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SECOND WORKSHOP ON MATHEMATICS IN INDUSTRY

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AN INTRODUCTION TO FREE BOUNDARY PROBLEMS

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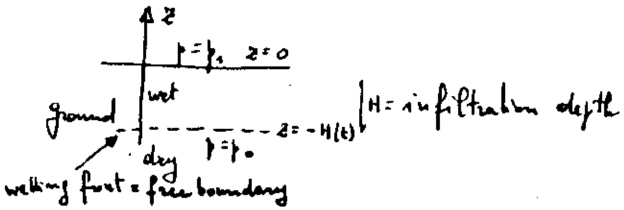
An Introduction to Free Boundary Problems

I. Examples

1. A simple model for water infiltration. (Green-Ampt, 1911)



Darcy's law : $\vec{v} = -\kappa\,(\nabla p + \rho\vec{g})$

incompressibility $\operatorname{div}\vec{v} = 0 \Rightarrow \nabla^2 p = 0$ in the wet region.

The velocity of the moving front is

$$-\dot{H} = -\kappa\left(\frac{p_1 - p_0}{H} + \rho g\right)$$

Separating the variables and integrating

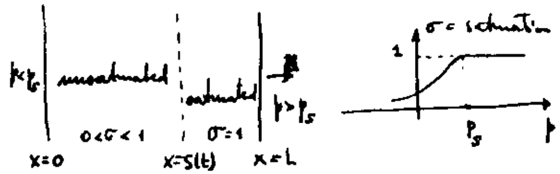
$$H - b\ln\left(1 + H/b\right) = a t$$

with $b = \dfrac{p_1 - p_0}{\rho g}$, $a = \kappa\rho g$

For small times $H \simeq \left[2\kappa(p_1 - p_0)t\right]^{1/2}$,
for large times $H \simeq \kappa\rho g\, t$.

<u>Remark</u> : this is a free boundary problem for the o.d.e. $p''(z) = 0$.
All the characteristic features of a f.b.p. are present, including nonlinearity.

2. Flows in partially saturated media.



In Darcy's law the hydraulic conductivity κ is some function of σ.

Mass balance : $\dfrac{\partial\sigma}{\partial t} = \nabla\cdot(\kappa\nabla h)$, $h = p + \rho g z$ (hydraulic head)

For simplicity we neglect gravity and we write (one dimension)

$$\frac{\partial\sigma}{\partial t} = \frac{\partial}{\partial x}\left[\kappa(p)\frac{\partial p}{\partial x}\right].$$

Introducing

$$u = \int_{p_s}^{p} \kappa(\eta)\,d\eta \qquad \begin{cases} u < 0 : \text{unsaturated} \\ u > 0 : \text{saturated} \end{cases}$$

$$a(u) = \left[\sigma'(p)/\kappa(p)\right]^{-1}_{p = p(u)}$$

we get

$$(1) \qquad a(u)\,u_{xx} - u_t = 0 \quad , \quad u < 0$$

$$(2) \qquad u_{xx} = 0 \quad , \quad u > 0$$

If $u = u_0 > 0$ is prescribed at the saturated (external) boundary, since $u = 0$ at the interface $x = s(t)$, from (2) we derive

$$u = u_0\,\frac{x - s(t)}{L - s(t)}$$

in the saturated zone.

The continuity of velocity across the interface $x=s(t)$ implies the continuity of p_x, i.e. of u_x. This motivates the free boundary conditions

(3) $$u(s(t),t) = 0$$

(4) $$u_x(s(t),t) = \frac{u_0}{L - s(t)}$$

The corresponding free boundary problem consists in finding a pair (s,u) such that

- s is continuous in some interval $[0,T]$
- u is continuous in the closure of the domain $D = \{(x,t) : 0<x<s(t),\ 0<t<T\}$
- u_x is continuous up to $x=s(t)$
- eq. (1) is satisfied in D
- the free boundary conditions (3), (4) are satisfied for $t \in (0,T)$

and satisfying the initial conditions

(5) $$s(0) = s_0 \in (0,1)$$

(6) $$u(x,0) = u_0(x) < 0 \quad , \ 0<x<s_0$$

in addition to some boundary condition at $x=0$.

Remark. The free boundary conditions are of Cauchy type.

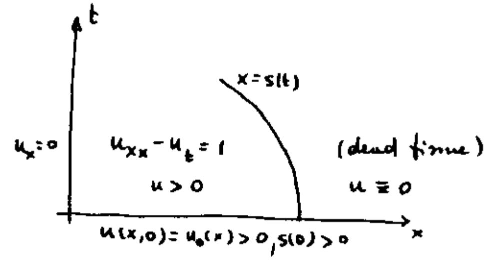
Remark. The statement above defines a classical solution of the problem.

