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SIX FREE BOUNDARY PROBLEMS FOR THE HEAT-DIFFUSION EQUATION

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INTRODUCTION .

By using approximate and analytic methods we obtain an answer to six free boundary problems for the heat–diffusion equation [Ta4] :

(a) By using explicit solutions :

(I) We give a generalized Lamé–Clapeyron solution for a one–phase Stefan problem with a particular type of sources. Necessary and sufficient conditions are given in order to characterize the source term which provides a unique solution.

(II) We give formulas for the determination of some unknown thermal coefficients of a semi-infinite material through a phase-change process. We consider that the conductivity is an affine (i.e. variable) function of the temperature.

(III) We give a generalized Neumann solution for a simple mushy zone model with two parameters for the two–phase Stefan problem for a semi–infinite material with equal mass densities in both solid and liquid phases, and constant thermal coefficients.

(b) By using a theoretical approach :

(IV) We give a local result in time for the existence and uniqueness of the solution of the free boundary problem in the shrinking core model for noncatalytic gas–solid reactions. We impose free boundary conditions which generalize Wen and Langmuir conditions.

(c) By using approximate methods :

(V) We give a new proof of the exponentially fast asymptotic behavior of the solutions in heat conduction problems with absorption by using a variant of the heat balance integral method.

(VI) We give a growth absorption model for the root surface through an absorption mechanism. For low concentrations the resultant equations have been analytically solved by the quasi–stationary method. This solution is used to compute growth of root radius.

PART I. We consider the following singular free boundary problem for the heat equation : Find the free boundary $x = s(t) > 0$, defined for $t > 0$ and $s(0) = 0$, and the temperature $\theta = \theta(x,t) > 0$, defined $0<x< s(t)$, $t> 0$, such that they satisfy the following conditions [MeTa](For β=0, we have the Lamé–Clapeyron problem [LaCl]) :

$$\begin{aligned} &\rho\, c\, \theta_t - k\, \theta_{xx} = \frac{\rho\, h}{t}\, \beta\left(\frac{x}{2a\sqrt{t}}\right) \quad , \ 0 < x < s(t) \ , \ t > 0 \ , \\ &\theta(0,t) = B > 0 \ , \ t > 0 \ , \\ (1) \qquad &\theta(s(t),t) = 0 \ , \quad k\, \theta_x(s(t),t) = -\, \rho h\, \dot{s}(t) \ , \ t > 0 \ , \\ &s(0) = 0 \ , \end{aligned}$$

for a given source function $g(x,t) = \frac{\rho\, h}{t}\, \beta(x/2at)$, fixed face temperature $B>0$ and constant thermal coefficients $k > 0$ (thermal conductivity), $\rho > 0$ (mass density), $c>0$ (specific heat), and $h > 0$ (latent heat of fusion). We denote by $a^2 = \frac{k}{\rho\, c} > 0$ the diffusion coefficient and $\mathrm{Ste} = \frac{B\, c}{h} > 0$ the Stefan number.

THEOREM 1: An explicit solution of (1), as function of β, is given by

$$\theta(x,t) = B \left\{ 1 - \frac{\sqrt{\pi}}{\mathrm{Ste}}\, \xi\, \exp(\xi^2)\, \mathrm{erf}(\eta) + \right.$$

$$(2) \qquad \left. + \frac{4}{\mathrm{Ste}} \int_0^{\eta} \left(\int_r^{\xi} \beta(y)\, \exp(y^2)\, dy \right) \exp(-r^2)\, dr \right\} ,$$

$$s(t) = 2\, a\, \xi\, \sqrt{t} \ , \ \eta = \frac{x}{2\, a\, \sqrt{t}} \in (0,\xi) \ ,$$

where the number $\xi > 0$ is a solution of the equation

$$(3) \qquad F(x,\beta) = \frac{\mathrm{Ste}}{\sqrt{\pi}} \ , \quad x > 0 \ ,$$

with

$$\begin{aligned} &F(x,\beta) = F_0(x) - 2 \int_0^x \exp(r^2)\, \mathrm{erf}(r)\, \beta(r)\, dr \ , \\ (4) \qquad & \\ &\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-u^2)\, du \ , \quad F_0(x) = x\, \exp(x^2)\, \mathrm{erf}(x) \ . \end{aligned}$$

