The Problem of Free and Moving Boundary for Root Growth, Nutrient Uptake and Other Applications

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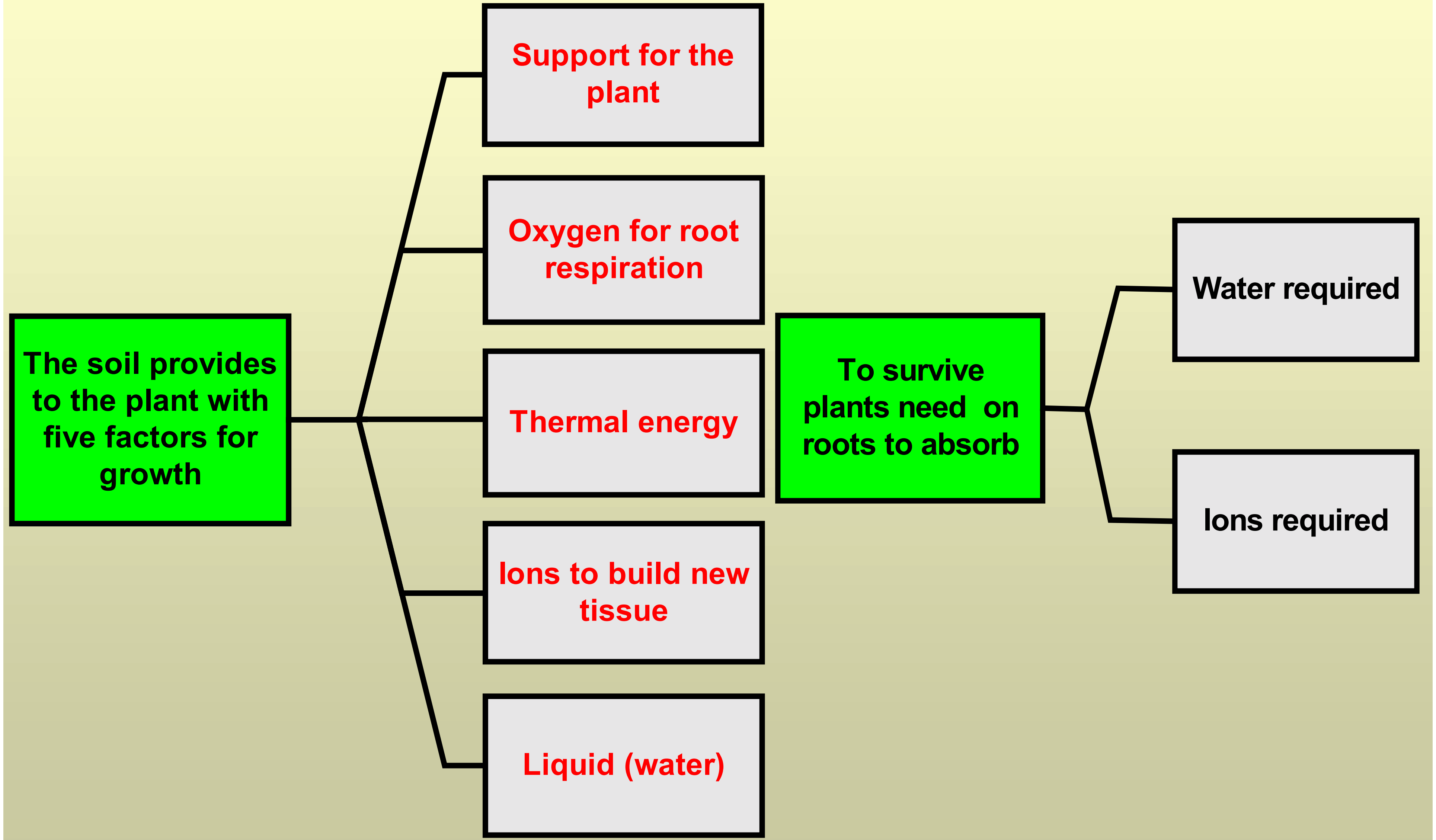
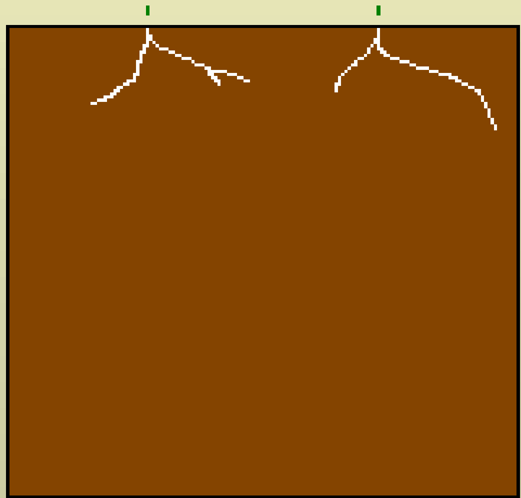
ARGENTINA

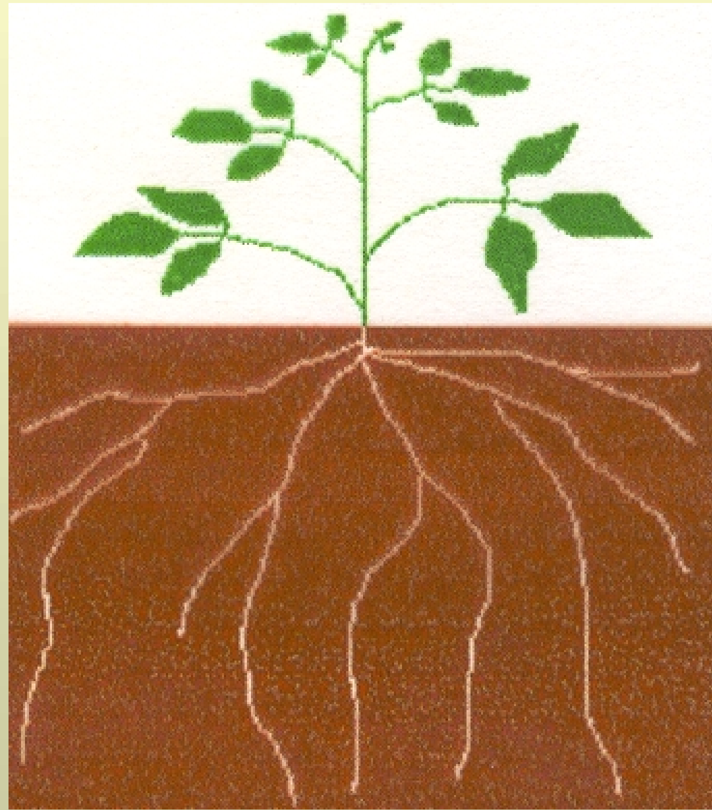
Root growth. A short introduction



Root growth introduction

The germination results in the development of shoots upwards and roots downwards. As the roots move through the soil they find a growing source of ions and water

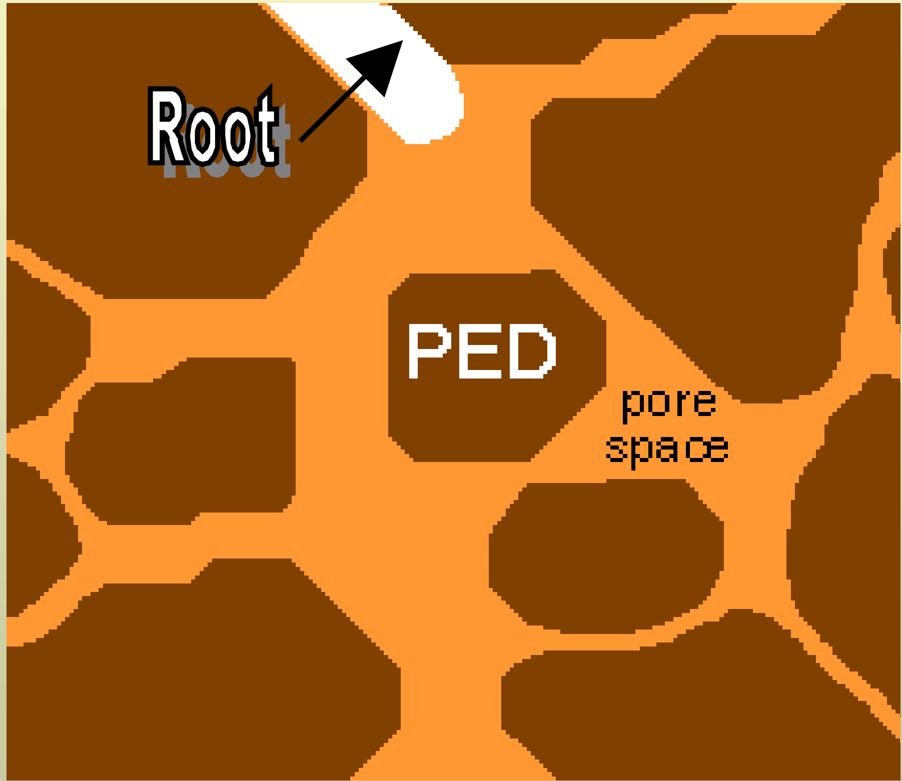




Root growth introduction

The roots grow in the path of minor resistance and they extend in the porous spaces of soil. The roots change their directions when they find Peds which are aggregates of resistant soil

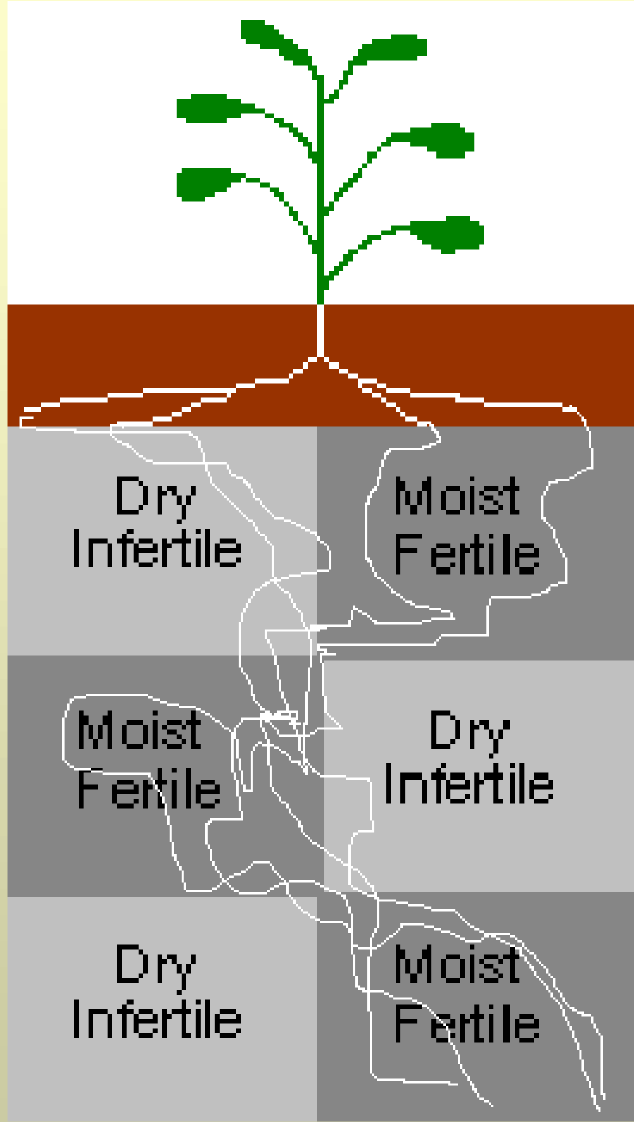
Root path



Root growth introduction

Besides, following the path of minor resistance, roots also grow where the media is better. Here the roots avoid the dry and arid soil while they grow in the moist and fertile soil

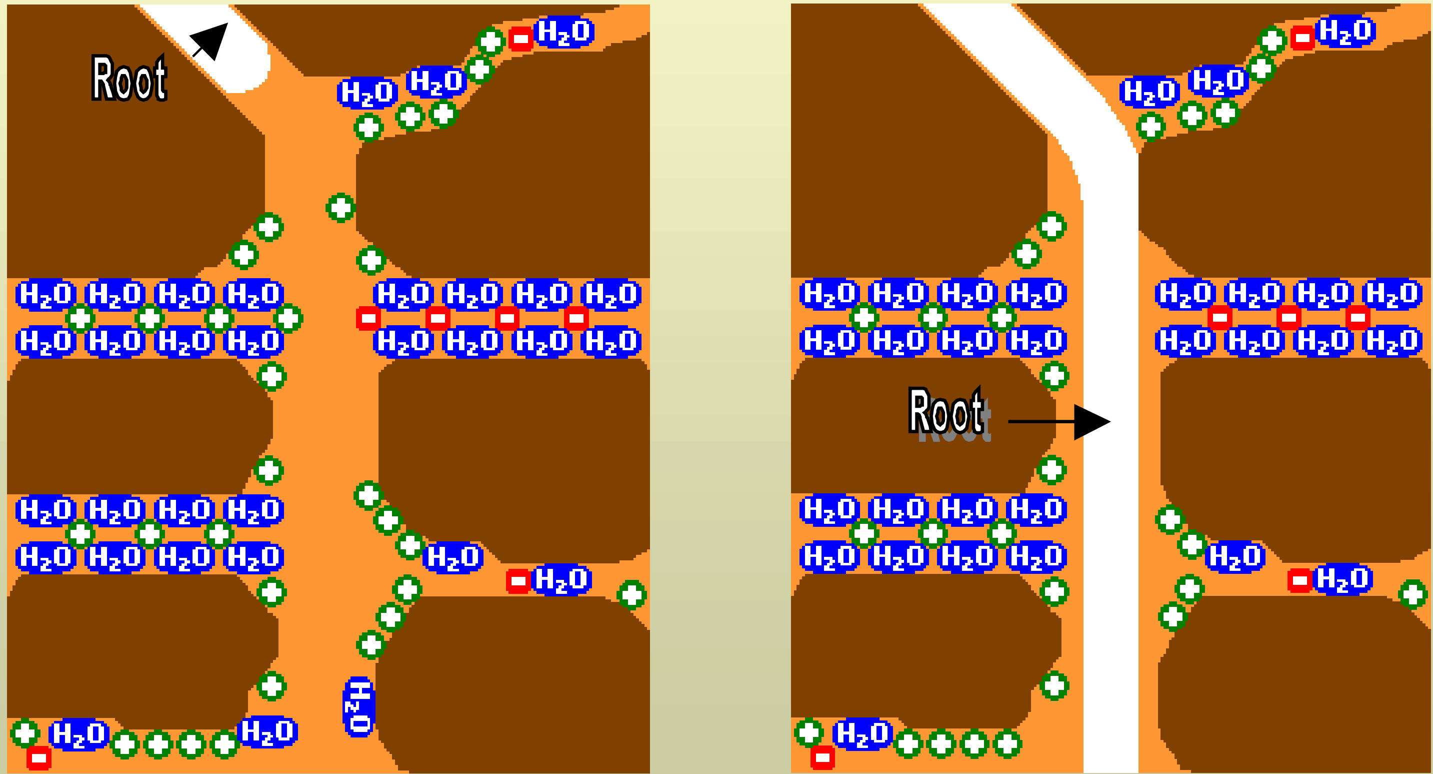
As the roots absorbs and dries the source of water and adjacent ions to them, fortuitously extends through the root zone. In the majority of the annual and horticultural cultivation, the radical systems will penetrate to a depth of 1 meter or more



Root enviromment

Root growth Introduction : Nutrient uptake

The root incorporates adjacent ions, then it is important that ions move towards the root. As the root grows through the soil absorbs ions and water in direct contact with it.



INTERSECTION (≈1%)

Root growth introduction

As the water adjacent to the root is absorbed, a gradient of potential water is established which cause the water to move slowly towards the roots transporting ions. The process of ions moving towards the root with the movement of the water is called the *CONVECTIVE FLUX*

The convective flux depends on the ion concentration in solution and on the amount of water moved towards the root which is proportional to the plant respiration

The ions in soil solution diffuse slowly towards the root whether exists or not water moving towards it. The process is denominated *DIFFUSIVE FLUX*

ONLY IONS IN THE ROOT SURFACE ARE AVAILABLE FOR UPTAKE

Root growth introduction

NUTRIENT ABSORPTION

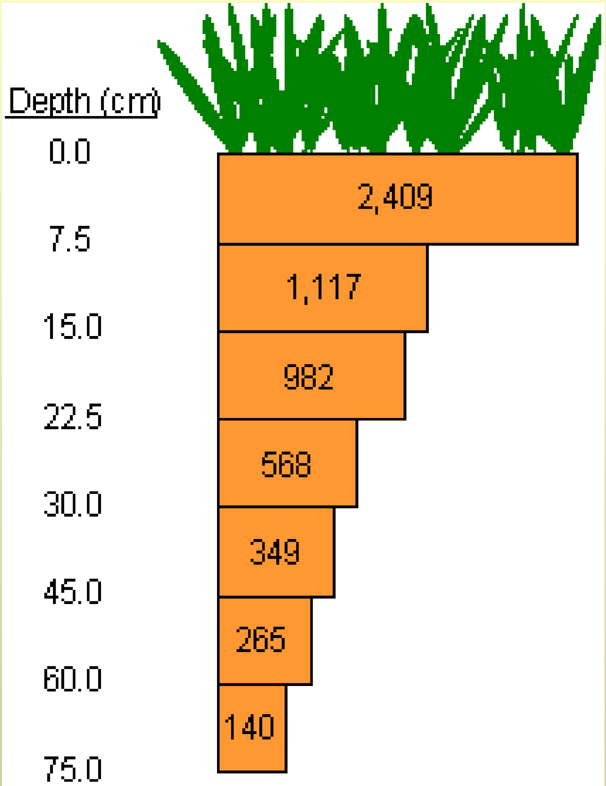
- **INTERSECTION** (nutrients which the plant finds by direct contact)
- **CONVECTIVE FLUX** (nutrients transported by water movement)
- **DIFFUSIVE FLUX** (nutrient movement through soil solution)

Root growth Introduction

ROOT DISTRIBUTION

The plant capacity to absorb water and ions is related to root length (area density of the root surface). Uptake is based on ions availability and root length

UPTAKE = Ions availability by root length (density of superficial area)



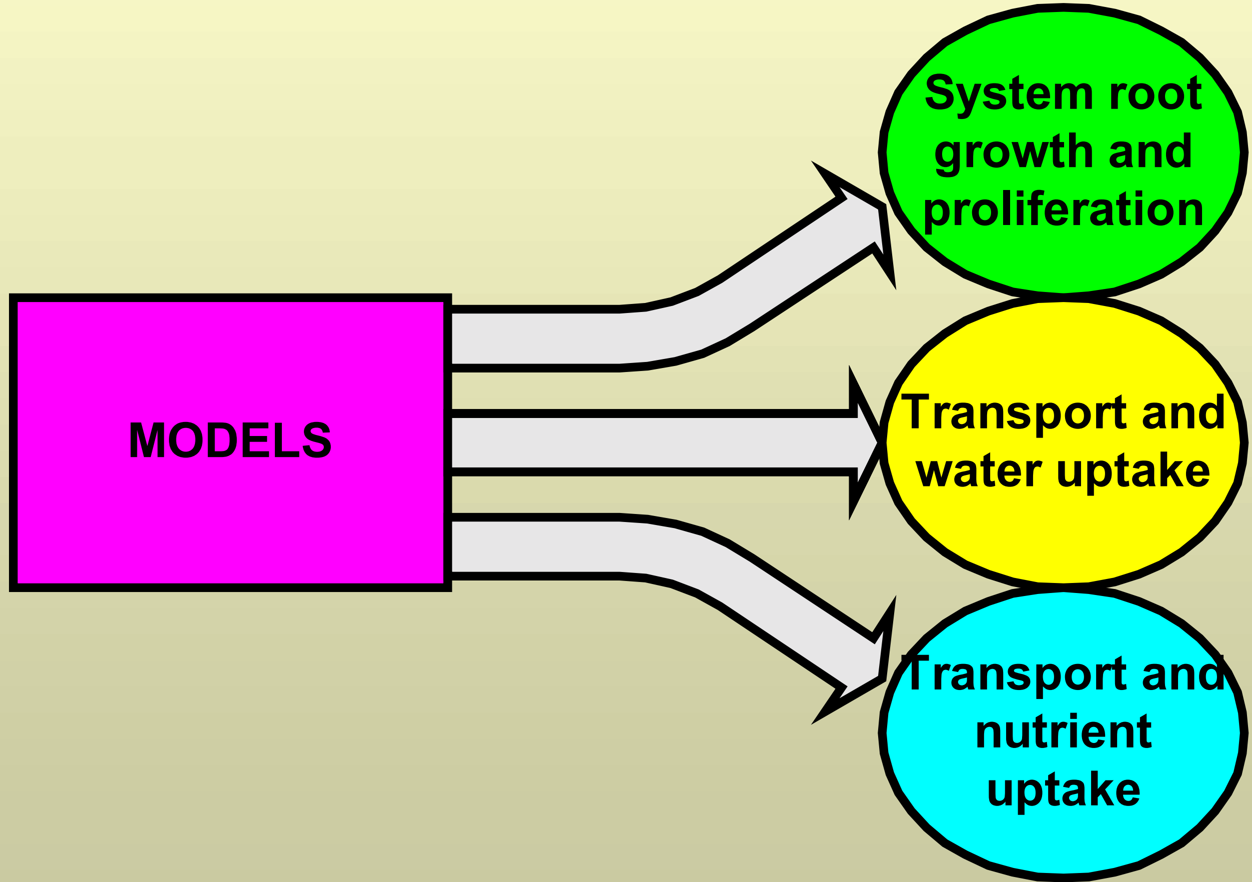
ROOT LENGTH

What total root length has a plant as wheat in 1 acre to a depth of 75 cm? Excluding hairs, the total length is 5830 miles = 9329 km.

