

## **MODELING NUTRIENT UPTAKE USING A MOVING BOUNDARY APPROACH COMPARISON WITH THE BARBER-CUSHMAN MODEL**

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### **Abstract**

Single nutrient uptake by a growing root system is often estimated by the Barber-Cushman model. The model solves the coupled equations of transport in the soil and absorption of nutrient by roots in fixed domains. This study was conducted to determine whether a moving boundary model, accounting for increasing root competition, could improve predictions of nutrient uptake. Our model includes assumptions of the Barber-Cushman model and the moving boundary approximation. The model predicts nutrient uptake by coupling nutrient flux to roots and nutrient absorption on a variable domain in time. The model output was compared with measured uptake of Mg, K, P and S by various crops and soils by using experimental data obtained from the literature. Predicted Mg, K and P uptake by pine seedlings were close to the observed for K and P but out of, Mg, yet the predicted uptake showed deviations similar to those of the Barber-Cushman model. Predicted S uptake by wheat in different soils was better at least in ten out of eighteen measured cases. The model prediction was also compared with measured K uptake by three maize hybrids grown on typic Hapludult of Río Cuarto, Argentina, in a growth chamber. The moving boundary model appears to provide a better description of coupling between transport, absorption of nutrient and root growth and improve the prediction for nutrient uptake in some tests.

Nutrient uptake has been evaluated through diffusive and mass flow models which are based on numerical approximation in fixed domains of differential transport equations in soils coupled with absorption kinetics by roots (Cushman, 1979; Barber, 1995). These models estimate the nutrient concentration at the root-soil interface and the resulting nutrient uptake. Other models assume the root surface behaves like a zero-sink, therefore nutrient uptake is determined by the rate of nutrient supply to the root surface by mass flow and diffusion. In these models, the radius of finite cylindrical soil volume assigned to each root declines with increasing root density (Hoffland, 1990). In other models, analytical solutions (Nye and Tinker, 1977) were used for calculating the volume of the soil allocated to each root and the concentration at root surface including a depletion zone that increased with time until it reached the non-transfer boundary (Smethurst, 1993). Recently, we have formulated free boundary models for root growth (Reginato et al., 1990, 1991, 1993a), i.e., analytical models through which it is possible to compute nutrient concentration at the root-soil interface and root growth rate (a priori an unknown function of time). This fact allows us to postulate a new model of nutrient uptake due to the transport and absorption of ions from a more dynamic point of view. This new model differs from our previous ones as the root growth rate is now plugged in as known function of time, the same as the Barber-Cushman model. Thus, the goal of the present work is to evaluate a moving boundary model for nutrient uptake which takes into account an increasing root competition for nutrient uptake from the soil by a growing root system combining ion transport, absorption kinetics and root growth simultaneously.

A one-dimensional model is considered, i.e., a single cylindrical root in a soil where it is assumed that the conditions of moisture, light and temperature are controlled (like in a growth chamber). With these assumptions, the following one-dimensional nutrient uptake model through a moving boundary problem to one phase (the soil) (Crank, 1984, Tarzia, 1988) in cylindrical coordinates is proposed:

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

$$C(r, 0) = \varphi(r), \quad s_o \leq r \leq R_o \quad [1-b]$$

$$-Db \frac{\partial}{\partial r} C(R(t), t) + v_o C(R(t), t) = 0, \quad 0 < t < T \quad [1-c]$$

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

$$R(t) = R_o \sqrt{\frac{l_o}{l(t)}}, \quad 0 < t < T \quad [1-e]$$

where  $r$  is the radial distance from the root axis [m],  $t$  is the time [s];  $T$  is the maximum time for which the system has solution [s];  $C_u$  is the concentration for which the net influx is null [ $\text{mol m}^{-3}$ ];  $v_o$  is the mean effective velocity of soil solution at root surface [ $\text{m s}^{-1}$ ];  $b$  is the buffer power,  $D$  is the effective diffusion coefficient [ $\text{m}^2 \text{s}^{-1}$ ],  $k_a (= J_m / K_m)$  is the absorption power of nutrient [ $\text{m s}^{-1}$ ];  $J_m$  is the maximum influx at infinite concentrations [ $\text{mol m}^{-2} \text{s}^{-1}$ ];  $K_m$

