

## ON THE FREE BOUNDARY PROBLEM FOR THE MICHAELIS-MENTEN ABSORPTION MODEL FOR ROOT GROWTH

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**The root surface as an absorption mechanism and its growth is studied, and a growth absorption model is proposed, i.e., the free boundary Michaelis-Menten model. Differences in nutrient availability and transport between the root surface and the rhizosphere are studied through the mechanism of absorption which manifests itself in the limit expression of Michaelis-Menten kinetics for low concentrations. The resultant equations are analytically solved by the quasi-stationary method with two interface boundary conditions and boundary and initial conditions. The solution is used to compute growth of root radius. Several examples of concentration distribution curves in soil and interface root-soil as a function of root radius are plotted. The parameters which are varied are the root absorption power, flux velocity, transpiration rate, rhizosphere soil solution concentration, diffusion coefficient, and buffer power.**

Many methods exist for studying the mechanism involved in nutrient uptake. One of the most promising methods is the mathematical model, which can be a satisfactory method of modelling the plant-root system by use of the partial differential equation for convective and diffusive flow to a root (Claassen and Barber, 1966; Nye and Marriot, 1969; Cushmann, 1979, 1980, 1982). In general, these models have not considered computing root growth, but rather they have assumed young roots to be growing at exponential rates (Claassen and Barber, 1966; Cushmann, 1980, 1982). In the past, various devices and models have been proposed and analyzed with the purpose of interpreting growing process as a free boundary problem for the heat-diffusion equation [Lame and Clayperon, 1831; Stefan, 1889; Carslaw and Jaeger, 1959; Crank, 1975; Tarzia, 1988). In this article we compute the free boundary (the root-soil interface) a priori unknown through the quasi-stationary method (Stefan 1889; Carslaw and Jaeger, 1959). We obtain an analytical solution for the nutrient interface concentration and the interface position (the free boundary).

### ANALYSIS ( THE FREE BOUNDARY MODEL)

Before developing the present model for the nutrient flow to a root, we make several assumptions, which are the following:

The porous medium is homogeneous and isotropic,  
 Moisture conditions are maintained at a steady state,  
 Nutrient uptake occurs at the root surface of the absorption zone,  
 The roots are smooth cylinders,  
 The rate of uptake can be described by a Michaelis-Menten type equation,  
 The nutrient transport occurs via convection and diffusion in the radial direction only (the latter takes place in soil solution phase only),  
 The rate of influx at infinite concentration ( $J_m$ ) and the Michaelis Menten constant ( $K_m$ ) are independent of the velocity of soil water at the root ( $v_o$ ), and the diffusion coefficient ( $D$ ) is independent of the flux,  
 $D$  and the buffer power  $b$  ( $b = \frac{dC}{dC_i}$  where  $C$  is the total diffusable ion and  $C_i$  is the ion concentration in soil solution) are independent of concentration,  
 The root system parameters are not changed by root age ( $k = \frac{J_m}{K_m} = \text{constant}$ ),  
 The velocity of water is not affected by nutrient concentration,  
 Production or depletion of nutrient by microbial or other activity is null,  
 All parameters  $D, b, k$  are independent of temperature, in the temperature range normally encountered in root growth,  
 The net uptake of nutrient is totally available for growth,  
 Root hairs do not affect nutrient uptake.  
 With the above assumptions, the partial differential equation for mass and diffusive transport of nutrient to the root (Cushman, 1979, 1980) is given (in cylindrical coordinates) by:

$$D C_{rr} + \left[ D + \frac{v_0 s_0}{b} \right] \frac{C_r}{r} = C_t \quad (1)$$

where:  $C = C_i$  is the ion concentration in soil solution,  $C_r = \frac{\partial C}{\partial r}$ ,  $C_{rr} = \frac{\partial^2 C}{\partial r^2}$ ,  $C_t = \frac{\partial C}{\partial t}$ ,  $r$  the position coordinate,  $t$  the time,  $D$  is the effective diffusion coefficient;  $v_0$  the velocity of flux solution at the root surface;  $b$  the buffer power, and  $s_0$  the initial radius.