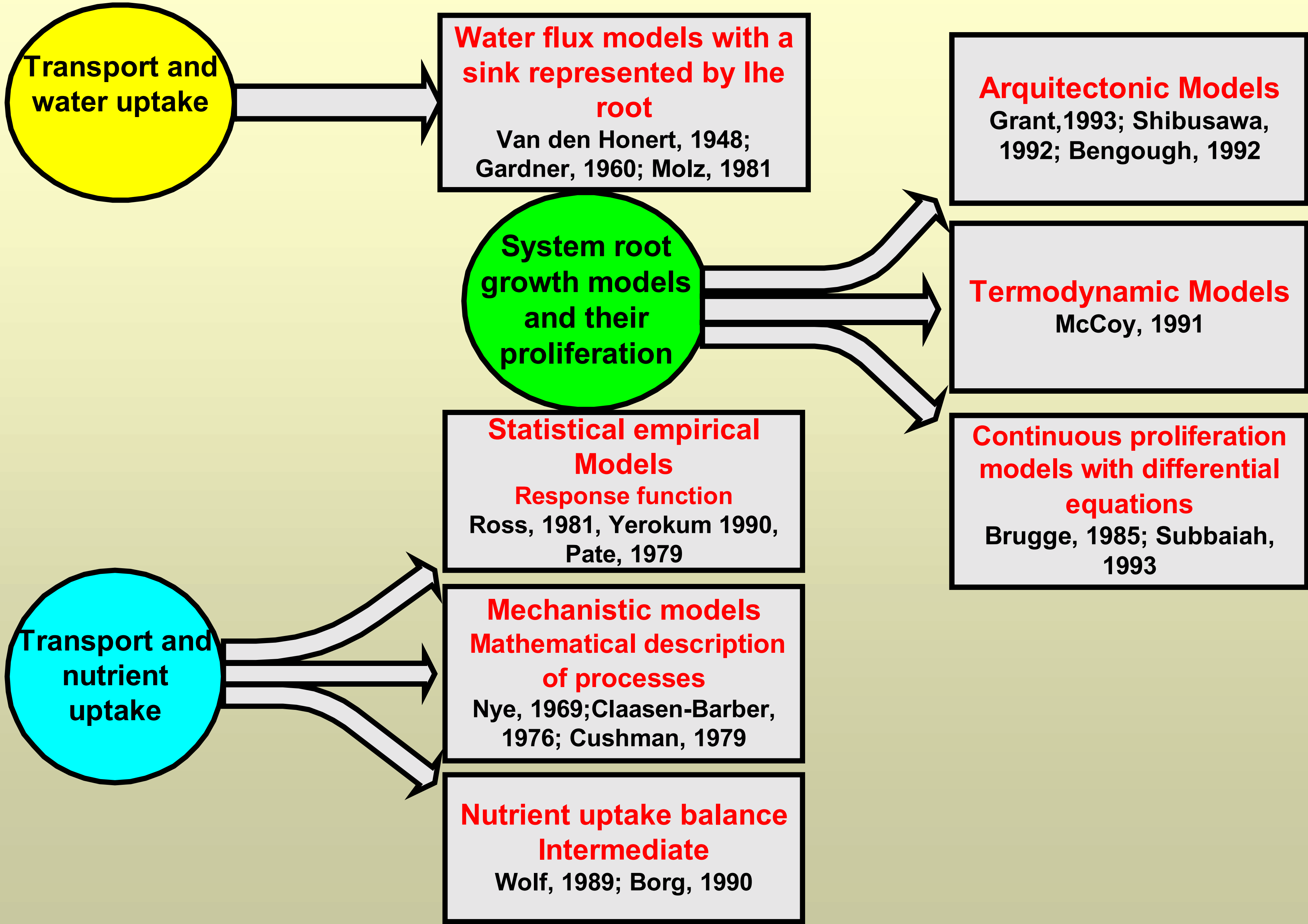
UPTAKE OF WATER AND IONS IS DEPENDENT ON ROOT LENGTH (SURFACE AREA DENSITY) AND AS IT INCREASES, THE ABSORPTION OF WATER AND IONS INCREASES TOO

Models related to root growth

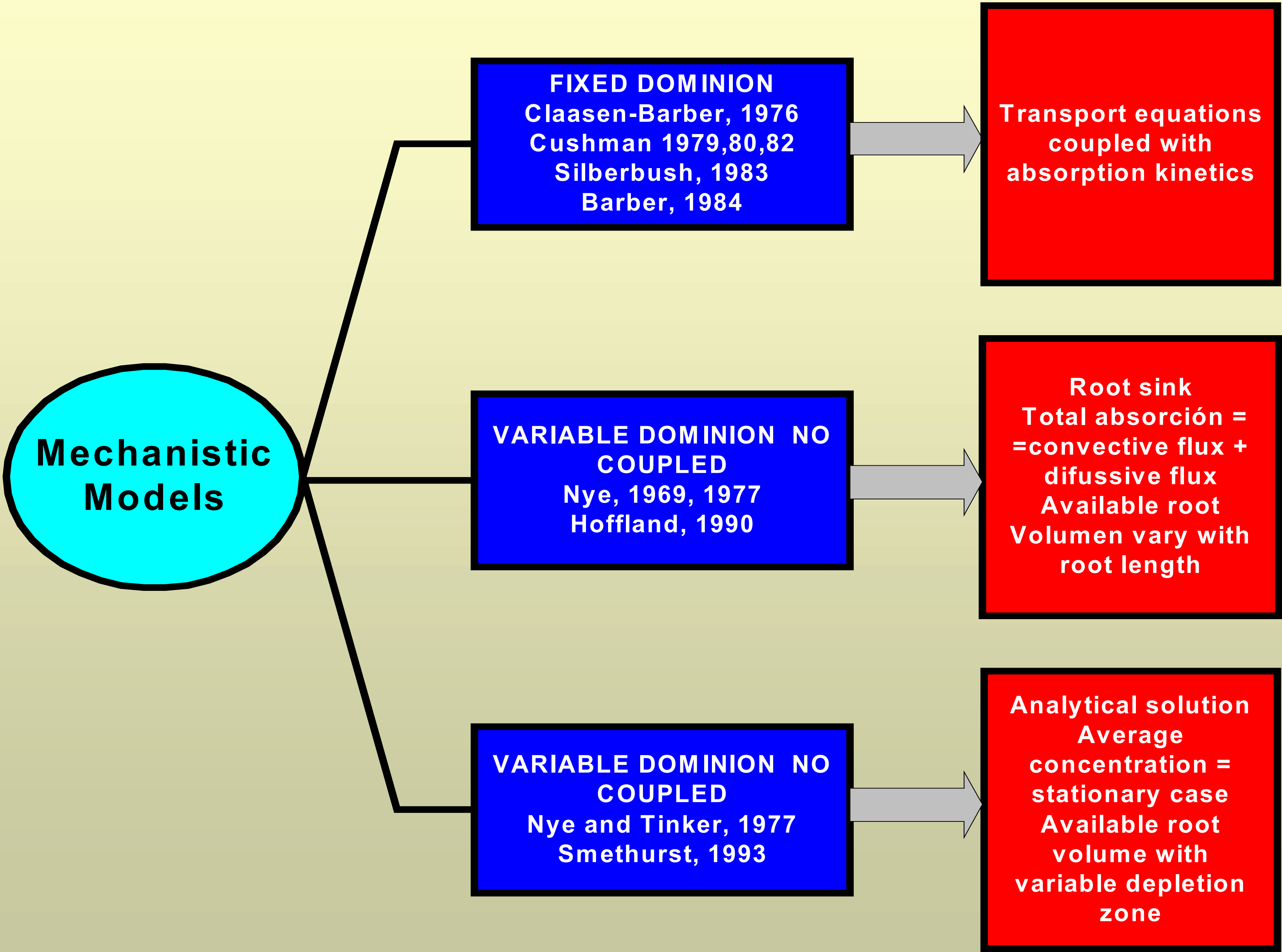
The crop functioning optimization is obtained through models simulation which predict the system behavior or subsystem during the growth period



Root growth, water and nutrient uptake models

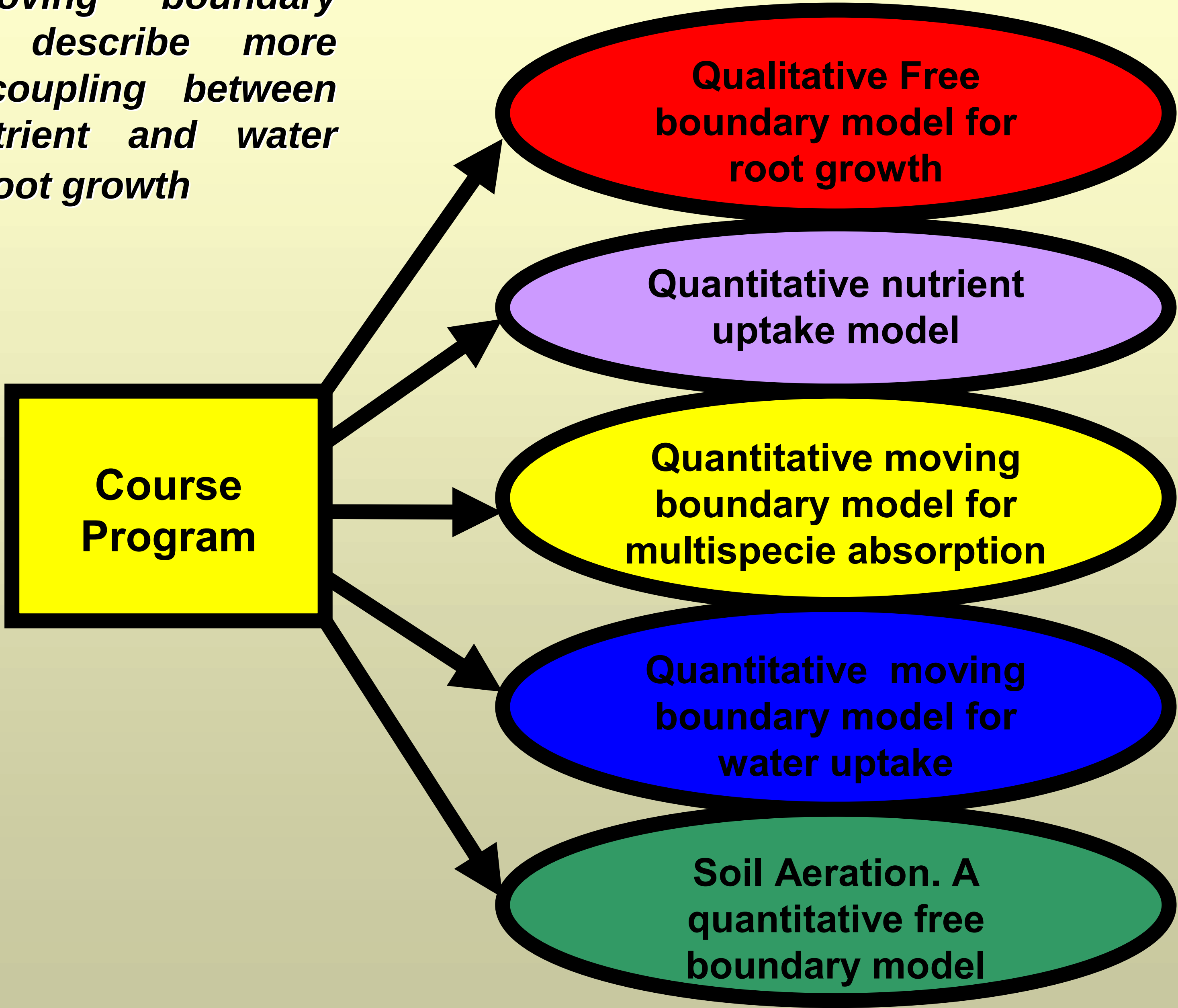


Transport and absorption of nutrient. Mechanistic models



Free and moving boundary models

Free and moving boundary problems can describe more precisely the coupling between transport, nutrient and water absorption and root growth



What Are The Free Boundary Problems?

Although you perhaps no imagine it, you live surrounded by phenomena that involve problems of "free boundary”, which go from:

the small things of daily life as:

the way in which a cube of ice goes changing form and size in a water glass, or the way in which a jet of milk is spread in a cup of coffee

to varied and important industrial processes like

Steel continuous casting, freezing and defrosting of food, solidification of plastics, solidification of pavements, etcetera.

as well as medical applications

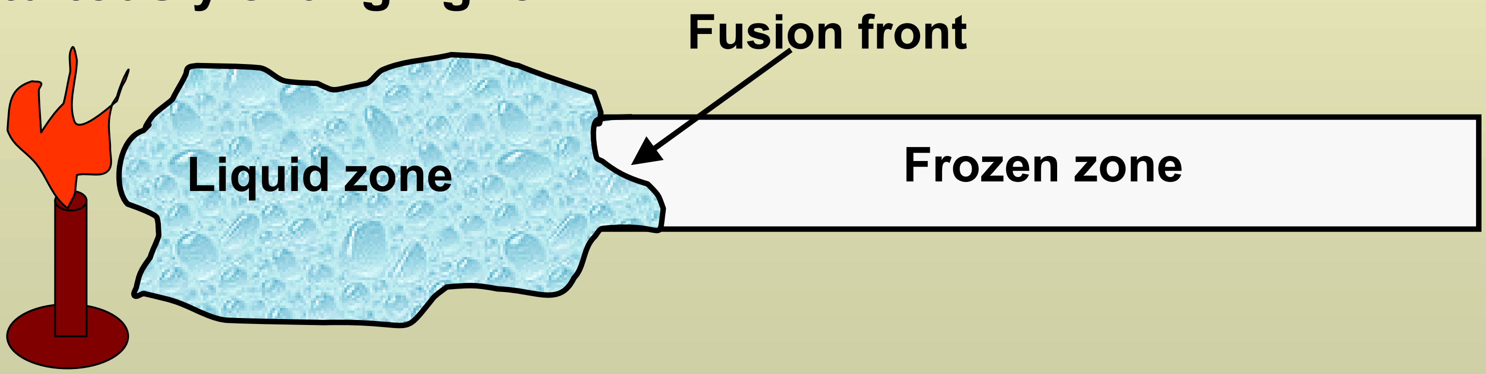
diffusion-consumption of oxygen in live tissues, for the treatment of tumors by means of radiations.

To agronomical applications

Root growth

But, what are the problems of free boundary, and why do we call them so?

Nothing better that analyzing an example. If an ice bar contained in a receptacle is heated in one of its ends, it will begin to melt from an end and it will go advancing a "front of fusion”. In every moment later it will be a zone still frozen (the more distant of the heat source), other in liquid state, and a surface of contact between both regions, (or which is the same a boundary that separates them). With time the liquid phase will occupy a bigger space each time, for which such boundary will move and fortuitously changing form.



The free boundary name comes of, in each moment; the location and form of this boundary are unknown.

But, what are the problems of free boundary, and why we call them so?

The physical-mathematical problem consists in predicting which will the position of that boundary be at every moment, and which will the temperature in each point of the bar be.

This problem (denominated *Stefan problem*) constitutes only one of the types of free boundary problems, and it appears in industries such as:

Steel (steel continuous casting),

Refrigerator (freezing or defrosting of foods),

Metallurgical (solidification of binary alloys, metals welding),

Plastic (solidification of diverse products)

Nuclear technology (prevention of accidents due to fusion of radioactive material)

Civil engineering (solidification of moist soils)

Solar energy (architecture), etcetera.

Other classes of "free boundary"

that don't correspond to a front of change of state, are those which appears, for example, in problems of:

Chemical engineering:

diffusion-gasoline reaction-solid, processes of oxidation, poisoning of catalysts.

Hydraulics:

case of the porous dike.

Ecology:

propagation of fires, propagation of stains of petroleum in water, growth of species, storm fronts, melting of glaciers

Electronic:

semiconductors.

