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Finite Differences and Integral Balance Methods Applied to Nutrient Uptake by Roots of Crops

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The nutrient uptake by growing roots of crops is studied. An approximation by a moving boundary model is given and a solution through the integral balance method is obtained. Other solutions through the front-fixing method and the application of the finite differences method in its explicit and implicit versions are obtained. Moreover, an additional solution through the front-tracking and explicit finite differences method is obtained. The algorithms are applied to compute K, Mg and P uptake by pine seedlings. The results obtained for the four methods are compared with experimental results as with predictions of other well known models based on fixed domains such as the Barber-Cushman model.

Keywords Moving Boundary Model, Integral Balance Method, Front Fixing and Finite Differences Model

1. INTRODUCTION

Nutrient uptake has been evaluated through diffusion and mass flux models, which are based on numerical approximations in fixed domain through transport differential equations coupled with root absorption kinetics [1, 2]. These models estimate the nutrient concentration in the root-soil interface and consequently the resultant nutrient uptake. Other models assume that the surface of the root behaves like a sink; therefore the nutrient uptake is determined by the rate of the nutrient supplied by mass and diffusion flux. In these models, the radius of the volume of cylindrical finite shell assigned to each root decreases when root density increases [3]. In other models analytical solutions have been used in order to compute the volume of soil assigned to each root [4], and the concentration on root surface including an increasing depletion zone with time until is reached the limit of not-transference [5]. Recently, free boundary models for root growth have been formulated [6–8], that is, analytic models through which it is possible to compute the nutrient concentration in the root-soil interface and to estimate a qualitative law of root growth (a function of the time, a priori, unknown). Based upon these models a new model of nutrient uptake due to the transport and absorption of ions from a more dynamic viewpoint has been proposed. This model, in contrast to the free boundary model, now introduces the root growth rate as a known function of time. Thus, the objective of this work is to evaluate a moving boundary model of nutrient uptake, which takes into account a growing root system. It is considered to be a one-dimensional model, that is, a single cylindrical root in the soil for which the conditions of humidity, light and temperature are assumed to be controlled (as in a growth chamber). With this hypothesis, we propose the following method to compute nutrient uptake through a moving boundary model to one phase (the soil) in cylindrical coordinates: [9, 10]

$$D\frac{\partial^2 C}{\partial r^2} + D(1+\varepsilon_o)\frac{1}{r}\frac{\partial C}{\partial r} = \frac{\partial C}{\partial t}, \quad s_o < r < R(t), \quad 0 < t < T \tag{1}$$

$$C(r,0) = \varphi(r), \quad s_o \le r \le R_o \tag{2}$$

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$$-Db\frac{\partial}{\partial r}C(R(t),t)+v_oC(R(t),t)=0,\quad 0<t<T \tag{3}$$

$$Db\frac{\partial}{\partial r}C(s_o,t)+v_oC(s_o,t)=\frac{k_a[C(s_o,t)-C_u]}{1+\frac{k_a[C(s_o,t)-C_u]}{J_m}},\quad 0<t<T \tag{4}$$

$$R(t)=R_o\sqrt{\frac{l_o}{l(t)}},\quad 0<t<T \tag{5}$$

where r is the radial distance from the axis of the root [cm]; t is the time [s]; T is the maximum time for which there is solution [s]; C_u is the threshold concentration from which influx stops [mol cm^{-3}]; v_o is the effective velocity of flux solution on the root [cm s^{-1}]; b is the buffer power [dimensionless]; D is the diffusion coefficient [cm^2 s^{-1}]; k_a ($= J_m/K_m$) is the nutrient absorption power [cm s^{-1}]; J_m is the maximum influx [mol cm^{-2} s^{-1}]; K_m is the concentration for which the influx is $J_m/2$ [mol cm^{-3}]; $R(t)$ is the half distance between roots axis [cm]; $\varphi(r)$is the initial concentration profile in $[s_o, R_o]$ [mol cm^{-3}]; R_o is the initial half distance between root axis [cm]; s_o is the root radius [cm]; $l(t)$ is the root length as a function of time [cm]; l_o is the initial root length [cm]. $\varepsilon_o = v_os_o/Db$ is a dimensionless parameter. Equation (1) is the transport equation of ions in soil and Eq. (2) corresponds to the profile of initial concentrations. Equation (3) represents a null flux on $R(t)$. Equation (4) represents the mass balance on the root surface and the Eq. (5) represents the moving boundary $R(t)$ as a function of the instantaneous root length $l(t)$, which is known a priori.