THEOREM 2: Let β be a continuous real function on $\mathbb{R}^+$ such that $x\beta(x)$ is locally integrable on $\mathbb{R}^+$. Define the function Z by

$$\begin{aligned} &Z = Z_\beta(x) = \exp(x^2)\, \mathrm{erf}(x)\, [\, \psi_0(x) - \beta(x)\,] \ , \ x > 0 \ , \\ (5) \qquad & \\ &\psi_0(x) = \tfrac{1}{2} + x^2 + \tfrac{x}{\sqrt{\pi}}\, G(x) \ ; \ G(x) = \frac{\exp(-x^2)}{\mathrm{erf}(x)} \ , \end{aligned}$$

which is continuous and locally integrable on $\mathbf{R}^+$. If the function Z satisfies the following conditions

$$(6) \qquad Z(x) > 0 \ , \ \forall\, x \in (\nu, +\infty) \quad \text{and} \quad \int_0^{+\infty} Z(t)\, dt = +\infty \ ,$$

where $\nu = \nu_Z \geq 0$ is defined by

$$(7) \qquad \nu = \operatorname{Inf} \left\{ x \geq 0 \,/\, \int_0^x Z(t)\, dt > 0 \right\},$$

then for any Ste > 0, there exists a unique $\xi = \xi(\text{Ste}) > 0$ which is the solution of the equation (3) for the given function β. Conversely, if for the given function β the equation (3) has a unique root $\xi = \xi(\text{Ste}) > 0$ for any Ste > 0 then there exists a continuous and locally integrable function Z on $\mathbf{R}^+$ satisfying (6) and (7) such that

$$(8) \qquad \beta(x) = \psi_0(x) - Z(x)\, G(x) \quad (= \beta_Z(x)) \ , \ x > 0 \ .$$

Moreover in any case the root $\xi > \nu$.

Remark 1: We can also study the particular case

$$(9) \qquad 0 < \text{Ste} \ll 1 \ , \ \beta(x) \approx \beta(0) < 1$$

which is related to the corresponding quasi–steady state free boundary problem.

Part II . We consider the following one–phase solidification problem for a semi-infinite material with an overspecified condition on the fixed face :

$$(1) \qquad \begin{aligned} & \rho\, c\, T_t = (k(T)\, T_x)_x \ , && 0 < x < s(t) \ , t > 0, \\ & s(0) = 0 \ , \\ & T(0,t) = T_o < T_f \ , t > 0 \ , \\ & T(s(t),t) = T_f \ , t > 0 \ , \\ & k(T_f)\, T_x(s(t),t) = \rho\, h\, \dot{s}(t) \ , t > 0 \ , \\ & k(T_o)\, T_x(0,t) = \frac{q_o}{\sqrt{t}} \ , t > 0 \ , \end{aligned}$$

where $T = T(x,t)$ is the temperature, $\rho > 0$ es the mass density, h is latent heat of fusion, $c > 0$ is the specific heat, $x = s(t)$ is the phase-change front, T_f is the phase-change temperature (T_o is a reference temperatur), $k = k(T) = k_o\, [1 + \beta (T-T_o)/(T_f-T_o)]$ [ChSu, Lu] is the thermal conductivity, $\alpha_o = k_o/\rho c$ is the diffusion coefficient at reference temperature T_o , and coefficients $\beta > 0$, $q_o > 0$.

In [Ta7, Ta8] we obtain one or two thermal coefficients, for the case $k = k_o$ (i.e. $\beta \equiv 0$), and we give formulas for the unknown coefficients. We consider here the general case $\beta \neq 0$. The problem consists in finding the :

1) temperature $T = T(x,t)$ and two thermal coefficients ($x = s(t)$ is a moving boundary [Ta4], i.e., known a priori),

2) temperature $T = T(x,t)$, the phase-change front $x=s(t)$ and a thermal coefficient ($x = s(t)$ is a free boundary [Ta4], i.e., unknown a priori).

