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K^+ Uptake by Root Systems Grown in Soil Under Salinity: I. A Mathematical Model

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Abstract. A novel theoretical model is proposed for K^+ uptake by intact root systems from saline soil considering interactions with Na^+, Ca^{2+} and Mg^{2+}. The model assumes radial movement of ions towards the root governed by advection and diffusion flux mechanisms, and chemical exchange of the four cations according to Gapon isotherms, with Cl^- as the accompanying anion. Influx of K^+ to the root surface is assumed as a function of its concentration in the soil solution at the root. This influx is governed by a saturable-cooperative term and a linear term for low and high K^+ concentrations, respectively. Influx of Na^+, above a critical value of its concentration, increases linearly with its concentration in the soil solution at the root surface. Uptake of Ca^{2+} is controlled by the balance between influxes of anions and cations, which induces efflux of H^+ or HCO_3^-, and interacts with calcite in a calcareous soil. The model may provide information about the behavior of ions at the root-soil interface which cannot be measured *in situ*.

Key words. Cation exchange, cation interaction, Gapon isotherms, K^+ uptake, H^+ efflux, mathematical model, mineral nutrition, soil salinity.

Nomenclature

$\mathring{a}^\beta$	ion's effective diameter
C^β	($\equiv \Delta^{\rho^\beta_f}$), concentration of β-component in water
C^β_0	initial concentration of the β-component
$C^I_{r_0}$	concentration at the root surface of the I ion
$C^I_{r_1}$	concentration at the external boundary
$C^{Na}_{cr.}$	critical concentration for Na^+ influx to the root surface
CEC	cation exchange capacity
$\mathbf{D}^\beta_{h\eta}$	hydrodynamic dispersion of the β-component in the η-phase
$\mathbf{D}^\beta_\eta$	mechanical dispersion of the β-component in the η-phase
$D^{*\beta}_\eta$	the molecular diffusion of the β-component of the η-phase
$\mathbf{D}^\beta_f$	diffusion coefficient of the β-component in water
f	as subscript, symbol for fluid ($\equiv l$ or g)
$f^\beta_{\tau\to\upsilon}$	rate of transfer of a β-component from a τ-phase to a υ one
F^β	mass of the β-component on the solid phase
g	as subscript, symbol for gaseous phase
h	as superscript, Hill's cooperativity index for K^+ influx
$\mathbf{J}^\beta_{h\eta}$	hydrodynamic dispersion flux of the mass of the β-component in the η-phase
$\mathbf{J}^\beta_\eta$	mechanical dispersion flux of the mass of the β-component in the η-phase
$\mathbf{J}^{*\beta}_\eta$	molecular diffusion flux of the mass of the β-component in the η-phase
$J^I_{r_0}$	influx at the root surface of the I ion
J_{max}	maximal influx of K^+
K_a	apparent Michaelis–Menten coefficient for K^+ influx
K_i	selectivity coefficients of the exchange reactions
$K^{N^{n+}}_{M^{m+}}$	equilibrium coefficient for exchange reaction
l	as subscript, symbol for liquid phase
r	radial distance

P_m^β	permeability of root membrane for β-component
r_0	root radius
r_1	radius of external boundary
$R^{I\beta}$	retardation factor of the β ion in equation for I ion
s	as subscript, symbol for solid phase
S_η	saturation of η-phase
t	time
t_0	initial time
T	simulation time
T_l	factor of tortuosity
v	water radial velocity
v_0	water radial velocity at the root surface
$\mathbf{v}_\eta$	mass-weighted velocity of the η-phase
Z^β	valence of ion β

Greek Letters

α	coefficient of linear change of K^+ influx with respect to high concentrations
α'	coefficient of linear change of Na^+ influx with the concentration
β	as superscript, symbol for component (i.e. ions)
γ^β	activity coefficient of the β-component
θ_f	volumetric content of the f-phase
η	as subscript, symbol for phase
ϕ	porosity
λ	ionic strength of the solution
Γ_η^β	rate of production of the β-component within/on the η-phase
ρ_η^β	mass density of a β-component in a η-phase.