2. THE INTEGRAL BALANCE METHOD

The model is solved applying the method of the integral balance for which the differential equation (1) is integrated in the variable r on the domain $[s_o, R(t)]$ [8, 11]. Using a similar methodology to that used in processes of phase change, the following expression is proposed for $C(r, t)$:

$$C(r,t)=\varphi(r)\left[1+\beta(t)\left(1-\frac{r}{R(t)}\right)^2\right] \tag{6}$$

with:

$$\varphi(r)=C_Re^{-\varepsilon(R_o-r)},\quad \varepsilon=\frac{v_o}{Db}=\frac{\varepsilon_o}{s_o} \tag{7}$$

where C_R is the initial concentration of ion in solution on $r = R_o$ [mol cm^{-3}]. The expression (6) for the concentration verifies the initial condition (2) taking into account $\beta(0) = 0$ and the condition of contour (3). After algebraic elementary manipulations and taking into account the particular case of a linear longitudinal growth, given by $l(t) = l_o + kt$, we obtain the following differential equation for $\beta(t)$:

$$\begin{cases}\dfrac{d\beta(t)}{dt}=\dfrac{F_2(R(t),\beta(t))}{F_1(R(t))},\quad \beta(0)=0\\ R(t)=R_o\sqrt{\dfrac{l_o}{l_o+kt}}\end{cases} \tag{8}$$

where the real functions F_1 and F_2 were given in previous works [12].

The system (8) is solved by using the Runge-Kutta method for ordinary differential equations, and a computer program written in FORTRAN. Nutrient uptake can be obtained from the following formula [13], which is a modified version of the Cushman formula [1].

$$U=2\pi s_ol_o\int_{\tau=0}^{\tau=t_{\max}}J_c(\tau)\,d\tau+2\pi s_o\int_{\tau=0}^{\tau=t_{\max}}\left[\int_{\tau=t}^{\tau=t_{\max}}J_c(\tau)\,d\tau\right]\dot{l}(\tau)\,d\tau \tag{9}$$

$$J_c(\tau)=\frac{k_a[C(s_o,\tau)-C_u]}{1+\frac{k_a[C(s_o,\tau)-C_u]}{J_m}} \tag{10}$$

where $J_c(\tau)$ is the influx, $\dot{l}(\tau)$ it is the longitudinal growth velocity and U is calculated from $\tau = 0$ to $\tau = t_{\max}$.

3. THE METHOD OF FRONT-FIXING AND FINITE DIFFERENCES

Another method to obtain the solution of the mathematical model (1)–(5) is applying the immobilization of the domain or front fixing method and the subsequent application of finite differences in their explicit version. In order to fix the domain $[s_o, R(t)]$ to the interval [0, 1] we carry out the following transformation:

$$\begin{cases}y=\dfrac{r-s_o}{R(t)-s_o},\quad t=t\\ \Psi(y,t)=C(r,t)\end{cases} \tag{11}$$

obtaining for the problem (1)–(5) the following equations and conditions:

$$A_1(t)\psi_{yy}(y,t)+B(y,t)\psi_y(y,t)=\psi_t(y,t),\quad 0\le y\le 1,\quad 0<t<T \tag{12}$$

$$\Psi(y,0)=\varphi(y[R_o-s_o]+s_o),\quad 0\le y\le 1 \tag{13}$$

$$-A(t)b\Psi_y(1,t)+v_o\Psi(1,t)=0,\quad 0<t<T \tag{14}$$

$$A(t)b\Psi_y(0,t)+v_o\Psi(0,t)=\frac{k_a[\Psi(0,t)-\Psi_u]}{1+\frac{k_a[\Psi(0,t)-\Psi_u]}{J_m}},\quad 0<t<T \tag{15}$$

$$R(t)=R_o\sqrt{\frac{l_o}{l_o+kt}} \tag{16}$$

where $\Psi_u = C_u$ and $\dot{R}(t)$ represents the derivative of $R(t)$ with respect to t, and

$$A(t) = \frac{D}{R(t) - s_o}, \quad A_1(t) = \frac{A(t)}{R(t) - s_o} \tag{17}$$

$$B(y,t) = \frac{D_1 + s_o \dot{R}_1(t) y + R_1(t)\dot{R}_1(t) y^2}{R_1^2(t) y + s_o R_1(t)} \tag{18}$$

where $D_1 = D(1 + \varepsilon_o)$, $R_1(t) = R(t) - s_o$.