Agronomy:

root growth of crops, nutrient and water uptake, anaerobiosis

Introduction to the Stefan problem and its applications

In 1831, Lamé and Clapeyron studied the problem of the solidification for cooling of a liquid globe (earth) in the following way. The earth is supossed to be a sphere that verifies the following hypothesis:

1) originally it was liquid and composed of a single substance, which it found to the temperature of fusion

2) it cools in the space and it solidifies from the exterior surface inwards, which rapidly takes a media temperature constant, $\theta_o < \theta_f$

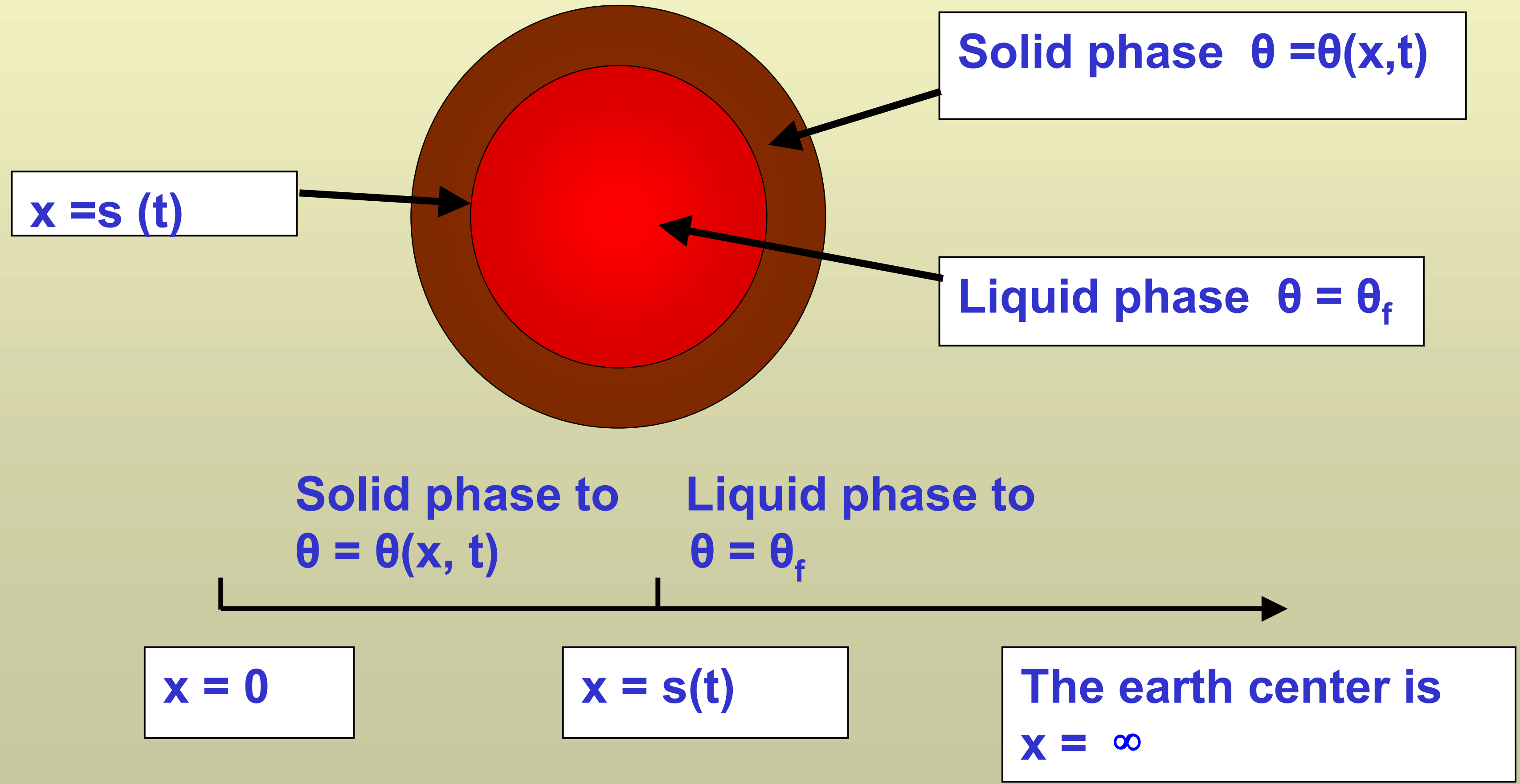
3) the solid cortex already formed in our days has not a considerable thickness compared to the terrestrial radius, and then it is obtained that:

a) the thickness of the solid part that covers our earth increases proportionally to $\sqrt{t}$, where t is the time since the beginning of solidification

b) the knowledge of the age of the solid part of the earth depends on numerous coefficients that can be easily obtained from the experience. These coefficients depend only on the solid phase.

The Lame-Clayperon problem

Really, below the hypothesis given previously, Lamé and Clayperon solves the problem of the solidification of a material partly-infinite, represented by x > 0, that initially is in liquid phase to their temperature of fusion and that in the extreme x = 0 is cooled to a temperature θ_o lower to that of fusion.



The mathematical model of Lamé and Clayperon

From a mathematical viewpoint, the problem can be outlined in the following way: To find the function s = s(t) (free boundary that separates the solid phase from the liquid phase and that it is to constant temperature) defined by t > 0 with s(0) = 0, and the temperature so that it satisfies the following conditions:

$$\theta = \begin{cases} \theta = \theta(x,t) & \text{if} \quad 0 < x < s(t), \quad & t > 0 \\ \theta_f & \text{if} \quad s(t) \leq x, \quad & t > 0 \end{cases}$$

so that it satisfies the following conditions:

$$\begin{cases} \text{i) } \rho c \dfrac{\partial \theta}{\partial t} = k \dfrac{\partial^2 \theta}{\partial x^2}, \quad 0 < x < s(t), & t > 0 \\ \text{ii) } \theta(0,t) = \theta_o > \theta_f, & t > 0 \\ \text{iii) } \theta(s(t),t) = \theta_f, & t > 0 \\ \text{iv) } k \dfrac{\partial \theta(s(t),t)}{\partial x} = \rho \lambda \dfrac{ds(t)}{dt}, & t > 0 \\ \text{v) } s(0) = 0 & \end{cases}$$

Properties of free boundary problem

It must be remarked that the problem is named *to a phase* because, in our case, the liquid phase finds to constant temperature and equal to the temperature of the phase change

The Stefan problem *is not linear* in spite of the apparent linearity of the conditions i)-v). In effect, if (iii) it is derived respect to t, it is obtained that:

$$\frac{\partial\theta(s(t),t)}{\partial x}\frac{ds(t)}{dt}+\frac{\partial\theta(s(t),t)}{\partial t}=0, \qquad t>0$$

then, the Stefan condition (iv) is transformed to

$$k\left[\frac{\partial\theta(s(t),t)}{\partial x}\right]^2=-\rho l\frac{\partial\theta(s(t),t)}{\partial t}=-\frac{\lambda k}{c}\frac{\partial^2\theta(s(t),t)}{\partial x^2}$$

which indicates that the problem is not linear.

Types of boundary problems

The Stefan problem is a free boundary problem for the heat equation of the explicit type. In general, the problems that are outlined for the heat equation or diffusion are classified in the following way

$$\text{boundary problems}\begin{cases}\text{fixed}\\[2em] \text{moving}\\[2em] \text{free}\begin{cases}\text{explicit type}\\ \text{implicit type}\end{cases}\end{cases}$$

The *fixed boundary problem* for the heat equation (diffusion) are those that are studied in the dominion (x_1,x_2) x (0,t).

The *moving boundary problems* for the heat equation (diffusion) are those that are studied in the dominion $(s_1(t), s_2(t))$ x (0,T) with $s_1(t) < s_2(t)$ functions given in (0,t), that is to say, that the space dominion of the unknown functions is variable with time by means of a law of movement known a priori

Free boundary problems explicit and implicit

The *free boundary problems* for the heat equation are those for which the space dominion of the unknown functions to compute is variable as a function of time through a movement law unknown a priori (Lamé and Clayperon)

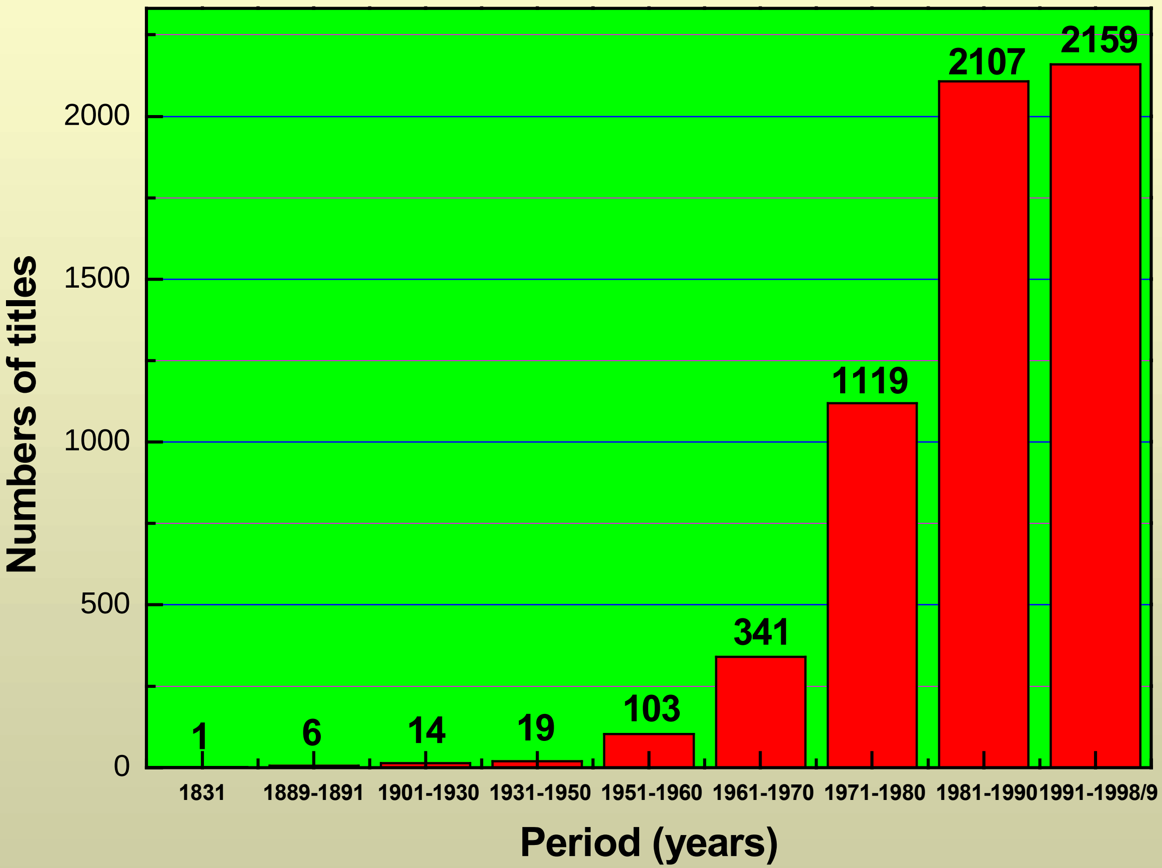
The *free boundary problems* are *explicit* or *implicit* if the free boundary velocity appears explicitly in the conditions that are imposes on that boundary, e.i, if s = s(t) appears explicitly in the condition iv). Instead, if this velocity is not present, the free boundary is implicit (difussion-consumption of oxigen in alives tissues, anaerobiosis)

Bibliography on free and moving boundary

Bibliography (Database) on moving and free boundary problems for the heat-diffusion equation, particularly regarding the Stefan and related problems contains 5869 titles referring to:

588 scientific Journals,
122 books,
88 symposia
30 collections,
59 thesis and
247 technical reports.

It tries to give a comprehensive account of the western existing mathematical-physical-engineering literature on this research field.



The free boundary for root growth

Many methods exist for studying the mechanism involved in nutrient uptake. These methods model 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

In the past, various 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;

The Root Growth Model. Model assumptions

- The soil is homogeneous and isotropic,
- Moisture conditions are maintained constant
- Nutrient uptake occurs at root surface
- The roots are smooth cylinders,
- Uptake is described by the Michaelis-Menten equation,
- The nutrient transport occurs via convection and diffusion in the radial direction only
- Parameters (Jm) and (Km) are independent from the velocity of soil water at the root (vo)
- The diffusion coefficient (D) is independent of flux,
- D and the buffer power b are independent of concentration,
- The root system parameters are not changed by root age (k = Jm/Km = 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 from temperature,
- The net uptake of nutrient is totally available for growth,
- Root hairs do not affect nutrient uptake.

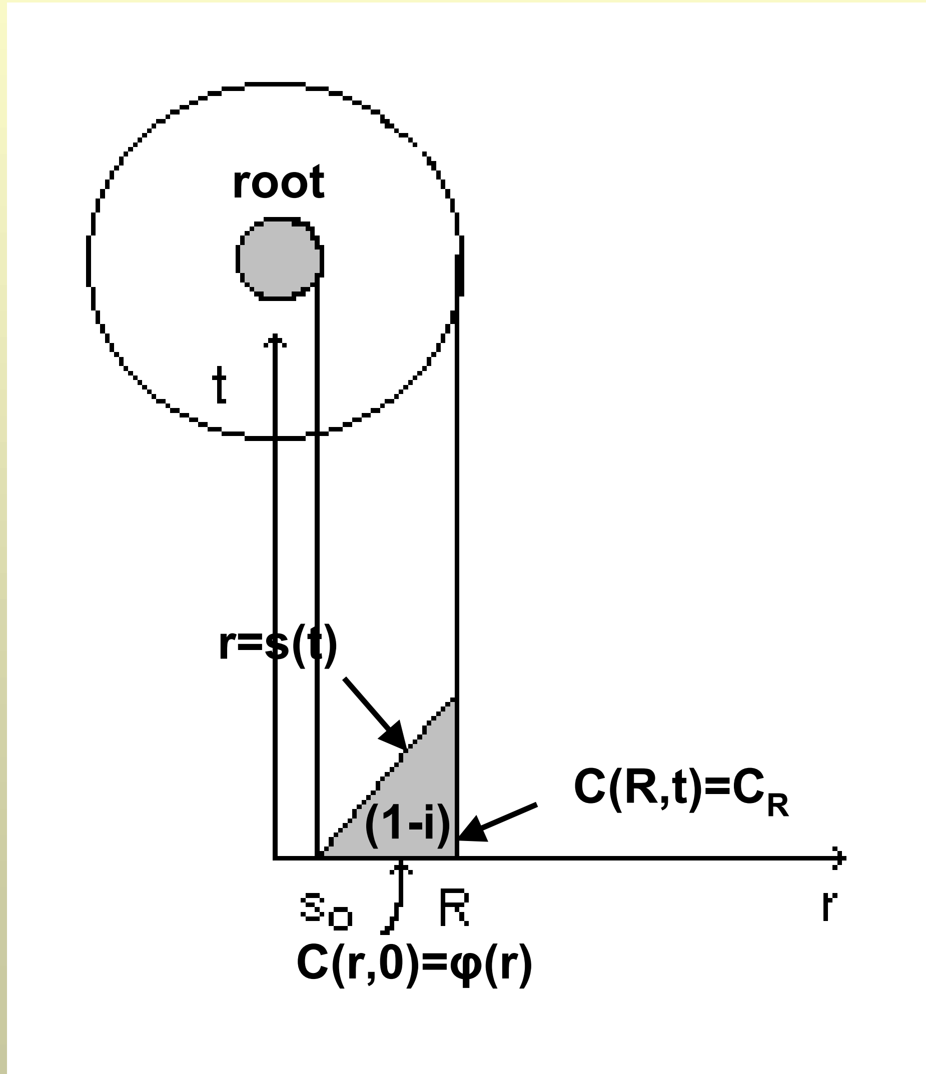
Root growth model

With the above assumptions, the root growth model is given (in cylindrical coordinates) by:

$$
1)\quad \begin{cases}
\text{i)}\ \ D\dfrac{\partial^2 C}{\partial r^2} + \dfrac{D(1+\varepsilon)}{r}\dfrac{\partial C}{\partial r} = \dfrac{\partial C}{\partial t}, & s(t) < r < R, \qquad 0 < t < T \\
\text{ii)}\ \ C(r,0) = \varphi(r), & s_o \le r \le R \\
\text{iii)}\ \ C(R,t) = C_R, & 0 < t < T \\
\text{v)}\ \ Db\dfrac{\partial C(s(t),t)}{\partial r} + v_o C(s(t),t) = \dfrac{k_a C(s(t),t)}{1+\dfrac{k_a C(s(t),t)}{J_m}} - E = & \\
\text{vi)}\ \ \dfrac{k_a C(s(t),t)}{1+\dfrac{k_a C(s(t),t)}{J_m}} - E = aC(s(t),t)\dfrac{ds(t)}{dt}, & 0 < t < T \\
\text{vi)}\ \ s(0) = s_o, & 0 < s_o < R
\end{cases}
$$

A schematic diagram for root growth model

A schematic diagram of free boundary problem is given in the following outline:



Analytical solution. The quasistationary method

In this method it is assumed that the soil concentration is that corresponding to stationary case in the interval (s(t),R). Then the problem is reduced to solve the equation:

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

With the conditions (ii, iii, iv and v).The solution of the problem by low

concentrations $\left(k_a C(s(t),t)/\left(1+k_a C(s(t),t)/J_m\right) \cong k_a C(s(t),t)\right)$ is given by:

$$\boxed{C(r,t) = \beta(t) - \frac{\alpha(t)}{r^{\varepsilon}}, \qquad s(t) < r < R, \qquad t > 0}$$

Where:

$$\alpha(t) = \left[\frac{1}{Db}\right]\frac{\left[(k-v_o)C_R - E\right]}{\dfrac{\varepsilon}{s(t)^{\varepsilon+1}} + \dfrac{(k-v_o)}{Db}\left[\dfrac{1}{\dot{s}(t)^{\varepsilon}} - \dfrac{1}{R^{\varepsilon}}\right]}, \quad \beta(t) = C_R + \frac{\alpha(t)}{R^{\varepsilon}},$$

$$\varphi(r) = C_R - \frac{\left[(k-v_o)C_R - E\right]}{\dfrac{v_o}{s_o^{\ \varepsilon}} + (k-v_o)\left[\dfrac{1}{s^{\varepsilon}(t)} - \dfrac{1}{R^{\varepsilon}}\right]}\left[\frac{1}{r^{\varepsilon}(t)} - \frac{1}{R^{\varepsilon}}\right]$$

The quasistationary method

And s(t) is the only solution of the following Cauchy problem:

$$\boxed{\begin{array}{ll} \dfrac{ds(t)}{dt} = F(s(t)), & t > 0 \\ s(0) = s_o \in (0,R) & \end{array}}$$