is the concentration at which influx is  $J_m/2$  [mol m<sup>-3</sup>];  $R(t)$  is the variable half distance between root axes at time  $t$  [m],  $\varphi$  is the initial concentration defined in  $[s_o, R(t)]$  [mol m<sup>-3</sup>],  $R_o$  is the initial half distance between root axes [m],  $s_o$  is the root radius [m],  $l(t)$  is the root length as a function of time [m], and  $l_o$  is the initial root length [m]. The parameter  $\varepsilon_o$  is given by

$$\varepsilon_o = \frac{v_o s_o}{Db} \text{ [dimensionless]}. \text{ In our model, all coefficients are assumed to be constant. Equation}$$

(1-a) represents the ion transport equation in the soil. Condition (1-b) corresponds to the initial concentration and Condition (1-c) is the boundary condition representing null flux on the moving boundary  $R(t)$  that is a priori a known function of time. Condition (1-d) represents the mass balance at the root surface where the ions arriving are incorporated through absorption kinetics. Equation (1-e) gives us the moving  $R(t)$  as a function of the instantaneous root length  $l(t)$ , which is known a priori. Expression (1-e) is obtained assuming a fixed volume of soil and relating  $R(t)$  with the instantaneous root length (which is a special function according to method used to estimate longitudinal root growth, i.e., linear, exponential, sigmoid, etc.) (See Appendix A.). Equation [1-e] characterizes the moving boundary approximation and replaces a second equation in [1-d], which was postulated, in our previous free boundary models.

The model is solved by applying the integral balance method (Goodman, 1958, Reginato et al., 1993b). So, the partial differential equation (1-a) is integrated in variable  $r$  on the domain  $(s_o, R(t))$ . Moreover, by using an analogous methodology as used in phase-change processes, the following expression for  $C(r, t)$  is proposed:

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

$$\text{with:} \quad \varphi(r) = C_R e^{-\varepsilon(R_o - r)}, \quad \varepsilon = \frac{v_o}{Db} = \frac{\varepsilon_o}{s_o} \quad [3]$$

where  $C_R$  is the initial ion concentration in soil solution at  $r = R_o$  [mol m<sup>-3</sup>]. Expression [2] for the concentration verifies the initial (1-b) by taking  $\beta(0)=0$  and boundary (1-c) conditions. So, after some elementary and long manipulations, and taking into account the particular case of an linear root growth, the following differential equation for  $\beta(t)$  was obtained (see Appendix B.):

$$\frac{d\beta(t)}{dt} = \frac{F_2(R(t), \beta(t))}{F_1(R(t))}, \quad \beta(0) = 0 \quad [4]$$

$$\text{with:} \quad R(t) = R_o \sqrt{\frac{l_o}{l_o + kt}}$$

The system [4] is solved through the Runge-Kutta method for ordinary differential equations, which was implemented in a FORTRAN program on a personal computer.

Total nutrient uptake can be obtained from the following formula (See Reginato, Tarzia, 2000), which is a modified version of the Cushman formula (Cushman, 1979; Claasen and Barber, 1976).

$$U = 2\pi s_o l_o \int_{t=0}^{t=t_{\max}} J_c(t) dt + 2\pi s_o \int_{t=0}^{t=t_{\max}} \left[ \int_{t=t}^{t=t_{\max}} J_c(t) dt \right] \dot{l}(t) dt \quad [5]$$

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

where  $J_c(t)$  is the influx,  $\dot{l}(t)$  is the longitudinal root rate growth and  $U$  is computed from  $t = 0$  to  $t = t_{max}$ .

