16e

20-26 08 1998

Congrès Mondial de Science du Sol
World Congress of Soil Science
Bodenkundlicher Weltkongress
Congreso Mundial de la Ciencia del Suelo

HOMME
MAN
MENSCH
HOMBRE

SOL
SOIL
BODEN
SUELO

FRANCE
Montpellier
Le Corum | Palais des congrès

Nutrient Uptake through a Moving Boundary Model. Comparative results with the Barber-Cushman Model Assimilation des éléments nutritifs d'après un modèle à limites mobiles – Comparaison avec les résultats du modèle de Barber-Cushman

REGINATO Juan Carlos (1), **TARZIA Domingo Alberto** (2)

(1) Dpto. Química-Física, Fac. Cs. Exactas, Universidad Nacional de Río Cuarto, Ruta 36 Km 601, (5800) Río Cuarto, Córdoba, Argentina
(2) Dpto. Matemática, Fac. Cs. Empresariales, Universidad Austral, Paraguay 1950, (2000), Rosario, Argentina

The uptake of a single nutrient for root of crops is studied through a moving boundary model, which differ of previous models that solve the problem in fixed domains. The equations of the model are solved through the Integral Balance method. Theoretical and experimental results are compared for the potassium uptake for three hybrids of maize (Dekalb 762, Tilkara Funks and Capitán Ciba). The model has been also tested with experimental data extracted of the literature in order to compute and compare the nutrient uptake of various nutrients in different crops and soils. It is obtained a better prediction with respect to only one nutrient though of the same way that for previous models some deviations persists in certain cases.

Analysis

The nutrient uptake has been evaluated through models that solve differential equations of transport in soils (diffusive and mass flows) coupled with absorption kinetics. These equations are solved on fixed domains (Cushman, 1979, Barber et al., 1984) through which the nutrient concentration at root-soil interface and the resulting nutrient uptake are estimated. Moreover, the formulation of free boundary problems allows to postulate a model of nutrient uptake due to the transport and absorption of ions from a dynamic point of view (Reginato et al, 1990, 1991, 1993a). The goal of the present work is to evaluate a moving boundary model (root growth known a priori) for the nutrient uptake. A one-dimensional model is considered, i.e., a single cylindrical root in the soil where all the nutrients arriving at the root surface are assumed to be used for root growth. It is also assumed that the conditions of moisture, light and temperature are controlled (like in a growth chamber), i.e. the model coefficients are constant.

1

With these assumptions, the following one-dimensional root growth model through a moving boundary problem to one phase (the soil) (Crank, 1984; Tarzia, 1988) in cylindrical coordinates is proposed:

$$DC_{rr} + D(1+\varepsilon_o)\frac{C_r}{r} = C_t, \qquad s(t) < r < s(t)+R-s_o, \qquad 0 < t < T \qquad (1\text{-}a)$$

$$C(r,0) = \varphi(r), \qquad\qquad s_o \leq r \leq R \qquad\qquad (1\text{-}b)$$

$$-DC_r(s(t)+R-s_o,t) + v_0 C(s(t)+R-s_o,t) = 0, \qquad 0 < t < T \qquad (1\text{-}c)$$

$$t),t) \quad v \; C(s(t),t) \; \frac{k \left[C(s(t),t) \quad C \right]}{1 \; \dfrac{k \left[C(s(t),t) \quad C \right]}{J}} \quad aC(s(t),t)s(t), \; 0 \quad t \quad T \quad (1\text{-}d)$$

