view of (5.4) when K_1 increase, the amount of K^+ in the exchange complex decreases and its uptake by root decreases as well. The obtained results indicate that for a K_1 change ratio of 0.25 and 4, the difference of Ca^{2+} uptake was 3%, while 2.5% for K^+ uptake. In the case of Mg^{2+} and Na^+, K_1 had even a less influence on their uptake. Sensitivity of the model to K_2 is negligible for all cations, yet some effect is noticeable on Na^+ uptake (Figure 4). We note that an increase in Na^+ uptake follows the increase in K_2. The explanation may be the same as in the case of the influence of K_1 on Ca^{2+} uptake.

The influence of the selectivity coefficient K_3 (isotherm of $Ca^{2+} \Leftrightarrow K^+$) on K^+ uptake is more pronounced than that of K_1 and K_2, but, less significant than that of v_0, θ, D^{*K} and J°_{max} (Figure 1b). An increase of K_3 decreases the soil selectivity to K^+. This causes a decrease in the amount of K^+ on the exchange complex which in return, reduces its availability for root uptake.

We found that parameter of maximum K^+ influx (J^0_{max}) was the second most influential (after r_0) in dominating K^+ uptake (Figure 1a). As J^0_{max} increases, the influx of K^+ increases too, but not linearly. Note that for large values of J^0_{max} its influence reaches an asymptotic value. This can be explained due to the fact that a depletion zone is formed very quickly near the root surface. This depletion is associated with a high affinity of root to K^+ influx and a limited rate of ion supply. Uptake of potassium may be increased by its diffusive or advective transport to the root. Nutrient uptake for other ions is less sensitive to changes in J^0_{max}. Yet when J^0_{max} is raised, it somewhat increases the value of J^{Ca} (Figure 2).

The apparent Michaelis–Menten constant (K_a) had appreciable influence, on predicted K^+ uptake. As K^0_a increases, K^+ uptake decreases. The increase of K_a may be achieved through the parameters K^0_a or λ_2 (see (26)). Their influence on J^K is shown on Figure 1b. Unlike K_a, the cooperativity index (h^0) had an opposite effect on K^+ uptake. An increase of h^0 raised J^K (Figure 1b). Other parameters of K^+ influx, i.e. λ_1, λ_3 and α had very little impact on predicted potassium uptake. Coefficient of linear change of sodium influx (α'), had an effect only on Na^+ uptake. As α' increases, J^{Na} increases in linear proportion as expected from (9)

(Figure 4). We found that α' had no influence on other ion uptake because of low soil selectivity to Na^+.

Following Figures 2, 3 and 5, we note that an increase in P_m^I or decrease in $C_{r_0}^I$ will raise J^I ($I \equiv$ Ca, Mg, Cl). The influence of the increase in $C_{r_0}^I$ on the uptake of the latter I-components, complies with the magnitude of difference between this concentration and the concentration at root surface ($C^I(r_0, t)$).

In order to study the influence of NaCl concentration in soil solution on K^+ uptake, we made simulations with high initial concentrations of Na^+ and Cl^-. Note that the effect of Na^+ concentration on K^+ uptake is formulated in (25) to (27). In our example increasing the initial Na^+ and Cl^- concentrations up to 100 mmol L^{-1}, reduced somewhat linearly K^+ uptake by a factor of 3.2.

The model provides information about pH changes at the root surface. On the one hand, if the soil is calcareous, dissolution or precipitation of $CaCO_3$ may occur, affecting pH changes (Nye, 1984; Nye and Ameloko, 1987). On the other hand, a higher proportion of cation over anion influx, results in an increase in H^+ efflux and a pH decrease. In Figure 6 predicted pH changes are depicted for soil with and without dissolution and precipitation of $CaCO_3$. It is demonstrated that in calcareous soil, the pH changes are rather small. The phenomena may be explained by the fact that the balance between cations and anions in soil solution due to their uptake, is compensated by $CaCO_3$ dissolution or precipitation. Changes of pH, without $CaCO_3$, are more significant and depend on the influx intensity of anion and cations. A growth in the difference between the sum of cations concentration and concentration of Cl^-, causes an increase in pH. Similarly, a lessening in this difference will cause a decrease in pH. This is exemplified at the first time instant when a steep rate of K^+ influx yields a decrease in the aforementioned difference and resulted in a fall of pH (Figure 6). Afterwards a pH decrease slows down because of a lower rate of K^+ influx.

