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Workshop on Mathematical Modelling of Energy and Mass Transfer Processes, and Applications

Domingo A. Tarzia

Rodolfo H. Mascheroni (Eds.)

Departamento de Matemática, Rosario, Argentina

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SERIE A: CONFERENCIAS, SEMINARIOS Y TRABAJOS DE MATEMÁTICA

No. 15

WORKSHOP ON MATHEMATICAL MODELLING OF ENERGY AND MASS TRANSFER PROCESSES, AND APPLICATIONS

Domingo A. Tarzia – Rodolfo H. Mascheroni (Eds.)

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Rosario, Diciembre 2008

Within the frame of activities planned for the Project PAV2003-00120: Applications and Interdisciplinary Integration of Mathematics, Subproject # 5: Mathematics and Physics: "Modeling and Mathematical Analysis of the Heat and Mass Transfer and its Applications", financed by the National Agency of Scientific and Technological Promotion of Argentina (ANPCyT), the VII School on Energy and Mass Transfer, Free Boundary Problems and Applications (Rosario, November 28 – December 3, 2005) and the TEM2005-Workshop on Mathematical Modelling of Energy and Mass Transfer Processes and Applications (Rosario, December 5-7, 2005) achieved in Rosario, Argentina. The scientific committee was integrated by Juan C. Gottifredi (INIQUI (CONICET–UNSa), Salta), Rodolfo H. Mascheroni (CIDCA (CONICET–UNLP), La Plata), Rubén Piacentini (IFIR (CONICET–UNR), Rosario) and Domingo A. Tarzia (CONICET–UA, Rosario, Coordinator). The local organizing committee was integrated by Adriana C. Briozzo (UA, Rosario, Coordinator), Eduardo Luccini (IFIR (CONICET–UNR), Rosario), María F. Natale (UA, Rosario), Mariela Olguin (UA-UNR, Rosario), Eduardo A. Santillan Marcus (UA, Rosario) and María C. Sanziel (UNR, Rosario).

The goals of these events were:

- Physical-chemical treatment and mathematical modeling of energy and mass transfer problems related to diverse applications.
- Theoretical and numerical study of parabolic and elliptical differential equations with constant and temperature variable thermal coefficients, and Volterra integral equations, and also of variational inequalities involved in these processes.
- Entailment and accomplishment of agreements with research groups and/or other Argentine and foreign basic and applied research institutions of international level, in which analogous problems to those proposed in the Project are studied in order to induce a useful scientific interaction.
- Formation of Doctors and young researchers in the energy and mass transfer applied mathematical techniques, of fundamental importance in a great number of practical applications.

The VII School on Energy and Mass Transfer, Free Boundary Problems and Applications has consisted of eight courses:
Course 1: "Modelling and Simulation in Food Technology", by Rodolfo H. Mascheroni – Viviana O Salvadori (CIDCA (CONICET–UNLP), La Plata);
Course 2): "Nonlinear Diffusion Equations: Applications, Models and Solutions", by Philip Broadbridge (Australian Mathematical Sciences Institute, University of Melbourne, Australia);
Course 3: "Numerical Analysis of Parabolic Equations", by Ricardo Durán (UBA–CONICET, Buenos Aires);
Course 4: "Inverse Problems in Heat Conduction: Regularization Methods", Rubén D. Spies (IMAL (CONICET–UNL), Santa Fe);
Course 5: "The Blow-up Problem for Semi Linear and Quasilinear Parabolic Equations", by Arturo De Pablo (Univ. Carlos III de Madrid, Leganés, España);
Course 6): "Differential Equations: Perturbation Technics and Superposition" by Juan C. Gottifreddi (INIQUI (CONICET –UNSa), Salta);
Course 7: "Moving and Free Boundary Problems for the One-Dimensional Heat Equation" by Domingo A. Tarzia (CONICET–Univ. Austral, Rosario);
Course 8: "Energy and Mass Transfer in Photo Reactors. Application to Advanced Oxidation Processes for the Reduction of the Environmental Pollution" by Orlando M. Alfano (INTEC (CONICET–UNL), Santa Fe).

The Workshop on Mathematical Modelling of Energy and Mass Transfer Processes and Applications (TEM2005) has consisted of lectures and communications.