$$s(t) = s_o \sqrt{e^{kt}}, \qquad\qquad 0 < t < T \qquad\qquad (1\text{-}e)$$

Where: $C_r = \partial C/\partial r$, $C_{rr} = \partial^2 C/\partial r^2$, $C_t = \partial C/\partial t$, **r** is the radial distance from the root axis [cm], **t** is the time [sec]; **T** is the maximum time for which the system has solution [sec]; C_u is the minimum concentration under which growth is stopped [mol/cm^3]; v_O is the mean effective velocity of soil solution on root surface [cm/sec]; **b** is the buffer power, **D** is the diffusion coefficient, k_a ($= J_m / K_m$) is the root absorption power of nutrient [cm/sec]; **R** is the half distance between roots, [cm], φ is the initial concentration profile [mol/cm^3]; **a** is the stequiometric coefficient [dimensionless], **s(t)** is the root radius as a function of the time t, $\dot{s}(t) = \dfrac{ds(t)}{dt}$ is the radial root growth rate, **k** is the root rate constant [1/sec], and s_o is the root initial radius [cm]. The parameter ε_o is given by $\varepsilon_o = \dfrac{v_o s_o}{Db}$. Equation (**1-a**) represents the ion transport equation in soil. Equation (**1-b**) is the initial concentration profile and Equation (**1-c**) is the boundary condition representing null flux (can input water but not nutrients). Equations (**1-d**) represent the mass balance at the root surface where the ions arriving are incorporated through absorption kinetic. Equation (**1-e**) gives us the moving boundary **s (t)** (the root radius) which is known a priori. The expression (**1-e**) is obtained assuming fixed volume of soil and relating the root radius with the root length (which is a especial function according to the method for to estimate the longitudinal root growth **l(t)**, i.e., linear, exponential, sigmoid, etc.) through the following expression (See **Appendix A.**):

$$s(t) = s_o \sqrt{\frac{l(t)}{l_o}} \qquad\qquad (2)$$

The model is solved applying the integral balance method (Reginato et al., 1993b, 1997a). So, the partial differential equation (**1-a**) is integrated in variable r on the domain (**s (t), s (t)+R-s_o**) and the following expression for **C(r, t)** is proposed:

$$C(r,t) = \varphi(r,t)\left[1 + \frac{\beta(t)}{R^2}(s(t)+R-s_0-r)^2\right] \qquad\qquad (3)$$

$$\varphi(r,t) = A(t)e^{\varepsilon r}, \qquad A(t) = C_R e^{-\varepsilon[s(t)+R-s_o]}, \qquad \varepsilon = \frac{v_0}{Db} = \frac{\varepsilon_0}{s_0} \qquad (4)$$

2

with: $$\varphi(\mathbf{r}) = \varphi(\mathbf{r},0) = C_R e^{-\varepsilon(R-r)}$$

which verify the initial **(1-b)** by taking $\beta(0) = 0$ and boundary **(1-c)** conditions. So, after some elementary but tedious manipulations, the following differential equation for $\beta(t)$ was obtained:

$$\frac{d\beta(t)}{dt} = \frac{\dfrac{DF_1}{A(t)} + D(1+\varepsilon_o)\{F_2 + F_3 + F_4\} - \dfrac{k}{2}s(t)\{F_5 + F_6 + F_7\}}{\{F_8 + F_9 + F_{10}\}} R^2 \quad (5)$$

$$s(t) = s_o\sqrt{e^{kt}}, \qquad\qquad\qquad \beta(0) = 0$$

where:

$$F_1 = C_R\left[\varepsilon - \varepsilon e^{-\varepsilon(R-s_o)}\left[1 + \frac{\beta(t)}{R^2}(R-s_o)^2\right] + e^{-\varepsilon(R-s_o)}\frac{2\beta(t)}{R^2}(R-s_o)\right]$$

$$F_2 = \left[\varepsilon + \varepsilon\frac{\beta(t)}{R^2}(s(t)+R-s_0)^2 - \frac{2\beta(t)}{R^2}(s(t)+R-s_0)\right].$$

$$\cdot\begin{bmatrix}
\ln\dfrac{(s(t)+R-s_o)}{s(t)} + \varepsilon(R-s_o) + \dfrac{\varepsilon^2}{4}\left[(s(t)+R-s_o)^2 - s^2(t)\right] + \\[2mm]
+\dfrac{\varepsilon^3}{18}\left[(s(t)+R-s_o)^3 - s^3(t)\right] + \dfrac{\varepsilon^4}{96}\left[(s(t)+R-s_o)^4 - s^4(t)\right] + \\[2mm]
+\dfrac{\varepsilon^5}{600}\left[(s(t)+R-s_o)^5 - s^5(t)\right] + \dfrac{\varepsilon^6}{4320}\left[(s(t)+R-s_o)^6 - s^6(t)\right] + \\[2mm]
+\dfrac{\varepsilon^7}{35280}\left[(s(t)+R-s_o)^7 - s^7(t)\right] + \dfrac{\varepsilon^8}{322560}\left[(s(t)+R-s_o)^8 - s^8(t)\right] + \\[2mm]
\dfrac{\varepsilon^9}{3265920}\left[(s(t)+R-s_o)^9 - s^9(t)\right]
\end{bmatrix}$$

$$F_3 = \frac{2\beta(t)}{R^2}[1-\varepsilon(s(t)+R-s_0)]\frac{\left[e^{\varepsilon(s(t)+R-s_o)} - e^{\varepsilon s(t)}\right]}{\varepsilon}$$