With:

$$F(s) = \frac{k}{a}\left[1 - \alpha_3 (H(s)\right], \quad H(s) = \frac{\left[1 + \alpha_2 G(s)\right]}{\left[1 + \alpha_1 G(s)\right]}, \quad G(s) = s\left[1 - \left(\frac{s}{R}\right)^{\varepsilon}\right]$$

$$\alpha_1 = \frac{E}{v_o s_o C_R}, \quad \alpha_2 = \frac{(k - v_o)}{v_o s_o}, \quad \alpha_3 = \frac{E}{k C_R} = \frac{C_u}{C_m} > 0$$

$$\boxed{C(s(t), t) = \frac{C_R}{H(s(t))} \quad (= C(s(t))), \quad t > 0}$$

The quasistationary method

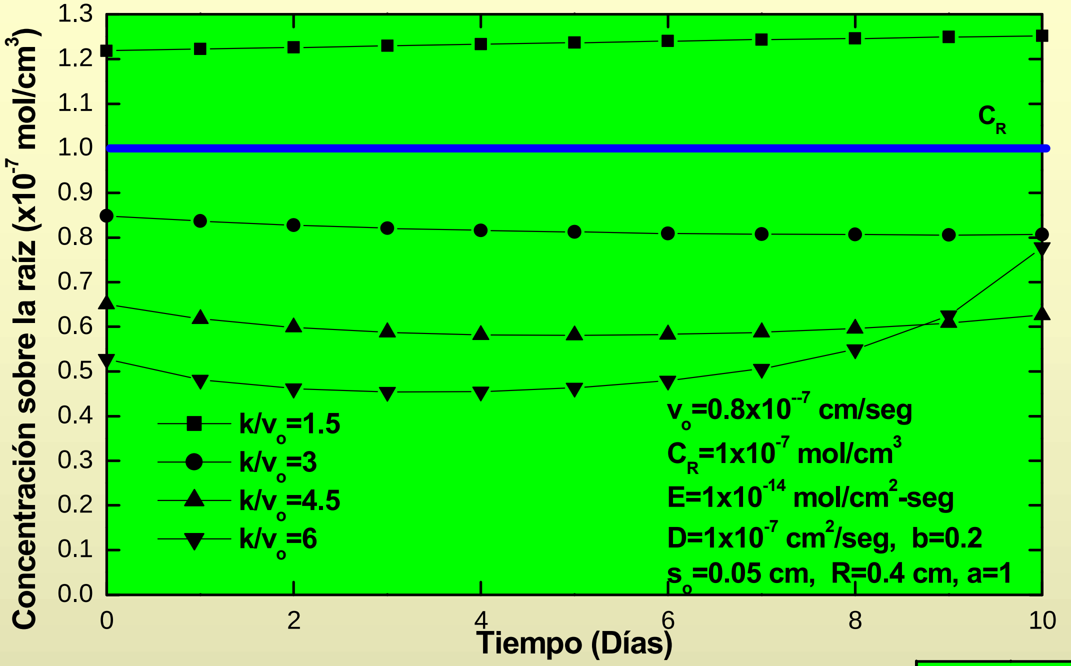
Let γ be the parameter defined by: $\gamma = \dfrac{E}{(k - v_o)C_R} = \dfrac{\alpha_1}{\alpha_2}$. It can prove that if

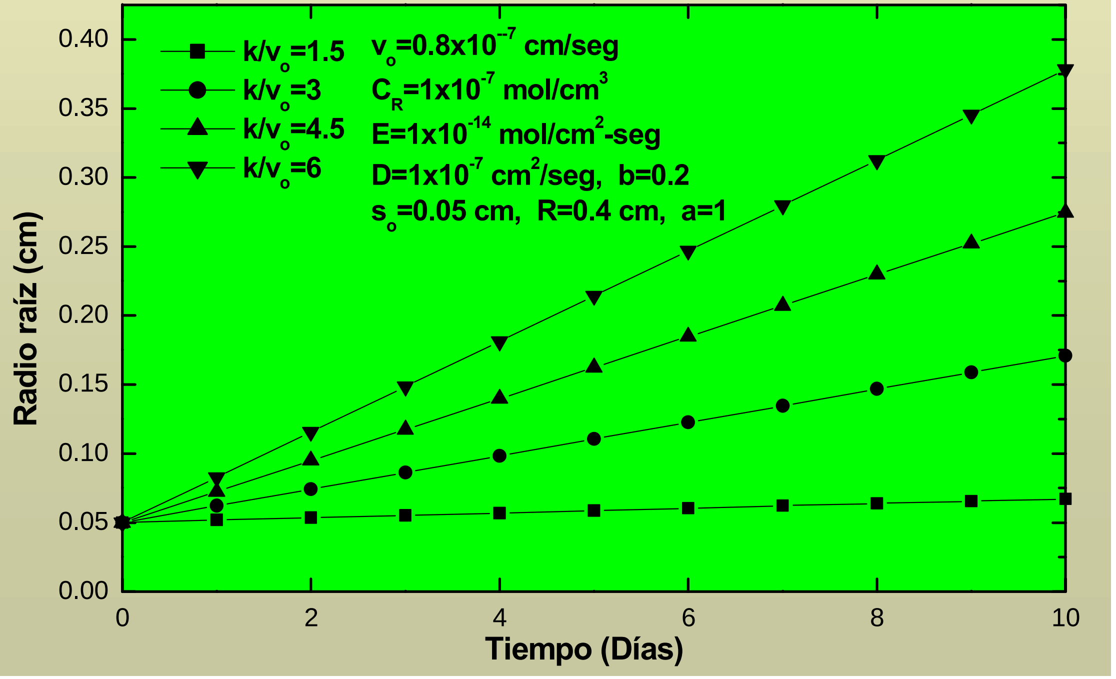
$$\gamma \text{ is } \begin{cases} <1 \quad \Rightarrow \quad C(s(t)) < C_R \quad \text{then absorption power } k \quad v_o \text{ and there is no counterdiffusion} \\ =1 \quad \Rightarrow \quad C(s(t)) \text{ remains constant} \\ >1 \quad \Rightarrow \quad C(s(t)) > C_R \text{ because k is small and root can not absorbs all the nutrient and there is counterdiffusion} \end{cases}$$

and

$$\boxed{\frac{1}{\alpha_3} \geq \frac{1+\alpha_2 R}{1+\alpha_1 R} \Rightarrow \dot{s}(t) > 0}$$

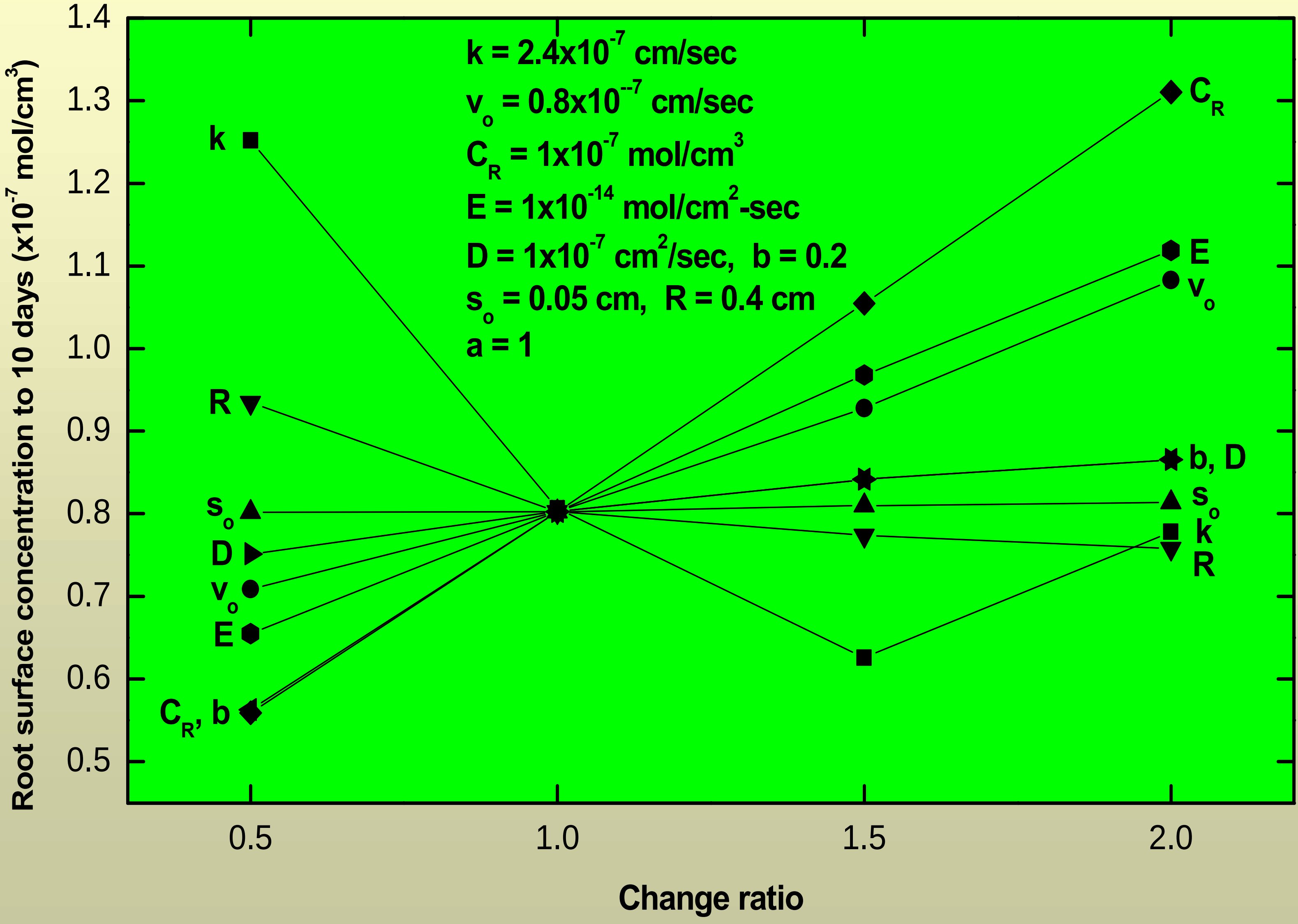
Quasi-stationary method solution



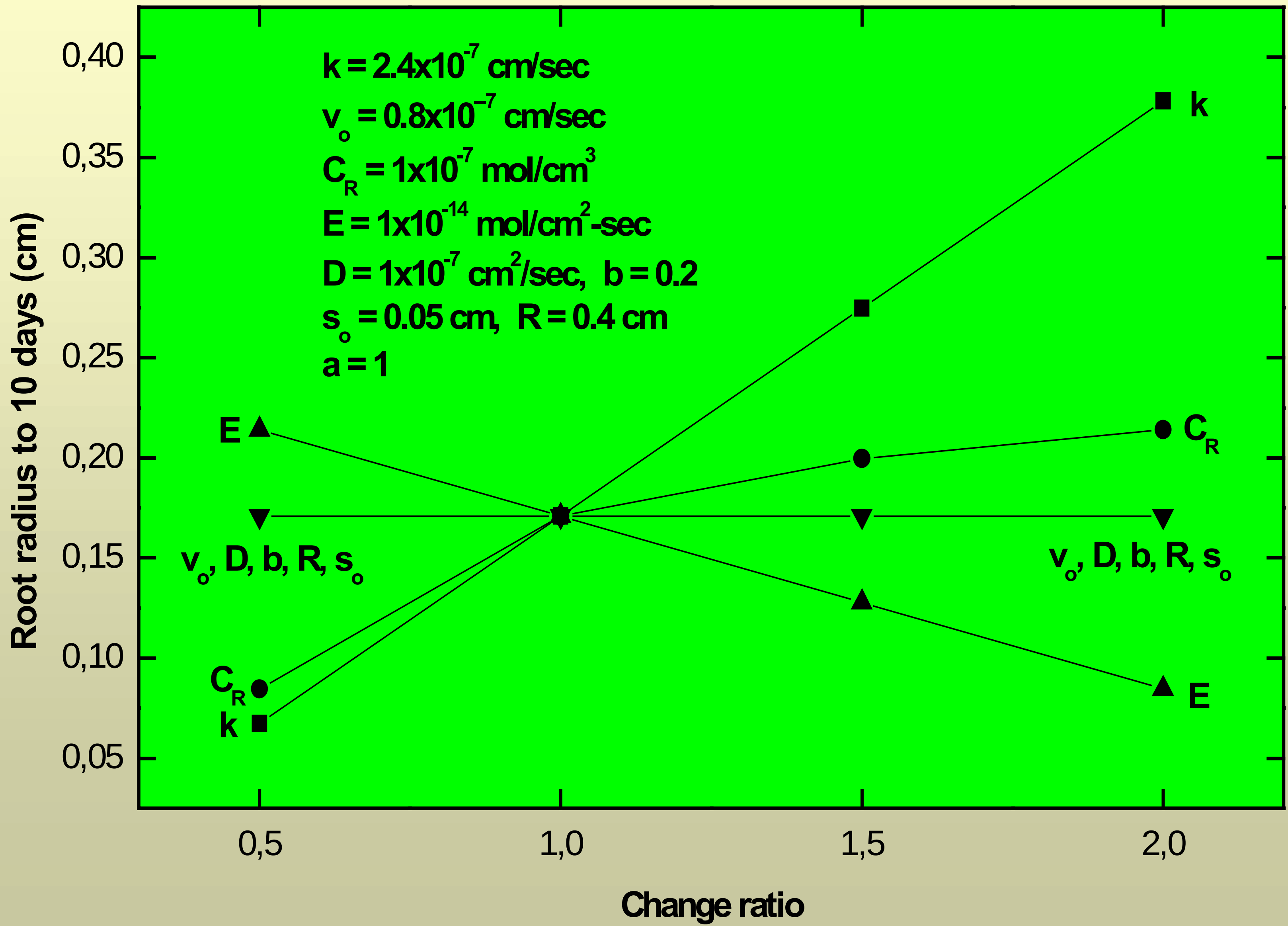


The quasistationary method

Effect of system parameters



The quasistationary method



Approximated solution. The integral balance method

To solve the problem (1- i, ii,iii,iv, and vi), i.e., C = C(r,t) (specially C=C(s(t),t) and the free boundary r = s(t)) we integrate the differential equation (1-i) in r on the dominion (s(t),r):

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

And it is proposed that: $\boxed{C(r,t) = \varphi(r)\left[1+\beta(t)(R-r)\right]}$

That verifies

$$C(r,0) = \varphi(r) \Leftrightarrow \beta(0) = 0$$

$$C(R,t) = C_R \Leftrightarrow \varphi(R) = C_R$$

Replacing C(r,t)

in $\int_{s(t)}^{R} C(r,t)dr$

we obtain:

$$2)\ \begin{cases} \int_{s(t)}^{R} C_t(r,t)dr = D\left[C_r(R,t) - g(\alpha(t))\right] + \\ \qquad + D(1+\varepsilon)\left[\dfrac{C_R}{R} - \dfrac{\alpha(t)}{s(t)} + \int_{s(t)}^{R} \dfrac{C(r,t)}{r^2}dr\right],\quad t>0 \\ \dot{s}(t) = f(s(t)),\quad t>0,\quad s(0)=0 \end{cases}$$

The balance integral method solution

Replacing $\varphi(r) = C_R + A\left[1 - \left(\frac{R}{r}\right)^{\varepsilon}\right]$ **in 2) we obtain the following ordinary differential equations system:**

$$\begin{cases} \dfrac{d\beta(t)}{dt} = F_1(F_2 + F_3 + F_4 + F_5 + F_6 + F_7), & \beta(0) = 0 \\ \dfrac{ds(t)}{dt} = \dfrac{1}{a}\left[k - \dfrac{E}{\varphi(s(t)\left[1 + \beta(t)\left(r - s(t)\right)\right]}\right], & s(0) = s_o \end{cases}$$

The balance integral method solution

Where:

$$A=\frac{E-(k-v_o)C_R}{k\left[1-\left(\frac{R}{s_o}\right)^{\varepsilon}\right]-v_o},$$

$$A_1=\left\{\left(C_R+A\right)\left[R-s(t)\right]+\frac{AR^{\varepsilon}s^{(1-\varepsilon)}(t)-AR}{(1-\varepsilon)}\right\}$$

$$A_2=\left\{\frac{C_R+A}{2}\left(R^2-s^2(t)\right)+\frac{AR^{\varepsilon}s^{(2-\varepsilon)}(t)-AR^2}{(2-\varepsilon)}\right\}$$

$$F_1=\frac{D}{RA_1-A_2},$$

$$F_2=\frac{A\varepsilon}{R}-C_R\beta(t)-\frac{1}{Db}\left[\varphi(s(t)\left[1+\beta(t)(R-s(t))\right](k-v_o)-E\right],$$

$$F_3=(1+\varepsilon)\frac{C_R}{R}-(1+\varepsilon)\frac{\varphi(s(t)\left[1+\beta(t)(R-s(t))\right]}{s(t)},$$

$$F_4=(1+\varepsilon)\left(C_R+A\right)(1+\beta(t)R)\left[\frac{1}{s(t)}-\frac{1}{R}\right],$$

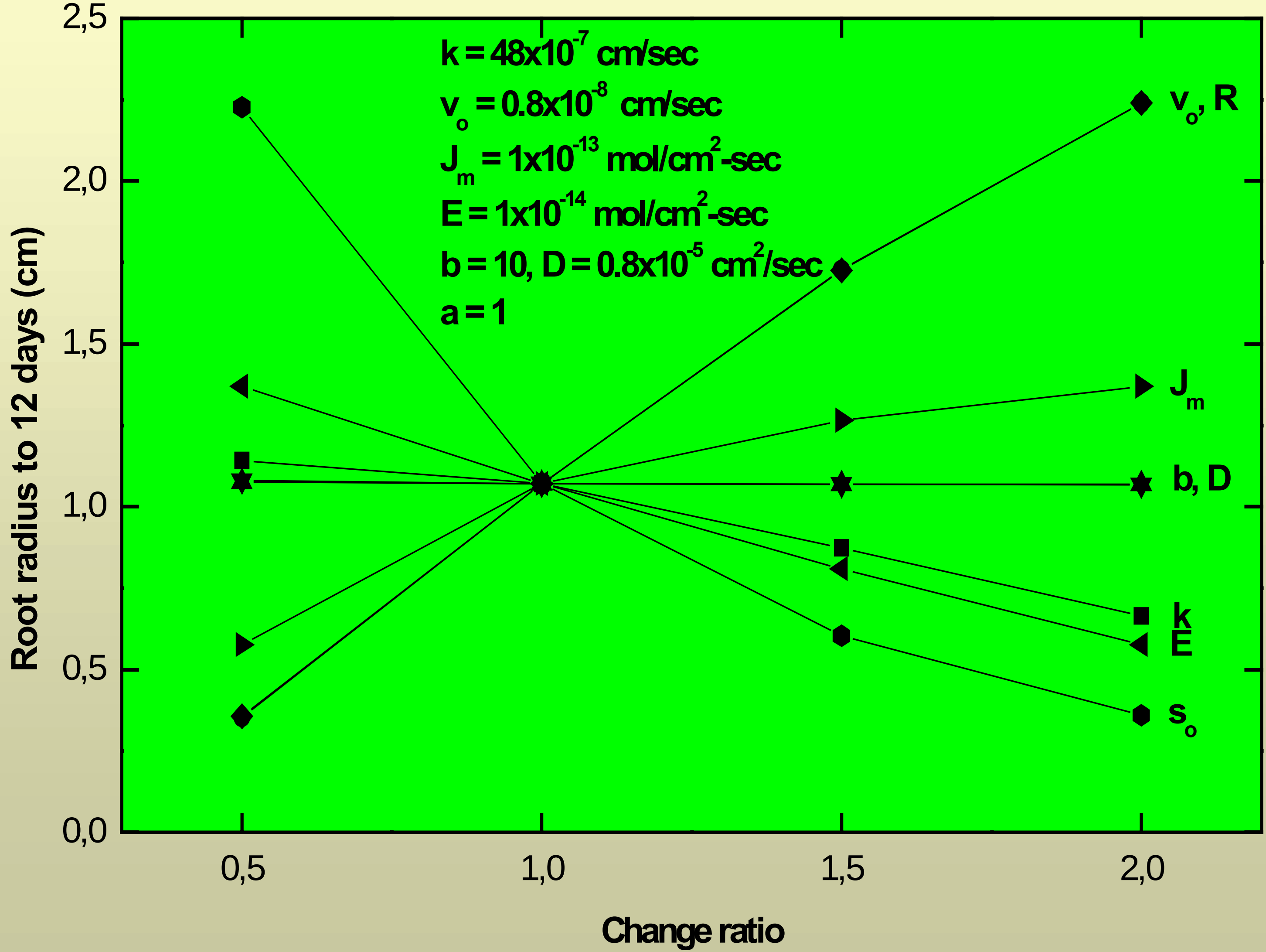
$$F_5=-(1+\varepsilon)\beta(t)\left(C_R+A\right)\ln\left(\frac{R}{s(t)}\right),$$