Lectures:
1) Mahdi Boukrouche (Univ. de Saint Etienne, Saint Etienne, France), "On a nonisothermal nonnewtonian lubrication problem with Tresca law. Existence and asymptotics of solutions".
2) Philip Broadbridge (Australian Mathematical Sciences Institute, University of Melbourne, Australia), "Exact solution of nonlinear boundary value problems for surface diffusion".

3) Alberto Cassano (INTEC (CONICET–UNL), Santa Fe), "Modeling and experimental verification of the degradation of trichloro-ethylene in air streams employing a fixed bed photocatalytic reactor made of glass fiber meshes coated with TiO_2".
4) Arturo De Pablo (Univ. Carlos III, Leganés, España), "Blow-up for the porous medium equation with a localized reaction"
5) Julio Deiber (INTEC (CONICET–UNL), Santa Fe), "Modeling fluid flow and heat transfer in consolidated and saturated porous media ".
6) Manuel Elgueta (P. Universidad Catolica de Chile), "Difusión no local"
7) Hugo Grossi (Univ. Nac. de Luján, Luján), "Evaluación de la irradiación solar global incidente en la superficie terrestre en Argentina: estado del conocimiento".
8) Pablo Marino (FUDE/FISI–SIDERCA, Buenos Aires), "La aplicación de modelos numéricos al control de hornos de recalentamiento de acero".
9) Nelson Moraga (Fac. de Ingeniería, Univ. de Santiago de Chile, Santiago, Chile), "Mathematical modeling and numerical simulation of energy and mass transfer processes with finite volume method".
10) Rubén Piacentini (IFIR (CONICET–UNR), Rosario), "Modelización matemática y mediciones de radiaciones solares".
11) Sergio Preidikman (Fac. de Ingeniería, UNRC, Río Cuarto), "Developing Nonlinear Models for Aeroelastic Behavior".
12) José Antonio Rabi (Univ. São Paulo, Brasil), "Mathematical modelling and numerical simulation of radon-222 exhalation from phosphogypsum-bearing materials and its air-borne concentration".
13) Juan Carlos Reginato (UNRC, Río Cuarto), "Some aspects on the dynamical modeling of nutrient uptake for root crops"
14) Amelia Rubiolo, (INTEC (CONICET–UNL), Santa Fe), "Multicomponent diffusion during salting and ripening cheeses".
15) Luis Saravia (INENCO (CONICET–UNSa), Salta), "Solar systems development in the Argentinian Northwest".
16) Ricardo Simpson (Univ. Técnica Federico Santa María, Valparaíso, Chile), "Simple, practical, and efficient on-line correction of process deviations: batch retort operations".
17) Luis T. Villa (INIQUI (CONICET–UNSa), Salta), "Some considerations on the well posedness model formulation of a immersion frying process in hot oil applied to natural potato"
18) Noemí Zaritzky (CIDCA (CONICET–UNLP), La Plata), "Modelado matemático de la transferencia de energía en los procesos de calentamiento y descongelación por microondas".

Communications:

TEM in Foods:
* R. Lozano (Salta), A. Boucíguez (Salta), M. A. Lara (Rosario), "Control de temperaturas en productos agrícolas utilizando sustancias de cambio de Fase"
* M. C. Olguin, M. A. Medina, M. C. Sanziel, D. A. Tarzia (Rosario), "Análisis del comportamiento de la solución al problema de Stefan con respecto a la variación en las propiedades físicas de una sustancia"
* L.A. Campañone, A. Paola, R. H. Mascheroni (La Plata), "Modelado y simulación de la transferencia de energía y materia durante el calentamiento de alimentos en hornos microondas".
* R. Lespinard, P. R. Salgado, R. H. Mascheroni (La Plata), "Modelado de la transferencia de calor en alimentos particulados en medio liquido, envasados en frascos de vidrio"
* D. F. Olivera, V. O Salvadori (La Plata), "Empleo de un software comercial en la simulación de la cocción de alimentos en hornos convectivos"
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Publications:
From these activities, lectures from Arturo De Pablo and Mahdi Boukrouche were published on MAT-Serie A #12 (2006) and MAT-Serie A #16 (2009) respectively. Here in MAT-Serie A #15 (2008) four communications received during 2007 and accepted on March 2008 are published.