Taking into account the idea of the model used for the shrinking core problem for noncatalytic gas-solid reactions (Wen, 1968; Tarzia and Villa, 1990), we propose the following free boundary problem for root growth (An extensive bibliography for moving and free boundary problems for the heat-diffusion equation is given in Tarzia, 1988:

$$\begin{aligned}
 & \text{i)} \quad D C_{rr} + D \alpha_0 \frac{C_r}{r} = C_t, \quad s(t) < r < R, \quad t > 0, \\
 & \text{ii)} \quad C(r, 0) = \Phi(r), \quad s_0 \leq r \leq R \\
 & \text{iii)} \quad C(R, t) = C_\infty > 0, \quad t > 0, \\
 & \text{iv)} \quad D b C_r(s(t), t) + v_0 C(s(t), t) = \frac{k C(s(t), t)}{1 + \frac{k C(s(t), t)}{J_m}} - E = a C(s(t), t) \dot{s}(t) \\
 & \text{v)} \quad s(0) = s_0, \quad 0 < s_0 < R
 \end{aligned} \quad (2)$$

where: i) is the Cushman equation [4,5], ii) and iii) are the initial and boundary conditions respectively, iv) are the interface conditions representing the mass nutrient balance, and v) is the initial radius.

with the conditions (2-LC:ii,iii,iv,v) which are called the quasi-stationary method for low concentrations (QSMCLC).

The two free boundary conditions (2-LC:iv) can be written by:

$$C_r(s(t),t) = g(C(s(t),t)) \quad , \quad t > 0 \quad (5)$$

$$\dot{s}(t) = f(C(s(t),t)) \quad , \quad t > 0 \quad (6)$$

where functions  $g$  and  $f$  are given by:

$$g(C) = \frac{1}{D b} [(k - v_0) C - E] \quad (7)$$

$$f(C) = \frac{1}{a} \left[ k - \frac{E}{C} \right] \quad (8)$$

which satisfy the following properties:

$$f(C) > 0 \Leftrightarrow C > C_p = \frac{E}{k} \quad (9)$$

$$g(C) > 0 \Leftrightarrow C > C_m = \frac{E}{(k-v_0)} \quad , \quad (C_m > C_p) \quad (10)$$

The solution of (QSMLC) problem is given by (see appendix A.):

$$C(r,t) = \beta(t) - \frac{\alpha(t)}{r^\epsilon} \quad , \quad s(t) < r < R, t > 0 \quad (11)$$

where:

$$\alpha(t) = \left[ \frac{1}{D b} \right] \frac{[(k - v_0)C_\infty - E]}{\frac{\epsilon}{s(t)^{1+\epsilon}} + \frac{(k-v_0)}{D b} \left[ \frac{1}{s(t)^\epsilon} - \frac{1}{R^\epsilon} \right]} \quad (12)$$

$$\beta(t) = C_\infty + \frac{\alpha(t)}{R^\epsilon} \quad (13)$$

$$\Phi(r) = C_\infty - \frac{[(k - v_0)C_\infty - E]}{\frac{v_0}{s_0^\epsilon} + (k - v_0) \left[ \frac{1}{s_0^\epsilon} - \frac{1}{R^\epsilon} \right]} \left[ \frac{1}{r^\epsilon} - \frac{1}{R^\epsilon} \right] \quad (14)$$

and  $s(t)$  is the unique solution of the following Cauchy problem (see Appendix B.):

$$\dot{s}(t) = F(s(t)) \quad , \quad t > 0 \quad (15)$$

$$s(0) = s_0 \in (0, R)$$

with:

$$F(s) = \frac{k}{a} [1 - \alpha_3 H(s)] \quad (16)$$

$$H(s) = \frac{[1 + \alpha_2 G(s)]}{[1 + \alpha_1 G(s)]} \quad , \quad G(s) = s \left[ 1 - \left( \frac{s}{R} \right)^\epsilon \right] \quad (17)$$

$$\alpha_1 = \frac{E}{v_0 s_0 C_\infty} > 0 \quad , \quad \alpha_2 = \frac{(k - v_0)}{v_0 s_0} > 0 \quad , \quad \alpha_3 = \frac{E}{k C_\infty} = \frac{C_p}{C_\infty} > 0 \quad (18)$$

Therefore, we obtain, after some elementary manipulations, that the interface concentration is given by the following expression:

$$C(s(t),t) = \frac{C_\infty}{H(s(t))} (= C(s(t))) \quad , \quad t > 0 \quad (19)$$

that is, the interface concentration does not depend explicitly on variable  $t$ .