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

$$F_7=-AR^{\varepsilon}\left[1+\beta(t)R\right]\left[\frac{1}{s^{\varepsilon+1}(t)}-\frac{1}{R^{\varepsilon+1}}\right].$$

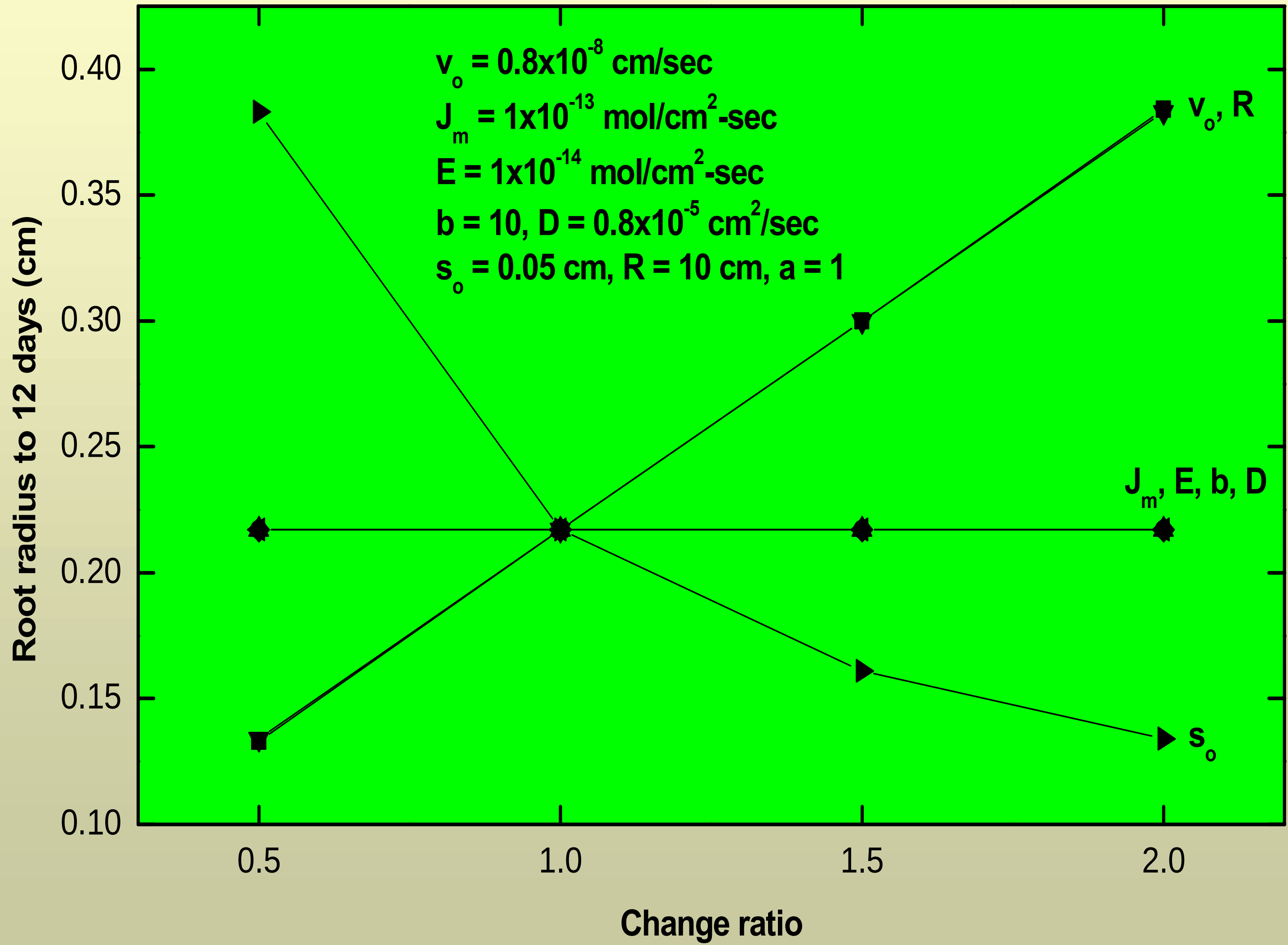
The balance integral method solution

Low concentrations



The balance integral method solution

High concentrations



Root Growth models conclusions

From the comparison of the theoretical results of the model for the effects on the growth in low and high concentrations we conclude that: ***absorption kinetic in low concentrations is more efficient than the same mechanism for high concentrations.***

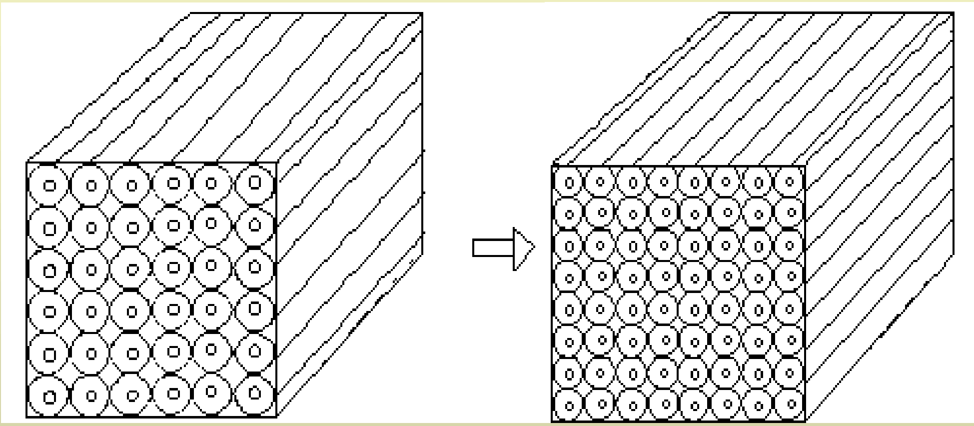
From the comparison of the diagrams of parametric sensibility for immobile ions in low concentrations obtained by means of the quasi-stationary method and the integral balance we conclude that the qualitative behavior is the same and we obtain numeric similar values and of the same order of magnitude ***although the integral balance method offers us more detail of the effect of the parameters which we cannot appreciate in the case of the quasi-stationary.***

From the comparison of the sensibility diagram that results from the integral balance method we can see the effect of the initial radius on the growth, result that was not obtained by the quasi-stationary method, ***thus showing the great sensibility of the integral balance method.***

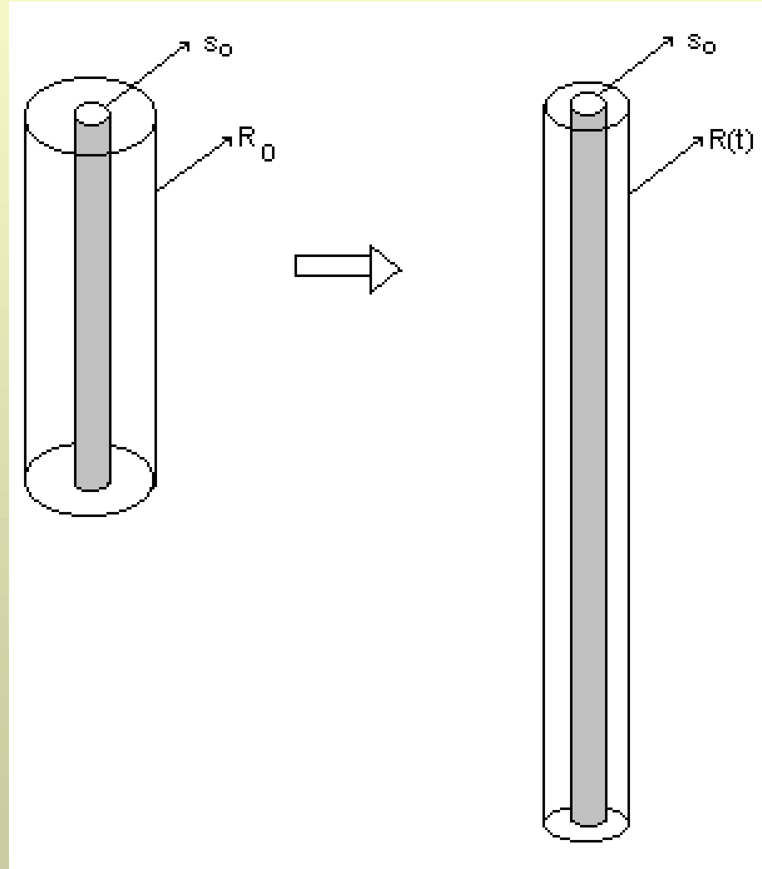
The nutrient uptake model

For ***ROOT GROWTH***, we compute C = C(s(t),t) and r = s(t) unknown a priori as solution of a ***free boundary model***.

Now, for ***NUTRIENT UPTAKE***, we will compute $C = C(s_o,t)$ as solution of a ***moving boundary model***, where r = R(t) is known a priori. The situation is:



t = 0 t = t



t = 0 t = t

The mathematical model

We propose the following moving boundary model, we resembles the free boundary model:

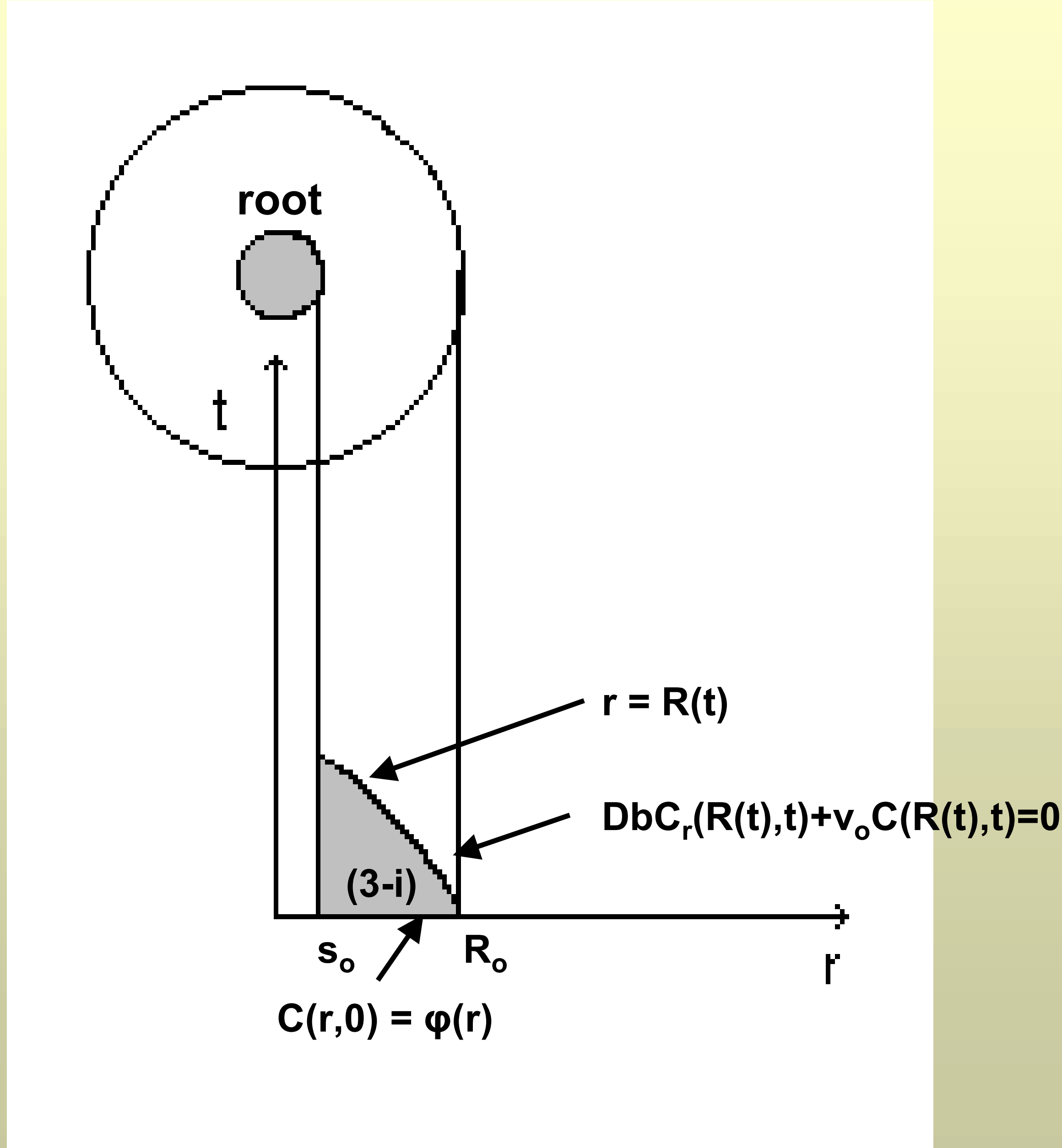
$$
3)\ \begin{cases}
\text{i)}\ D\dfrac{\partial^2 C}{\partial r^2}+\dfrac{D}{r}\left(1+\dfrac{v_o s_o}{Db}\right)\dfrac{\partial C}{\partial r}=\dfrac{\partial C}{\partial t}, & s_o<r<R(t),\quad 0<t<T\\
\text{ii)}\ C(r,0)=\varphi(r), & s_o\le r\le R_o\\
\text{iii)}\ Db\dfrac{\partial C(R(t),t)}{\partial r}+v_o C(R(t),t)=0, & 0<t<T\\
\text{iv)}\ Db\dfrac{\partial C(s_o,t)}{\partial r}+v_o C(s_o,t)=\dfrac{k_a\left[C(s_o,t)-C_u\right]}{1+\dfrac{k_a\left[C(s_o,t)-C_u\right]}{J_m}} & \\
\text{v)}\ R(t)=R_o\sqrt{\dfrac{I_o}{I(t)}}, & 0<t<T\\
\text{with:}\quad I(t)=\begin{cases} I_o(1+kt)\ \ [\text{linear growth}]\\ \text{or}\\ I_o e^{kt}\qquad [\text{exponential growth}]\end{cases}
\end{cases}
$$

The last condition for R(t) is obtained assuming that:

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

$$\pi I(t)\left[R^2(t)-s_o^2\right]=\pi I_o\left[R_o^2-s_o^2\right]-\pi s_o^2\left[I(t)-I_o\right]$$

A schematic diagram



The nutrient uptake model solution

The solution is obtained by applying the integral balance method. Thus, (3-i) is integrated in variable r on the domain (s_o,R(t)) and it is proposed that:

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

With:

$$\varphi(r) = C_R e^{-\varepsilon(R_o - r)}, \qquad \varepsilon = \frac{v_o}{Db} = \frac{\varepsilon_o}{s_o}$$

After elementary manipulations, we obtain:

$$\begin{cases} \dfrac{d\beta(t)}{dt} = \dfrac{F_2(R(t),\beta(t))}{F_1(R(t))}, \\ R(t) = R_o\sqrt{\dfrac{I_o}{I(t)}} \end{cases} \qquad \beta(0) = 0$$

The functions F_i

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

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

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

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

The functions F_i are given by:

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

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

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

$$G_5 = \left[D(1+\varepsilon_o)\ \left(\varepsilon + \varepsilon\beta(t) - \frac{2\beta(t)}{R(t)}\right)\right]\ C_R e^{-\varepsilon R_o}.$$
$$\cdot \left[\ln\frac{R(t)}{s_o} + \varepsilon[R(t) - s_o] + \frac{\varepsilon^2}{4}[R^2(t) - s_o^2] + \frac{\varepsilon^3}{18}[R^3(t) - s_o^3] + \frac{\varepsilon^4}{96}[R^4(t) - s_o^4] + \right.$$
$$+ \frac{\varepsilon^5}{600}[R^5(t) - s_o^5] + \frac{\varepsilon^6}{4320}[R^6(t) - s_o^6] + \frac{\varepsilon^7}{35280}[R^7(t) - s_o^7] +$$
$$\left. + \frac{\varepsilon^8}{322560}[R^8(t) - s_o^8] + \frac{\varepsilon^9}{3265920}[R^9(t) - s_o^9] \right]$$

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

Computing the nutrient uptake

Once the concentration on the root surface $C(s_o,t)$ has been obtained we must compute the nutrient uptake by a system whose dominion is variable (By adding the resultant fluxes for every moment of time on the variable superficial area of the root)

Total nutrient uptake can be obtained from the following formula

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

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

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

Computing the nutrient uptake

First increment: $$\Delta U_o = 2\pi s_o l_o J_o \Delta t$$

Second increment: $$\Delta U_1 = 2\pi s_o l_o J_1 \Delta t + 2\pi s_o \Delta l_1 J_1 \Delta t$$

$$\Delta U_2 = 2\pi s_o l_o J_2 \Delta t + 2\pi s_o \Delta l_1 J_2 \Delta t + 2\pi s_o \Delta l_2 J_2 \Delta t$$

$$\Delta U_n = 2\pi s_o l_o J_n \Delta t + 2\pi s_o \Delta l_1 J_n \Delta t + 2\pi s_o \Delta l_2 J_n \Delta t + .. + 2\pi s_o \Delta l_n J_n \Delta t$$

$$\Delta U = \sum_{i=1}^{n} \Delta U_i = 2\pi s_o \left[\sum_{i=1}^{n} l_o J_i \Delta t + \sum_{i=1}^{n} \Delta l_1 J_i \Delta t + \sum_{i=2}^{n} \Delta l_2 J_i \Delta t + .. + \sum_{i=n}^{n} \Delta l_n J_i \Delta t \right]$$

And, taking the limit when $\Delta t \rightarrow 0$, we deduce:

$$\Delta U = 2\pi s_o l_o \int_0^{t_{max}} J(s)dt + 2\pi s_o \int_{l_o}^{l(t_{max})} \left[\int_t^{t_{max}} J(s)ds \right] dl(t) =$$

$$= 2\pi s_o l_o \int_0^{t_{max}} J(s)dt + 2\pi s_o \int_0^{t_{max}} \left[\int_t^{t_{max}} J(s)ds \right] \dot{l}(t)dt$$

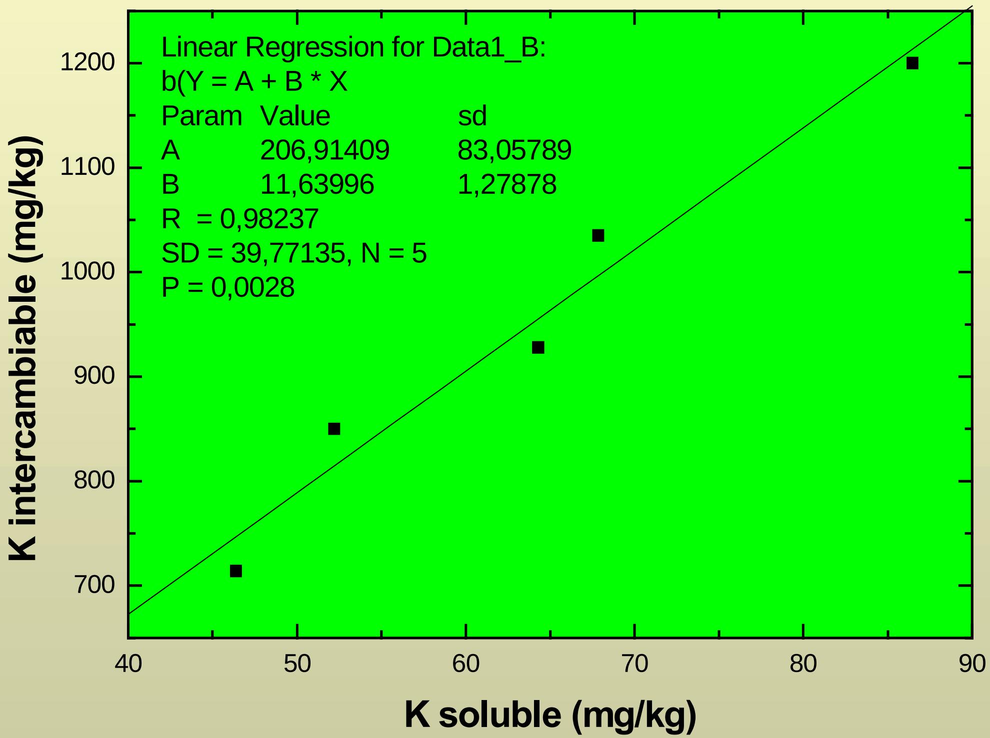
where the first term represents the uptake for the initial root volume of length l_o, the second term represents the uptake for the successive growing volume elements and $\dot{l}(t) = dl(t)/dt$ is the root growth rate at instant t.