Special Symbols

[...]	activity
$(...)^{N^+}$	as superscript, N-valent cation
$(...)^{N^-}$	as superscript, N-valent anion
$\Leftrightarrow$	designator for a two-direction chemical reaction

1. Introduction

Salinity of the root growth medium may reduce plant growth as a result of two mechanisms (Greenway and Munns, 1980); (a) osmotic effect, and (b) nutritional disorders. The latter even occurs in relatively low salt concentrations. Interactions between nutritional cations like K^+, NH_4^+ and Ca^{2+} with Na^+ were investigated mainly in nutrient solutions (Greenway and Munns, 1980). Cotton (*Gossypium hirsutum* L.) cultivars varied in their selectivity of K^+/Na^+ ratio according to their salinity tolerance (Läuchli and Stelter, 1982). Similar results were obtained with rice cultivars, *Oryza sativa* L. (Qadar, 1988; Arjunan and Chandrasekaran, 1988). Uptake of K^+ was suppressed by Na^+, but not by a similar concentration of polyethylene glycol (PEG); the addition of Ca^{2+} resulted in a K^+ uptake similar to the no-Na^+ control (Kawasaki *et al.*, 1983). In addition, the ratio between Na^+ and Ca^{2+} affects the root elongation rate (Howard and Adams, 1965; Greenway and Munns, 1980) which, in return, may control the ion uptake by the plant (Barber and Silberbush, 1984). It is impossible, however, to measure these mechanisms *in situ* at the root-soil interface. A mathematical model which describes the interactions among these ions in the soil and their uptake by the plant, may be a most powerful tool to study the effect of salinity on root nutrient uptake in time and space (Clarkson 1985; Grove and Bouldin, 1988; Rengel and Robinson, 1990). The existing models (Baldwin *et al.*, 1973; Claassen and Barber, 1976; Cushman, 1979) treat only one ion at a time, and do not account for interactions between ions, as is required in the case of nutrient uptake from a saline medium. The recent model of Bouldin (1989) treats interactions among ions in the soil, both cations and anions. However, this model over-simplifies

the nature of ion uptake by roots, and does not account for interaction between ions during uptake, which is essential in our case. The model of Bar-Tal *et al.* (1991) accounted for pH changes in the rhisophere, but aimed at Zn^{2+} and Zn^{2+} uptake chemistry in the soil. The proposed model is aimed at simulating K^+ uptake by a root system grown in soil in the presence of Na^+, Ca^{2+}, and Mg^{2+}, and to provide information of their changes at the soil-root interface.

2. The Mathematical Model

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

- Three phases (superscript η): solid (s), liquid (l), and gaseous (g).
- Five components (subscript β, $\beta \equiv K^+, Na^+, Ca^{2+}, Mg^{2+}, Cl^-$), all of which are dissolved matter in the liquid.

Our objective is to write the complete set of macroscopic equations that are required to model the mass transport of the above phases and components. Obviously, this set should also include momentum balance equations as well as constitutive equations that describe the behavior of specific materials. In our model, we assume that

[2.1] The entire system is under isothermal conditions.

[2.2] The dominant cations, relevant to describe root uptake of K^+ from saline soil, are Na^+, Ca^{2+}, and Mg^{2+}, with Cl^- as the accompanying anion.

[2.3] Precipitation and dissolution of ion species is negligible (except of that at the root surface, which will be treated separately).

[2.4] Roots are assumed to be lumped into a smooth cylinder (i.e. without root hairs or mycorrhizal hyphae), with a constant radius r_0.

Let us write the mass balance equations for an individual component (β):

(a) *Dissolved Matter in a Fluid* ($\eta \equiv f$) *Phase* ($f \equiv l, g$)

$$\frac{\partial}{\partial t}(\phi S_f \rho_f^\beta) = -\nabla[\phi S_f(\rho_f^\beta \mathbf{v}_f + \mathbf{J}_{hf}^\beta)] + f_{\tau\to\upsilon}^\beta + \phi S_f \rho_f \Gamma_f^\beta, \tag{1}$$

where $\mathbf{J}_{h\eta}^\beta$ = (macroscopic) flux of hydrodynamic dispersion of the mass of the β-component in the η-phase

$f_{\tau\to\upsilon}^\beta$ = rate of transfer of a β-component from a τ-phase to a υ-one, per unit volume of porous medium (i.e. $f_{l\to g}^\beta$ denotes the rate of transfer of β through the interface between the fluid phases l and g).

Γ_η^β = rate of production of the β-component within/on the η-phase, per unit mass of the later.

The flux $\mathbf{J}^{\beta}_{h\eta}$, including the fluxes due to mechanical dispersion, $\mathbf{J}^{\beta}_{\eta}$, and due to molecular diffusion, $\mathbf{J}^{*\beta}_{\eta}$, of the β-component, with

$$\mathbf{J}^{\beta}_{h\eta} = -\mathbf{D}^{\beta}_{h\eta}\nabla\rho^{\beta}_{\eta} \tag{2}$$

in which

$$\mathbf{D}^{\beta}_{h\eta} = \mathbf{D}^{\beta}_{\eta} + D^{*\beta}_{\eta} \tag{3}$$

denotes the coefficient of hydrodynamic dispersion of the β-component in the η-phase. It is the sum of the coefficients of mechanical dispersion, $\mathbf{D}^{\beta}_{\eta}$, and that of molecular diffusion in a porous medium, $D^{*\beta}_{\eta}$.