We consider a uniform grid in the space and in the time of the rectangular domain $[0, 1] \times [0, t_{\max}]$, where $t_{\max} < T$, with steps Δy in the space and Δt in the time respectively. It is noted:

$$\begin{cases} y_j = j\,\Delta y, \quad j = 0, \ldots, M \quad con \quad M\Delta y = 1 \\ t^n = n\,\Delta t, \quad n = 0, \ldots, N \quad con \quad N\Delta t = t_{\max} \\ \Psi(y_j, t^n) = \Psi_j^n\text{: } \Psi \text{ value in the point } y_j \text{ to time } t^n \end{cases} \tag{19}$$

where the points (y_i, t^n) are the nodes of the discrete domain.

We apply the explicit finite differences method for problem (12)–(16): forwards in the time derivative and centered in the space for the spatial second derivative, i.e:

$$\frac{\partial \psi(y_j, t^n)}{\partial t} \cong \frac{\psi(y_j, t^n + \Delta t) - \psi(y_j, t^n)}{\Delta t}$$

$$\frac{\partial^2 \psi(y_j, t^n)}{\partial y^2} \cong \frac{\psi(y_j + \Delta y, t^n) - 2\psi(y_j, t^n) + \psi(y_j - \Delta y, t^n)}{\Delta y^2}$$

Taking into account the sign of the coefficient $B(y_j, t^n)$ we discretize the spatial first derivative with backwards differences if $B_j^n < 0\,(B_j^n = B(y_j, t^n))$, i.e.

$$\frac{\partial \psi}{\partial y}(y_j, t^n) \cong \frac{\psi(y_j, t^n) - \psi(y_j - \Delta y, t^n)}{\Delta y}$$

or forward differences if $B_j^n > 0$, i.e.

$$\frac{\partial \psi(y_j, t^n)}{\partial y} \cong \frac{\psi(y_j + \Delta y, t^n) - \psi(y_j, t^n)}{\Delta y}.$$

When $B_j^n < 0$ the discretization of the Eq. (12) is given by:

$$\Psi_j^{n+1} = \left[B_j^n \frac{\Delta t}{\Delta y} - 2A_1^n \frac{\Delta t}{\Delta y^2} + 1 \right] \Psi_j^n + \left[A_1^n \frac{\Delta t}{\Delta y^2} \right] \Psi_{j+1}^n + \left[A_1^n \frac{\Delta t}{\Delta y^2} - B_j^n \frac{\Delta t}{\Delta y} \right] \Psi_{j-1}^n \tag{20}$$

with:

$$\Delta t \leq \frac{\Delta y^2}{2A_1^n - B_j^n \Delta y} \quad \forall n \tag{21}$$

where $A_1^n = A_1(t^n)$. The condition (21) is obtained by imposing that the coefficient of Ψ_j^n is positive, in order to guarantee that Ψ_j^{n+1} is a positive number.

When $B_j > 0$ the discretization of the Eq. (12) results:

$$\Psi_j^{n+1} = \left[-B_j^n \frac{\Delta t}{\Delta y} - 2A_1^n \frac{\Delta t}{\Delta y^2} + 1 \right] \Psi_j^n + \left[A_1^n \frac{\Delta t}{\Delta y^2} \right] \Psi_{j-1}^n + \left[A_1^n \frac{\Delta t}{\Delta y^2} + B_j^n \frac{\Delta t}{\Delta y} \right] \Psi_{j+1}^n. \tag{22}$$

Similarly we obtain

$$\Delta t \leq \frac{\Delta y^2}{2A_1^n + B_j^n \Delta y} \quad \forall n \tag{23}$$

The values B_j^n for the different nutrients considered can be positive and/or negative according to the point and the time considered. Because of this, in each case we can apply the corresponding iterative formulae (20) or (22).