Among the unknown thermal coefficients we have k_o, β, c, ρ, h. Moreover, the coefficients q_o and $T_o > 0$ must be known from the experimental phase-change process. The solution is given by [Ta9] :

$$(2) \qquad \begin{aligned} &T(x,t) = T_o + (T_f - T_o)\, \Phi_\delta(\eta) \ , \quad \eta = \frac{x}{2\sqrt{\alpha_o t}} \ , \\ &s(t) = 2\, \lambda \sqrt{\alpha_o t} \ , \end{aligned}$$

where the three unknown coefficients must satisfy the following system of equations :

$$(3) \qquad \begin{aligned} &\beta = \delta\, \Phi_\delta(\lambda) \ , \\ &[1 + \delta\, \Phi_\delta(\lambda)]\, \frac{\Phi_\delta{}'(\lambda)}{\lambda\, \Phi_\delta(\lambda)} = \frac{2}{Ste} \ , \\ &\frac{\Phi_\delta{}'(0)}{\Phi_\delta(\lambda)} = \frac{2\, q_o}{(T_f - T_o)\sqrt{k_o \rho c}} \ , \end{aligned}$$

where $Ste = c(T_f - T_o)/h > 0$ is the Stefan number and $\Phi_\delta = \Phi_\delta(x)$ is error modified function which is the unique solution of the following differential problem :

$$(4) \qquad \begin{aligned} &[(1 + \delta\, y(x))\, y'(x)]' + 2\, x\, y'(x) = 0 \\ &y(0^+) = 0 \ , \ y(+\infty) = 1 \ . \end{aligned}$$

We obtain formulas for the determination of some thermal coefficients.

<u>THEOREM 1</u>: For the determination of the coefficients λ, β, c we obtain that : If

$$(5) \qquad \frac{\rho\, h\, k_o\, (T_f - T_o)}{2\, q_o^2} < 1$$

then we have

$$(6) \qquad \beta = \beta(\lambda) = \delta\, \Phi_\delta(\lambda) \ ,$$

$$(7) \qquad c = c(\lambda) = \frac{4\, q_o^2}{\rho\, k_o\, (T_f - T_o)^2}\, \frac{(\Phi_\delta(\lambda))^2}{(\Phi_\delta{}'(0))^2} \ ,$$

and $\lambda > 0$ is the unique solution of the equation

$$F_1(x) = \frac{\rho\, h\, k_o\, (T_f - T_o)}{2\, q_o^2} (\Phi_\delta'(0))^2\, F_2(x)\,, \qquad (8)$$

$$x > 0\,,$$

where functions F_1 and F_2 are defined by

(9) $$F_1(x) = [\, 1 + \delta\, \Phi_\delta(x)\,]\; \Phi_\delta'(x)$$

(10) $$F_2(x) = \frac{x}{\Phi_\delta(x)}\,.$$

PART III. We consider a semi—infinite material with mass density equal in both solid and liquid phases and the phase—change temperature at 0°C. We generalize the mushy zone model given for the one—phase Lamé—Clapeyron (Stefan) problem in [SoWiAl] (See also [Fa, Ta3]) to the two—phase case [Ta6]. Three distinct regions can be distinguished, as follows :

H_1) The liquid phase, at temperature $\theta_2=\theta_2(x,t)>0$, occupying the region $x>r(t)$, $t>0$.

H_2) The solid phase, at temperature $\theta_1=\theta_1(x,t)<0$, occupying the region $0<x<s(t)$, $t>0$.

H_3) The mushy zone, at temperature 0 , occupying the region $s(t) < x < r(t)$, $t > 0$. We make two assumptions on its structure following the paraffin case [SoWiAl] (the parameter ϵ and γ are characteristics of the phase—change material) :

a) The material in the mushy zone contains a fixed fraction ϵh (with constant $0 < \epsilon < 1$) of the total latent heat h .

b) The width of the mushy zone is inversely proportional (with constant $\gamma>0$) to the temperature gradient at the point $(s^-(t), t)$.

THEOREM 1: If the phase—change semi—infinite material is initially in liquid phase at the constant temperature $\theta_0 > 0$ and a constant temerature $-D < 0$ is imposed on the fixed face $x = 0$, then we obtain the following results :

(i) We obtain an exact solution of the Neumann type for $\theta_1(x,t)$, $\theta_2(x,t)$, $s(t)$ and $r(t)$ as functions of the initial and boundary temperature θ_0 and D, mushy zone parameters ϵ and γ, and thermal coefficients of the material.

(ii) We obtain an analogous property to (i) if we replace in the hypothesis (H3b) the temperature gradient at the point $(s^-(t),t)$ (i.e. $\theta_{1_x}(s(t),t)$) by the temperature gradient at the point $(s^+(t),t)$ (i.e. $\theta_{2_x}(r(t),t)$).