(b) *Dissolved Matter on the Solid ($\eta = s$) Phase*

On the solid phase, the movement of the adsorbate is by advection only. Hence, the mass balance equation reduces to

$$\frac{\partial}{\partial t}[(1-\phi)\rho_s F^{\beta}] = -\nabla\cdot[(1-\phi)\rho_s F^{\beta}\mathbf{v}_s] + f^{\beta}_{l\to s} + (1-\phi)\rho_s\Gamma^{\beta}_{s}, \tag{4.1}$$

where F^{β} denotes the mass of the β-component on the solid, per unit mass of the latter, and $f^{\beta}_{l\to s}$ denotes the rate of transfer of the β-component from liquid to solid, due to adsorption.

Equations (1) and (4.1) include unknown rates of interphase transfers. However, since

$$f^{\beta}_{l\to g} = -f^{\beta}_{g\to l}, \qquad f^{\beta}_{g\to s} = -f^{\beta}_{s\to g},$$

these rates can be eliminated from the balance equations by summing up the equations for the same component in all the phases.

While carrying out the summation of equations, let us further assume that

[2.5] The solid matrix remains undeformable and immobile at the macroscopic level as well as with a constant density, i.e. $\rho_s = \text{constant}$, and $\mathbf{v}_s = 0$.

[2.6] The gaseous phase is practically immobile, i.e. $\mathbf{v}_g = 0$.

[2.7] The porosity as well as the soil volumetric content of f-phase, θ_f, conditions remain constants, i.e. $\phi = \text{const.}$

$$\theta_l = \phi S_l = \text{const.}; \qquad \theta_g = \phi S_g = \text{const.}$$

[2.8] The dispersion flux is negligible due to the low average velocity of water, i.e. $\mathbf{D}^{\beta}_{h\eta} \cong D^{*\beta}_{\eta}$.

The effective diffusion in the soil for the β-component is calculated according to Nye and Marriott (1969) as

$$D^{*\beta}_{l} = \mathbf{D}^{\beta}_{l}\, T_l, \tag{4.2}$$

where D_l^β denotes the diffusion coefficient of β-component in water and T_l denotes a correction factor for the tortuosity of the diffusion path in soil (Barraclough and Tinker, 1981; So and Nye, 1989).

[2.9] The β-components are assumed not volatile, hence their concentration in the gas phase remains constant.

[2.10] Being an anion, the Cl^- component does not undergo adsorption.

In view of (1) to (4) and [2.5] to [2.10], we obtained the following mass balance equation for the ion components:

(a) For the Cl^-*-component in liquid*

$$\frac{\partial}{\partial t}(\theta_l \rho_l^{Cl}) = -\nabla\cdot[\theta_l(\rho_l^{Cl}\mathbf{v}_l - D_l^{*Cl}\nabla\rho_l^{Cl})] + \theta_l\rho_l\Gamma_l^{Cl} \tag{5}$$

(b) For *dissolved matter in liquid and solid* (i.e. the cationic species)

$$\frac{\partial}{\partial t}[\theta_l\rho_l^\beta + (1-\phi)\rho_s F^\beta] = -\nabla\cdot[\theta_l(\rho_l^\beta\mathbf{v}_l - D_l^{*\beta}\nabla\rho_l^\beta)] + \theta_l\rho_l\Gamma_l^\beta + (1+\phi)\rho_s\Gamma_s^\beta. \tag{6}$$

The amounts of dissolved matter in the liquid, expressed as ρ_l^β, and on the solid, expressed by F^β, are not independent, they are related to each other by a relationship referred to as an adsorption isotherm.

In the case considered herein, we refer to reversible reaction between negative (-1) exchange sites on the solid and M and N cations with charges of m^+ and n^+, respectively. The reaction is of the form

$$mN^{n+} + n(MXm)_s \Leftrightarrow nM^{m+} + m(NXn)_s$$

in which N^{n+} denotes a cationic component in solution, $(NX_n)_s$ denotes the component in the adsorbed state on the solid (its concentration will then be $\rho_s F^{NX_n}$), M^{m+} denotes the exchangeable cation, initially on the solid $(MX_m)_s$, remaining in the liquid.