3. Another f.b.p. with Cauchy data.

Diffusion-consumption of oxygen in a living tissue.

u = normalised non-dimensional oxygen concentration

1 = " " rate of oxygen consumption



free boundary conditions

$$u(s(t),t) = 0 \qquad \text{(continuity)}$$

$$u_x(s(t),t) = 0 \qquad \text{(no oxygen exchange)}$$

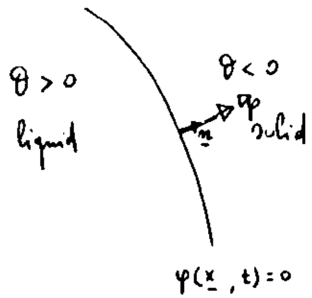
Remark. In the examples seen so far the free boundary is characterised by the discontinuity of some quantity which is relevant to the physical problem:

Ex.1 σ (saturation) jumps from 1 (saturated soil) to 0 (dry soil).

Ex.2 $\sigma'(p)$ can be discontinuous, in any case the governing equation is parabolic on one side of the f.b. and elliptic on the other.

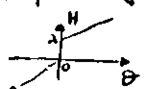
Ex.3 The oxygen consumption rate jumps to 1 (living tissue) to 0 (dead tissue).

4. Change of phase (Stefan problem)



, $\varphi \in C^1$

The jumping quantity is enthalpy



$H = \int_0^\theta c(\xi)\,d\xi + \lambda h(\theta)$ [h = Heaviside]

$\theta = 0$ (rescaled melting point) at the interface

Heat diffusion

$$c(\theta)\frac{\partial\theta}{\partial t} = \nabla\cdot\left[k(\theta)\nabla\theta\right]$$

in each phase.

Heat balance (Stefan) condition at the interface

$$\underline{n}\cdot\left[-k\nabla\theta\right]_L^S = \left[H\right]_L^S \underline{v}\cdot\underline{n}$$

$[\ ]_L^S$ = jump, H = enthalpy, $\underline{v}$ front velocity

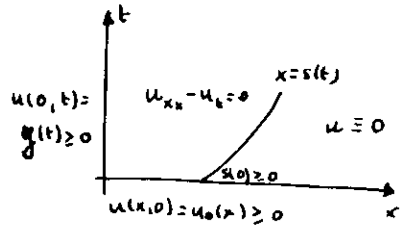
Note that $[H]_L^S = -\lambda$ (latent heat)

Writing $\underline{n} = \nabla\varphi/|\nabla\varphi|$

$$\left[k^S\nabla\theta^S - k^L\nabla\theta^L\right]\cdot\nabla\varphi = -\lambda\frac{\partial\varphi}{\partial t}$$

~~The Stefan problem~~ One space dimension : $\varphi = x - s(t)$

a) One-phase : melting of ice at 0°C



u = normalized non-dimensional temperature

x, t rescaled variables

$u = 0$ melting point

Free boundary conditions $[\, s \in C^1(0,T) \cap C([0,T]) \,]$

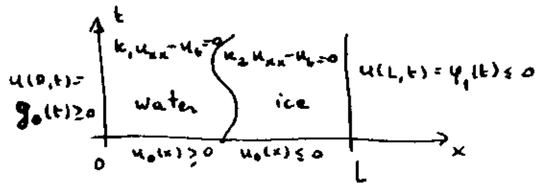
$$u(s(t), t) = 0 \qquad \text{(continuity)}$$

$$-u_x(s(t), t) = \lambda\,\dot{s}(t) \qquad \text{(Stefan condition = heat balance)}$$

(λ is associated to latent heat, $\lambda = 1$ with suitable rescaling)

<u>Remark</u> : the f.b. is monotone.

b) Two-phase problem



Free boundary conditions

$$u(s(t)-, t) = u(s(t)+, t) = 0$$

$$k_2 u_x(s(t)+, t) - k_1 (s(t)-, t) = \lambda\,\dot{s}(t)$$

5. Generalizations of Stefan problems.

We can state a Stefan-like problem for a more general parabolic equation, with more general conditions on the known boundary, and also with more general free boundary conditions.