The initial concentration profile given by the condition (14) transforms in:

$$\Psi(y_j, 0) = \varphi(y_j[R_o - s_o] + s_o), \quad \forall\, j \tag{24}$$

The boundary condition on $y = 1$ is approximated with backward differences and therefore the condition (14) results:

$$\Psi(1, t^n) = \frac{Db\,\Psi(1 - \Delta y, t^n)}{Db - v_o \Delta y\ R_1(t^n)} \tag{25}$$

with

$$\Delta y < \frac{Db}{v_o(R_o - s_o)} \tag{26}$$

that insures $\Psi(1, t^n) > 0$, for all n.

The boundary condition on $y = 0$ is approximated with forward differences and a quadratic equation for $\Psi(0, t^n)$ is obtained. This quadratic equation is given by:

$$\alpha(t^n)\Psi^2(0, t^n) + \beta(t^n)\Psi(0, t^n) + \gamma(t^n) = 0 \tag{27}$$

where the coefficients α, β and γ are given by:

$$\alpha(t^n) = v_o - \frac{A(t^n)b}{\Delta y} < 0, \tag{28}$$

$$\beta(t^n) = \frac{A(t^n)b}{\Delta y}\Psi(\Delta y, t^n) + \left(v_o - \frac{A(t^n)b}{\Delta y} \right)(K_m - \Psi_u) - J_m \tag{29}$$

$$\gamma(t^n) = (K_m - \Psi_u)\frac{A(t^n)b}{\Delta y}\Psi(\Delta y, t^n) + J_m \Psi_u \tag{30}$$

The second degree Eq. (27) verifies that the discriminant and the independent term are positive, and the coefficient of the term of second degree is negative; therefore, the product of the two roots of the second degree Eq. (27) is negative, and then the two roots have different signs. Since we work with concentrations we will take only positive results.

The unique positive root of the Eq. (27) is given by the following expression:

$$\Psi(0, t^n) = \frac{\beta + \sqrt{\beta^2 + 4\gamma(-\alpha)}}{2(-\alpha)} \tag{31}$$

which is positive for all β value.

Finally, the discretization of the moving boundary expression (16) results:

$$R(t^n) = R_o\sqrt{\frac{l_o}{l_o + kt^n}}, \quad \forall n. \tag{32}$$

The obtained results are shown in Table 2 in column MBM-FFEFDM by using data parameters extracted from literature [16]. The input parameters are shown in Table 1.

The problem (12)–(16) is also discretized by the finite differences method in their implicit full version. So the equations and conditions (12)–(16) are approximated by the finite differences method similar to the previous case and the following equations for the inside nodes are obtained:

$$\begin{aligned}\Psi_j^n = &\left[B_j^{n+1}\frac{\Delta t}{\Delta y} - A_1^{n+1}\frac{\Delta t}{\Delta y^2}\right]\Psi_{j-1}^{n+1} \\ &+ \left[1 + 2A_1^{n+1}\frac{\Delta t}{\Delta y^2} - B_j^{n+1}\frac{\Delta t}{\Delta y}\right]\Psi_j^{n+1} \\ &- \left[A_1^{n+1}\frac{\Delta t}{\Delta y^2}\right]\Psi_{j-1}^{n+1}\end{aligned} \tag{33}$$

if $B_j^{n+1} < 0$;

$$\begin{aligned}\Psi_j^n = &\left[-A_1^{n+1}\frac{\Delta t}{\Delta y^2}\right]\Psi_{j-1}^{n+1} \\ &+ \left[1 + 2A_1^{n+1}\frac{\Delta t}{\Delta y^2} + B_j^{n+1}\frac{\Delta t}{\Delta y}\right]\Psi_j^{n+1} \\ &- \left[A_1^{n+1}\frac{\Delta t}{\Delta y^2} + B_j^{n+1}\frac{\Delta t}{\Delta y}\right]\Psi_{j+1}^{n+1}\end{aligned} \tag{34}$$

if $B_j^{n+1} > 0$.