## MATERIALS AND METHODS

Three maize hybrids (Dekalb 762, Capitán Ciba y Tilkara Funks) were grown in cylindrical pots with 1.6 kg. of typic Hapludult from Río IV, Córdoba, Argentina in a growth chamber at 26 °C. The whole pot experiment consisted of four replicates with 15 plants in each pot for the three hybrids. At emergence, 5 days after germination [DAG], plants were harvested to determine initial potassium and root length. The plants were harvested 11 DAG, dried at 70 °C, digested by wet-combustion and analyzed for potassium by flame photometry (Jackson, 1964).

### Determination of Model Parameters

Soil and plant parameters for K uptake simulation were estimated as follows:

**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 hr. (Adams, 1974). Buffer power  $b$  and diffusion coefficient  $D$  were determined as described by Kovar and Barber (1990). Flux velocity  $v_o$  was determined by dividing the total water uptake of the plant in each pot within a given time, by the mean root surface area within the same given time:  $v_o = W (\ln S - \ln S_o) / (t - t_o)(S - S_o)$ . Total water uptake  $W$  was obtained by subtracting the water loss due to evaporation from the total water loss due to evapotranspiration

**Root parameters:** The exponential root growth rate  $k$  was calculated from root length as a function of time by  $k = (\ln l(t) - \ln l_o) / (t - t_o)$ . The linear growth rate was calculated from the relation  $k = (l(t) - l_o) / (t - t_o)$ . The mean root radius  $s_o$  was calculated from the root length and fresh weight by:  $s_o = [Weight\ Fresh / \pi \cdot Root\ length]^{1/2}$  assuming a root tissue density of 1 g cm<sup>-3</sup>. Half distance between roots axes,  $R_o$ , was calculated by:  $R_o = [Soil\ Volume / \pi \cdot Root\ Length]^{1/2}$ . Root length,  $l$ , was measured by the line-intersect method (Tennant, 1975).

**Kinetics Uptake parameters:**  $J_m$ ,  $K_m$ ,  $C_u$  and  $k_a$  were determined by analysis of potassium depletion curves in a nutritive solution from which roots absorb nutrients (Claassen and Barber, 1974).

Soil and plant parameters used in the moving boundary model are listed in Table 1.

Table 1. Soil and plant parameters used in the moving boundary model

Parameter	Hybrid		
	Capitán Ciba	Dekalb 762	Tilkara Funks
Exponential root growth rate $k$ , s <sup>-1</sup>	1.066 x 10 <sup>-6</sup>	9.63 x 10 <sup>-7</sup>	8.59 x 10 <sup>-7</sup>
Mean water influx rate at root surface $v_o$ , m s <sup>-1</sup>	1.26 x 10 <sup>-8</sup>	2.24 x 10 <sup>-8</sup>	1.15 x 10 <sup>-8</sup>
Mean root radius $s_o$ , m	5 x 10 <sup>-4</sup>	3.8 x 10 <sup>-4</sup>	3.4 x 10 <sup>-4</sup>

Initial root length $l_o$ , m	1.8	2.41	2.05
Initial half distance between roots axes $R_o$ , m	$1.27 \times 10^{-2}$	$1.14 \times 10^{-2}$	$1.24 \times 10^{-2}$
Soil buffer power $b$ , dimensionless	11.6	11.6	11.6
Effective diffusion coefficient for the ion in soil $D$ , $\text{m}^2 \text{s}^{-1}$	$6.827 \times 10^{-12}$	$6.827 \times 10^{-12}$	$6.827 \times 10^{-12}$
Maximum influx rate at high concentrations $J_m$ , $\text{mol m}^{-2} \text{s}^{-1}$	$1.316 \times 10^{-6}$	$6.752 \times 10^{-6}$	$4.744 \times 10^{-6}$
Absorption power $k_a$ , $\text{m s}^{-1}$	$1 \times 10^{-6}$	$3.57 \times 10^{-6}$	$2.584 \times 10^{-6}$
Ion concentration in soil solution below which influx ceases $C_u$ , $\text{mol m}^{-3}$	$2.183 \times 10^{-2}$	$1.5 \times 10^{-3}$	$9.9 \times 10^{-4}$
Initial concentration of ion in the soil solution $C_R$ , $\text{mol m}^{-3}$	8.4	8.4	8.4

## RESULTS AND DISCUSSION

The results obtained for the potassium uptake of the three maize hybrids are presented in Table 2. The values obtained represent good results.