For instance the condition $u(s(t),t)=0$ can be replaced by

(•) $$u(s(t),t) = f(s(t),t),$$

f being a prescribed function of x and t. The Stefan condition (one phase) can be substituted by

(∘) $$\dot s(t) = \psi(s, t, u_x)$$

or even by condition of higher order, like

(∘∘) $$\dot s(t) = \psi(s, t, u, u_x, u_{xx})$$

or

(∘∘∘) $$\dot s(t) = \psi(s, t, u, u_x, u_{xx}, u_{xxx}),$$

all coming from physical problems.

When applying higher order f.b. conditions we may have to replace (•) by a condition involving u_x (if we use (∘∘)) or even u_{xx} (if we use (∘∘∘)).

Remark : another type of generalization of the "simple" Stefan problem is just to suppress the identification of phases with the sets $\{u>0\}$, $\{u<0\}$. In such a case the free boundary may not coincide with the whole set $\{u=0\}$.

6. Relationship between free boundary problems with Cauchy data and Stefan-like problems.

This section refers to one-dimensional problems only.

Consider the following f.b.p. with Cauchy data

$$(CP)\quad \begin{cases} u_{xx} - u_t = q(x,t), & 0<x<s(t),\ 0<t<T \\ s(0) = s_0 \geq 0 & \\ u(x,0) = h(x), & 0<x<s_0 \\ u(0,t) = \varphi(t), & 0<t<T \\ u(s(t),t) = f(s(t),t), & 0<t<T \\ u_x(s(t),t) = g(s(t),t), & 0<t<T, \end{cases}$$

assuming all the data are smooth.

We observe that a Stefan type free boundary condition contains an explicit information on the function $s(t)$. This is of great advantage in looking for a classical solution.

For this reason it is useful to see when (CP) is amenable to a problem of Stefan type.

Let us consider the following three cases

(a) $g(x,t) \neq f_x(x,t)$, $x \geq 0$, $0 \leq t \leq T$,

(b) $g(x,t) = f_x(x,t)$, $f_{xx} - f_t \neq q$, $x \geq 0$, $0 \leq t \leq T$,

(c) $g(x,t) = f_x(x,t)$, $f_{xx} - f_t = q$, $x \geq 0$, $0 \leq t \leq T$.

It is easy to see that in cases (a), (b) the problem is equivalent to a Stefan type problem (provided some compatibility conditions are fulfilled), while in case (c) it is ill-posed.

Indeed, assume (a) is satisfied. We can (formally) write the following problem for the function

$$v(x,t) = u_x(x,t):$$

$$\text{(I)}\quad \begin{cases} v_{xx} - v_t = q_x, & 0<x<s(t),\ 0<t<T, \\ s(0)=s_0 \geq 0 & \\ v(x,0) = h'(x), & 0 \leq x \leq s_0 \\ v_x(0,t) = \dot\varphi(t) + q(0,t), & 0<t<T, \\ v(s(t),t) = g(s(t),t), & \\ (f_x - g)\dot s = v_x(s(t),t) - \left[f_t(s(t),t) + q(s(t),t)\right]. & \end{cases}$$

If we are able to find a solution (s,v) of (I), we can get a solution (s,u) of (CP) by means of the transformation

$$\text{(A)}\quad u(x,t) = -\int_x^s v(\xi,t)\,d\xi + f(s(t),t)$$

The required compatibility conditions are

$$h(s_0) = f(s_0,0), \quad h(0) = \varphi(0), \quad h'(s_0) = g(s_0,0)$$

<u>Remark</u>. The coefficient $f_x - g$ plays the role of a "latent heat"

Assuming (b), we set

$$w(x,t) = u_{xx}(x,t)$$

and formally derive the following system

$$\text{(II)}\quad \begin{cases} w_{xx} - w_t = q_{xx}, & 0<x<s(t),\ 0<t<T \\ s(0)=s_0 & \\ w(x,0) = h''(x), & 0 \leq x \leq s_0 \\ w(0,t) = \dot\varphi(t) + q(0,t), & 0<t<T \\ w(s(t),t) = f_t(s(t),t) + q(s(t),t), & 0<t<T \\ \left[f_{xx} - f_t - q\right]_{x=s(t)} \dot s(t) = w_x(s(t),t) - \left[f_{xt} + q_t\right]_{x=s(t)}. & \end{cases}$$

After solving (II), the pair (s,u) solving (CP) can be obtained by means of

$$\text{(B)}\quad u(x,t) = \int_x^{s(t)} \int_\eta^{s(t)} w(\xi,t)\,d\xi\,d\eta - (s(t)-x)\,f_x(s(t),t) + f(s(t),t),$$

with usual compatibility conditions $[h'(s_0) = f_x(s_0,0)]$

<u>Remark</u>. The role of latent heat is now played by $f_{xx} - f_t - q$.