$$F_4 = \varepsilon\frac{\beta(t)}{R^2}\frac{\left[e^{\varepsilon(s(t)+R-s_o)}\left[\varepsilon(s(t)+R-s_o)-1\right] - e^{\varepsilon s(t)}(\varepsilon s(t)-1)\right]}{\varepsilon^2}$$

$$F_5 = \left[-\varepsilon\left(1+\frac{\beta(t)}{R^2}\right)(s(t)+R-s_o)^2 + \frac{2\beta(t)}{R^2}(s(t)+R-s_o)\right]\frac{\left[e^{\varepsilon(s(t)+R-s_o)} - e^{\varepsilon s(t)}\right]}{\varepsilon}$$

$$F_6 = \frac{2\beta(t)}{R^2}[\varepsilon(s(t)+R-s_o)-1]\frac{\left[e^{\varepsilon(s(t)+R-s_o)}\left[\varepsilon(s(t)+R-s_o)-1\right] - e^{\varepsilon s(t)}(\varepsilon s(t)-1)\right]}{\varepsilon^2}$$

$$F_7 = -\varepsilon\frac{\beta(t)}{R^2}\frac{\left[e^{\varepsilon(s(t)+R-s_o)}\left[\varepsilon^2(s(t)+R-s_o)^2 - 2\varepsilon(s(t)+R-s_o)+2\right] - e^{\varepsilon s(t)}(\varepsilon^2 s^2(t) - 2\varepsilon s(t)+2)\right]}{\varepsilon^3}$$

$$F_8 = (s(t)+R-s_o)^2\frac{\left[e^{\varepsilon(s(t)+R-s_o)} - e^{\varepsilon s(t)}\right]}{\varepsilon}$$

$$F_9 = -2(s(t)+R-s_o)\frac{\left[e^{\varepsilon(s(t)+R-s_o)}\left[\varepsilon(s(t)+R-s_o)-1\right] - e^{\varepsilon s(t)}(\varepsilon s(t)-1)\right]}{\varepsilon^2}$$

$$F_{10} = \frac{\left[e^{\varepsilon(s(t)+R-s_o)}\left[\varepsilon^2(s(t)+R-s_o)^2 - 2\varepsilon(s(t)+R-s_o)+2\right] - e^{\varepsilon s(t)}(\varepsilon^2 s^2(t)-2\varepsilon s(t)+2)\right]}{\varepsilon^3}$$

The system **(5)** is solved through the Runge-Kutta method for ordinary differential equations.
The uptake nutrient can be obtained from the following formula (See Reginato, Tarzia, 1997b), which is a modified version of the Cushman´ formula (Cushman, 1979; Claasen and Barber. 1976).

$$U(t) = 2\pi s_o \int_0^{t_{max}} \left[\int_0^t \frac{k_a\left[C(s(t),t)-C_u\right]}{1+\frac{k_a\left[C(s(t),t)-C_u\right]}{J_m}} ds \right] \dot{l}(t)dt \qquad (6)$$

where $k_a[C(s(t),t)-C_u]/(1+k_a[C(s(t),t)-C_u]/J_m)$ is the influx and $\dot{l}(t)$ the longitudinal root rate growth.

Materials and Methods

Three hybrids of maize (Dekalb 762, Capitán Ciba y Tilkara Funks) grown in pots with 1.6 kg. of soil Typic Hapludoll of Río IV, Córdoba, Argentina during 11 days in growth chamber to 26 $^\circ$ C. At emergence (5 DAG) plants were harvested to determine initial potassium and root length. Later, plants were harvested 11 DAG, dried at 70 $^\circ$C to determine potassium uptake through acid digestion (Jackson, 1964) and flame photometry.
 In order to predict the potassium uptake it has made measurements of parameters that are used as data input to the present model. *Soil parameters*: Values of C_R (initial soil solution concentration of potassium) were obtained by analyzing aliquots of displaced solution from soil columns equilibrated at field capacity for 24 h. (Adams, 1974) The buffer power b and the diffusion coefficient D were determined as described by Kovar and Barber (1990). *Root parameters*: The flux velocity v_o was determined by dividing the total water uptake of the plant, which was obtained by subtracting the water loss due to evaporation from the total water loss due to evapotranspiration each pot within given time, by the mean root surface area within given time: $v_o = W(\ln S - \ln S_o)/(t - t_o)(S - S_o)$. The root rate constant, k, was calculated from root length as a function of time by: $k = (\ln l(t) - l_o)/(t-t_o)$ assumed an exponential growth; the root radius s_o was calculated from the length and fresh weight of by: $s_o =$ [Weight Fresh / 1. Root length] $^{1/2}$; the half distance between roots, R, was calculated by: R = [Soil Volume / 1. Root Length] $^{1/2}$. Root length, l, was measured by a line-intersect method (Tennant, 1975). *Kinetics parameters*: J_m, K_m, C_u y k_a are determined by analysis of potassium depletion curves in nutritive solution of which absorb nutrients the roots (Claassen y Barber, 1974).