Moreover, If we replace the constant temperature $-D < 0$ by a heat flux of the type $q_0\, t^{-\frac{1}{2}}$ (with $q_0 > 0$) on the fixed face $x = 0$, then we obtain the following results :

(iii) There exists an exact solution $\theta_1^*(x,t)$, $\theta_2^*(x,t)$, $s^*(t)$ and $r^*(t)$ of the Neumann type of the mushy zone model, as functions of θ_0 , q_0 , ϵ ,γ and the thermal coefficients of the material, if and only if the coefficient q_0 satisfies the inequality

$$(1) \qquad q_0 > \frac{\gamma\, k_1}{2\, a_2\, \eta_0} ,$$

where $\eta_0 = \eta_0(\epsilon, \gamma, \theta_0, h, k_1, k_2, c_2) = \eta_0\Big(\theta_0\, c_2 \,/\, h\, (1-\epsilon)\, ,\, \gamma\, k_1\, c_2 \,/\, h\, k_2\, (1-\epsilon)\Big) > 0$ is the unique positive zero of a given function G.

Moreover, for the solution given in (i), the inequality for q_0 turns into

$$(2) \qquad f\left(\frac{\sigma}{a_1}\right) < \frac{2\, D\, \eta_0}{\gamma} \left(\frac{k_2\, c_1}{\pi\, k_1\, c_2}\right)^{1/2}$$

where $\sigma > 0$ is the coefficient that characterizes the first free boundary $s(t) = 2\, \sigma \sqrt{t}$ of the two−phase mushy zone model.

(iv) If $q_0 = \gamma\, k_1 \,/\, 2\, a_2\, \eta_0$, then there exists an exact solution for $\theta_2^*(x,t)$, $r^*(t)$ and $s^*(t) = 0$ for the corresponding one−phase mushy zone model (the solid phase there does not exist). If $0<q_0<\gamma k_1/2 a_2 \eta_0$, then there does not exist an exact solution of the Neumann type for the corresponding mushy zone model.

Remark 1: For the particular case $\gamma = 0$, that is the mushy zone model is identical to the classical Neumann model [CaJa, Ru, Ta2], we find the inequality $q_0 > k_2\, \theta_0 \,/\, a_2 \sqrt{\pi}$ [Ta1] to obtain a phase−change problem.

PART IV. We shall analyze a mathematical model of an isothermal noncatalytic diffusion−reaction process of a gas A with a solid slab S. The solid has a very low permeability and semi−thickness R along the gas diffusion direction[TaVi]. Since 1960, various devices and models, either phenomenological or structural, have been proposed and analyzed with the purpose of interpreting gas−solid reaction process [BeLeWa, Bi, Do, FrBi, Le, SzEvSo, We]. We assume the solid is chemically attacked from the surface $y = R$ with a quick and irreversible reaction of order $\nu > 0$ with respect to the gas A and zero order with respect to the solid S. We also assume that the solid has uniform and constant composition. As a result of the chemical reaction an inert layer is formed which is permeable to the gas and the process will exhibit a free boundary (the reaction front) as described in [We]. The corresponding mathematical scheme (Wen's model) is formulated as follows (in a dimensionless form):

$$\text{i)} \quad u_{xx} - u_t = 0 \quad \text{in } D_T ,$$

$$\text{ii)} \quad u(0, t) = v_0 , \quad 0 < t \le T ,$$

$$(1) \qquad \text{iii)} \quad u_x(s(t), t) = -\, u^{\nu}(s(t), t) , \quad \text{iv)} \quad u_x(s(t), t) = -\, \dot{s}(t) , \quad 0<t\le T ,$$

$$\text{v)} \quad s(0) = b > 0 , \qquad \text{vi)} \quad u(x, 0) = \Psi(x) , \quad 0 \le x \le b ,$$

where

(2) $D_T = \{ (x, t) / 0 < x < s(t) , 0 < t \leq T \}$.

We can consider the following generalized free boundary conditions :

(3) i) $u_x(s(t), t) = g(u(s(t), t))$, ii) $\dot{s}(t) = f(u(s(t), t))$, $0 < t \leq T$,

where f and g are real functions which satisfy

(4a) i) $f>0$, $f'>0$ in $\mathbb{R}^+$ and $f(0)=0$, ii) $g<0$, $g'<0$ in $\mathbb{R}^+$ and $g(0)= 0$.

Functions f and g may be defined in $\mathbb{R}$ but we are only interested in positive arguments of them as it will be seen below. Moreover, we shall assume that f and g are Lipschitz functions in $[\frac{v_0}{2}, v_0]$ with constants f_0 and g_0 respectively, i.e.