THE CLASSICAL ONE-PHASE STEFAN PROBLEM WITH TEMPERATURE-DEPENDENT THERMAL CONDUCTIVITY AND A CONVECTIVE TERM

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Abstract

We study a one-phase Stefan problem for a semi-infinite material with temperature-dependent thermal conductivity and a convective term with a constant temperature boundary condition or a heat flux boundary condition of the type $-q_0/\sqrt{t}$ ($q_0 > 0$) at the fixed face $x = 0$. We obtain in both cases sufficient conditions for data in order to have a parametric representation of the solution of the similarity type for $t \geq t_0 > 0$ with t_0 an arbitrary positive time. We improve the results given in Rogers-Broadbridge, ZAMP, 39 (1988), 122-129 and Natale-Tarzia, Int. J. Eng. Sci., 41 (2003), 1685-1698 obtaining explicit solutions through the unique solution of a Cauchy problem with the time as a parameter and we also give an algorithm in order to compute the explicit solutions.

Key words : Stefan problem, free boundary problem, moving boundary problem, phase-change process, nonlinear thermal conductivity, fusion, solidification, similarity solution.

2000 AMS Subject Classification: 35R35, 80A22, 35C05

I. Introduction.

We consider Stefan problems for a semi-infinite region $x > 0$ with temperature-dependent thermal conductivity and a convective term with phase change temperature $\theta_f = 0$ [16]. In all of them is required to determine the evolution of the moving phase separation $x = s(t)$ and the temperature distribution $\theta(x, t)$. The modeling of this kind of systems is a problem with a great mathematical and industrial significance. Phase-change

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problems appear frequently in industrial processes an other problems of technological interest [1],[2],[8] - [14],[17]. A large bibliography on the subject was given in [27]. We consider one-phase Stefan problems in fusion process with nonlinear heat conduction equations.

Owing to [19], [24] we consider the following free boundary (fusion process) problem

$$\rho c\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial x}\left(k(\theta,x)\frac{\partial\theta}{\partial x}\right)-v(\theta)\frac{\partial\theta}{\partial x}\ ,\ 0<x<s(t)\ ,\ t>0 \tag{1}$$

$$k(\theta(0,t),0)\frac{\partial\theta}{\partial x}(0,t)=-\frac{q_0}{\sqrt{t}}\ ,\ q_0>0\ ,\ t>0 \tag{2}$$

$$k\left(\theta\left(s(t),t\right),s(t)\right)\frac{\partial\theta}{\partial x}\left(s(t),t\right)=-\rho l\overset{\bullet}{s}(t)\ ,\ t>0 \tag{3}$$

$$\theta\left(s(t),t\right)=0\ ,\ t>0\ ,\ s(0)=0 \tag{4}$$

where the thermal conductivity $k(\theta,x)$ and the velocity $v(\theta)$ are given by

$$v(\theta)=\rho c\frac{d}{2\left(a+b\theta\right)^2}\quad,\quad k(\theta,x)=\rho c\frac{1+dx}{\left(a+b\theta\right)^2} \tag{5}$$

and c,ρ and l are the specific heat, the density and the latent heat of fusion of the medium respectively, all of them are assumed to be constant with positive parameters a,d and real parameter b. This kind of nonlinear thermal conductivity or diffusion coefficients was considered in numerous papers, e.g. [3, 6, 7, 15, 20, 21, 25]. The nonlinear transport Eq.(1) arises in connection with unsaturated flow in heterogeneous porous media. If we set $d=0$ and $b=0$ in the free boundary problem $(1)-(5)$ then we retrieve the classical one-phase Lamé-Clapeyron-Stefan problem. The first explicit solution for the one-phase Stefan problem was given in [16]. Here $-q_0/\sqrt{t}$ denotes the prescribed flux on the boundary $x=0$ which is of the type imposed in [26]. We will determine which conditions on the parameters of the problem must be satisfied in order to have an instantaneous phase-change process.

In Section II we consider the free boundary problem $(1)-(4)$ with the nonlinear heat coefficients (5) under the hypotheses $b>0$ and $a>bl/c$, or $b<0$. We follow [19, 24] and we improve [19] in the sense that the existence of the explicit solution of the problem $(1)-(5)$ is obtained through the unique solution of the Cauchy problem $(55)-(56)$ in the spatial variable and the time t is a parameter for $t\geqslant t_0>0$ where t_0 is an arbitrary positive time. This explicit solution can be obtained as a function of a parameter δ which is given as the unique solution of the transcendental Eq. (38) . We also give an algorithm in order to compute the explicit solution for the temperature $\theta=\theta(x,t)$ and free boundary $x=s(t)$.