Let us assume,

[2.11] Instantaneous equilibrium for the ions exchange reactions.

Thus, according to the law of mass action, we obtain

$$K_{M^{m+}}^{N^{n+}} = \frac{[NX_n]^m[M^{m+}]^n}{[N^{n+}]^m[MX_m]^n}, \tag{7.1}$$

in which $K_{M^{m+}}^{N^{n+}}$ denotes the equilibrium coefficient for the exchange reaction, and the bracketed terms represent activities. These activities can be related to the molar concentrations by

$$[\beta] = \gamma^\beta\rho_\eta^\beta, \tag{7.2}$$

where γ^β denotes the activity coefficient of the β-component. It can be evaluated according to the Debye–Hückel relation (at a temperature of 20°C)

$$\gamma^\beta = 10^{-\left(\frac{0.5(Z^\beta)^2(\lambda)^{0.5}}{1+0.327\cdot 10^{+8}\partial^\beta(\lambda)^{0.5}}\right)+0.041\lambda}, \tag{7.3}$$

where Z^β denotes the valence of ion β, ∂^β (cm) denotes the ion's 'effective diameter', and λ denotes the ionic strength of the solution, given by

$$\lambda = \frac{1}{2}\sum_{(\beta)} \rho_\eta^\beta (Z^\beta)^2. \tag{7.4}$$

In the case considered, the reversible ion exchange reactions are

$$\tfrac{1}{2}Ca^{2+} + (Mg^{2+})_{s0.5} \Leftrightarrow Mg^{2+} + (Ca^{2+})_{s0.5}, \tag{8.1}$$

$$\tfrac{1}{2}Ca^{2+} + (K^+)_s \Leftrightarrow K^+ + (Ca^{2+})_{s0.5}, \tag{8.2}$$

$$\tfrac{1}{2}Ca^{2+} + (Na^+)_s \Leftrightarrow Na^+ + (Ca^{2+})_{s0.5}, \tag{8.3}$$

$$\tfrac{1}{2}Mg^{2+} + (K^+)_s \Leftrightarrow K^+ + (Mg^{2+})_{s0.5}, \tag{8.4}$$

$$\tfrac{1}{2}Mg^{2+} + (Na^+)_s \Leftrightarrow Na^+ + (Mg^{2+})_{s0.5}, \tag{8.5}$$

$$K^+ + (Na^+)_s \Leftrightarrow Na^+ + (K^+)_s. \tag{8.6}$$

However, in writing expressions for the equilibrium coefficients, we alternatively use Gapon's concept (Robbins *et al.*, 1980; Fischer, 1990) for the selectivity coefficients K_i ($i = 1, 2, 3$) which rewrites the reactions per unit electrical charge. Hence, the equivalent to (7.1) is in the form

$$\left(\frac{\gamma^{Ca}\rho_l^{Ca}}{\gamma^{Mg}\rho_l^{Mg}}\right)^{1/2}\frac{F^{\frac{1}{2}Mg}}{F^{\frac{1}{2}Ca}} = K_1, \tag{9.1}$$

$$\frac{\gamma^{Na}\rho_l^{Na}}{(\gamma^{Ca}\rho_l^{Ca})^{1/2}}\frac{F^{\frac{1}{2}Ca}}{F^{Na}} = K_2, \tag{9.2}$$

$$\frac{\gamma^{K}\rho_l^{K}}{(\gamma^{Ca}\rho_l^{Ca})^{1/2}}\frac{F^{\frac{1}{2}Ca}}{F^{K}} = K_3. \tag{9.3}$$

Note that in writing (9) we have assumed that,

[2.12] The activity coefficients of the adsorbed substances are approximately equal to unity.

Actually, the reason for rewriting the ion exchange reactions via Gapon's convection is to allow an additional relation concerning the cation exchange capacity CEC (assumed to be constant),

$$CEC = F^{\frac{1}{2}Ca} + F^{\frac{1}{2}Mg} + F^{Na} + F^{K}. \tag{10}$$

The CEC originates from the surplus of negative over positive electrostatic charges on the clay surfaces. The soil is considered well-buffered so that variations in pH

causing changes of the hydroxyl groups on the clay would yield a minimal effect on the net charge. We also neglect the effect of alkalinization that may influence the thickness of the electrical double layer at the clay surfaces, which, in return, changes the stability of the soil aggregates and the cation adsorbing characteristics. Based on the above, the anion exchange capacity (AEC) is minor (i.e., practically no adsorption of anions), which allows us to neglect diffusion due to electric potential.