For Ca^{2+}, Mg^{2+} and Cl^- we assumed passive root uptake mechanism and proposed two kinds of boundary conditions at $r = r_0$: (1) diffusion through root surface (see (10.1)), and (2) ion uptake by root with an advective transport (see (10.2)). In the latter condition there is no selectivity for the uptake of Ca^{2+}, Mg^{2+} and Cl^- and their influx depends on the water radial velocity, moisture content and the concentration of these components near root surface (see (24)). Strictly speaking this may be regarded as a nonrealistic boundary condition. Yet, our simulation shows that this may be useful when there is no information related to the parameters P_m^I and $C_{r_0}^I$ which appear in (10.1). For example, when applying condition (10.1), we received uptake intensities (J^I) of 0.603, 0.112 and 0.263 ($\times 10^{-4}$) mmol/cm root length for Ca^{2+}, Mg^{2+} and Cl^-, respectively. These flux intensities became 0.365, 0.139, 4.380 ($\times 10^{-4}$) for the above ions when using the condition (10.2). Therefore we note that for Ca^{2+} and Mg^{2+} the differences between the evaluated ion uptake intensities, are minor. For Cl^-, the difference is very big because of its high concentration in soil solution.

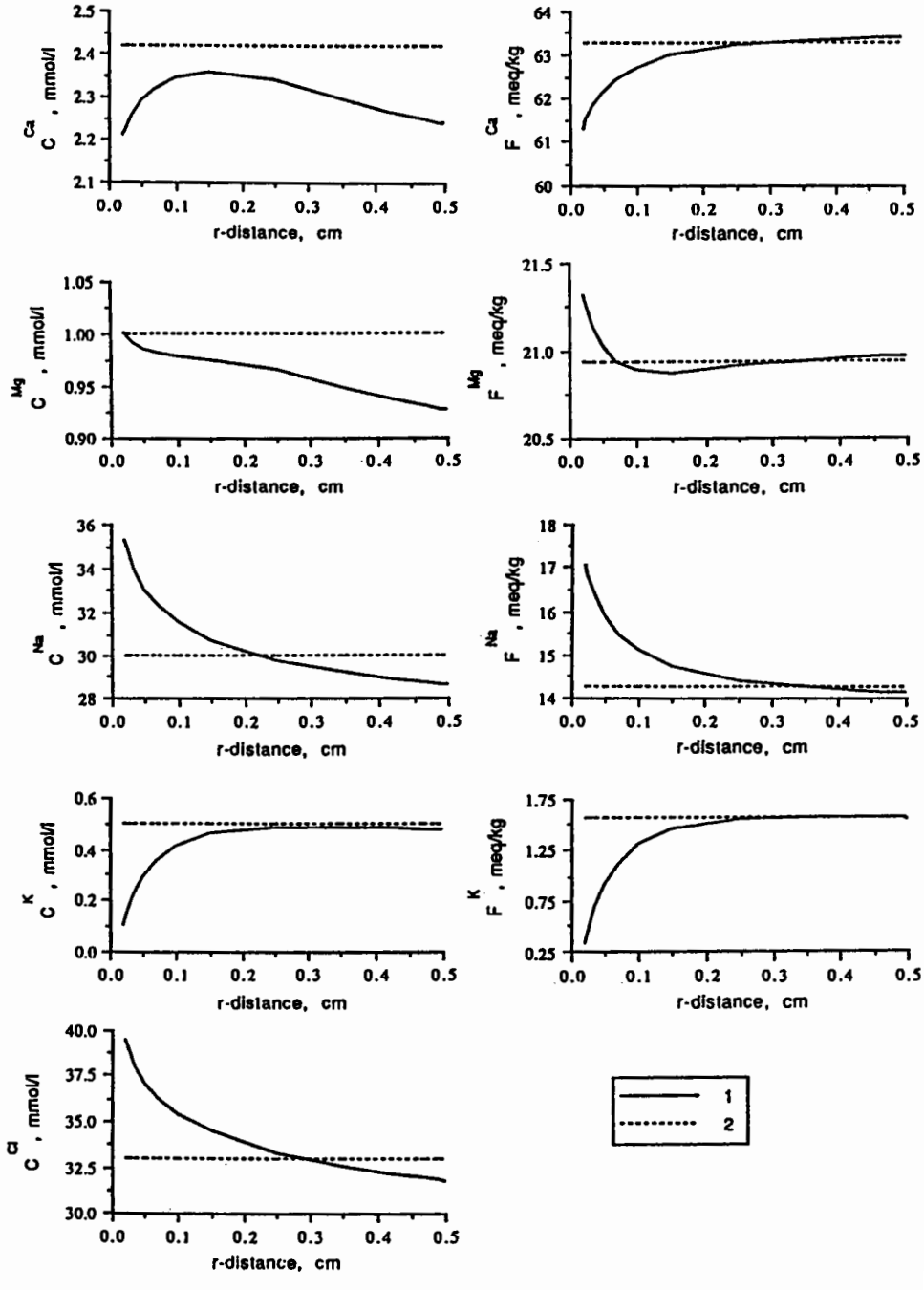

Fig. 7. Distribution of components versus spatial coordinate: 1-after 10 days, 2-initial.

Figure 7 depicts the distribution of ions in the soil solution and on the exchange complex versus the spatial distance after 10 days period. We notice a depletion for Ca^{2+} and K^+ and an increase for other ions near root surface. Such behavior is determined by the water radial velocity, the reactions between the components in liquid, solid and gaseous phase, and the parameters of ion uptake. Thus in our example the depletion of Ca^{2+} in the soil solution was caused by its uptake and precipitation into $CaCO_3$. On the exchange complex, Ca^{2+} was substituted by Mg^{2+} and Na^+ due to an increase of their concentration in soil solution. This increase in Mg^{2+} and Na^+ (as well as in Cl^-) concentration occurs because