Experimental method. Input data

Determination of soil parameters

Values of the initial concentration of nutrient in solution C_R were obtained analyzing aliquots of solution moved from columns of soil balanced to field capacitance for 24 hours (Adams, 1974, Hesse, 1971).

The buffer power b and the diffusion coefficient D was obtained by means of the of Kovar and Barber technique (1990). The following figure illustrates the obtained relation between the interchangeable nutrient (K) and the soluble nutrient (K)



The diffusion coefficient D was obtained after the buffer power had been computed by means of the following expression (Nye, 1966; Wietholter, 1983)):

$$D = \frac{D_w f\theta}{b}$$

Experimental method. Input data

where D_w is the nutrient diffusion coefficient of potassium in water (1.98x10-5 cm2/s, Parsons, 1958), (θ is the content of water (soil to field capacitance (θ =0.2) and f (dimensionless) is a factor of tortuousness or continuity (Porter, 1960). For soils varying from loamy To sandy and with 0.2<θ<0.4, f can numerically be considered equal to θ (Barraclough, 1981), hence the previous expression for the coefficient of diffusion results:

$$\boxed{D = \frac{D_w \theta^2}{b}}$$

The flux speed v_o was obtained dividing the total water taken for the plant W for a given time (which was obtained subtracting the water lost due to evaporation from the total water lost due to evapotranspiration in each pot) by the media root surface during that same time:

$$\boxed{v_o = \frac{W}{(t_2 - t_1)\bar{S}_{(t_2 - t_1)}} = \frac{W(\ln S_2 - \ln S_1)}{(S_2 - S_1)(t_2 - t_1)}}$$

where:

$$\bar{S} = \frac{1}{(t_2 - t_1)} \int_{t_1}^{t_2} S_o e^{kt} dt$$

Experimental method. Input data

Determination of root parameters

- The root growth rate k was obtained from the knowledge of the root length as a function of time by means of the expression (assuming an exponential or linear growth, condition generally valid for vegetative growth (Claassen, 1986)):

$$\boxed{k = \frac{\ln l(t) - \ln l(t_o)}{t - t_o}}$$ exponential growth

$$\boxed{k = \frac{l(t) - l(t_o)}{t - t_o}}$$ linear growth

- The root radius was obtained from the root length and the fresh mass root *m* by means of the expression (assuming a root density ρ=1):

$$\boxed{s_o = \sqrt{\frac{M}{\pi \rho l}}}$$

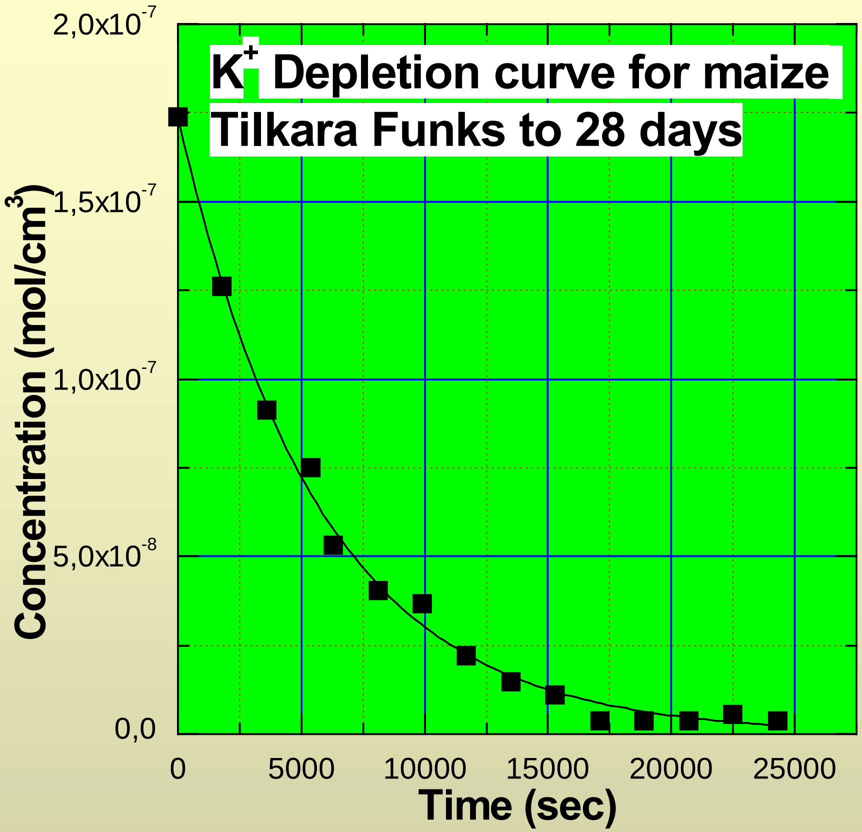
- The inter-root distance was obtained from the volume of soil V_s and root length l by means of the following expression (Barber, 1984):

$$\boxed{R = \sqrt{\frac{V_s}{\pi l}}}$$

Experimental method. Input data

Determination of kinetic parameters

- J_m, K_m, k_a and C_u were obtained through the analysis of K^+ depletion curves in nutritive solution from which the roots absorbed potassium (Claassen and Barber, 1974).



The parameters k_a, K_M, J_m, C_u and E were obtained from the values of the concentration at initial time C(0), the first derived ($\alpha = dC(0)/dt$), the second derived ($\beta = d^2C(0)/dt^2$) and the value of concentration at infinite ($\gamma = C(\infty)$) which can be obtained from the graphic C versus time. The expressions obtained for k_a, K_M , J_m, C_u and E are:

Experimental results. Determination input data

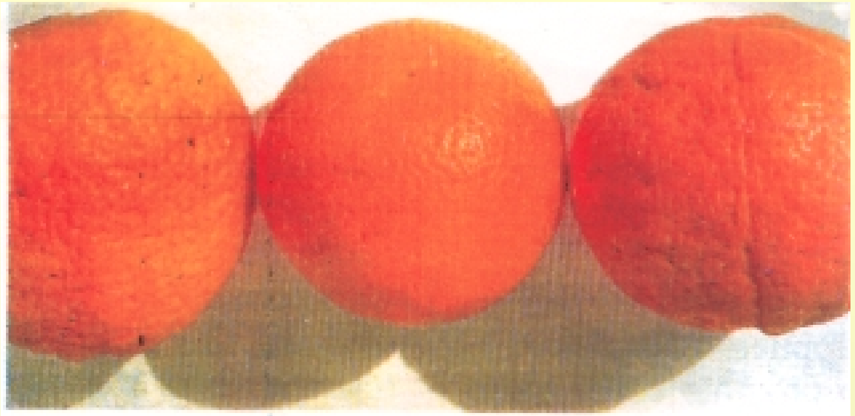
$$E=\frac{\alpha}{A\left[\frac{\beta C_o}{\alpha^2}\left(\frac{C_o}{\gamma}-1\right)-1\right]},\qquad J_m=\frac{\gamma\beta}{A\alpha}\frac{\left(\frac{C_o}{\gamma}-1\right)^2}{\left[\frac{\beta C_o}{\alpha^2}\left(\frac{C_o}{\gamma}-1\right)-1\right]\left[1-\frac{\beta\gamma}{\alpha^2}\left(\frac{C_o}{\gamma}-1\right)\right]}$$

$$K_M=\gamma\frac{\left[\frac{\beta C_o}{\alpha^2}\left(\frac{C_o}{\gamma}-1\right)-1\right]}{\left[1-\frac{\beta\gamma}{\alpha^2}\left(\frac{C_o}{\gamma}-1\right)\right]},\qquad k_a=\frac{\beta\left(\frac{C_o}{\gamma}-1\right)^2}{A\alpha}\frac{1}{\left[\left(\frac{\beta C_o}{\alpha^2}\right)\left(\frac{C_o}{\gamma}-1\right)-1\right]^2}$$

The value of C_u is obtained from the values of k_a, J_m and E from the consideration of a null flux when the concentration takes the threshold value under which there is no growth

$$\frac{k_a C_u}{1+\frac{k_a C_u}{J_m}}-E=0 \quad\Rightarrow\quad C_u=\frac{E}{k_a\left(1-\frac{E}{J_m}\right)}$$

Nutrient effects on quality of food

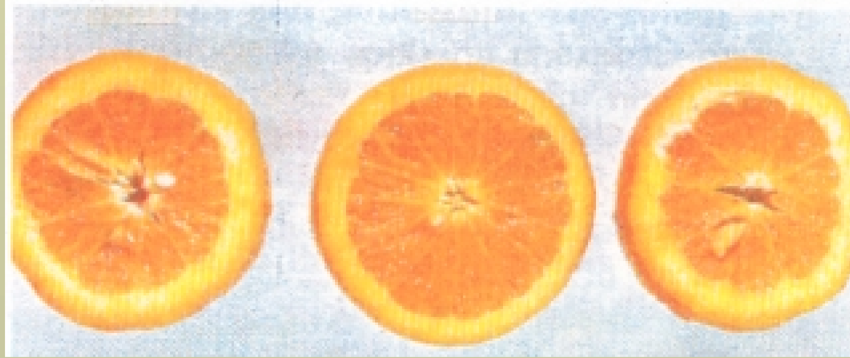


R. Weir

Too much nitrogen and low phosphorus can adversely affect fruit appearance and quality. The oranges on the left and right received high levels of nitrogen fertiliser and no phosphorus. This caused the fruit to be misshapen and the rind to be coarse and roughly textured. The fruit in the centre received a moderate but sufficient level of nitrogen and adequate phosphorus.

The two outer cut dissected fruit show thickened rinds, open centres and coarse flesh, caused by high nitrogen and no phosphorus. The thin-skinned fruit in the centre received adequate phosphorus and a moderate nitrogen level.

M. Hill



Nutrient uptake and the Finite Differences method

The method of front-fixing and finite differences

The solution of the mathematical model (3) is also obtained applying the dominion Immobilization or front fixing method and the subsequent application of finite differences. To immobilize the dominion $[s_o,R(t)]$ taking it to the interval [0,1] we carry out the following transformation:

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

$$4)\begin{cases} \text{i)}\ \dfrac{D\Psi_{yy}(y,t)}{[R(t)-s_o]^2} + \left\{\dfrac{D(1+\varepsilon_o)+s_o\dot{R}(t)y+[R(t)-s_o]\dot{R}(t)y^2}{[R(t)-s_o]^2\,y+s_o[R(t)-s_o]}\right\}. \\ .\Psi_y(y,t)=\Psi_t(y,t) \qquad 0\le y\le 1,\quad 0<t<T \\ \text{ii)}\ \Psi(y,0)=\varphi(y[R_o-s_o]+s_o), \qquad 0\le y\le 1 \\ \text{iii)}\ -\dfrac{Db}{[R(t)-s_o]}\Psi_y(1,t)+v_o\Psi(1,t)=0, \qquad 0<t<T \\ \text{iv)}\ \dfrac{Db}{[R(t)-s_o]}\Psi_y(0,t)+v_o\Psi(0,t)=\dfrac{k_a[\Psi(0,t)-\Psi_u]}{1+\dfrac{k_a[\Psi(0,t)-\Psi_u]}{J_m}}, \quad 0<t<T \\ \text{v)}\ R(t)=R_o\sqrt{\dfrac{I}{I(t)}} \end{cases}$$

Nutrient uptake and the finite differences method

The obtained equations (4) are approximated by finite differences, forwards in time, centered in the space for the second derived and forwards and back, for the derived first. For it, we propose:

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

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

When $B_j < 0$ (: $B(y,t)$ value in the node (j,n)) the first derived is approximated with differences backwards and the first equation results:

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

When $B_j > 0$ the first derived is approximated with differences forwards and then the first equation results:

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

Nutrient uptake and the explicit finite differences method

Now, our problem (4) Result in:

$$
4)\begin{cases}
\text{If } B_j < 0 \\
\text{i) } \Psi_j^{n+1} = \left[B_j^n \dfrac{\Delta t}{\Delta y} - 2A_1^n \dfrac{\Delta t}{\Delta y^2} + 1\right]\Psi_j^n + \left[A_1^n \dfrac{\Delta t}{\Delta y^2}\right]\Psi_{j+1}^n + \left[A_1^n \dfrac{\Delta t}{\Delta y^2} - B_j^n \frac{\Delta t}{\Delta y}\right]\Psi_{j-1}^n \\
\text{with} \quad \Delta t \le \dfrac{\Delta y^2}{2A_1^n - B_j^n \Delta y} \quad \forall n \\
\text{If } B_j > 0 \\
\text{i) } \Psi_j^{n+1} = \left[-B_j^n \dfrac{\Delta t}{\Delta y} - 2A_1^n \dfrac{\Delta t}{\Delta y^2} + 1\right]\Psi_j^n + \left[A_1^n \dfrac{\Delta t}{\Delta y^2}\right]\Psi_{j-1}^n + \left[A_1^n \dfrac{\Delta t}{\Delta y^2} + B_j^n \dfrac{\Delta t}{\Delta y}\right]\Psi_{j+1}^n \\
\text{with} \quad \Delta t \le \dfrac{\Delta y^2}{2A_1^n + B_j^n \Delta y} \quad \forall n \\
\text{ii) } \Psi(y_j, 0) = \varphi(y_j[R_o - s_o] + s_o), \quad \forall j \\
\text{iii) } \Psi(1, t^n) = \dfrac{Db\Psi(1-\Delta y, t^n)}{Db - v_o \Delta y\, R_1(t^n)} \\
\text{iv) } \alpha(t^n)\Psi^2(0,t^n) + \beta(t^n)\Psi(0,t^n) + \gamma(t^n) = 0 \\
\text{with:} \qquad \alpha(t^n) = v_o - \dfrac{A(t^n)b}{\Delta y} < 0, \quad \gamma(t^n) = \left(K_m - \Psi_u\right)\dfrac{A(t^n)b}{\Delta y}\Psi(\Delta y, t^n) + J_m\Psi_u \\
\qquad\qquad \beta(t^n) = \dfrac{A(t^n)b}{\Delta y}\Psi(\Delta y, t^n) + \left(v_o - \dfrac{A(t^n)b}{\Delta y}\right)(K_m - \Psi_u) - J_m \\
\text{v) } R(t^n) = R_o\sqrt{\dfrac{I_o}{I(t^n)}}, \quad \forall n.
\end{cases}
$$

Explicit Finite Differences

Nutrient uptake and the implicit finite differences method

The problem (3) approximated by finite differences backwards in the time, centered in the space for the second derived and forwards and back according to the sign of B(y,t) for the first derived:

Implicit Finite Differences

The equations of the problem (5) constitute a system of linear equations whose matrix of coefficients results to be a tridiagonal matrix

$$
5)\left\{\begin{array}{l}
\text{i) } \Psi_j^n = \left[B_j^{n+1}\dfrac{\Delta t}{\Delta y} - A_1^{n+1}\dfrac{\Delta t}{\Delta y^2}\right]\Psi_{j-1}^{n+1} + \left[1+2A_1^{n+1}\dfrac{\Delta t}{\Delta y^2} - B_j^{n+1}\dfrac{\Delta t}{\Delta y}\right]\Psi_j^{n+1} - \\
\qquad -\left[A_1^{n+1}\dfrac{\Delta t}{\Delta y^2}\right]\Psi_{j-1}^{n+1} \\
\text{i) } \Psi_j^n = \left[-A_1^{n+1}\dfrac{\Delta t}{\Delta y^2}\right]\Psi_{j-1}^{n+1} + \left[1+2A_1^{n+1}\dfrac{\Delta t}{\Delta y^2} + B_j^{n+1}\dfrac{\Delta t}{\Delta y}\right]\Psi_j^{n+1} - \\
\qquad -\left[A_1^{n+1}\dfrac{\Delta t}{\Delta y^2} + B_j^{n+1}\dfrac{\Delta t}{\Delta y}\right]\Psi_{j+1}^{n+1} \\
\text{ii) } \Psi(y_j,0) = \varphi(y_j[R_o - s_o] + s_o), \quad \forall j \\
\Psi(1,t^{n+1}) - \dfrac{Db}{Db - v_o \Delta y\, R_1(t^{n+1})}\Psi(1-\Delta y, t^{n+1}) = 0 \\
\Psi(0,t^{n+1}) + \dfrac{1}{\left[\dfrac{v_o \Delta y}{A^{n+1} b} - 1\right]}\Psi(1,t^{n+1}) = \dfrac{k_a}{\left[v_o - \dfrac{A^{n+1} b}{\Delta y}\right]}\dfrac{\left[\Psi(0,t^n) - \Psi_u\right]}{\left[1 + \dfrac{k_a\left[\Psi(0,t^n) - \Psi_u\right]}{J_m}\right]} \\
\text{v) } R(t^n) = R_o\sqrt{\dfrac{I_o}{I(t^n)}}, \quad \forall n.
\end{array}\right.
$$