In view of (9) and (10) and following Robbins *et al.* (1980), we may now express the equilibrium adsorption isotherms, F^I, of the I ion, in the form

$$F^{\frac{1}{2}Ca} = \frac{(\rho_l^{Ca})^{1/2}}{d}(CEC), \tag{11.1}$$

$$F^{\frac{1}{2}Mg} = K_1^* \frac{(\rho_l^{Mg})^{1/2}}{d}(CEC), \tag{11.2}$$

$$F^{Na} = \frac{1}{K_2^*}\frac{\rho_l^{Na}}{d}(CEC), \tag{11.3}$$

$$F^{K} = \frac{1}{K_3^*}\frac{\rho_l^{K}}{d}(CEC), \tag{11.4}$$

where

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

$$K_1^* = K_1\frac{(\gamma^{Mg})^{0.5}}{(\gamma^{Ca})^{0.5}}, \qquad K_2^* = K_2\frac{(\gamma^{Ca})^{0.5}}{\gamma^{Na}}, \qquad K_3^* = K_3\frac{(\gamma^{Ca})^{0.5}}{\gamma^{K}}.$$

In considering the mass balance expression in (6), we continue and assume that

[2.13] The β-component mass does not change due to the rate of production caused by chemical reaction nor by influx or efflux. Decay or degradation of the component in the fluid phase is negligible.

[2.14] Plane radial flow with radial symmetry and

$$\frac{\partial}{\partial r}(rv) = 0, \tag{12}$$

where r denotes the radial distance from the center of the root cross-section, and v denotes the water radial velocity.

In view of [2.13] and [2.14], we now rewrite (5) and (6) for $C^\beta(\equiv \rho_l^\beta)$ the β-component concentration in water (omitting the l subscript).

$$\frac{\partial}{\partial t}C^{Cl} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD^{*Cl}\frac{\partial C^{Cl}}{\partial r} + v_0 r_0 C^{Cl}\right], \tag{13}$$

$$\frac{\partial}{\partial t}C^I + \frac{1-\phi}{\theta_l}\rho_s\frac{\partial F^I}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD^{*I}\frac{\partial C^I}{\partial r} + v_0 r_0 C^I\right]; \quad I \equiv \text{K, Ca, Mg, Na,} \tag{14}$$

where v_0, denotes the water radial velocity at the root surface ($r = r_0$).

In view of (9) and (11), we now express $\partial F^I/\partial t$, in the form

$$\frac{\partial F^I}{\partial t} \cong \sum_{\beta=1}^{4} A^{I\beta}\frac{\partial C^\beta}{\partial t}, \quad I, \beta = 1, 2, 3, 4, \tag{15.1}$$

$$A^{I\beta} = \begin{cases} -\dfrac{1}{a_I a_\beta}\dfrac{F^I F^\beta}{C^\beta(\text{CEC})}, & \text{if } I \neq \beta, \\ \dfrac{1}{a_I^2}\dfrac{F^I}{C^I}\left(1 - \dfrac{F^I}{\text{CEC}}\right), & \text{if } I = \beta, \end{cases} \tag{15.2}$$

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

Note that in writing (15) we have also assumed that

$$\frac{\partial \gamma^\beta}{\partial t} \ll \gamma^\beta. \tag{16}$$

Thus, by virtue of (13)–(15), we may write a general mass balance equation, in the form

$$\sum_{\beta=1}^{5} R^{I\beta}\frac{\partial C^I}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD^{*I}\frac{\partial C^I}{\partial r} + v_0 r_0 C^I\right] \tag{17}$$

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

$$R^{I\beta} = \left\{\begin{array}{ll} \dfrac{1-\phi}{\theta_l}\rho_s A^{I\beta}, & \text{if } I \neq \beta \\ 1 + \dfrac{1-\phi}{\theta_l}\rho_s A^{I\beta}, & \text{if } I = \beta \end{array}\right\} I, \beta = 1, 2, 3, 4, \tag{18.1}$$

$$R^{55} = 1, \qquad R^{5\beta} = R^{I5} = 0, \qquad I, \beta = 1, 2, 3, 4. \tag{18.2}$$

The transport equation (17) is to be solved for each of the β-component concentrations (C^β) subject to

Initial Conditions:

$$C^\beta_{(r,t_0)} = C^\beta_{0(r)}, \tag{19}$$

where t_0 denotes the initial time.

Boundary Conditions:

Boundary conditions are supplied at the root surface ($r = r_0$) and at the external radius ($r = r_1$).