of the low P_m^I ($I \equiv$ Mg, Cl) and α' values. A high affinity of the root to potassium, which makes its advection-diffusion in the soil the limiting factor to K^+ influx, causes the depletion of K^+ in the soil around the root. In this respect, the lower K^+ concentration at the root is expected (Silberbush and Barber, 1983). This is also consistent with experiments reported by Claassen *et al.* (1986). As for the other ions, which accumulated at the root surface, the answer is less clear. Accumulation of Mg^{2+} was simulated also by Kelly *et al.* (1992), using the one-component Barber–Cushman model in a non-saline soil. Sodium is being actively excluded by roots (Schubert and Läuchli, 1990), and Ca^{2+}, Mg^{2+} and Cl^- are absorbed rather passively when the concentration is not low. Yet, we still miss the adequate techniques to measure effect in situ, at the soil-root interface.

5. Conclusion

A numerical algorithm was developed to solve a set of nonlinear transport equations describing multicomponent nutrient uptake into root. The model emphasizes adsorption due to cations exchange mechanism, dissolution and precipitation of $CaCO_3$ and pH changes near root surface controlled by the cation-anion influx balance. The model also accounts for various boundary conditions at the root zone (passive and active influx) as well as at the external boundary (continues and no ionic supply). A sensitivity analysis was exercised to assess the influence of various soil and root parameters on nutrient uptake. It was found that K^+ uptake was most sensitive to changes of root radius. The next most influential parameters were maximal influx of K^+ (J_{max}^0), soil moisture (θ) and effective diffusion coefficient (D^{*K}). The uptake of other ions was also sensitive to changes of root radius, root surface permeabilities, concentration of those ions at the inner side of the root surface and soil moisture. The model allows the prediction of pH changes near root. Experiments for estimating model parameters as well as validation, are to be reported in a future publication.