<u>Remark</u>. If the differential equation is e.g. of the type

$$a(u)\,u_{xx} - u_t = 0$$

(see Ex. 2), we can still differenciate the free boundary conditions along the free boundary $x = s(t)$ in order to let $\dot s$ appear explicitly. This technique leads to the higher order free boundary conditions previously mentioned.

<u>Remark</u>. Note that in the reduced problems (I) and (II) the "phase" is not identifiable by any inequality, that is to say that there is no quantity playing the role of a "melting point".

Finally, let us assume that (C) is satisfied and try to iterate the procedure, observing that (II) is now a problem with Cauchy data:

$$w_{xx} - w_t = q_1 ,$$
$$w(s(t),t) = f_1 ,$$
$$w_x(s(t),t) = g_1 ,$$

with $q_1 = q_{xx}$, $f_1 = f_t + q$, $g_1 = f_{xt} + q_x$.

We immediately realize that

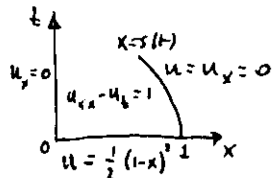
$$f_{1x} = g_1 , \quad f_{1xx} - f_{1t} = q_1$$

i.e. the new data still satisfy (C). Therefore (CP) will not be reducible to any Stefan type problem.

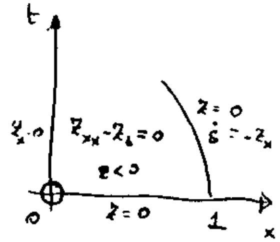
In such a case it is not difficult to find examples showing that (s,u) cannot depend continuously on the data.

Remark: importance of compatibility conditions.

Consider the oxygen diffusion-consumption problem

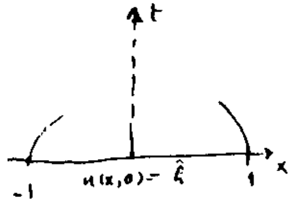


Here the data are such that u_x is not continuous at the origin. If we apply the procedure of reduction to a Stefan problem we get that the pair (s,z) with $z = u_{xx} - 1 = u_t$ formally satisfies the Stefan problem

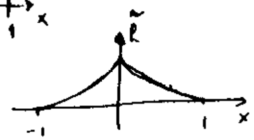


but is obviously singular at the origin (otherwise we would have the trivial solution $z=0$, $s=1$).

As a matter of fact, if we reflect the domain about the t-axis, the initial datum $\tilde{\ell}$ for the original problem



has the form



$$\tilde{\ell} = \begin{cases} \frac{1}{2}(1-x)^2 , & x>0 \\ \frac{1}{2}(1+x)^2 , & x<0 \end{cases}$$

and $\tilde{\ell}'$ is discontinuous. This produces a singularity of u_{xx} of the same type of the fundamental solution of the heat equation.

However the problem possesses a unique classical solution.

Remark. Singularities occurring at the point $(s(0),0)$ may have much more serious consequences (they may even imply non-existence). Therefore proving existence of a solution of (CP) usually requires strong conditions on $\ell(x)$ at $x=s(0)$.

II. SOME SIMPLE RESULTS

1. Self-similar solution for the one-phase Stefan problem.

A self-similar solution of the heat equation $u_{xx}-u_t=0$ is a solution depending on x and t through the ratio $\frac{x}{2\sqrt{t}}$.
It is easily verified that the function

$$v(x,t)=\int_0^{\frac{x}{2\sqrt{t}}} e^{-\rho^2}\,d\rho$$

meets such a requirement.

Let us try to construct a self similar solution for the heat equation satisfying the free boundary conditions

$$u(s(t),t)=0,\quad u_x(s(t),t)=-\dot{s}.$$

If the basic structure of u is the same as v, then we expect that $x=s(t)$ has to be a parabola

$$s(t)=c\sqrt{t},$$

since v is constant along such a curve (where we want u to be zero).
Let us compute

$$v_x(s(t),t)=\frac{1}{2\sqrt{t}}e^{-c^2/4}$$

and compare it with

$$\dot{s}(t)=\frac{c}{2\sqrt{t}}.$$

We get

$$\dot{s}(t)= c\, e^{c^2/4}\, v_x(s(t),t).$$

Therefore we are led to the following choice of u

$$u(x,t)=-c\,e^{c^2/4}\{v(x,t)-v(s(t),t)\},$$

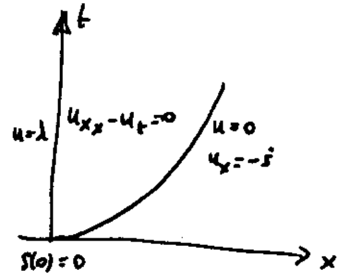
i.e.