At the Root Surface ($r = r_0$),

Absorption of ions at the root surface is characterized by different mechanisms. Accordingly, such mechanisms dictate specific boundary conditions for each ion:

$$\theta_l D^{*I} \frac{\partial C^I}{\partial r} + \theta_l v_0 C^I = J^I_{r_0}, \quad I \equiv \text{K, Ca, Mg, Na, Cl,} \tag{20}$$

where $J^I_{r_0}$ denotes the uptake flux at $r = r_0$ for the I ion.

The influx $J^I_{r_0}$ is assumed to be passive when concerning Ca^{2+}, Mg^{2+}, and Cl^- components (Mengel and Kirkby, 1987). In this case, we can take into consideration two kinds of boundary conditions. One which is diffusion through the root membrane,

$$J^I_{r_0} = -P^I_m(C^I_{r_0} - C^I), \quad I \equiv \text{Ca, Mg, Cl,} \tag{21.1}$$

where $P^I_{r_0}$ and $C^I_{r_0}$ denote the permeability of the root membrane and the concentration inside the root for the I ion, respectively. Those parameters may be time-dependent.

The second choice concerns the domination of the advective flux, namely

$$J^I_{r_0} = \theta_l v_0 C^I, \quad I = \text{Ca, Mg, Cl.} \tag{21.2}$$

In view of (20), this in return would mean that

$$\frac{\partial C^I}{\partial r} = 0, \quad I = \text{Ca, Mg, Cl.} \tag{21.3}$$

Influx of the K^+ component

$$J^{\text{K}}_{r_0} = \left[\frac{(C^{\text{K}})^h}{(K_a)^h + (C^{\text{K}})^h}\right] J_{\max} + \alpha C^{\text{K}}, \tag{22}$$

where $J_{\max}$ denotes maximal flux uptake (influx), K_a denotes the apparent Michaelis–Menten coefficient (i.e., concentration when $J^{\text{K}}_{r_0} = \frac{1}{2}J_{\max}$), h denotes the cooperative (Hill) power index (Bernard, 1968), and α denotes the linear change of influx with respect to relatively high (above 0.2 mM) concentrations (Kochian and Lucas, 1988). There is a debate as to the exact nature of K^+ influx at high concentrations (Jensen *et al.*, 1987; Nissen, 1988). However, since the major limitations for K^+ uptake by a root grown in soil are the root system geometry (length and mean radius) and soil parameters, rather than influx parameters of the root surfaces (Silberbush and Barber, 1983; Clarkson, 1985), such as assumption is reasonable for practical purposes.

The influx $J^{\text{K}}_{r_0}$ is influenced by C^{Na} at $r = r_0$. This constitutes the functional relations $[J_{\max}(C^{\text{Na}}), K_a(C^{\text{Na}}), h = h(C^{\text{Na}}), \alpha(C^{\text{Na}})]$ that can be found empirically (Silberbush and Ben-Asher, 1987, 1989).

Influx of the Na^+ component:

$$J^{\text{Na}}_{r_0} = \begin{cases} 0; & C^{\text{Na}} \leqslant C^{\text{Na}}_{\text{cr.}}, \\ \alpha' C^{\text{Na}}; & C^{\text{Na}} > C^{\text{Na}}_{\text{cr.}}, \end{cases} \tag{23}$$

where $C^{Na}_{cr.}$ denotes a critical Na^+ concentration and α' (constant under the assumption of no aging of roots) denotes the linear change of influx associated with C^{Na}.

Boundary Concentration for the Ca-*component*:
This boundary condition is governed by the efflux (from the root surface) of either H^+ or HCO_3^- components (or their organic equivalents) which balances the difference between the sums of anions' and cations' influxes. The pH adjustment was shown to be actively affected by the root system (Mengel and Kirkby, 1987; Schubert and Mengel, 1989).

For calculation of the changes in HCO_3^-, CO_3^{2-}, and H^+ concentrations we use the equation of electroneutrality

$$2C^{Ca} + 2C^{Mg} + C^{Na} + C^{K} - C^{Cl} - 2C^{CO_3} - C^{HCO_3} = 0. \tag{24}$$

In writing (24), we have assumed that C^{H} and C^{OH} are small.