References

Baldwin, J. P., Nye, P. H., and Tinker, P. B., 1973, Uptake of solutes by multiple root systems from soil. III. A model for calculating the solute uptake by a randomly dispersed root system developing the finite volute of soil, *Plant and Soil* **37**, 621–635.

Bar-Tal, A., Bar-Yosef, B., and Chen, Y., 1991, Validation of the model of the transport of zinc to an artificial root, *J. Soil Sci.* **42**, 399–411.

Bouldin, D. R., 1989, A multiple ion uptake model, *J. Soil Sci.* **40**, 309–319.

Bouldin, D. R., Miyasaka, S. C., and Grunes, D. L., 1992, Cation accumulation by winter wheat forage: II. Correlation with multi-ion model, *J. Plant Nutr.* **15**, 1081–1097.

Claassen, N. and Barber, S. A., 1976, Simulation model for nutrient uptake from soil by a growing plant root system, *Agron. J.* **68**, 961–964.

Claassen, N., Syring, K. M., and Jungk, A., 1986, Verification of a mathematical model by simulating potassium uptake from soil, *Plant and Soil* **95**, 209–220.

Cushman, J. N., 1979, Analytical solution to solute transport near root surfaces for low initial concentration: I. Equation development, *Soil Sci. Soc. Am. J.* **43**, 1087–1092.

Garrels, R. M. and Christ, C. L., 1965, *Solutions, Minerals, and Equilibria*, Harper & Row, New York.

Jurinak, J. J., 1984, Salt-affected soils: Thermodynamic aspects of the soil solution, in I. Shainberg and J. Shalhevet (eds.), *Soil Salinity Under Irrigation: Processes and Management*, Ecological Studies 51, Springer-Verlag, Berlin, pp. 15–31.

Kelly, J. M., Barber, S. A., and Edwards, G. S., 1992, Modeling magnesium, phosphorus and potassium uptake by loblolly pine seedlings using a Barber– Cushman approach, *Plant and Soil* **139**, 209–218.

Nye, P. H., 1984, On estimating the uptake of nutrients solubilized near roots or other surfaces, *J. Soil Sci.* **35**, 439–446.

Nye, P. H., and Ameloko, A. Y., 1987, Predicting the rate of dissolution of lime in soil, *J. Soil Sci.* **38**, 641–649.

Rengel, Z. and Robinson, D. L., 1990, Modelling magnesium uptake from an acid soil. II. Barber–Cushman model, *Soil Sci. Soc. Am. J.* **44**, 1195–1200.

Samarskii, A. A., 1977, *Theory of Finite Difference Schemes* (in Russian: '*Teoriya raznostnih skhem*'), Moscow, Nauka.

Schubert, S. and Läuchli, A., 1990, Sodium exclusion mechanisms at the root surface of two maize cultivars, *Plant and Soil* **123**, 205–209.

Silberbush, M. and Barber, S. A., 1983, Sensitivity analysis of parameters used in simulating K uptake with a mechanistic mathematical model, *Agron. J.* **75**, 851–854.

Silberbush, M. and Ben-Asher, J., 1987, The effect of salinity on parameters of potassium and nitrate uptake of cotton, *Comm. Soil Plant Anal.* **18**, 65–81.

Silberbush, M. and Ben-Asher, J., 1989, The effect of NaCl concentration on NO_3^-, K^+ and orthophosphate-P influx to peanut roots, *Scientia Hortic.* **39**, 279–287.

Silberbush, M., Sorek, S. and Yakirevich, A., 1993. K^+ uptake by root systems grown in soil under salinity: I. A mathematical model, *Transport in Porous Media* **11**, 101–116.

Van Rees, K. C. J., Comerford, N. B., and McFee, W. W., 1990, Modelling potassium uptake by slash-pine seedlings from low-potassium-supplying soils, *Soil. Soc. Am. J.* **54**, 1413–1421.