Table 2. Potassium uptake by three maize hybrids: observed vs. predicted uptake by the moving boundary model.

Hybrid	K-uptake ( $\text{mmol pot}^{-1}$ )	
	Observed	Predicted
DEKALB 762	0.1685	0.213
TILKARA FUNKS	0.293	0.325
CAPITAN CIBA	0.304	0.287

For a more exhaustive analysis, the model was also tested with experimental data extracted from the literature. Thus, uptake of Mg, K and P for loblolly pine seedlings during 180 days in a modified A horizon soil mesic Typic Hapludult (Kelly et al., 1992), was estimated. The comparison between the Barber-Cushman prediction using the NUTRIENT UPTAKE program (Oates and Barber, 1987) and the estimation of the present model, i.e., the moving boundary model, assuming a linear root growth with time is shown in Table 3.

Table 3. Mg, K and P uptake by pine seedling: observed vs. predicted by Barber-Cushman and moving boundary models

Nutrient	Observed uptake ( $\text{mmol pot}^{-1}$ )	Predicted uptake ( $\text{mmol pot}^{-1}$ )			
		Barber-Cushman Model (1)		Moving Boundary Model (2)	
		Error (†)		Error (†)	
Mg	1.617	0.625	61.3	0.680 (*)	57.1
K	6.663	6.285	5.6	6.653 (*)	0.15
P	1.332	1.185	11	1.302 (*)	2.25

(1) Source: Kelly et al. 1992

(2) Source: Present paper

(†) Relative error = [(Observed uptake - predicted uptake)/Observed uptake] x 100.

(\*) The value obtained by the moving boundary model represents a better prediction

Predicted uptakes improved in all cases, although for Mg uptake the same deviations showed by the Barber-Cushman model persisted, probably because high  $J_m$  values obtained from solution studies are responsible for underprediction of Mg uptake by crops (Rengel et al., 1990). Thus, both models can be improved taking into account  $J_m$  values obtained from soil studies. The nutrient uptake predicted by our model can be improved in its theoretical aspects. In this respect, the limitation of these models is that both consider the absorption of only one nutrient explicitly without taking into account the simultaneous absorption of ions and the possible coupling with other ions in the absorption. This last fact suggests the need for a model that simultaneously takes into account the interactions among nutrients, as for example, by using competitive kinetic absorption.

Moreover, the model is tested with data of S uptake by wheat grown on Norwood silt loam (Typic Hapludalf) and Mhoon silty clay loam (Typic Fluvaquent) for a period of 24 and 17 days, respectively, under glasshouse conditions (Delgado and Amacher, 1997). The NUTRIENT UPTAKE program (Oates and Barber, 1987) and the present model were used for the input data. The predicted uptakes using a linear root growth are shown in Table 4.

Table 4. S uptake by wheat: observed vs. predicted by Barber-Cushman and moving boundary models

Crop (Soil)	Observed Uptake (mmol pot <sup>-1</sup> )	Predicted uptake (mmol pot <sup>-1</sup> )			
		Barber-Cushman Model (1)		Moving Boundary Model (2)	
			Error (†)		Error (†)
Wheat (Norwood +)	0.02557	0.004678	81.7	0.00749 (*)	70.7
	0.0287	0.02969	3.4	0.02684	6.5
	0.0452	0.05925	31	0.0532 (*)	17.7
	0.06923	0.09355	35.1	0.0746 (*)	7.75
	0.08358	0.1294	54.8	0.099 (*)	18.4
Wheat (Norwood)	0.01091	0.004678	57.1	0.00822 (*)	24.6
	0.0234	0.03119	33.3	0.02966 (*)	26.7
	0.0452	0.0701	55	0.06599 (*)	46
	0.0561	0.106	88.9	0.08624 (*)	53.7
	0.0977	0.145	48.4	0.1141 (*)	16.8
Wheat (Mhoon +)	0.08576	0.09048	5.5	0.01247	85.3
	0.1356	0.2089	54	0.01383	89.8
	0.229	0.3071	34	0.01477	93.5
	0.2426	0.4288	76.7	0.01577	93.5
Wheat (Mhoon)	0.0555	0.02807	49.4	0.01913	65.5
	0.08358	0.05519	33.9	0.03627	56.6
	0.0764	0.08731	14.3	0.05137	32.7
	0.08358	0.1185	41.8	0.06883 (*)	17.6