$$u(x,t)=c\,e^{c^2/4}\int_{\frac{x}{2\sqrt{t}}}^{c/2} e^{-\rho^2}\,d\rho.$$

This is called Neumann's solution.
It value at $x=0$ is constant

$$u(0,t)\equiv\lambda = c\,e^{c^2/4}\int_0^{c/2}e^{-\rho^2}\,d\rho,$$

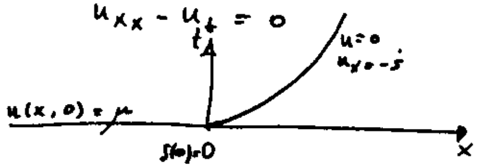
so it solves the Stefan problem



Moreover, since $\lim_{t\downarrow 0} u(x,t)$ for $x<0$ is

$$u(x,0)\equiv\mu = c\,e^{c^2/4}\int_{-\infty}^{c/2}e^{-\rho^2}\,d\rho,$$

also constant, the same function solves the following initial value Stefan problem

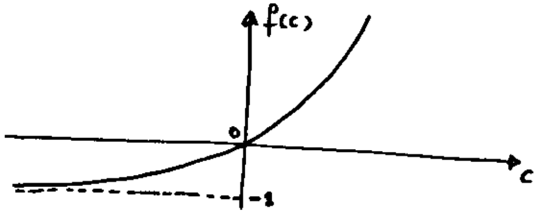


Now we have found u given c, i.e. given the free boundary (so we have solved the inverse problem).

The direct problem would be e.g.: given μ, find c.

We can solve this problem looking at the diagram of the function

$$f(c) = c\, e^{c^2/4} \int_{-\infty}^{c/2} e^{-\rho^2} d\rho$$



and conclude that we find a unique value of c for

$$\mu > -1$$

<u>Questions</u>: what is the meaning of the problem when $\mu \in (-1,0)$?
does any solution exist for $\mu \leq -1$?

2. The "supercooled" problem.

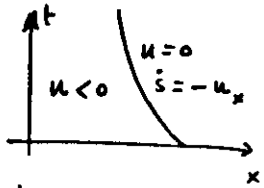
In the usual one-phase melting problem $(u>0)$ the Stefan condition is $\dot s = -u_x$.

In the solidification problem $(u<0)$ the Stefan condition is $\dot s = u_x$.

melting solidification

In both cases the phase change front is monotonically increasing: this is an immediate consequence of the maximum principle and of the so-called boundary point principle, in agreement with the physical interpretation.

For the same reason in the following situation



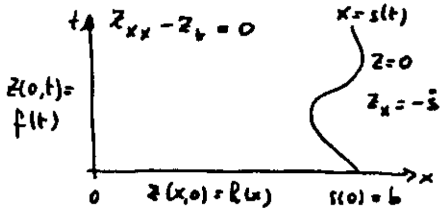
the free boundary is decreasing. This corresponds to change the sign of latent heat in the solidification process. If we still like to interpret the problem in terms of change of phase, we should say that we are solidifying a supercooled liquid.

<u>Remark</u>: it makes more sense to look at this problem as originating e.g. from the oxygen-consumption scheme.

<u>Remark</u>: note that for Neumann's solution $\mu<0 \Rightarrow c<0$.

3. A nonexistence result.

Let us consider the Stefan problem



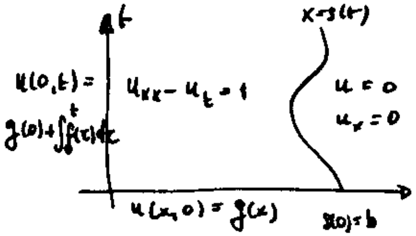
(SP)

where we make no sign assumptions on the data f, h, which are just supposed to be bounded and piecewise continuous.

The transformation

$$u(x,t)=\int_x^{s(t)}\int_\xi^{s(t)}[z(y,t)+1]\,dy\,d\xi \quad , \; 0\le x\le s(t)$$

provides the solution of the associated oxygen diffusion-consumption problem



(ODC)

with
$$g(x)=\int_x^b\int_\xi^b[h(y)+1]\,dy\,d\xi$$

THEOREM. If for some $\sigma>0$ we have

(*) $\qquad g(x)\le 0 \quad \text{for} \quad x\in(b-\sigma,\sigma)$,

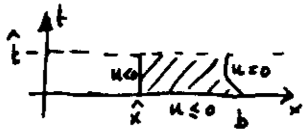
then (SP) [(ODC)] has no solution.