TABLE 1
Stability conditions for the various finite difference methods

Method	Stability condition
Explicit with Front Fixing (a)	$\frac{\Delta t}{\Delta y^2} < \frac{[R(t_{\max})-s_0]^2 s_0}{2Ds_0+[R(t_{\max})-s_0]D(1+\varepsilon_0)}$
Implicit with Front Fixing (b)	$\Delta y < \frac{Db}{v_0(R_0-s_0)}$
Explicit with Front-tracking (c)	$\frac{\Delta t}{\Delta y^2} \le \frac{1}{2D}, \quad \Delta y < \frac{Db}{v_o}$

The initial condition (13) is transformed by (24) and the boundary conditions are given by

$$\Psi(1, t^{n+1}) - \frac{Db}{Db - v_o\Delta y\ R_1(t^{n+1})}\Psi(1-\Delta y, t^{n+1}) = 0 \tag{35}$$

$$\begin{aligned}&\Psi(0, t^{n+1}) + \frac{1}{\left[\frac{v_o\Delta y}{A^{n+1}b} - 1\right]}\Psi(1, t^{n+1}) \\ &\quad = \frac{k_a}{\left[v_o - \frac{A^{n+1}b}{\Delta y}\right]}\frac{\left[\Psi(0, t^n) - \Psi_u\right]}{\left[1 + \frac{k_a[\Psi(0,t^n)-\Psi_u]}{J_m}\right]}\end{aligned} \tag{36}$$

The conditions (33)–(36) and (24) constitute a system of linear equations whose coefficients conform a tridiagonal matrix. The obtained results are shown in Table 2 in column MBM-FFIFDM for Mg, K and P.

4. THE FRONT-TRACKING AND EXPLICIT FINITE DIFFERENCES METHOD

The front-tracking method is a variable space grid method. We take the number of space intervals between $y = s_o$ and $y = R(t)$ constant and equal to M for all time. Thus, $\Delta y = \frac{R(t)-s_o}{M}$ is different in each time step. The moving boundary is always on the Mth grid line. The problem given by the Eqs. (1)–(5) is discretized considering forward differences and centered differences for the temporal and space derivatives, respectively. Considering $r = y$ and $C(r, t) = \psi(y, t)$, and keeping the

TABLE 2
Input data parameters used for predicted K, P and Mg uptake for pine seedlings

Parameter	P	Mg	K
Absorption power k_a ($= J_m/K_m$) (cm/s)	1.67e-5	1.31e-5	4.66e-5
Flux velocity v_o (cm/s)	5.66e-7	5.66e-7	5.66e-7
Root radius s_o (cm)	3.5e-2	3.5e-2	3.5e-2
Interoot radius R_o (cm)	2	2	2
Diffusion coefficient D (cm^2/s)	8.17e-7	1.45e-7	3.29e-6
Buffer power b (dimensionless)	5.84	1.32	10.55
Soil concentration C_R (mol/cm^3)	1.9e-7	1.35e-6	2.7e-7
Minimum concentration C_u (mol/cm^3	6e-10	1e-10	1e-10
Maximum influx J_m ($mol/cm^2 - s$)	2.68e-12	1.29e-13	1.4e-12
Length growth velocity k (cm/s) (Linear growth)	1.62e-4	1.62e-4	1.62e-4
Initial length l_o (cm)	285	285	285

notation of the previous sections, Eq. (1) results:

$$D\Psi_{yy} + D(1+\varepsilon_o)\frac{1}{y}\Psi_y = \Psi_t, \quad s_o < y < R(t), \quad 0 < t < T \tag{37}$$

whose approximation is given by:

$$\begin{aligned}\frac{\Psi(y_j, t^n + \Delta t) - \Psi(y_j, t^n)}{\Delta t} &= D\left[\frac{\Psi(y_j + \Delta y, t^n) - 2\Psi(y_j, t^n) + \Psi(y_j - \Delta t, t^n)}{(\Delta y)^2}\right] \\ &+ \frac{D(1+\varepsilon_0)}{y_j}\left[\frac{\Psi(y_j + \Delta y, t^n) - \Psi(y_j - \Delta y, t^n)}{2\Delta y}\right]\end{aligned} \tag{38}$$