(4b) i) $\exists\, f_0 > 0 \,/\, | f(v_2) - f(v_1) | \leq f_0 | v_2 - v_1 |$, $\forall v_1 , v_2 \in [\frac{v_0}{2}, v_0]$,

ii) $\exists\, g_0 > 0 \,/\, | g(v_2) - g(v_1) | \leq g_0 | v_2 - v_1 |$, $\forall v_1 , v_2 \in [\frac{v_0}{2}, v_0]$.

We remark here that functions f and g , defined by

(W) $g(x) = - x^{\nu}$ $(= - f(x))$ $(x \geq 0 , \nu > 0)$

satisfy conditions (4ai, ii). A different choice of g in (3i) is considered in [Do]; It is a Langmuir type condition : the chemical reaction rate is given by

(L) $g(x) = - \dfrac{a\, x^n}{b + c\, x^n}$ $(= - f(x))$, a, b, c = const. > 0 , n > 0 .

which also verifies conditions (4aii) for all constants a, b, c, n > 0 . We remark here that the (L) condition reduces to a (W) condition when c = 0 .

Firstly, we study an auxiliary moving boundary problem. We generalize the results obtained in [FaPr1, FaPr2] changing the nonlinear condition on the fixed face x = 0 by other one on the moving boundary x = s(t) , given by (3i). Secondly, we study the Wen–Langmuir free boundary model for noncatalytic gas–solid reactions that consists in finding T > 0 , x = s(t) and u = u(x, t) such that they satisfy conditions (3). We prove that there exists a unique solution for a sufficiently small T > 0 . Moreover, the solution is given through the unique fixed point, in an adequate Banach space, of the following contraction operator F_2 : For $s = s(t) \in C^0([0,T])$ we define

(5) $$F_2(s)\,(t) = \int_0^t f(v(s(\tau), \tau))\, d\tau$$

where v is the solution of problem (1i–ii–iv) and (3i).

Here we exploit some techniques recently used in [CoRi, FaMePr] for sorption of swelling solvents in polymers.

PART V. We give a new and explicit estimate for the asymptotic behavior of the solutions of the problem:

$$(1) \qquad \begin{array}{ll} \text{i)} & L(u) = u_t - u_{xx} + \lambda^2 u_+^p = 0 \ , \ x > 0 \ , \ t > 0 \ , \\ \text{ii)} & u(0,t) = 1 \ , \ t > 0 \ , \qquad \text{iii)} \ u(x,0) = U_0(x) \geq 0 \ , \ x > 0 \ , \end{array}$$

for a class of functions $U_0 = U_0(x)$ corresponding to the initial condition (1iii), and parameters $p > 0$ and $\lambda > 0$. We denote with x_+ the positive part of x, that is $x_+ = \text{Max}\,(0,x)$. If $0 < p < 1$, it is well known [Di, St] that equation (1i) has a stationary solution corresponding to datum (1ii), which has compact support in $[0,+\infty)$ and is given by

$$(2) \qquad u_\infty(x) = \left(1 - \frac{\lambda}{I}\, x\right)_+^{\frac{2}{1-p}} \ , \ I = I(p) = \frac{\sqrt{2(1+p)}}{1-p} \ .$$

In the case $0 < p < 1$ and $U_0 \leq u_\infty$, the solution $u = u(x,t)$ of (1) satisfies

$$(3) \qquad 0 < u(x,t) < u_\infty(x,t) \ , \ 0 < x < \frac{I}{\lambda} \ , \ t > 0 \ ,$$

because of the comparison principle for equation (1i) [Be]. This means that $u(t) = u(.;t)$ has compact support in variable x for any $t > 0$ and

$$(4) \qquad s(t) = \text{Sup}\ \{\, x > 0 \ / \ u(x,t) > 0 \,\} \ , \ t > 0 \ ,$$

is a free boundary which is moving with finite speed for $t > 0$.

We shall give an estimate of how fast the free boundary s(t) tends to its limit $\frac{I}{\lambda}$ as $t \to +\infty$ [Ta5]. The estimate we get implies that this convergence is exponentially fast in time, in a similar form to the one given in [RiTa]. The purpose of the present part is to show how this result can be obtained in a different way to [RiTa] by using the Goodman heat balance integral method [Go]. To prove that we use an approximate solution given and motivated by the heat balance integral method with the innovation property (7) which fixes appropiately the asymptotic limit of the corresponding approximate free boundary. This approximate solution to (1), approaches exponentially fast the stationary solution $u_\infty = u_\infty(x)$ when $U_0 \leq u_\infty$ and $0 < p < 1$ for all $\lambda > 0$.