In Section III we consider the free boundary problem $(1),(3)-(4)$ with the nonlinear heat coefficients (5) and the temperature boundary condition (62) (with θ_0 is a constant temperature given on the fixed boundary $x=0$) instead of the heat flux condition (2)

under the hypotheses $a > 0, d > 0, b < 0$ and $a + b\theta_0 > 0$. We improve [19] obtaining the explicit solution through the unique solution of the Cauchy problem (92) − (93) in the spatial variable and the time t is a parameter for $t \geqslant t_0 > 0$ where t_0 is an arbitrary positive time. In this case, the explicit solution can be also obtained as a function of a parameter β which is the unique solution of the Eq. (85) . We also give an algorithm to compute the temperature $\theta = \theta(x,t)$ and free boundary $x = s(t)$. Other problems with nonlinear thermal coefficients in this subject are also given in [4, 5, 18, 22, 23].

II. Solution of the free boundary problem with heat flux condition on the fixed face.

We consider the problem (1) − (4) . Taking into account (5) we can put our problem as

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}\left(\frac{1+dx}{(a+b\theta)^2}\frac{\partial \theta}{\partial x} + \frac{d}{2b\,(a+b\theta)}\right)\ ,\ 0 < x < s(t)\ ,\ t > 0 \tag{6}$$

$$\frac{1}{(a+b\,\theta\,(0,t))^2}\frac{\partial \theta}{\partial x}(0,t) = -\frac{q_0^*}{\sqrt{t}}\ ,\ t > 0 \tag{7}$$

$$\frac{1+ds(t)}{a^2}\frac{\partial \theta}{\partial x}\,(s(t),t) = -\alpha \overset{\bullet}{s}(t)\ ,\ t > 0 \tag{8}$$

$$\theta\,(s(t),t) = 0\ ,\ t > 0\ ,\ s(0) = 0 \tag{9}$$

where $\alpha = \dfrac{l}{c}$, $q_0^* = \dfrac{q_0}{\rho c}$ and $a, d \in \mathbb{R}^+, b \in \mathbb{R}$.

If we define the transformations in the same way as in [20], [24]

$$\begin{cases} y = \dfrac{2}{d}\left[(1+dx)^{\frac{1}{2}} - 1\right] \quad , \quad \overline{S}(t) = \dfrac{2}{d}\left[(1+ds(t))^{\frac{1}{2}} - 1\right] \\ \overline{\theta}(y,t) = \theta(x,t) \end{cases} \tag{10}$$

we obtain the following free boundary problem

$$\frac{\partial \overline{\theta}}{\partial t} = \frac{\partial}{\partial y}\left(\frac{1}{\left(a+b\overline{\theta}\right)^2}\frac{\partial \overline{\theta}}{\partial y}\right)\ ,\ 0 < y < \overline{S}(t)\ ,\ t > 0 \tag{11}$$

$$\frac{1}{\left(a+b\,\overline{\theta}\,(0,t)\right)^2}\frac{\partial \overline{\theta}}{\partial y}(0,t) = -\frac{q_0^*}{\sqrt{t}}\ ,\ t > 0 \tag{12}$$

$$\frac{1}{a^2}\frac{\partial \overline{\theta}}{\partial y}\left(\overline{S}(t),t\right) = -\alpha \overset{\bullet}{\overline{S}}(t)\ ,\ t > 0 \tag{13}$$

$$\overline{\theta}\left(\overline{S}(t),t\right)=0\ ,\ t>0\ \ ,\ \ \overline{S}(0)=0 \tag{14}$$

Then, we define the new transformation

$$\begin{cases} y^*=y^*(y,t)=\int\limits_{S(t)}^{y}\left(a+b\overline{\theta}\left(\sigma,t\right)\right)d\sigma+\left(-\alpha b+a\right)\overline{S}(t) \\ \theta^*(y^*,t^*)=\dfrac{1}{a+b\overline{\theta}(y,t)}\ \ ,\ \ t^*=t \\ S^*(t^*)=y^*\Big|_{y=\overline{S}(t)}=\left(-\alpha b+a\right)\overline{S}(t). \end{cases} \tag{15}$$