The solution of Cauchy problem is computed numerically by the Runge-Kutta method for ordinary differential equations. Figures 2a, 2b, 2c, 2d, 2e, 2f and 3a, 3b, 3c, 3d represent results for the interface concentration  $C(s,t)$  vs.  $s$  and the interface position  $s(t)$  vs.  $t$  respectively as a function of the dimensionless parameter  $k/v_0$ .

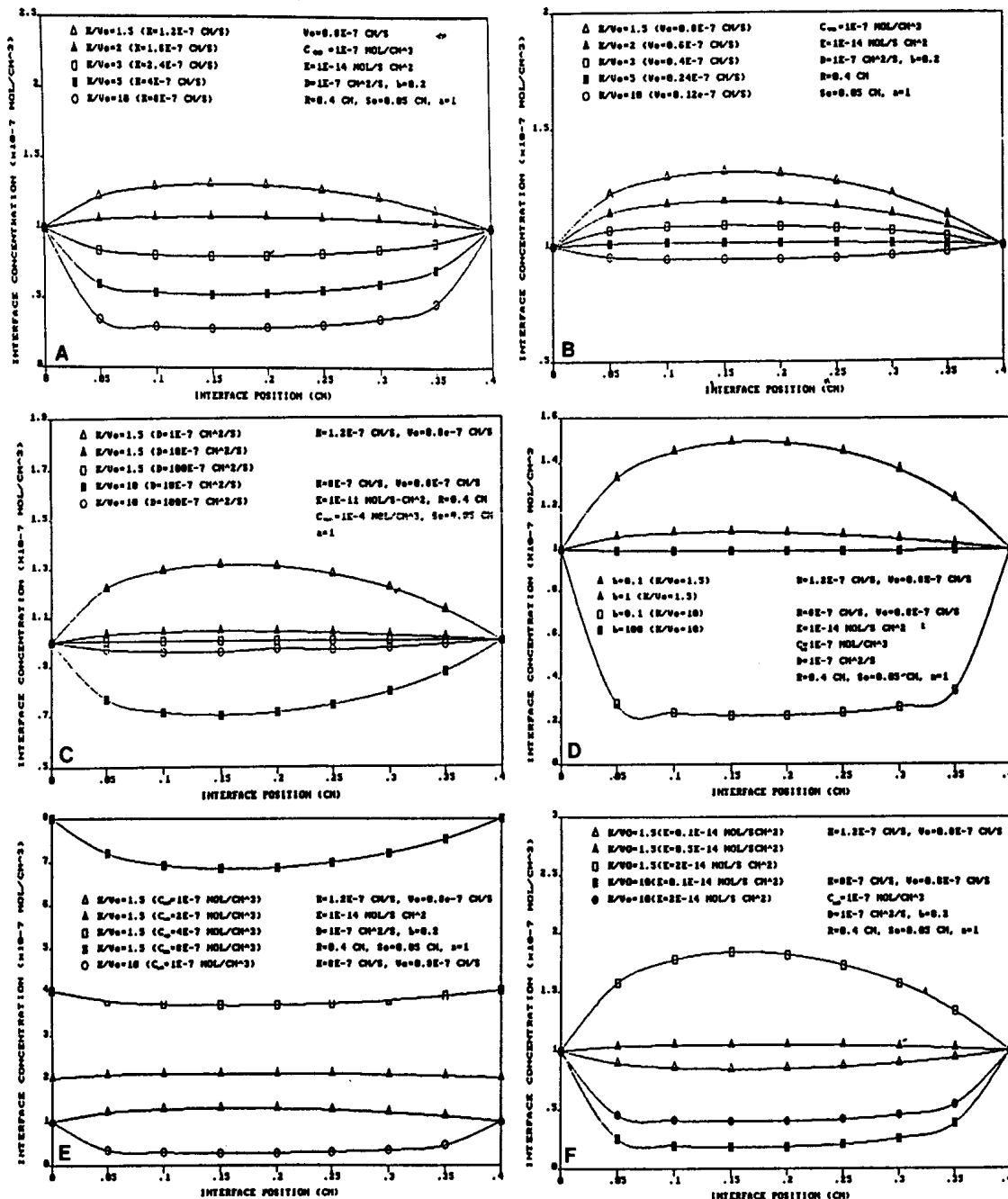


FIG. 2. a) Interface concentration versus root radius as a function of root absorption power. b) Interface concentration versus root radius as a function of flux solution velocity at root surface. c) Interface concentration versus root radius as a function of effective diffusion coefficient. d) Interface concentration versus root radius as a function of buffer power. e) Interface concentration versus root radius as a function of constant rhizosphere soil solution concentration. f) Interface concentration versus root radius as a function of constant efflux.