The method of finite explicit differences that follows the moving boundary

$$
6)\begin{cases}
\text{i) } \Psi_j^{n+1} = D\dfrac{\Delta t}{(\Delta y)^2}\left[\Psi_{j+1}^n + \Psi_{j-1}^n\right] + \left[1 - 2D\dfrac{\Delta t}{(\Delta y)^2}\right]\Psi_j^n + \\
\qquad + B_j \dfrac{\Delta t}{2\Delta y}\left[\Psi_{j+1}^n - \Psi_{j-1}^n\right] \\
\text{ii) } \Psi_j^0 = \Psi(y_j) = \varphi(y_j), \quad s_o \le y \le R_o \\
\text{iii) } \Psi(R(t), t^n) = \dfrac{Db}{Db - v_o \Delta y}\Psi(R(t) - \Delta y, t^n), \qquad 0 < t^n < T \\
\text{iv) } \left[v_o - \dfrac{Db}{\Delta y}\right]\Psi^2(s_0, t^n) + \\
+ \left[\dfrac{Db}{\Delta y}\Psi(s_0 + \Delta y, t^n) + \left[v_o - \dfrac{Db}{\Delta y}\right][k_m - \Psi_u] - J_m\right]\Psi(s_0, t^n) + \\
+ [k_m - \Psi_u]\dfrac{Db}{\Delta y}\Psi(s_0 + \Delta y, t^n) + J_m \Psi_u = 0 \\
\text{v) } R(t^n) = R_o\sqrt{\dfrac{I_o}{I(t^n)}}, \quad \forall n.
\end{cases}
$$

Finite Differences with variable grid

Results for a fixed domain method and four moving boundary methods

Ion	Observed Uptake (mmol / pot)	Predicted uptake (mmol / pot)									
		Barber-Cushman Model		Moving Boundary Model (Integral Balance)		Moving Boundary Model (Front fixing / Explicit Finite Differences)		Moving Boundary Model (Front fixing / Implicit Finite Differences)		Moving Boundary Model (Dom. Var. / Explicit Finite Differences)	
	(†)		(*) 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
(*) Percent relative error

Competitive Ion Absorption

We study the problem when two ions are present and our interest is to analize the ***sinergism*** and ***antagonism*** effects

$$
3)\ \begin{cases}
\text{ion 1} \begin{cases}
\text{i)}\ D_1 \dfrac{\partial^2 C_1}{\partial r^2} + \dfrac{D_1}{r}\left(1 + \dfrac{v_o s_o}{D_1 b_{\partial 1}}\right)\dfrac{\partial C_1}{\partial r} = \dfrac{\partial C_1}{\partial t}, & s_o < r < R(t), \quad 0 < t < T \\
\text{ii)}\ C_1(r,0) = \varphi_1(r), & s_o \le r \le R_o \\
\text{iii)}\ D_1 b_1 \dfrac{\partial C_1(R(t),t)}{\partial r} + v_o C_1(R(t),t) = 0, & 0 < t < T
\end{cases} \\
\text{ion 2} \begin{cases}
\text{iv)}\ D_2 \dfrac{\partial^2 C_2}{\partial r^2} + \dfrac{D_2}{r}\left(1 + \dfrac{v_o s_o}{D_2 b_2}\right)\dfrac{\partial C_2}{\partial r} = \dfrac{\partial C_2}{\partial t}, & s_o < r < R(t), \quad 0 < t < T \\
\text{v)}\ C_2(r,0) = \varphi_2(r), & s_o \le r \le R_o \\
\text{vi)}\ D_2 b_2 \dfrac{\partial C_2(R(t),t)}{\partial r} + v_o C_2(R(t),t) = 0, & 0 < t < T
\end{cases} \\
\begin{cases}
\text{vii)}\ D_1 b_1 \dfrac{\partial C_1(s_o,t)}{\partial r} + v_o C_1(s_o,t) = \dfrac{k_{a1}\left[C_1(s_o,t) - C_{u1}\right]}{1 + \dfrac{k_{a1}\left[C_1(s_o,t) - C_{u1}\right]}{J_{m1}} + \dfrac{k_a\left[C_2(s_o,t) - C_{u2}\right]}{J_{m2}}} \\
\text{viii)}\ D_2 b_2 \dfrac{\partial C_2(s_o,t)}{\partial r} + v_o C_2(s_o,t) = \dfrac{k_{a2}\left[C_2(s_o,t) - C_{u2}\right]}{1 + \dfrac{k_{a1}\left[C_1(s_o,t) - C_{u1}\right]}{J_{m1}} + \dfrac{k_a\left[C_2(s_o,t) - C_{u2}\right]}{J_{m2}}}
\end{cases} \\
\text{ix)}\ R(t) = R_o \sqrt{\dfrac{I_o}{I(t)}}, \qquad\qquad 0 < t < T
\end{cases}
$$

Future perpectives

Subjects in development

Simultaneous multispecie nutrient uptake contemplating effects of interaction in the transport as well as in the absorption (competence of ions for the transporter), problem already suggested by some authors (Rengel, 1993).

- Moving boundary models for water uptake at one and two phases, of which some initial sketches have been presented through a free boundary model at one phase for water uptake in loamy soils
- Study of anaerobiosis of spherical aggregates of soil.

Water flux

The Darcy flux per root length unit is: $$v = -\pi r k(\Psi)\frac{\partial \Psi}{\partial r}$$

The continuity equation is $$2\pi\frac{\partial \theta}{\partial t} = -\frac{\partial v}{\partial r}$$

$$\frac{\partial \theta}{\partial t} = \frac{d\theta}{d\Psi}\frac{\partial \Psi}{\partial t} = C(\Psi)\frac{\partial (\Psi)}{\partial t}$$

but $$\Psi = \Psi_0 \theta^{-b} \qquad \theta = \left(\frac{\Psi}{\Psi_0}\right)^{-1/b}$$ (experimental)

then $$C(\Psi) = \frac{d\theta}{d\Psi} = \frac{d}{d\Psi}\left(\frac{\Psi}{\Psi_o}\right)^{-1/b} = \Psi_o^{1/b}\frac{d\left(\Psi^{-1/b}\right)}{d\Psi} = -\frac{\Psi_o^{1/b}}{b}\Psi^{-1/b-1}$$

$$-\frac{\partial v}{\partial r} = 2\pi\frac{\partial \theta}{\partial t} = 2\pi C(\Psi)\frac{\partial \Psi}{\partial t} = -2\pi\frac{\Psi_0^{\frac{1}{b}}}{b}\Psi^{-\frac{1}{b}-1}\frac{\partial \Psi}{\partial t}$$

$$\boxed{\frac{\partial v}{\partial r} = 2\pi\frac{\Psi_0^{\frac{1}{b}}}{b}\Psi^{-\frac{1}{b}-1}\frac{\partial \Psi}{\partial t}}$$

Water flux

But deriving v with respect to r:

$$\frac{\partial v}{\partial r} = \pi\left[k(\Psi)\frac{\partial \Psi}{\partial r} + rk(\Psi)\frac{\partial^2 \Psi}{\partial r^2} + r\frac{\partial}{\partial \Psi}k(\Psi)\left(\frac{\partial \Psi}{\partial r}\right)^2\right]$$

Experimentally, we known:

$$k(\Psi) = k_0\Psi^{-n} \quad \Rightarrow \quad \frac{\partial}{\partial \Psi}k(\Psi) = -k_0 n\Psi^{-n-1}$$

Replacing in the previous equation

$$\frac{\partial v}{\partial r} = \pi k_0\Psi^{-n}\left[\frac{\partial \Psi}{\partial r} + r\frac{\partial^2 \Psi}{\partial r^2} - \frac{rn}{\Psi}\left(\frac{\partial \Psi}{\partial r}\right)^2\right].$$

Now, our continuity equation results:

$$2\pi\frac{\Psi_0^{\frac{1}{b}}}{b}\Psi^{-\frac{1}{b}-1}\frac{\partial \Psi}{\partial t} = \pi k_0\Psi^{-n}\left[\frac{\partial \Psi}{\partial r} + r\frac{\partial^2 \Psi}{\partial r^2} - \frac{rn}{\Psi}\left(\frac{\partial \Psi}{\partial r}\right)^2\right]$$

Finally

$$\boxed{\frac{\partial \Psi}{\partial t} = \alpha\Psi^{\frac{1}{b}+1-n}\left[\frac{\partial \Psi}{\partial r} - \frac{rn}{\Psi}\left(\frac{\partial \Psi}{\partial r}\right)^2 + r\frac{\partial^2 \Psi}{\partial r^2}\right], \qquad \text{with} \quad \alpha = \frac{k_0 b}{2\Psi_0^{\frac{1}{b}}}}$$

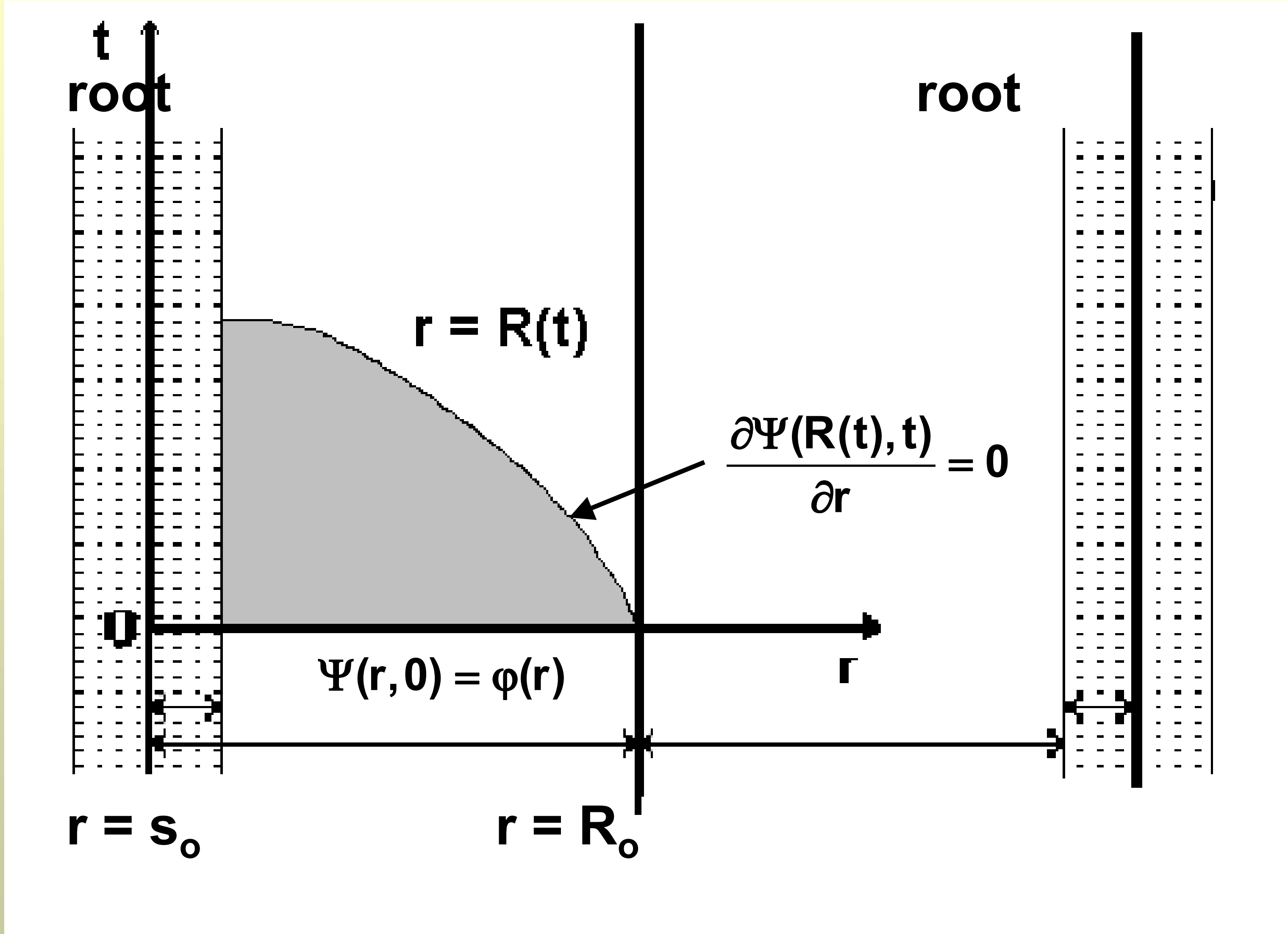
That is a differential equation with fractional coefficients (n and b which are obtained experimentally)

The moving boundary model for water uptake

In a similar way to nutrient uptake, we propose the following moving boundary model for water uptake:

$$\begin{cases} \alpha \Psi^{\frac{1}{b}+1-n}\left[\frac{\partial \Psi}{\partial r} - \frac{rn}{\Psi}\left(\frac{\partial \Psi}{\partial r}\right)^2 + r\frac{\partial^2 \Psi}{\partial r^2}\right] = \frac{\partial \Psi}{\partial t}, \quad \text{with} \quad \alpha = \frac{k_o b}{2\Psi_o^{1/b}} \\ \qquad s_o < r < R(t), \quad 0 < t < T \\ \Psi(r,0) = \varphi(r), \qquad s_o \le r \le R_o \\ -\pi R(t) k\left(\Psi(R(t),t)\right)\frac{\partial \Psi(R(t),t)}{\partial r} = 0 \quad \left(\frac{\partial \Psi(R(t),t)}{\partial r} = 0\right), \quad 0 < t < T \\ -\frac{k_0\left(\Psi(s_0,t)\right)^{-n}}{l(t)}\frac{\partial \Psi(s_0,t)}{\partial r} = G\left(\Psi\left(s_0,t\right)\right), \quad 0 < t < T \\ R(t) = R_o\sqrt{\frac{l_o}{l(t)}}, \quad 0 < t < T \end{cases}$$

A schematic diagram:

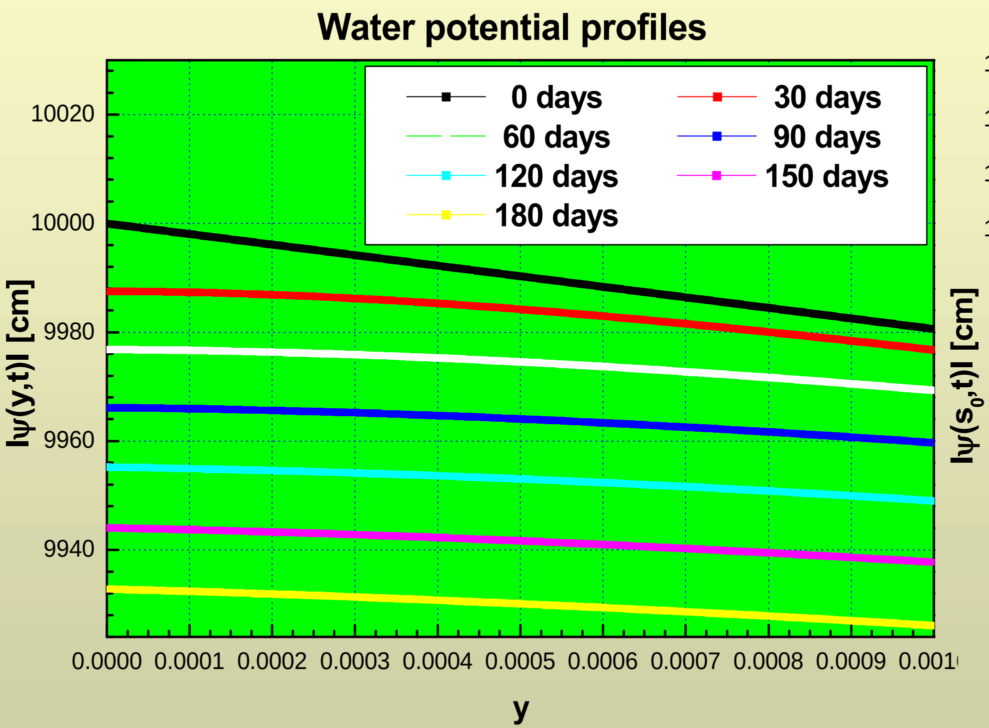


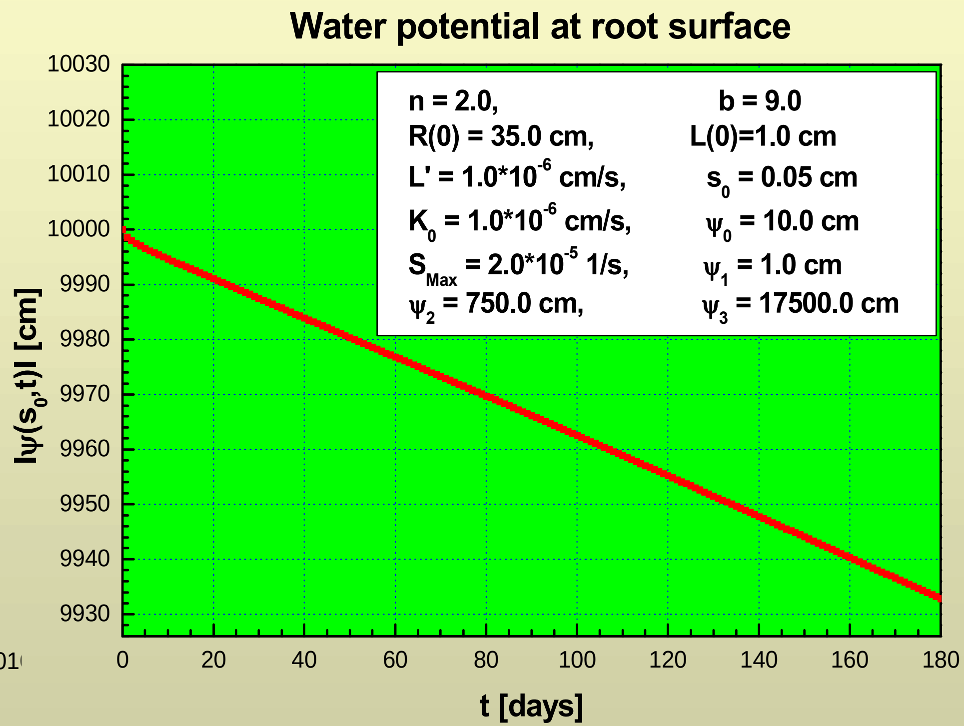
Solution: Front fixing and Finite Differences

$$y = \frac{r - s_0}{R(t) - s_0}, \qquad \tilde{t} = t, \qquad \Phi(y,\tilde{t}) = \Psi(r,t).$$

$$\begin{cases}
\text{i)}\ \dfrac{\partial \Phi}{\partial \tilde{t}} = \alpha \Phi^{\frac{1}{b}+1-n}\left[\left(\dfrac{1}{\delta(\tilde{t})} - \dfrac{\dot{R}(\tilde{t}) y \Phi^{n}}{\alpha \delta(\tilde{t})^2 \Phi^{\frac{1}{b}+1}}\right)\dfrac{\partial \Phi}{\partial y}\right] + \\
\qquad \Phi^{\frac{1}{b}+1-n}\left[-\dfrac{y\delta(\tilde{t}) + s_0}{\delta(\tilde{t})^2}\dfrac{n}{\Phi}\left(\dfrac{\partial \Phi}{\partial y}\right)^2 + \dfrac{y\delta(\tilde{t}) + s_0}{\delta(\tilde{t})^2}\dfrac{\partial^2 \Phi}{\partial r^2}\right], & 0 < y < 1, \quad 0 < t < T \\
\text{ii)}\ \Phi(y,0) = \varphi(y), & 0 < y < 1 \\
\text{iii)}\ \dfrac{\partial \Phi(1,t)}{\partial y} = 0, & 0 < y < 1 \\
\text{iv)}\ -\dfrac{k_0}{I(t)\delta(\tilde{t})\left(\Phi(0,\tilde{t})\right)^{n}}\dfrac{\partial \Phi(0,t)}{\partial y} = G\left(\Phi\left(0,\tilde{t}\right)\right) & 0 < t < T \\
\text{v)}\ R(t) = R_o\sqrt{\dfrac{I_o}{I(t)}}, & 0 < t < T
\end{cases}$$

Water uptake. Predicted results for n = 2 (loamy soils)





Soil Aeration

The production of cultivations is affected by the insufficient oxygenation and the generation of carbon dioxide of microbial activity of the soils

Diverse authors have studied the mechanisms of the problems of aeration by means of simulation models in which differential equations are resolved on fixed dominions with varied initial conditions and contour.