In calcareous soils, with an opened $CaCO_3$(calcite)–$CO_{2(g)}$–H_2O system (constant $CO_{2(g)}$ pressure), the soil chemistry is governed by the relations

$$[H_2CO_3] = 10^{-1.46}[CO_2]. \tag{25.1}$$

The gaseous CO_2 partial pressure in soils is usually much higher than in the open atmosphere (Glinski and Stepniewski, 1985, pp. 89–100). A representative value, commonly used in soil models, is $[CO_2] = 10^{-2}$ (Bar) (Jurinak, 1984, p. 25).

$$[HCO_3^-] = 10^{-6.36}\frac{[H_2CO_3]}{[H^+]}, \tag{25.2}$$

$$[CO_3^{2-}] = 10^{-10.33}\frac{[HCO_3^-]}{[H^+]}, \tag{25.3}$$

$$[Ca^{2+}] = \frac{10^{-8.30}}{[CO_3^{2-}]}. \tag{25.4}$$

From (24) and (25), we obtain the equation for the C^{H} component

$$\sum_{n=0}^{4} b_n (C^{H})^n = 0, \tag{26}$$

where

$$b_0 = -\frac{10^{-18.15}[CO_2]}{\gamma^{CO_3}(\gamma^{H})^2}, \qquad b_1 = -\frac{10^{-7.82}[CO_2]}{\gamma^{H}\gamma^{HCO_3}},$$

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

Solving (26), we obtain C^{H} and, from (25.1)–(25.3), we can calculate concentrations of HCO_3^- and CO_3^{2-}. The concentration of Ca^{2+} is corrected by relation (25.4).

At the External Boundary of the Soil Cylinder ($r = r_1$)

A continuous supply of ion mass occurs at that boundary to keep the ion concentration constant at any time,

$$C^I_{r_1} = \text{const.}, \quad I \equiv Cl^-, Mg^{2+}, Ca^{2+}, Na^+, K^+, \tag{27}$$

When a supply of ion mass does not occur at the boundary, the flux is zero at any time,

$$D^{*I}\frac{\partial C^I}{\partial t} + v_0 C^I = 0, \quad I \equiv Cl^-, Mg^{2+}, Ca^{2+}, Na^+, K^+. \tag{28}$$

3. Summary of the Equations and Variables

At this stage, we have stated all the governing equations, initial and boundary conditions, constitutive relations, and definitions included in our model. Altogether, the state variables and the equations are listed in Table I. The various initial and boundary conditions are presented in Table II.

Table I. Summary of complete model of K^+ uptake under salinity for each of the β-components

Equations	Dependent variables
Mass balance equation in the soil-water system (17)	C^β,
Function for diffusion in the soil (4.2)	$D^{*\beta}$,
Definition of retardation term (18)	R^β
Constitutive relation for the adsorption isotherm (11)	F^β
Activity coefficient (7.5)	γ^β
Total: 5 equations	5 variables

Table II. Summary of initial and boundary conditions for the various β-components

Equations	Applied to components
Initial conditions (19)	Cl^-, Ca^{2+}, Mg^{2+}, Na^+, K^+
Influx uptake at the root surface, $r = r_0$	
(20), (21.1) or (21.3)	Ca^{2+}, Mg^{2+}, Cl^-
(21)	K^+
(22)	Na^+
Concentration at the root surface, $r = r_0$	
(26)	H^+
(25)	Ca^{2+}, HCO_3^-, CO_3^{2-}
Concentration or flux at the external boundary, $r = r_1$ (27), (28)	Cl^-, Ca^{2+}, Mg^{2+}, Na^+, K^+

4. Discussion

The complexity of salinity effects on plants resulted in numerous approaches to this problem (Pasternak, 1987). Lack of knowledge as to the physiological aspects of salinity and practical convenience, introduced the concept of osmotic potential and, consequently, the electrical conductivity (EC) of water and the soil solution as indexes to salinity (Maas and Hoffman, 1977). Accumulated evidence shows that this concept is biased, and the major effect of saline media on plant metabolism and on plant growth is due to interactions among ions during their uptake (Papadopoulas and Rending, 1983; Singh *et al.*, 1990; Subbarao *et al.*, 1991; Akhavan-Kharazian *et al.*, 1991).

Simulation models are most useful for complex processes as soil-rhizosphere-root interactions (Clarkson, 1985; Jungk and Claassen, 1986). They may give us information that we cannot measure *in situ* (Rengel and Robinson, 1990; Bar-Tal *et al.*, 1991; Claassen *et al.*, 1986), although the experimental verification is not always satisfactory (Clarkson, 1985). The potential merit of such a model for simulation of the simultaneous movement of ions in the soil and uptake by plant roots is therefore a substantial step forward in plant mineral nutrition in general, and to the salinity effect on crops in particular. However, the existing models do not provide a satisfactory answer to this complexity. Some of them are based on assumptions that contradict the salinity case, like treating one ion only, or aimed at very low concentrations (e.g. Cushman, 1979). The model proposed by Bouldin (1989) was aimed at accounting for interaction among all the major nutrients in the soil and consequent pH changes at the root. However, this model neglected the interaction among ions during uptake, which is of major importance in the case of uptake from a saline medium.