Results and Discussion
The results obtained for the potassium uptake for the three mentioned hybrids are shown in the Table I.

Hybrids	Predicted Uptake (mmol)	Observed Uptake (mmol)
DEKALB 762	0.2023	0.1685
TILKARA FUNKS	0.2729	0.293
CAPITAN CIBA	0.2235	0.304

Table I. Potassium uptake for three hybrids of maize

Moreover, the model is tested with experimental data extracted of the literature. Thus, is estimated the uptake of Mg, K y P for loblolly pine seedlings during 180 days in a modified horizon A soil mesic Typical Hapludult (Kelly, Barber, Edwards, 1992). The comparison between the Barber-Cushman prediction and the estimation of the present model by using a linear root growth is shown in Table II.

Nutrient	Observed Uptake (μmol)	Predicted Uptake. (Kelly-Barber) (μmol)		Predicted Uptake (Reginato-Tarzia) (μmol)	
			Er. (%)		Er. (%)
Mg	1617	625	61.3	680	57.1(*)
K	6663	6285	5.6	6653	0.15(*)
P	1332	1185	11	1302	2.25(*)

Table II. Mg, K y P uptake for pine seedlings. The data with asterisk showed a better prediction

The model is also tested with data corresponding the NO_3 uptake for wheat, rice and rape during 3 to 20 days in soils Paddy (derived from lacustrine deposits), Red (developed from Quaternary red clay) and Fluvo-aquic (developed on the alluvial deposits of the Huanghe River) (Xuan Jia-Xiang, Zhang Li-Gan y Zhu Wei-Min, 1991). The predicted uptakes using an exponential root growth are shown in the Table III.

Nutrient NO_3 (N)	Observed Uptake (μmol)	Predicted Uptake Xiang, Li-gan, Wei-min (μmol)		Predicted Uptake Reginato-Tarzia (μmol)	
			Er. (%)		Er. (%)
Wheat (Red)	189	208	10	157	16.9
Wheat (Paddy)	1263	974	22.9	1468	16.2(*)
Wheat (Fluvo)	2205	1847	16.2	1961.4	11(*)
Rice (Red)	514.2	640	24.5	740.1	43.9
Rice (paddy)	2517.1	2300	8.6	1661	34.2
Rape (Red)	190	300	57.9	179.1	5.73(*)
Rape (Fluvo)	401	350	12.7	351	12.4(*)

Table III. NO_3 uptakes for wheat, rice and rape.

Moreover, for this last case, the predicted uptake NO_3 for the model and the observed uptake are compared in the Figure 1.
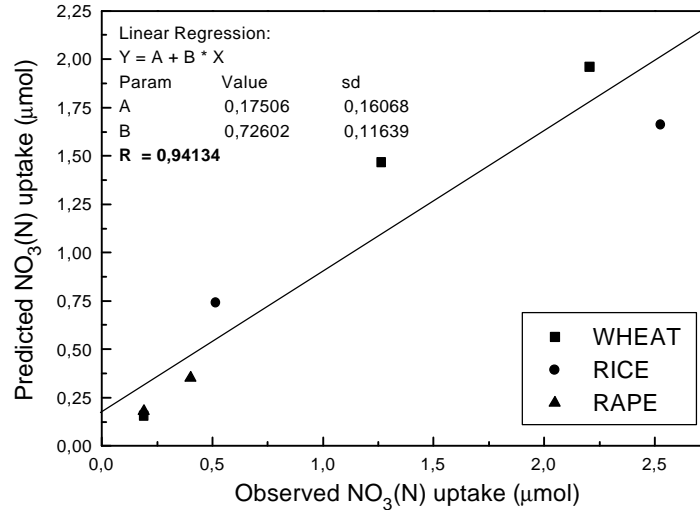
Figure 1. Comparison between predicted and observed NO_3 uptake

In spite of that the errors obtained are 7% (Tilkara), 20% (Dekalb) and 26% (Capitán) the validation of our model with experimental data of other authors shown a better prediction that the same authors using the Cushman-Barber model. The predictions are improved up to 30% more arriving up to 80% in some cases.