We consider a related problem to (1) which consists in finding the function $C = C(x,t)$ and the free boundary $s = s(t)$ such that they satisfy the following conditions :

$$(5) \qquad \begin{array}{ll} \text{i)} & C_t - C_{xx} + \lambda^2 C_+^p = 0 \ , \ 0 < x < s(t) \ , \ t > 0 \ , \\ \text{ii)} & C(0,t) = 1 \ , \ t > 0 \ , \quad \text{iii)} \ s(0) = 0 \ , \\ \text{iv)} & C(s(t),t) = 0 \ , \ t > 0 \ , \quad \text{v)} \ C_x(s(t),t) = 0 \ , \ t > 0 \ . \end{array}$$

Taking into account the heat balance integral method we replace equation (5i) by its integral in the variable x from 0 to s(t), we propose for the corresponding approximate problem the following expression for C, namely :

$$(6) \qquad C(x,t) = (1 - \frac{x}{s(t)})_+^{\alpha}$$

where s=s(t) is a function to be determined and $\alpha > 1$ is a parameter to be chosen so that

$$(7) \qquad \lim_{t\to\infty} s(t) = \frac{I(p)}{\lambda} .$$

THEOREM 1. Let $p \in (0,1)$ and $\lambda > 0$ be. If we apply Goodman heat balance integral method with the innovation property (7), we obtain the solutions $C_B = C_B(x,t)$ and $s_B = s_B(t)$ which are given respectively by (6) with

$$(8) \qquad s_B(t) = \frac{I}{\lambda}\left[1 - \exp(- \frac{2\lambda^2(3-p)t}{1+p}) \right]^{1/2} , \ t \ge 0 , \quad \alpha = \alpha(p) = \frac{2}{1-p} > 2.$$

We can define the following functions:

$$(9) \qquad u_1(x,t) = \left[1 - \frac{x}{s_1(t)} \right]_+^{\frac{2}{1-p}} , \quad s_1(t) = \frac{I}{\lambda}\left[1 - \exp(- \frac{2\lambda t}{I}) \right] .$$

If we consider the heat conduction problem with absorption (1), we obtain:

THEOREM 2. Let $0 < p < 1$, $\lambda > 0$ and $0 \le U_0 \le u_\infty$ in $\mathbb{R}^+$ be. If u=u(x,t) is a solution of (1) and s=s(t) is defined by (4), we have the following comparison properties :

$$(10) \qquad u_1(x,t) \le u(x,t) \le u_\infty(x) \ , \ 0 \le x \le \frac{I}{\lambda} \ , \ t > 0 \ ,$$

$$(11) \qquad s_1(t) \le s(t) \le \frac{I}{\lambda} \ , \ t \ge 0 \ ,$$

and the following estimates

$$(12) \qquad 0 < \frac{I}{\lambda} - s(t) \le \frac{I}{\lambda} - s_1(t) \le \frac{I}{\lambda}\exp(- \frac{2\lambda t}{I}) \ , \ t \ge 0 \ ,$$

$$(13) \quad 0 \le u_\infty^{\frac{1-p}{2}}(x) - u^{\frac{1-p}{2}}(x,t) \le u_\infty^{\frac{1-p}{2}}(x) - u_1^{\frac{1-p}{2}}(x,t) \le \frac{\exp(-\frac{2\lambda t}{I})}{1 - \exp(-\frac{2\lambda t}{I})},$$

$$x \in [0, \frac{I}{\lambda}] , \ t > 0 \ .$$

From now on, without loss of generality, we consider the case $\lambda = 1$, $0<p<1$ and $0 \le U_0 \le u_\infty$ in $\mathbb{R}^+$ in problem (1). The results obtained in [RiTa] are given by :

(14) $$s_0(t) \le s(t) \le I \ , \ t \ge 0 \ , \ (I = I(p) = \frac{\sqrt{2(1+p)}}{1-p})$$

(15) $$u_0(x,t) \le u(x,t) \le u_\infty(x) \ , \ 0 \le x \le I \ , \ t \ge 0 \ ,$$

where functions s_0 and u_0 are defined by (take $L_0 = 0$ and $m=1$ in [RiTa])