<u>Proof</u>. From (*) either $g\equiv 0$ in $(b-\sigma,\sigma)$ or $g(x_0)<0$ for some $x_0\in(b-\sigma,\sigma)$. In both cases there exist $\hat{x}$ and $\hat{t}$ such that

$$u(\hat{x},t)<0 \quad \text{for} \quad 0<t<\hat{t}$$

(when $g\equiv 0$ use the differential equation).

Now apply the (strong) maximum principle in the domain



and conclude that $u<0$ inside. Now the boundary point principle says that $u_x(s(t),t)$ must be positive for $t\in(0,\hat{t})$, thus contradicting the free boundary condition $u_x=0$. ∎

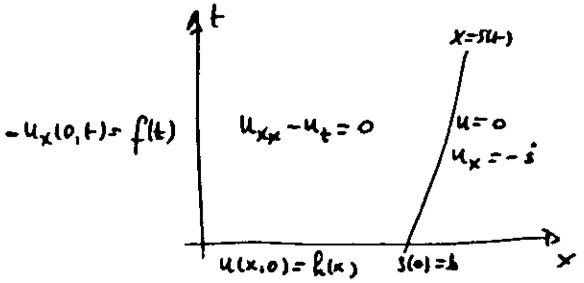
<u>Remark</u>: the result depends on the <u>local</u> behaviour of the function $g(x)$ near $x=b$.

<u>Remark</u>: a sufficient condition for $h(x)$ in order to get (*) is

(**) $\qquad h(x)\le -1 \quad \text{for} \quad x\in(b-\sigma,\sigma)$.

4. Monotone dependence and uniqueness.

We consider a Stefan problem of this type



$f \geq 0$, $h \geq 0$
and
either $f \not\equiv 0$ or $h \not\equiv 0$
$\Rightarrow u > 0$

Integrating the differential equation over the domain $0<x<s(\tau)$, $0<\tau<t$, we get the following equality

$$(\square) \qquad s(t) = b + \int_0^b h(x)\,dx + \int_0^t f(\tau)\,d\tau - \int_0^{s(t)} u(x,t)\,dx,$$

representing the overall thermal balance.

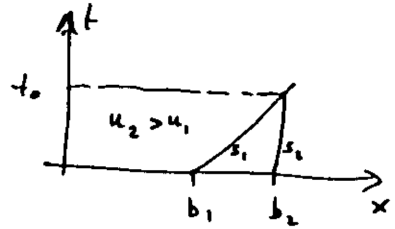
Let now (s_1,u_1) and (s_2,u_2) be solutions corresponding to the respective sets of data (f_1,h_1,b_1), (f_2,h_2,b_2).

We prove the following comparison result.

THEOREM. If $f_1 \leq f_2$, $h_1 \leq h_2$, $b_1 \leq b_2$ then $s_1 \leq s_2$.

<u>Proof</u>. Assume first $b_1<b_2$ and prove that $s_1<s_2$.

If the two boundaries meets for the first time at some point $t=t_0$, then we have $u_2>u_1$ for $0<x<s_1(t)$, $0<t<t_0$



by the maximum principle. Moreover $u_2=u_1=0$ at the point of intersection. We know that this implies $(u_2-u_1)_x\big|_{(s_1(t_0),t_0)}<0$, i.e. $u_{2x}<u_{1x}$ at $(s(t_0),t_0)$, implying in turn $\dot s_2(t_0)>\dot s_1(t_0)$. Thus t_0 cannot be the first intersection time and we have proved that $s_1<s_2$.

Now take $b_2=b_1$. Of course the above argument fails, but for any $\delta>0$ we can consider a solution (s_2^δ,u_2^δ) of the problem with data $(f_2, \tilde h_2, b_2+\delta)$, where $\tilde h_2(x)$ is $h_2(x)$ for $x\in(0,b_2)$ and is zero outside [it can be proved that such a solution always exists]. We have seen that

$$s_1<s_2^\delta, \quad s_2<s_2^\delta.$$

Let us now compare s_2 and s_2^δ. To this aim we use $(\square)$ and we get

$$s_2^\delta(t)-s_2(t) = \delta - \int_0^{s_2(t)} \{u_2^\delta(x,t)-u_2(x,t)\}\,dx - \int_{s_2(t)}^{s_2^\delta(t)} u_2^\delta(x,t)\,dx.$$

Since $u_2^\delta \geq 0$ and $u_2^\delta \geq u_2$ (maximum principle), we conclude that

$$s_2^\delta(t) \leq s_2(t)+\delta.$$

So we arrived at the following comparison

$$s_1(t) \le s_2(t) + \delta$$

which gives the desired result by letting δ tend to zero. ∎

COROLLARY. The problem considered cannot have more than one solution.