However, the nutrient uptake predicted by this model and the previous models is perfectible both experimentally as theoretically. For the last case, the difficulty of these models is that consider the absorption of only one nutrient no taking into account the simultaneous absorption any way the possible coupling with others ions in the absorption. We remark that our model and the Barber-Cushman display similar deviations for the magnesium uptake (Kelly-Barber). This last fact raising the need of a model that will simultaneously taking into account interactions between nutrients, by example, by using competitive kinetic absorption.

Appendix A. The expression **(2)** is obtained assuming that for the same time the root volume grown radially is equal to volume grown longitudinally, i.e., if s_o and l_o are the initial root radius and initial root length, we can write:

$$\mathbf{V}^{grown}_{longitudinally} = \mathbf{V}^{grown}_{radially}$$
$$\pi s_o^2 \left[l(t) - l_o \right] = \pi l_o \left[s^2(t) - s_o^2 \right]$$

Thus, after elementary manipulations the condition **(2)** is obtained.

References

Adams F. 1974. Soil Solution. In *"The Plant and its Environment"*. Ed. E.W. Carson. pp. 441-481. University Press of Virginia, Charlottesville, VA.

Barber, S.A. 1984. *"Soil nutrient bioavailability. A mechanistic approach"*. J. Wiley, New York.

Claassen, N.; Barber, S.A. 1974. *"A Method for Characterizing the Relation between Nutrient Concentration and Flux into Roots of Intact Plants"*. Plant Physiol. 54: 564-568

Claasen, N.; Barber, S.A. 1976. *"Simulation model for nutrient uptake from soil by a growing plant root system"*. Agron. J. 68: 961-964

Crank, J. 1984. *Free and Moving Boundary Problems*. Clarendon Press, Oxford

Cushman, J.H. 1979. *"An analytical solution to solute transport near root surfaces for low initial concentrations: I. Equation development"*, Soil Sc. Soc. Am. J. 43: 1087-1090

Jackson M. L. 1964. "Soil Chemical Analysis", Prentice Hall, Englewood Cliff, N. J. USA. 441-458.

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

Kovar, J.L.; Barber, S.A. 1990. *Potassium Supply Characteristics of Thirty-three Soil as Influenced by Seven Rates of Potassium*, Soil Sc. Soc. Am. J. 54: 1356-1361

Reginato, J.C.; Tarzia, D.A.; Cantero, A. 1990. *"On the free boundary problem for the Michaelis-Menten absorption model for root growth"* Soil Sc. 150: 722-729

Reginato, J.C.; Tarzia, D.A.; Cantero, A. 1991. *"On the free boundary problem for the Michaelis-Menten absorption model for root growth. High concentrations"*. Soil Sc. 152 (2): 63-71

Reginato, J.C.; Tarzia, D.A.; Dzioba, M.A. 1993a. *"Analytical study of the effect of some soil and plant parameters on root growth due to absorption of one mobile ion: A free boundary model"* Plant and Soil, 157: 185-196

Reginato, J.C.; Tarzia, D.A. 1993b. *"The balance integral method applied to root growth of crops"*. Int. J. of Eng. Sc., 31 (1): 61-70

Reginato, J.C.; Tarzia, D.A. 1997a. "Modeling the Nutrient Uptake through A Moving Boundary Model. Experimental Results and Comparison with the Barber-Cushman Model", submitted to Soil Sc. Soc. of America J.

Reginato, J. C., D. A. Tarzia. 1997b. *"A formula to compute the nutrient uptake for root growth"* submitted to Plant and Soil

Tarzia, D.A. 1988. *"A bibliography on moving-free boundary problems for the heat-diffusion equation. The Stefan Problem"*, Progetto Nazionale M.P.I."Equazioni di Evoluzione e applicazioni fisico-matematiche", Firenze, with 2528 references.

Tennant D. 1975. *"A test of modified line intersect method of estimating root length"*. J. Ecol. 63: 995-1001

Xuan Jia-Xiang, Zhang Li-Gan, Zhu Wei-Min, 1991. *Mechanistic Model for Predicting NO_3-N Uptake by Plants and Its Verification*. Pedosphere, 1 (2): 97-108