(16) $$s_0(t) = I\,[\,1 - \exp(-c_0 t)\,]^{1/2} , \ u_0(x,t) = [\,1 - \frac{x}{s_0(t)}\,]_+^{\frac{2}{1-p}} , \ c_0 = c_0(p) = 4(1-p) .$$

THEOREM 3. For any $0 < p < 1$, we obtain the following estimates:

(17) $$s_1(t) < s_0(t) \le s(t) \le I \ , \quad s_1(t) < s_0(t) < s_B(t) < I \ , \ t > 0 \ ,$$

and therefore

(18) $$| s(t) - s_B(t) | \le I - s_0(t) \le I - s_1(t) \le I \exp(-\frac{2t}{I}) \ , \ t > 0 .$$

Remark 1. The expression s_0 was obtained in [RiTa] by constructing a sub–solution of the problem (1) ($\lambda = 1$). Instead s_B was obtained by calculating the solution of an approximate problem to (1) through the heat balance integral method with the innovation property (7). Both expressions, s_0 and s_B , give us a fast asymptotic behavior in heat conduction problems with absorption (1), but at present we cannot say which is the better. For t large both expressions are equivalent because

(19) $$\lim_{t \to \infty} \frac{s_B(t)}{s_1(t)} = 1 \ , \ 0 < p < 1 .$$

COROLLARY 4. We also obtain

(20) $$u_1(x,t) \le u_0(x,t) \le u(x,t) \le u_\infty(x), \ u_1(x,t) \le u_0(x,t) \le C_B(x,t) \le u_\infty(x), \ 0 \le x \le I, \ t>0,$$

and therefore :

(21) $$| u^{\frac{1-p}{2}}(x,t) - C_B^{\frac{1-p}{2}}(x,t) | \le u_\infty^{\frac{1-p}{2}}(x,t) - u_1^{\frac{1-p}{2}}(x,t) \le u_\infty^{\frac{1-p}{2}}(x,t) - u_1^{\frac{1-p}{2}}(x,t) \le$$
$$\le \exp(-\frac{2t}{I}) , \ 0 < x < s_1(t) \ , \ t > 0 .$$

PART VI. 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 [CaBa, Cu1, Cu2]. In general, these models have not considered computing root growth, but rather they have assumed young roots to be growing at exponential rates .

We compute the free boundary (the root–soil interface) a priori unknown through the quasi–stationary method. We obtain an analytical solution for the nutrient interface concentration and the interface position (the free boundary). Taking into account the idea of the model used for the shrinking core problem for noncatalytic gas–solid reactions [TaVi], we propose the following free boundary problem for root growth [ReTaCa1, ReTaCa2] :

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

where: (1i) is the Cushman equation [Cu1,Cu2], (1ii) and (1iii) are the initial and boundary conditions respectively, and (1iv) are the interface conditions representing the mass nutrient balance. C is the ion concentration in soil solution, r is the position coordinate (in cylindrical coordinates), t is the time, D is the effective diffusion coefficient; v_0 is the velocity of flux solution at the root surface, b is the buffer power, and s_0 the initial radius. Function s(t) is the interface position (root radius), $\dot{s}(t) = \frac{ds(t)}{dt}$ is the interfase velocity, a is a stoichiometric coefficient, E is the constant eflux, k is the absorption power of root, R is the rhizosphere radius, and $\alpha_0 = 1 + \epsilon$, $\epsilon = v_0\, s_0/D\, b > 0$. $\Phi(r)$ is the initial concentration profile given by the equation (8).

Assuming low concentrations, the uptake nutrient given by Michaelis–Menten expression reduces to [ReTaCa1] :

$$(2)\qquad \frac{k\,C(s(t),t)}{1+\frac{k\,C(s(t),t)}{J_m}} \sim k\,C(s(t),t)\,.$$

The two free boundary conditions can be written by:

$$(3)\qquad C_r(s(t),t) = g(C(s(t),t))\ ,\quad \dot{s}(t) = f(C(s(t),t))\ ,\quad t>0\,,$$

where functions g and f are given by:

$$(4)\qquad g(C) = \frac{1}{D\,b}\left[(k - v_0)\,C - E\right]\ ,\quad f(C) = \frac{1}{a}\left[k - \frac{E}{C}\right]\,,$$

which satisfy the following properties:

$$(5)\quad f(C) > 0 \Leftrightarrow C > C_p = \frac{E}{k}\ ,\quad g(C) > 0 \Leftrightarrow C > C_m = \frac{E}{(k - v_0)}\,,\ (C_m > C_p).$$