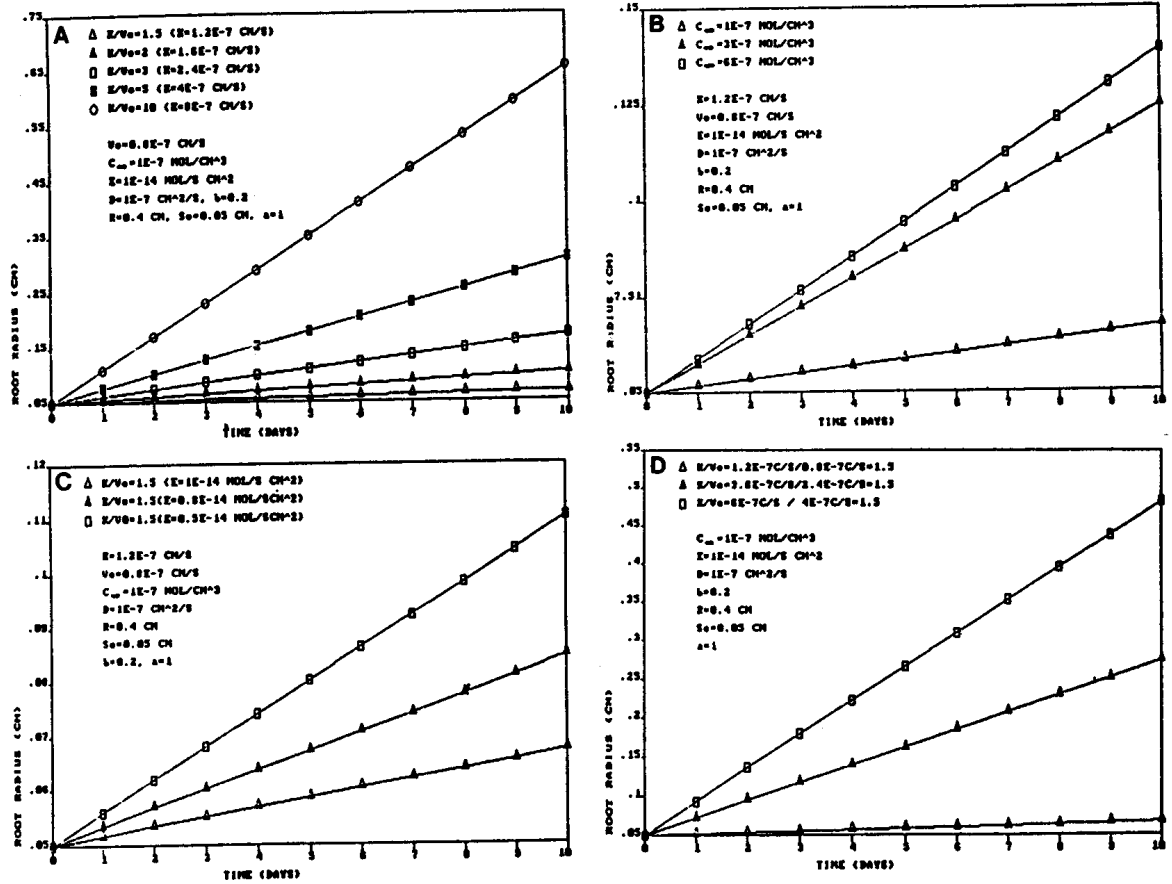


FIG. 3. a) Root radius versus time as a function of root absorption power. b) Root radius versus time as a function of constant rhizosphere soil solution concentration. c) Root radius versus time as a function of constant efflux. d) Root radius versus time as a function of root absorption power and flux solution velocity at root surface.

From the results of figs 2a., 2b., 2c. and 2d. we deduce that if the parameter  $k/v_0$  is small (e.g.: 1.5, 2) accumulation of nutrient is produced in the interface root-soil, then there is counterdiffusion and the root growth is low. On the other hand, for large values of  $k/v_0$  (e.g.: 10) the root growth is fast and the counterdiffusion is null. The limit value of  $k/v_0$  which produces the counterdiffusion effect depends on the remaining parameters.