By using the notation:

$$B(y_i) = B_j = \frac{D(1+\varepsilon_0)}{y_j} \tag{39}$$

we have:

$$\begin{aligned}\Psi_j^{n+1} &= D\frac{\Delta t}{(\Delta y)^2}\left[\Psi_{j+1}^n + \Psi_{j-1}^n\right] + \left[1 - 2D\frac{\Delta t}{(\Delta y)^2}\right]\Psi_j^n \\ &+ B_j\frac{\Delta t}{2\Delta y}\left[\Psi_{j+1}^n - \Psi_{j-1}^n\right]\end{aligned} \tag{40}$$

In this expression, in order to assure that all coefficients on the right-hand side are positive, we impose the condition:

$$1 - 2D\frac{\Delta t}{(\Delta y)^2} \geq 0 \tag{41}$$

which give us an upper bound for the temporal step, i.e.

$$\Delta t \leq \frac{(\Delta y)^2}{2D} \tag{42}$$

and

$$\Delta y < \frac{2D}{B_j} = \frac{2y_j}{1+\varepsilon_o}, \quad \forall j \tag{43}$$

i.e.

$$\Delta y < \frac{2s_o}{1+\varepsilon_o}. \tag{44}$$

The initial and boundary conditions (2) and (3) now result:

$$\Psi_j^0 = \Psi(y_j) = \varphi(y_j), \quad 0 \leq j \leq M, \quad j = 0, 1, \ldots, M \tag{45}$$

$$\begin{aligned}&-\frac{Db}{\Delta y}[\Psi(R(t^n), t^n) - \Psi(R(t^n) - \Delta y, t^n)] + v_o\Psi \\ &\times (R(t^n), t^n) = 0,\end{aligned} \tag{46}$$

therefore:

$$\Psi(R(t^n), t^n) = \frac{Db}{Db - v_o\Delta y}\Psi(R(t^n) - \Delta y, t^n), \quad n = 1, 2, \ldots, N \tag{47}$$

and we obtain that

$$\Psi(R(t^n), t^n) > 0 \Leftrightarrow Db - v_o\Delta y > 0 \Leftrightarrow \Delta y < \frac{\mathrm{Db}}{v_o} \tag{48}$$

The boundary condition on $y = 0$ now results:

$$\begin{aligned}&\Psi(s_0, t^n)\left[v_o - \frac{Db}{\Delta y}\right] + \frac{Db}{\Delta y}\Psi(s_0 + \Delta y, t^n) \\ &= \frac{J_m}{\frac{\Psi(s_0,t^n) - \Psi_u + k_m}{\Psi(s_0,t^n) - \Psi_u}}\end{aligned} \tag{49}$$

that is

$$\begin{aligned}&\left[\frac{Db}{\Delta y}\Psi(s_0 + \Delta y, t^n) + \left[v_o - \frac{Db}{\Delta y}\right][k_m - \Psi_u] - J_m\right]\Psi(s_0, t^n) \\ &+ \left[v_o - \frac{Db}{\Delta y}\right]\Psi^2(s_0, t^n) + [k_m - \Psi_u]\frac{Db}{\Delta y}\Psi(s_0 + \Delta y, t^n) \\ &+ J_m\Psi_u = 0\end{aligned} \tag{50}$$

In order to guarantee that the solution (concentration) in the different outlines of the finite differences methods is positive sufficient stability conditions for the space and temporal steps were obtained (see Appendix A). Table 1 shows the stability conditions that were used.

These conditions allow us to obtain a bound for the temporal step after fixing the space step with front fixing (a) and (b) and the space step by front-tracking (c) methods. In order to explain the best results for the integral balance method we plot the concentration in the root surface $C(s_o, t)$ vs. time (see Fig. 1) and the influx $J(s_o, t)$ vs. time (see Fig. 2) for K through the three methods (the front-tracking and explicit differences method is not considered due to the poor results obtained).