Keeping in mind the presence of aggregates of diverse forms in the soils and their effect in the transference of oxygen a model of radial diffusion-consumption in spherical aggregates physical and biologically homogeneous is proposed.

The diffusion in spherical aggregates is described by means of the Fick law with term of constant absorption and the anaerobiosis of an isolated aggregate can be estimated on the basis of certain data

Following the physical process that originates a mathematical model of free boundary for the diffusion and the consumption of oxygen in a spherical media is detailed

Soil Aeration

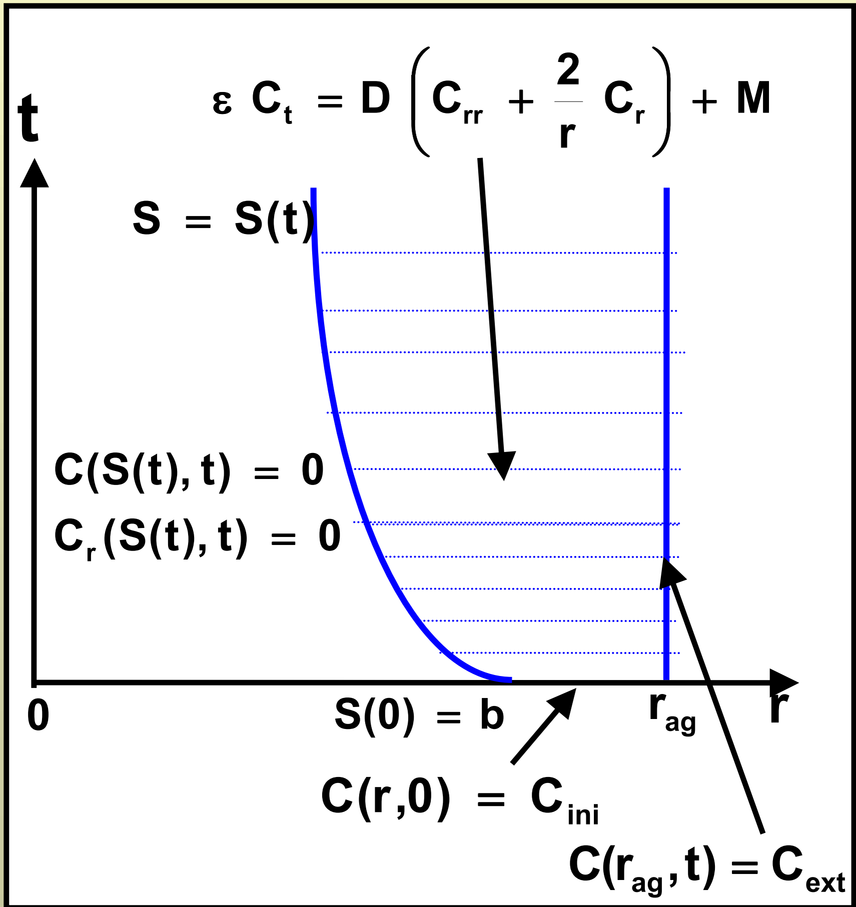
First (diffusive stage) **oxygen is diffused in such a way that part of it is absorbed and eliminated from the diffusion process. The concentration of oxygen in the fixed surface of the media is fixed. The first phase continues until it reaches a stationary state in which the oxygen doesn't penetrate any deeper in the media (*second phase: stationary stage*).**

The provision of oxygen is stopped and the media surface is isolated so that no oxygen can enter or leave. The media continues absorbing the inner available oxygen and therefore, the free boundary that establishes a separation between the zone of positive concentration and the zone of null concentration of oxygen respectively (and that marks the width of maximum penetration in the stationary case) begins to go back towards the isolated boundary (*third phase: consumption stage*).

The problem consists in localizing the movement of the free boundary and computes the distribution of oxygen in the spherical media.

Diffusive stage

Diffusive stage: Consist in to compute the transient concentration C = C(r,t) and the boundary of separation s = s(t) that satisfies the following problem of free parabolic boundary



$$
\begin{cases}
\varepsilon C_t = D\left(C_{rr} + \frac{2}{r} C_r\right) + M, & S(t) \le r \le r_{ag}, \\
 & t > 0 \\
C(r,0) = C_{ini}, & S(0) \le r \le r_{ag} \\
C(r_{ag}, t) = C_{ext}, & t > 0 \\
C(S(t),t) = C_r(S(t),t) = 0, & t > 0 \\
S(0) = b &
\end{cases}
$$

Stationary stage

Consist in deciding the stationary concentration C = C(r) and the free boundary s = s(t) that satisfies the following problem of free elliptic boundary

$$\begin{cases} -D\left(C'' + \dfrac{2}{r}C'\right) = M, \quad s \le r \le r_{ag}; \\ C(r_{ag}) = C_{ext}; \\ C(s) = C'(s) = 0. \end{cases}$$

Consumption stage

Consist in to compute the transient concentration C =C(r,t) and the boundary of separation s = s(t) that it satisfies the following problem of free parabolic boundary

$$\begin{cases} \varepsilon C_t = D\left(C_{rr} + \dfrac{2}{r}C_r\right) + M, \quad s(t) \le r \le r_{ag},\ t > 0; \\ C(r,0) = C^*(r), \quad s^* \le r \le r_{ag}; \\ C_r(r_{ag},t) = 0, \quad t > 0; \\ C(s(t),t) = C_r(s(t),t) = 0, \quad t > 0; \\ s(0) = s^* \end{cases}$$

Where:

C_{ini} >0 is the initial concentration of oxygen in the diffusive stage

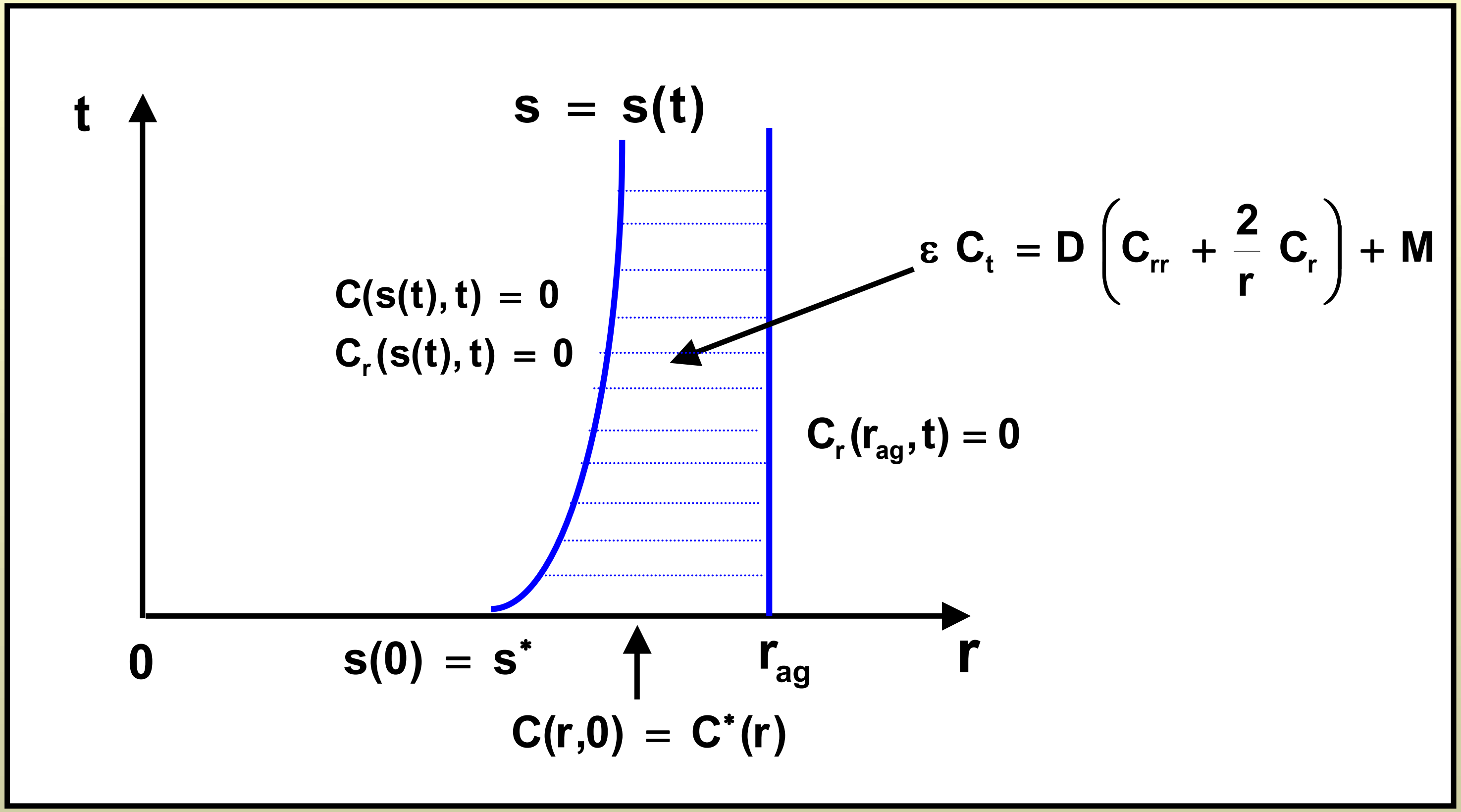
C_{ext} >0 is the external concentration of oxygen in the diffusive stage,

S = S(t) is the free boundary in the diffusive stage m,

s = s(t) is the free boundary in the stage of consumption m,

(C*,s*) is the solution of the stationary stage.

Consumption stage

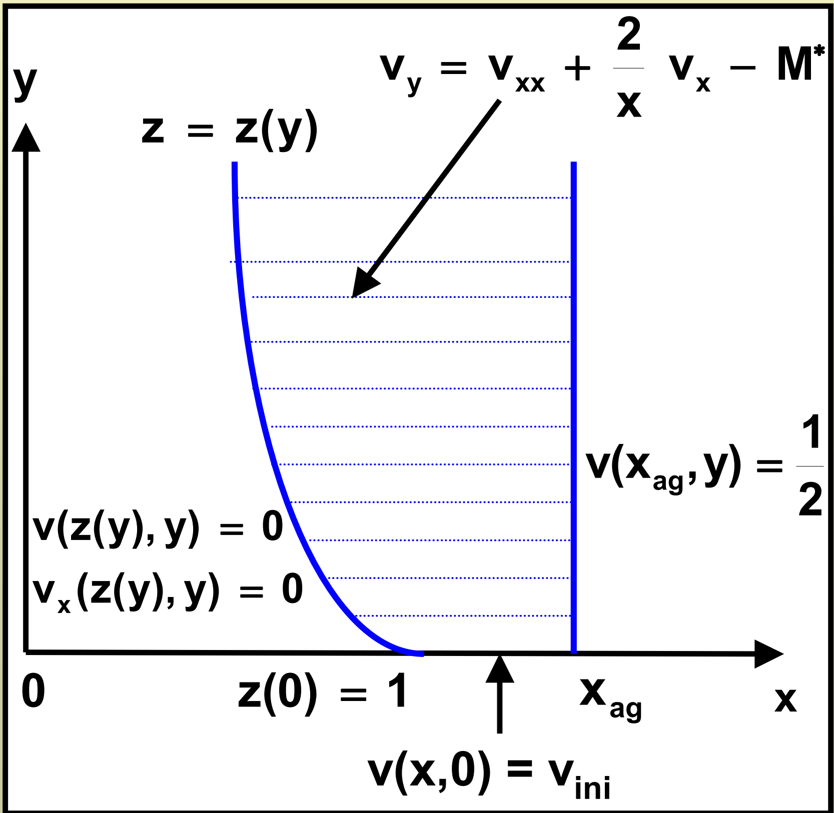


Stationary stage solution

A numeric algorithm based on the discretization method of lines is presented to approximate the solution of the diffusive stage. Carrying out the change of variables

$$x = \frac{r}{b}, \quad y = \frac{D\,t}{\varepsilon\, b^2}, \quad v = \frac{C}{2\,C_{ext}} \quad y \quad z(y) = \frac{S(t)}{b} \quad \left(\text{donde } b = S(0)\right)$$

The diffusive problem results:



$$\begin{cases} v_y = v_{xx} + \dfrac{2}{x} v_x - M^*, \quad z(y) \le x \le x_{ag}\ , \ y > 0; \\ v(x,0) = v_{ini}\ , \quad 1 \le x \le x_{ag}; \\ v(x_{ag}, y) = \dfrac{1}{2}\ , \quad y > 0; \\ v(z(y), y) = v_x(z(y), y) = 0, \quad y > 0; \\ z(0) = 1. \end{cases}$$

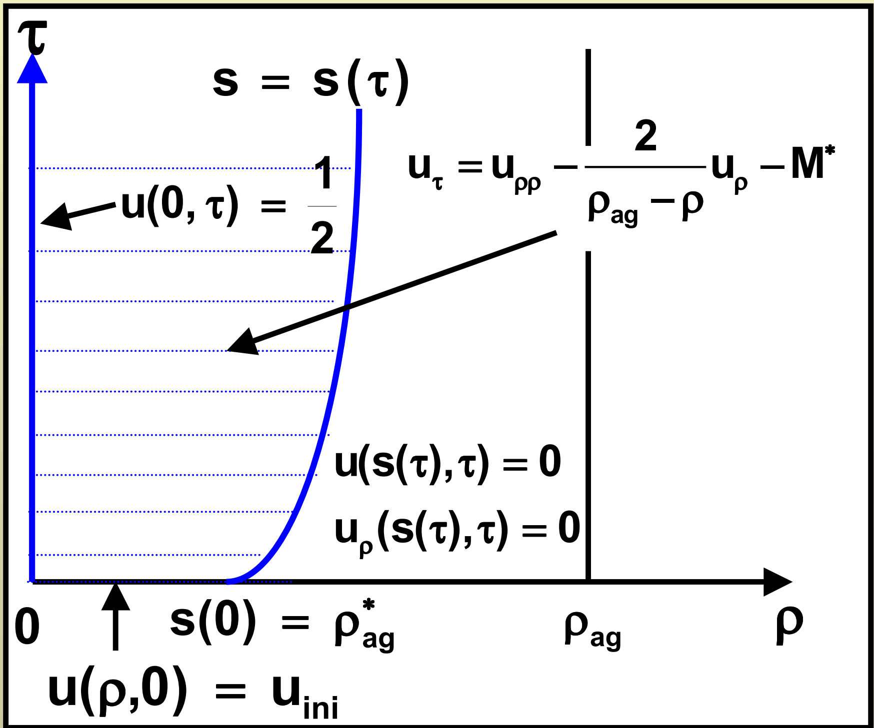
Stationary stage solution

Where: $M^* = \dfrac{b^2\,(-M)}{2\,D\,C_{ext}}$, $x_{ag} = \dfrac{r_{ag}}{b}$ y $v_{ini} = \dfrac{C_{ini}}{2\,C_{ext}}$

Carrying out a new change of variables:

$$\rho = x_{ag} - x \quad , \quad \tau = y \quad , \quad u(\rho,\tau) = v(x,y) = v(x_{ag} - \rho, \tau)$$

The diffusive problem results



$$\begin{cases} u_\tau = u_{\rho\rho} - \dfrac{2}{\rho_{ag} - \rho} u_\rho - M^*, & 0 \le \rho \le s(\tau),\ \tau > 0; \\ u(\rho,0) = u_{ini}, & 0 \le \rho \le \rho^*_{ag}; \\ u(0,\tau) = \dfrac{1}{2}, & \tau > 0; \\ u(s(\tau),\tau) = u_\rho(s(\tau),\tau) = 0, & \tau > 0; \\ s(0) = \rho^*_{ag^*} & \end{cases}$$

Where: $s(\tau) = \rho_{ag} - z(\tau)$ y $\rho^*_{ag} = \rho_{ag} - 1$ con $\rho_{ag} = x_{ag}$ y $u_{ini} = v_{ini}$.

Stationary stage solution

Fixing a step of constant time k, for each n = 0,1,2,... we define

$$\begin{cases} \tau_n = nk \\ s_n = s(\tau_n) \\ u_n(\rho) = u_n(\rho, \tau_n) \end{cases}$$

The time derivate is approximated backwards

$$u_\tau \approx \frac{u_n - u_{n-1}}{k}$$

and the differential equation

$$u_\tau = u_{\rho\rho} - \frac{2}{\rho_{ag} - \rho} u_\rho - M^*$$

adopt the following discrete form by using the method of lines

$$\frac{u_n - u_{n-1}}{k} = u_n'' - \frac{2}{\rho_{ag} - \rho} u_n' - M^*$$

Defining $q^2 = \frac{1}{k}$ and g_n the real function given by:

$$g_n(\rho) = \begin{cases} -M^* & \text{si} \quad n = 1 \\ -M^* + q^2 u_{n-1}(\rho) & \text{si} \quad n > 1 \end{cases}$$

Stationary stage solution

the diffusive problem is replaced by the following succession of problems of free boundary

$$\begin{cases} -u_n''(\rho) + \dfrac{2}{\rho_{ag} - \rho} u_n'(\rho) + q^2 u_n(\rho) = g_n(\rho), \quad 0 \le \rho \le s_n \\ u_n(0) = \dfrac{1}{2}; \\ u_n(s_n) = u_n'(s_n) = 0. \qquad\qquad n = 1, 2, 3, \ldots \end{cases}$$

Algorithm for the diffusive stage

Initial data

k, step of the time

E, tolerance.

s_1 and s_2 , initials values of the free boundary.

First step

$n = 1$

$s = s_1$

Subroutine to solve the problem by means of fourth order Runge -Kutta method (denoting the solution $u = u(p)$).

$u_1(p) = u(p)$

If $\left|u_1(0) - 1/2\right| < E$ then it ends.

Beginning of the iteration

$n = n + 1$

$s = s_n$

Subroutine to solve the problem by means of fourth order Runge -Kutta method (denoting the solution $u = u(p)$).

$u_n(p) = u(p)$

If $\left|u_1(0) - 1/2\right| < E$ then it ends

$$s_{n+1} = s_n - \left(u_n(0) - 1/2\right)\frac{s_n - s_{n-1}}{u_n(0) - u_{n-1}(0)}.$$

End of the iteration