From the results of Fig. 2e., it follows that if the nutrient concentration  $C_\infty$  increases or  $k/v_0$  is large then the counterdiffusion is null and the growth is faster. On the other hand, as shown in the fig. 2f. if  $E$  decreases or  $k/v_0$  is large, then the counterdiffusion is null and the root growth is faster.

Some of the above theoretical results have been observed from an experimental point of view (Barley, 1970; Nye and Tinker, 1977).

Let  $\gamma$  be the parameter defined by:

$$\gamma = \frac{E}{(k - v_0) C_\infty} \quad \left( = \frac{\alpha_1}{\alpha_2} \right)$$

We can prove that (see Appendix C):

- i)  $\gamma = \frac{E}{(k - v_0) C_\infty} < 1$  implies that  $C(s(t), t)$  has a minimum value because the absorption power  $k$  is large with

respect to  $v_o$  and there is no counterdiffusion.

$$\text{ii)} \quad \gamma = \frac{E}{(k - v_o) C_\infty} = 1 \quad \text{implies that } C(s(t), t) \text{ is constant.} \quad (20)$$

$$\text{iii)} \quad \gamma = \frac{E}{(k - v_o) C_\infty} > 1 \quad \text{implies that } C(s(t), t) \text{ has a maximum value because } k \text{ is small and the root can not absorb all the arriving nutrient and there is a counterdiffusion effect.}$$

These results agree with Cushmann's conclusions (Cushmann, 1979).

## CONCLUSIONS

We conclude from the model presented above that:

$s = s(t)$  increases when parameter  $k$  or  $C_\infty$  increases (Figures 3a, 3b).

$s = s(t)$  decreases when parameter  $E$  increases (Figure 3c).

$s = s(t)$  increases when parameter  $(k/v_o)$  increases and,  $k$  and  $v_o$  are large (Figure 3d).

$s = s(t)$  does not vary in function of the parameters  $v_o$ ,  $b$  and  $D$  because we did not have variations in the corresponding diagrams in a wide range of order of magnitude (1 to  $10^5$  for each).

$\dot{s} = \dot{s}(t)$  decreases when parameter  $\gamma$  increases, because from (15)-(18) we have for  $\dot{s}(t)$  the following representation in function of the parameter  $\gamma$ :

$$\dot{s} = \frac{k}{a} \left[ 1 - \frac{(k - v_o)}{k} \frac{G(s(t) + \frac{1}{\alpha_2})}{G(s(t) + \frac{1}{\gamma \alpha_2})} \right], \quad t > 0.$$

This conclusion agrees with the first three conclusions.

Finally, we can remark that the model presented in this paper gives us a qualitative approach (through a mathematical model) to root growth under the action of only one nutrient, with natural limitations in the real situation.

Moreover, these conclusions are useful for calibrating numerical models of the more complex nutrient transport and growth problems or they may be used to isolate the effects of the various parameters in the present model.

## APPENDIX

### Part A

The general solution of the second order ordinary differential equation (4) is given by:

$$C(r) = \beta - \frac{\alpha}{r^\epsilon} \quad (A1)$$

where  $\alpha$  and  $\beta$  are arbitrary constants.

Because the partial differential equation (4) should be solved in the variable interval  $r \in (s(t), R)$ , the coefficients  $\alpha$  and  $\beta$  must depend on the time  $t$ , that is, (12) and (13). After some elementary manipulations we deduce that  $\alpha(t)$ ,  $\beta(t)$  and  $s(t)$  are given by (12), (13) and (15) respectively.

*Part B*

From (16) we obtain that  $[F'(s) = \frac{dF}{ds}]$ :

$$F'(s) = - \frac{k \alpha_3}{a} \quad H'(s) = - \frac{k \alpha_3}{a} (\alpha_2 - \alpha_1) \frac{G'(s)}{[1 + \alpha_1 G(s)]^2} \quad (B1)$$

that is:

$$|F'(s)| \leq \frac{k \alpha_3}{a} |\alpha_2 - \alpha_1| \text{Max}(1, \epsilon) \quad (B2)$$

because:

$$\begin{aligned} G'(s) &= 1 - (1+\epsilon) \left[ \frac{s}{R} \right]^\epsilon, \quad G'(0) = 1, \quad G'(R) = -\epsilon \\ G''(s) &= - \frac{(1+\epsilon)}{R^\epsilon} \epsilon s^{\epsilon-1} < 0, \quad |G'(s)| \leq \text{Max}(1, \epsilon). \end{aligned} \quad (B3)$$

From (B2),  $F'$  is a bounded function and therefore, the Cauchy problem (15) has a unique solution.