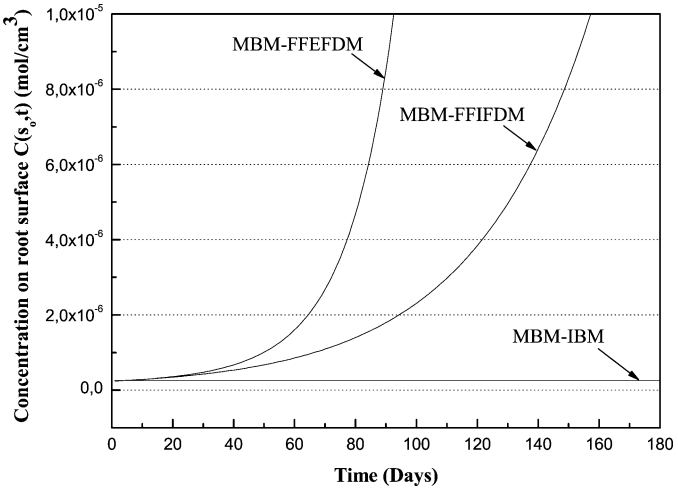

FIG. 1. Concentration on root surface $C(s_o, t)$ vs. time by the integral balance method and the finite differences methods in their explicit and implicit versions.

TABLE 3
Comparison of predictions of the moving boundary model respect to the Barber-Cushman model

		Predicted uptake (mmol/pot)									
Observed uptake (mmol/pot)		Barber-Cushman Model		MBM-IBM		MBM-FFEFDM		MBM-FFIFDM		MBM-FTEFDM	
	†	†	Error		Error		Error		Error		Error
Mg	1.617	0.625	61.3	0.680	57.1	0.18	88.9	0.763	52.8	0.687	57.5
K	6.663	6.285	5.6	6.653	0.15	7.33	9.96	7.272	9.15	0.582	91.3
P	1.332	1.185	11	1.302	2.25	1.41	6	1.409	5.84	0.683	51.5

(†)Source: Kelly et al., 1992 [16].
Column Error refers to: [(Observed uptake—Predicted uptake)/Observed uptake] $\times 100$.
Column MBM-IBM refers to Moving Boundary Model—Integral Balance Method.
Column MBM-FFEFDM refers to Moving Boundary Model—Front-Fixing and Explicit Finite Differences Method.
Column MBM-FFIFDM refers to Moving Boundary Model—Front-Fixing and Implicit Finite Differences Method.
Column MBM-FTEFDM refers to Moving Boundary Model—Front-Tracking and Explicit Finite Differences Method.

5. RESULTS

In order to evaluate the finite differences methods we compute K, P and Mg uptake for pine seedlings [16], using the input data parameters that are shown in Table 2. Table 3 shown the uptake predicted by these nutrients obtained by the Barber-Cushman model as well as those obtained by the moving boundary model in their four numerical solutions: the integral balance method and the finite differences method in their explicit and implicit versions with front-fixing and explicit version without front-fixing.

The obtained results are shown in Table 3 in column MBM-FTEFDM for Mg, K and P. The discretized equations by explicit finite differences method with front-tracking for the problem (1)–(5) and explicit and implicit methods with front-fixing of the domain for the problem (12)–(16) are solved by means of algorithms in Fortran language [15]. For the implicit finite differences method the usual subroutine TRIDAG was adapted to solve tridiagonal systems.

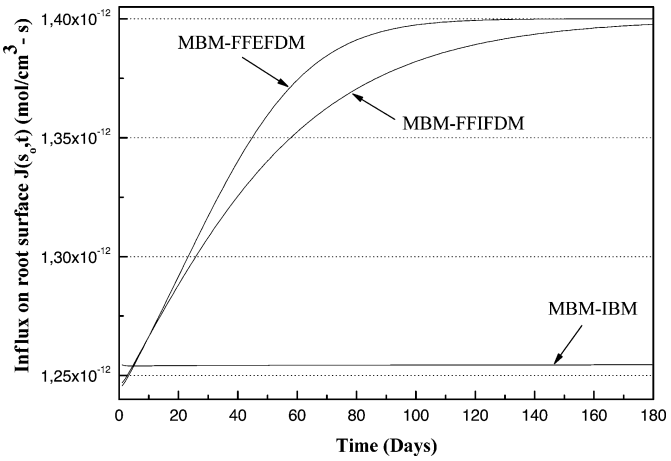

FIG. 2. Influx on root surface $J(s_o, t)$ vs. time by the integral balance method and the finite differences methods in their explicit and implicit versions.

From Table 3 the results show that for Mg all models render a poor prediction, probably due to the use of a high value for J_m obtained by means or experimental determinations of this parameter in nutritive solutions and not in soil [17]. However, for K and P, the integral balance method produces better results with respect to the one obtained by the finite differences methods; for example, for P we have a relative error 2,25% obtained by integral balance method in contrast to 5,84%, which is the best for implicit differences methods. For K, we obtain a similar result: 0,15% in contrast to 9,15%.