(1) Source: Delgado and Amacher, 1997 (We have extracted their predicted S uptake by using  $J_m$  obtained from soil studies)

(2) Source: Present paper

(†) Relative error = [(Observed uptake - predicted uptake)/Observed uptake] x 100.

(\*) The value obtained by the moving boundary model represents a better prediction

The moving boundary model provides a better prediction in ten cases for a total number of eighteen predictions. We remark that for Norwood soils the comparison between the predicted uptakes by the Barber-Cushman model and the predicted uptakes by our model shown that the present model overpredicts 1.27 times the observed uptakes while the Barber-Cushman model overpredicted 1.72 times the observed values. This fact is shown in Figure 1.

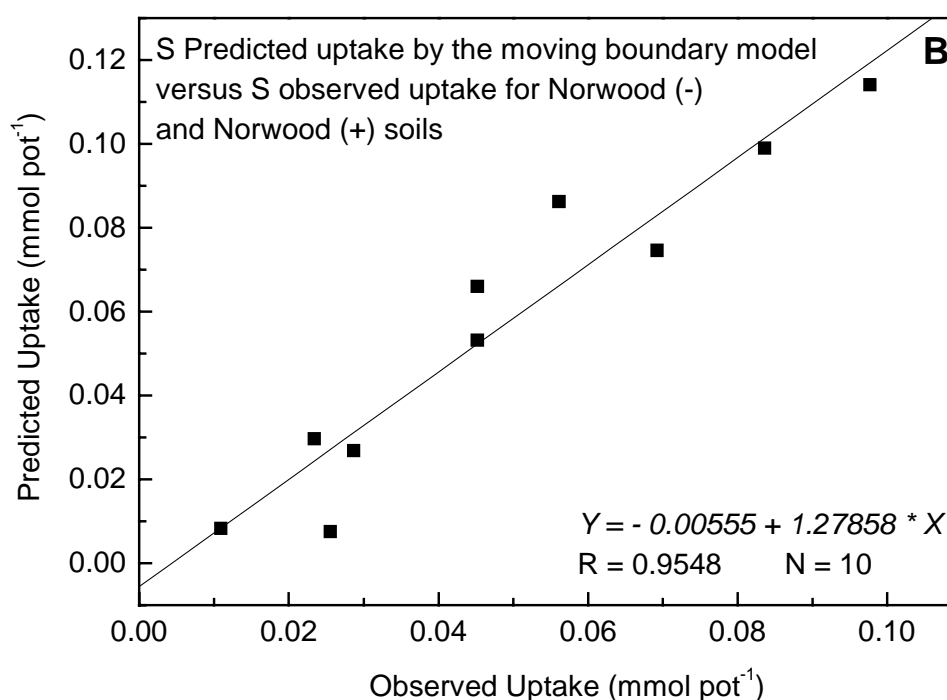
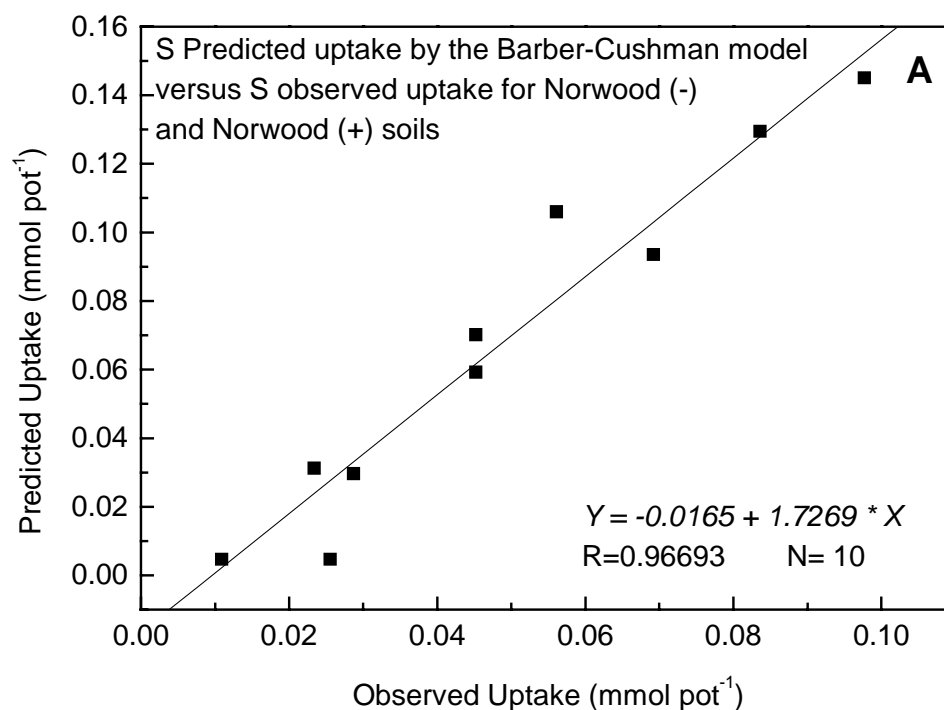