5. Existence and continuous dependence upon the data.

These are much harder questions which will not be treated here.

We just mention that techniques for showing existence are usually based on fixed point arguments. If e.g. we have to solve a f.b.p. with f.b. conditions of the type

$$u(s(t),t) = 0$$
$$\dot{s}(t) = \varphi(s(t), t, u_x(s(t),t))$$

we can look for the free boundary $x = s(t)$ as a fixed point of the following mapping:

(a) take a function $z(t)$ in a suitable subset X of $C^1(0,T)$

(b) solve the equation $v_{xx} - v_t = 0$, subjected to the same initial condition as u and to the same boundary condition at $x=0$, and such that $v(z(t),t) = 0$

(c) compute $v_x(z(t),t)$

(d) define the mapping $\mathcal{T} : z \to \rho$

$$\rho(0) = z(0) = s(0), \quad \dot{\rho}(t) = \varphi(z(t), t, v_x(z(t),t)).$$

Under suitable assumptions on the data it is possible to choose X and T in such a way that $\mathcal{T}$ is a contraction mapping from X to itself, thus proving existence and uniqueness for small times.

Then other questions come: can the solution be continued? if not, how does it behave near the extinction time?

6. Weak formulations.

The above technique generally works for one-dimensional problems only. For multidimensional problems it is preferable (when possible) to use a different formulation in which the free boundary conditions do not appear explicitly but are - so to speak - "hidden" in some singularity of the governing differential equation. This is often called a "weak formulation".

Here are two examples.

A) The oxygen diffusion-consumption problem.

Write the differential equation in the form

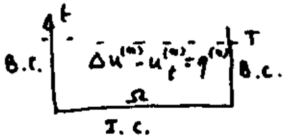
$$u_{xx} - u_t = g(u) \qquad , \; 0<x<1 \; , \; 0<t<T$$

where $g(u)=1$ if $u>0$ and $g(u)=0$ otherwise.

This is an equation with a discontinuous term so we need a slightly different definition of solution (i.e. u_{xx}, u_t need not be continuous over the rectangle $(0,1)\times(0,T)$).

More generally x can be a point in some bounded domain $\Omega \subset \mathbb{R}^n$ and Δu appears in the equation.

A typical method ~~f~~ for solving the problem is to consider a sequence $g^{(n)}(u)$ of smooth approximations ~~to~~ $g(u)$ and then solve



and show that the sequence $\{u^{(n)}\}$ is compact in some Banach space and in some sense. Next we perform a limit (in a suitable sense) along a convergent subsequence and we show that the limit function satisfies the weak version of the original problem.

B) The Stefan problem.

Making use of the enthalpy function we write the heat balance equation over the whole domain in the form

$$\frac{\partial h(\theta)}{\partial t} = \nabla \cdot [k(\theta)\nabla\theta] .$$

Of course, since $h(\theta)$ is not continuous this equation must be interpreted in a particular sense, usually called the "distributional sense".

Once again the way to handle it is to take smooth approximations $h^{(n)}$ to h, solve the corresponding nonlinear boundary value problems, show that the resulting sequence $\{\theta^n\}$ has some compactness property, etc.

Remark. After such generalized solutions are obtained one has to investigate their regularity and possibly get some information on the set $\{u=0\}$. This is usually an extremely hard task.

III THE DEAD CORE PROBLEM

1- Motivation : the diffusion-reaction system.

Assume we have a chemical substance diffusing through a medium and undergoing at the same time some chemical reaction.

Then if c denotes the concentration of the diffusing reactant and T denotes absolute temperature, we have the following mass and heat balance equations

(1)
$$\frac{\partial c}{\partial t} - D\Delta c = -A c^m e^{-E/RT}, \qquad c \geq 0,$$

(2)
$$C\frac{\partial T}{\partial t} - \kappa \Delta T = Q A c^m e^{-E/RT}, \qquad T > 0.$$

The right hand side of (1) describes the rate at which the chemical disappears because of the reaction : A is a positive constant (called pre-exponential factor), $m \geq 0$ is the order of the reaction, E is a positive constant (the activation energy) and R is the universal gas constant. The right hand side of (2) is the rate at which heat is released ($Q>0$) or absorbed ($Q<0$) in the reaction. If $Q=0$ the reaction is isothermal.