6. CONCLUSIONS

From Fig. 1 we conclude that the predicted concentration by the two differences methods increases very fast from 20 days while the predicted concentration by integral balance method increases according to the experimental results of K depletion. The final results (Table 3) correspond to the more representative values obtained (in order to compare, with the same values for temporal and space steps were taken for all methods if the stability conditions allowed it). As it can be seen, the front-tracking and explicit finite differences method produces poor results compared with those obtained by using the front fixing method. Notwithstanding, in the case of Mg uptake the front-tracking and explicit finite differences method produces similar results to the ones obtained by the integral balance method without indicating that, it is generally, an efficient method. Usually, when the boundary conditions are not constant, the front fixing method is applied at the beginning and then any variant of the finite differences method can be applied. In our case, the best approximation is the numerical integral balance method. We remark the importance of the choice of the adequate numerical method owing to their effects, e.g., on fertilization techniques.

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APPENDIX A STABILITY CONDITIONS

Stability Condition (a)

From Eqs. (21) and (23), we obtain:

$$\Delta t \le \frac{\Delta y^2}{2A_1^n + \left|B_j^n\right|\Delta y} \quad \forall n \tag{A.1}$$

and this condition must hold for all value of n and j. In order to assess this situation bounds for the functions $A_1(t)$ and $B(y,t)$ were obtained, i.e:

$$|B(y,t)| \le \max\left(\frac{D_1}{[R(t_{\max})-s_0]s_0}, \frac{2D_1 l_0[R(t_{\max})-s_0]-kR_0^3R(t_{\max})}{2R_0^2 l_0 s_0[R(t_{\max})-s_0]}\right)$$
$$\forall y \in [0,1]; \forall t \in [0, t_{\max}] \tag{A.2}$$

$$\frac{D}{[R_0-s_0]^2} \le A_1(t) \le \frac{D}{[R(t_{\max})-s_0]^2}$$
$$\forall t \in [0, t_{\max}]; R(t_{\max}) < s_0; t_{\max} < T \tag{A.3}$$

From (A.2) and (A.3) it is obtained:

$$2A_1^n + \Delta y\left|B_j^n\right| \le \frac{2D}{[R(t_{\max})-s_0]^2} + \max\left(\frac{D_1}{[R(t_{\max})-s_0]s_0}, \frac{2D_1 l_0[R(t_{\max})-s_0]-kR_0^3R(t_{\max})}{2R_0^2 l_0 s_0[R(t_{\max})-s_0]}\right) \tag{A.4}$$

Then the best value for $\frac{\Delta t}{\Delta y^2}$ is given by:

$$\frac{\Delta t}{\Delta y^2} < \frac{1}{\frac{2D}{[r_0-s_0]^2} + \max\left(\frac{D_1}{[r_0-s_0]s_0}, \frac{2D_1 l_0[r_0-s_0]-kR_0^3 r_0}{2R_0^2 l_0 s_0[r_0-s_0]}\right)},$$
$$r_0 = R(t_{\max}) \tag{A.5}$$

and finally replacing $r_0 = R(t_{\max})$ we obtain:

$$\frac{\Delta t}{\Delta y^2} < \frac{[R(t_{\max})-s_0]^2 s_0}{2Ds_0 + [R(t_{\max})-s_0]D(1+\varepsilon_0)} \tag{A.6}$$

Stability Condition (b)

This condition is obtained from boundary condition (25) due to:

$$\Psi(1,t^n) > 0 \leftrightarrow Db - v_o\Delta y[R(t^n)-s_0] > 0 \leftrightarrow \Delta y < \frac{Db}{v_o[R(t^n)-s_0]} (Db > 0) \tag{A.7}$$

therefore, is sufficient to consider

$$\Delta y < \min\left(\frac{1}{R(t^n)-s_0}\right)\frac{Db}{v_o} = \frac{Db}{v_o(R_0-s_0)} \tag{A.8}$$

with:

$$0 < R(t_{\max}) - s_0 \le R(t) - s_0 \le R_0 - s_0;$$
$$\forall t \varepsilon [0, t_{\max}], t < T$$