Figure 1. Comparison between predicted and observed S uptakes by: A) Barber-Cushman model, B) moving boundary model

For the Mhoon soils, the predictions are poor. On the other hand, for long periods of time as accounting for K, P and Mg our model makes better predictions. We remark that the validity of the root competition assumption for the soils considered in the tests is justified because the depletion radius ( $r_d = s_o + 2\sqrt{Dt}$  following Baldwin and Nye (1974)) equals to the instantaneous half distance between root axes  $R(t)$  in few days (Aprox. three or four days for the soils considered). Thus, the moving boundary model could be a good alternative method for the prediction of nutrient uptake.

### Appendix A.

The expression [1-e] is obtained assuming that the available soil volume at time  $t$  results from the difference between the available soil volume at initial time  $t = 0$  and the grown root volume at time  $t$ , i.e., if  $R_o$  is the initial half distance between roots,  $l_o$  is the initial root length and  $l(t)$  is the root length at time  $t$ , then we have

$$V_{soil}|_{t=t} = V_{soil}|_{t=0} - V_{root}|_{t=t}$$

that is

$$\pi l(t) [R^2(t) - s_o^2] = \pi l_o [R_o^2 - s_o^2] - \pi s_o^2 [l(t) - l_o]$$

Thus, after elementary manipulations the condition [1-e] is obtained.

### Appendix B

Integral balance method (Reginato et al., 1993b). The functions  $F_1$  and  $F_2$  are given by:

$$F_1(R(t)) = C_R e^{-\varepsilon R_o} \left\{ \frac{\left[ \frac{e^{\varepsilon R(t)} - e^{\varepsilon s_o}}{\varepsilon} - \frac{2}{R(t)} \frac{\left[ e^{\varepsilon R(t)} (\varepsilon R(t) - l) - e^{\varepsilon s_o} (\varepsilon s_o - l) \right]}{\varepsilon^2} \right]}{\frac{1}{R^2(t)} + \frac{\left[ e^{\varepsilon R(t)} (\varepsilon^2 R^2(t) - 2\varepsilon R(t) + 2) - e^{\varepsilon s_o} (\varepsilon^2 s_o^2 - 2\varepsilon s_o + 2) \right]}{\varepsilon^3}} \right\}$$

$$F_2(R(t), \beta(t)) = G_1 + G_2 + G_3 + G_4 + G_5$$

where:

$$G_1(R(t), \beta(t)) = D\varepsilon C_R e^{-\varepsilon(R_o - R(t))} + D\varepsilon C(s_o, t) - \frac{k_a}{b} \frac{[C(s_o, t) - C_u]}{1 + \frac{k_a [C(s_o, t) - C_u]}{J_m}}$$

$$\text{with: } C(s_o, t) = C_R e^{-\varepsilon(R_o - s_o)} \left[ 1 + \beta(t) \left( 1 - \frac{s_o}{R(t)} \right)^2 \right]$$

$$G_2(R(t), \beta(t)) = D(1 + \varepsilon_o) \frac{2\beta(t)}{R(t)} \left( \frac{1}{R(t)} - \varepsilon \right) C_R e^{-\varepsilon R_o} \frac{[e^{\varepsilon R(t)} - e^{\varepsilon s_o}]}{\varepsilon}$$



$$G_3(R(t), \beta(t)) = \frac{\beta(t)}{R^2(t)} \left[ D(1 + \varepsilon_o) \varepsilon - 2 \dot{R}(t) \right] C_R e^{-\varepsilon R_o} \frac{\left[ e^{\varepsilon R(t)} (\varepsilon R(t) - 1) - e^{\varepsilon s_o} (\varepsilon s_o - 1) \right]}{\varepsilon^2}$$

$$G_4(R(t), \beta(t)) = \frac{2\beta(t) \dot{R}(t)}{R^3(t)} C_R e^{-\varepsilon R_o} \frac{\left[ e^{\varepsilon R(t)} (\varepsilon^2 R^2(t) - 2\varepsilon R(t) + 2) - e^{\varepsilon s_o} (\varepsilon^2 s_o^2 - 2\varepsilon s_o + 2) \right]}{\varepsilon^3}$$

with:  $\dot{R}(t) = \frac{-kR(t)}{2(l_o + kt)}$

$$G_5 = \left[ D(1 + \varepsilon_o) \left( \varepsilon + \varepsilon \beta(t) - \frac{2\beta(t)}{R(t)} \right) \right] C_R e^{-\varepsilon R_o} \cdot$$

$$\cdot \left[ \ln \frac{R(t)}{s_o} + \varepsilon [R(t) - s_o] + \frac{\varepsilon^2}{4} [R^2(t) - s_o^2] + \frac{\varepsilon^3}{18} [R^3(t) - s_o^3] + \frac{\varepsilon^4}{96} [R^4(t) - s_o^4] + \right.$$

$$\left. + \frac{\varepsilon^5}{600} [R^5(t) - s_o^5] + \frac{\varepsilon^6}{4320} [R^6(t) - s_o^6] + \frac{\varepsilon^7}{35280} [R^7(t) - s_o^7] + \right.$$

$$\left. + \frac{\varepsilon^8}{322560} [R^8(t) - s_o^8] + \frac{\varepsilon^9}{3265920} [R^9(t) - s_o^9] \right]$$

The solution is found integrating the partial differential equation (1-a) in variable  $r$  over the domain  $(s_o, R(t))$  with  $C(r, t)$  given by the expression [3]. Thus, for linear root growth rate,  $l(t) = l_o + kt$ , the problem [1] reduces to:

$$\int_{s_o}^{R(t)} C_t(r, t) dr = D \int_{s_o}^{R(t)} C_{rr}(r, t) dr + D(1 + \varepsilon_o) \int_{s_o}^{R(t)} \frac{C_r(r, t)}{r} dr$$

$$R(t) = R_o \sqrt{\frac{l_o}{l_o + kt}}, \quad \beta(0) = 0$$

Computing the following integrals,  $\int_{s_o}^{R(t)} C_t(r, t) dr$ ,  $\int_{s_o}^{R(t)} C_{rr}(r, t) dr$  and  $\int_{s_o}^{R(t)} \frac{C_r(r, t)}{r} dr$  and taking into account that the integral for  $e^{\varepsilon r}/r$  is approximate by a Taylor polynomial of nine's order in variable  $r$  (Abramowitz, 1972), after elementary manipulations, we obtain system [4].

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