The statement of the problem is completed by giving information on c and on T for $t=0$ and at the boundary of the region where the reaction is taking place.

Now if we formally solve this system writing $|c|^m$ instead of c^m in (1), (2), we may find negative values for c. In such a case the solution looses its physical meaning.

Therefore its clear that the correct way of writing (1), (2) is to use $(c_+)^m$ on the right hand side. This will prevent c to become negative. However, if the reaction rate is strong enough c can vanish over some subregion, forming the so-called dead core. The boundary of the dead core is of course a free boundary.

We shall investigate the existence of the dead core in the simplest case : isothermal reaction ($Q=0$), one space dimension ($\Delta = \frac{\partial^2}{\partial x^2}$) and steady state ($\frac{\partial c}{\partial t}=0$).

2. The stationary dead core in one dimension for isothermal reactions.

Equation (1) reduces to

(3)
$$u_{xx} = \lambda u_+^m, \qquad u_+ = \max(0,u),$$

for some positive λ.

First we want to solve the boundary value problem

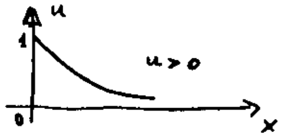
(4)
$$u(0) = 1, \qquad \lim_{x\to+\infty} u(x) = 0.$$

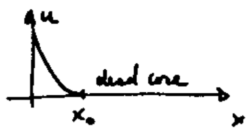
Note that since $u_{xx} \ge 0$, u_x has a limit for $x \to +\infty$ and owing to (4) such a limit must be zero.

Now we multiply eq. (3) by u_x and integrate w.r.t. x. As long as u is positive we get

(5) $$\frac{1}{2}\left[u_x^2(x) - u_x^2(0)\right] = \lambda\left(\frac{u^{m+1}}{m+1} - \frac{1}{m+1}\right)$$

We have two possibilities





In both cases it is clear that we can replace u^{m+1} by u_+^{m+1} and that the fact that both u and u_x go to zero as x goes to ∞ implies $\frac{1}{2}u_x^2(0) = \frac{\lambda}{m+1}$.

Moreover we observe that $u_x \le 0$ for any x. Therefore (5) takes the form

(6) $$u_x = -\left(\frac{2\lambda}{m+1}\right)^{1/2} u_+^{\frac{m+1}{2}}$$

As long as u is positive we can separate the variables and write

(7) $$\left(\frac{m+1}{2}\right)^{1/2}\int_u^1 \frac{dz}{z^{(m+1)/2}} = \lambda^{1/2} x .$$

Let us define

$$I = \lim_{u \downarrow 0}\left(\frac{m+1}{2}\right)^{1/2}\int_u^1 \frac{dz}{z^{(m+1)/2}}$$

We have $I = +\infty$ if $m \ge 1$, $I < +\infty$ if $m < 1$.

It means that if $m \ge 1$ the solution u can never attain the value zero, while if $m < 1$ u becomes zero at the point

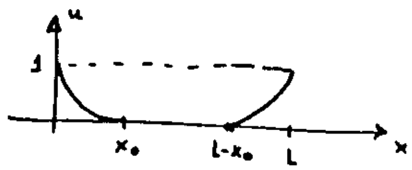
(8) $$x_0 = \lambda^{-1/2} I = \lambda^{-1/2}\,\frac{[2(m+1)]^{1/2}}{1-m} .$$

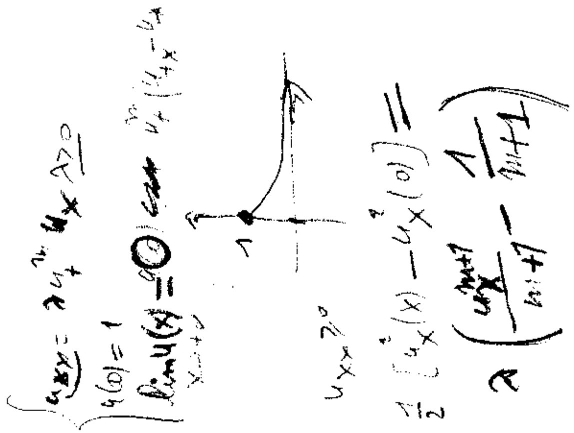
Of course $u \equiv 0$ for $x > x_0$.

If we now consider the boundary value problem for (3) in a bounded layer of thickness L

(9) $$u(0) = u(L) = 1$$

we will have a dead core provided that $L > x_0$:





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35 R 35