Influx parameters for the whole root system are assumed to be constant with age and location. This is a controversial assumption, since there is evidence that ions and water are absorbed nonuniformly along the roots (Eshel and Waisel, 1973). However, no unique pattern may be defined (Zobel, 1990). The practical way to treat this case is to assume average parameters along the roots which will be constant with time. Another effect which is disregarded is the influence of the K^+ content in the root tissue of K^+ influx (Siddiqi and Glass, 1982). This factor affects influx along a relatively wide range of K^+ concentrations in the root tissues (Siddiqi and Glass, 1982). It was recently shown (Fernando *et al.*, 1990) that drastic shifts from high to low K^+ concentration reduces its concentration in root and shoot tissues and causes an increase in K^+ influx. Changes in K^+ concentration in the root tissues, though, may not affect the K^+ influx unless the plant was supplied with extremely high amounts of K^+.

Net Na^+ influx is assumed to equal zero at low Na^+ concentration, and to increase linearly with the concentration above a critical concentration $C_{cr.}^{Na}$. At low Na^+ concentrations, active efflux balances passive influx (Jeschke, 1973), but Na^+ influx increases linearly with its external concentration (Kawasaki and Hori, 1968;

Silberbush and Ben-Asher, 1987), so above a certain concentration, a positive net influx occurs. The critical concentration $C_{cr.}^{Na}$ and the rate of influx increase, α', may be affected by Ca^{2+} and K^+ concentrations (Jeschke, 1973). However, in soils of arid and semi-arid zones, the Na^+ concentration in the soil solution is usually much higher than that of K^+ or Ca^{2+} concentrations (Reisenauer, 1966). The effect of the relevant range of concentrations of these cations on Na^+ influx parameters should be experimentally determined.

Influx of Ca^{2+} is assumed to be passive, namely, it depends only on mass-flow. This assumption is generally accepted, since the plant's needs for Ca^{2+} is usually supplied by mass-flow and root interception (Barber, 1984; Mengel and Kirkby, 1987). Also, the absorbing power of roots would not change much with Ca^{2+} concentration, except in very low concentrations (Rossi *et al.*, 1988). Concentrations of Ca^{2+} in plants and plant growth are affected mainly by $C^{Ca}/\Sigma C^I$ ($I \equiv K^+$, Na^+, Ca^{2+}, Mg^{2+}) ratio (Janzen and Chang, 1987; Carter and Webster, 1990), but Ca^{2+} influx to the root is unaffected (Lynch and Läuchli, 1985). The effect of salinity of plant Ca^{2+} is therefore by inhibiting Ca^{2+} translocation from the root to the shoot (Hansen and Munns, 1988), probably by inhibiting the radial movement of Ca^{2+} into the root xylem (Lynch and Läuchli, 1985). Since the motion of Ca^{2+} and Na^+ within the plant is not treated by this model, the above assumption is reasonable.

Chloride is assumed to be taken up by roots with the mass-flow, namely, passively (Mengel and Kirkby, 1987, p. 139). The difference between influxes of the absorbed anions and cations should be balanced by efflux, either of H^+ (when negative) or HCO_3^- (when positive), or their equivalents. This efflux should create a gradient of that ion from the root surface towards the soil bulk. If the soil is calcareous, dissolution or precipitation of $CaCO_3$ may occur (Nye, 1984; Nye and Ameloko, 1987). Magnesium carbonate is more soluble than calcite, so its precipitation is usually neglected in soils (Bresler *et al.*, 1982, p. 24). Indeed, the ion-balance is only in part the source for pH changes at the root surface. Proton release by plant roots may be a result of an active proton extrusion by ATPases (Bashan and Levanony, 1989; Schubert and Mengel, 1989). This activity may be controlled by plant metabolism as a reaction to some nutritional deficiencies like phosphorus (Grinsted *et al.*, 1982) or iron (Bienfait *et al.*, 1989). However, these effects cannot be quantified to be included in a simulation model, since very little is known as to their physiology. Therefore, the physiological effects on proton release by roots is disregarded.

The proposed model disregards physiological changes within the plant and their effects on the soil around the roots, and accounts for four cations and one anion only. Even so, this model is a meaningful advance in simulating plant nutrition under salinity.

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