*Part C*

From (17) and (19)  $\left[ C(s) = \frac{C_\infty}{H(s)} \right]$  we obtain that (Case  $\alpha_1 \neq \alpha_2$ ):

$$C'(s) = - \frac{C_\infty H'(s)}{[H(s)]^2} = - \frac{C_\infty (\alpha_2 - \alpha_1) G'(s)}{[1 + \alpha_1 G(s)]^2 [H(s)]^2} \quad (C1)$$

and:

$$C'(s) = 0 \Leftrightarrow G'(s) = 0 \Leftrightarrow s = R_0 = \frac{R}{[1 + \epsilon]^{\frac{1}{\epsilon}}}. \quad (C2)$$

From (C2) we can remark that the interface concentration has an extreme value at  $s = R_0$ . After some elementary manipulations we obtain:

$$\begin{aligned} C''(R_0) &= \frac{C_\infty (\alpha_2 - \alpha_1) \epsilon [1 + \epsilon]^{\frac{1}{\epsilon}}}{R [(1 + \alpha_1 G(R_0)) H(R_0)]^2} = d \alpha_2 \left[ 1 - \frac{E}{(k - v_0) C_\infty} \right] \\ &= d \alpha_2 (1 - \gamma), \end{aligned} \quad (C3)$$

where

$$d = \frac{C_\infty \epsilon [1 + \epsilon]^{\frac{1}{\epsilon}}}{R [(1 + \alpha_1 G(R_0)) H(R_0)]^2} > 0 \quad (C4)$$

and then we conclude (20).

## NOMENCLATURE AND UNITS

r:	Position (radius) coordinate	[ CM ]
t:	Time	[SEC ]



$J_m$ :	Rate of influx at infinite concentration	$\left[ \frac{\text{MOL}}{\text{SEC-CM}^2} \right]$
$K_m$ :	Michaelis Menten constant	$\left[ \frac{\text{MOL}}{\text{CM}^3} \right]$
$k$ :	Absorption power of root	$\left[ \frac{\text{CM}}{\text{SEC}} \right]$
$v_o$ :	Velocity of flux solution at root surface	$\left[ \frac{\text{CM}}{\text{SEC}} \right]$
$D$ :	Effective diffusion coefficient	$\left[ \frac{\text{CM}^2}{\text{SEC}} \right]$
$C$ :	Total diffusable ion concentration	$\left[ \frac{\text{MOL}}{\text{CM}^3} \right]$
$C_1$ :	Soil solution concentration	$\left[ \frac{\text{MOL}}{\text{CM}^3} \right]$
$C(s(t),t)$ :	Soil solution concentration at root-soil interface	$\left[ \frac{\text{MOL}}{\text{CM}^3} \right]$
$\Phi(r)$ :	Initial concentration profile	$\left[ \frac{\text{MOL}}{\text{CM}^3} \right]$
$C_\infty$ :	Constant rhizosphere soil solution concentration	$\left[ \frac{\text{MOL}}{\text{CM}^3} \right]$
$s_o$ :	Initial radius	$[ \text{CM} ]$
$E$ :	Constant efflux	$\left[ \frac{\text{MOL}}{\text{SEC-CM}^2} \right]$
$s(t)$ :	Instantaneous root radius	$[ \text{CM} ]$
$\dot{s}(t)$ :	Instantaneous velocity of root-soil interface	$\left[ \frac{\text{CM}}{\text{SEC}} \right]$
$R$ :	Rhizosphere radius	$[ \text{CM} ]$
$b$ :	Buffer power	DIMENSIONLESS
$a$ :	Stoichiometric coefficient	DIMENSIONLESS
$\alpha_1, \alpha_2$		$\left[ \frac{1}{\text{CM}} \right]$
$\alpha_o, \epsilon, \alpha_3, \gamma$		DIMENSIONLESS

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