The solution of the problem , by the quasi–stationnary method, is given by :

$$(6)\qquad C(r,t) = \beta(t) - \frac{\alpha(t)}{r^\epsilon}\quad ,\ s(t)<r<R\,,\ t>0\,,$$

where:

$$(7)\quad \alpha(t) = \left[\frac{1}{D\,b}\right]\frac{\left[(k - v_0)C_\infty - E\right]}{\frac{\epsilon}{s(t)^{1+\epsilon}} + \frac{(k - v_0)}{D\,b}\left[\frac{1}{s(t)^\epsilon} - \frac{1}{R^\epsilon}\right]}\ ,\quad \beta(t) = C_\infty + \frac{\alpha(t)}{R^\epsilon}\,,$$

$$(8) \qquad \Phi(r) = C_\infty - \frac{\left[(k - v_0)C_\infty - E\right]}{\frac{v_0}{{s_0}^\epsilon} + (k - v_0)\left[\frac{1}{{s_0}^\epsilon} - \frac{1}{R^\epsilon}\right]}\left[\frac{1}{r^\epsilon} - \frac{1}{R^\epsilon}\right]$$

and s(t) is the unique solution of the following Cauchy problem :

$$(9) \qquad \dot{s}(t) = F(s(t)) \,, \; t > 0, \qquad s(0) = s_0 \in (0,R) \,,$$

with:

$$(10) \quad F(s) = \frac{k}{a}\left[1 - \alpha_3\, H(s)\right] \,, \quad H(s) = \frac{\left[1 + \alpha_2\, G(s)\right]}{\left[1 + \alpha_1\, G(s)\right]} \,, \quad G(s) = s\left[1 - (\tfrac{s}{R})^\epsilon\right]$$

$$(11) \quad \alpha_1 = \frac{E}{v_0\, s_0\, C_\infty} > 0 \quad , \; \alpha_2 = \frac{(k - v_0)}{v_0\, s_0} > 0 \quad , \; \alpha_3 = \frac{E}{k\, C_\infty} = \frac{C_P}{C_\infty} > 0 \,.$$

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

$$(12) \qquad C(s(t),t) = \frac{C_\infty}{H(s(t))} \;\; (= C(s(t)\,) \quad , \quad t > 0 \,,$$

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

The solution of the problem (9) is computed numerically and the results are plotted for the interface concentration $C(s(t),t)$ vs. s and the interface position s(t) vs. t respectively as a function of the dimensionless parameter k/v_0 [ReTaCal]. We deduce that if the parameter k/v_0 is small (e.g.: 1.5 or 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. It follows that if the nutrient concentration C_∞ increases or k/v_0 is large then the counterdiffusion is null and the growth is faster. On the other hand, 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 [Ba, Wr].

Let γ be the parameter defined by:

$$(13) \qquad \gamma = \frac{E}{(k - v_0)\, C_\infty} \quad \left(= \frac{\alpha_1}{\alpha_2} \right).$$

We can prove that :

i) $\gamma < 1$ implies that $C(s(t),t)$ has a minimun value because the absorption power k is large with respect to v_0 and there is no counterdiffusion.

ii) $\gamma = 1$ implies that $C(s(t),t)$ is constant.

iii) $\gamma > 1$ implies that $C(s(t),t)$ has a maximun value because k 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 [Cu3].

Conclusions: We conclude from the model presented above that:

* $s = s(t)$ increases when parameter k or C_∞ increases.
* $s = s(t)$ decreases when parameter E increases.
* $s = s(t)$ increases when parameter (k/v_0) increases and, k and v_0 are large.
* $s = s(t)$ does not vary in function of the parameters v_0, 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 γ increases, because from (9)−(11) we have for $\dot{s}(t)$ the following representation in function of the parameter γ:

$$\dot{s}(t) = \frac{k}{a}\left[1 - \frac{(k - v_0)}{k}\,\frac{G(s(t)) + \frac{1}{\alpha_2}}{G(s(t)) + \frac{1}{\gamma\,\alpha_2}}\right], \qquad t > 0.$$

This conclusion agrees with the first three conclusions.

Finally, we can remark that the model presented here 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.

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