In order to obtain an alternative expression for y^* we compute

$$\begin{aligned} \frac{\partial y^*}{\partial t} &= -\left(a+b\overline{\theta}\left(\overline{S}(t),t\right)\right)\overset{\bullet}{\overline{S}}(t)+\int\limits_{S(t)}^{y}b\frac{\partial\overline{\theta}}{\partial t}\left(\sigma,t\right)d\sigma+\left(-\alpha b+a\right)\overset{\bullet}{\overline{S}}(t)= \\ &= -\alpha b\overset{\bullet}{\overline{S}}(t)+\int\limits_{S(t)}^{y}b\frac{\partial}{\partial\sigma}\left(\frac{1}{\left(a+b\overline{\theta}\left(\sigma,t\right)\right)^2}\frac{\partial\overline{\theta}}{\partial\sigma}\right)d\sigma= \\ &= -\alpha b\overset{\bullet}{\overline{S}}(t)+b\left(\frac{1}{\left(a+b\overline{\theta}\left(y,t\right)\right)^2}\frac{\partial\overline{\theta}}{\partial y}(y,t)-\frac{1}{a^2}\frac{\partial\overline{\theta}}{\partial y}(\overline{S}(t),t)\right)= \\ &= \frac{b}{\left(a+b\overline{\theta}\left(y,t\right)\right)^2}\frac{\partial\overline{\theta}}{\partial y}(y,t)= \end{aligned}$$

$$=\int\limits_{0}^{y}\frac{\partial}{\partial\sigma}\left(\frac{b}{\left(a+b\overline{\theta}\left(\sigma,t\right)\right)^2}\frac{\partial\overline{\theta}}{\partial\sigma}(\sigma,t)\right)d\sigma+\frac{b}{\left(a+b\overline{\theta}\left(0,t\right)\right)^2}\frac{\partial\overline{\theta}}{\partial y}(0,t) \tag{16}$$

$$=b\int\limits_{0}^{y}\frac{\partial\overline{\theta}}{\partial t}\left(\sigma,t\right)d\sigma-\frac{bq_0^*}{\sqrt{t}}\ \ , \tag{17}$$

then the new expression for y^* is given by

$$y^*(y,t)=\int\limits_{0}^{t}\left(\int\limits_{0}^{y}\frac{\partial}{\partial\sigma}\left(a+b\overline{\theta}\left(\sigma,\tau\right)\right)d\sigma-\frac{bq_0^*}{\sqrt{\tau}}\right)d\tau+\int\limits_{0}^{y}\left(a+b\overline{\theta}\left(\sigma,0\right)\right)d\sigma=$$

$$=\int\limits_{0}^{y}\left(a+b\overline{\theta}\left(\sigma,t\right)\right)d\sigma-2bq_0^*\sqrt{t}\ \ . \tag{18}$$

Now, applying (10) and (15) the problem (6) − (9) is transformed in a Stefan-like problem with a convective boundary condition given by [28]

$$\frac{\partial\theta^*}{\partial t^*}=\frac{\partial^2\theta^*}{\partial y^{*2}}\ ,\ -2bq_0^*\sqrt{t^*}<y^*<S^*(t^*)\ ,\ t^*>0 \tag{19}$$

$$\frac{\partial\theta^*}{\partial y^*}\left(-2bq_0^*\sqrt{t^*},t^*\right)=\frac{q_0^*b}{\sqrt{t^*}}\,\theta^*\left(-2bq_0^*\sqrt{t^*},t^*\right)\ ,\ t^*>0 \tag{20}$$

$$\frac{\partial\theta^*}{\partial y^*}\left(S^*(t^*),t^*\right)=\alpha^*\overset{\bullet}{S^*}(t^*)\ ,\ t^*>0 \tag{21}$$

$$\theta^*\left(S^*(t^*),t^*\right)=\theta_f^*\ ,\ t^*>0\ \ ,\ \ S^*(0)=0 \tag{22}$$

where

$$\alpha^*=\frac{\alpha b}{a\left(-\alpha b+a\right)}\qquad,\qquad\theta_f^*=\frac{1}{a}\,. \tag{23}$$

Then, if we introduce the similarity variable:

$$\xi^*=\frac{y^*}{\sqrt{2\gamma^*t^*}} \tag{24}$$

where γ^* is a dimensionless positive constant to be determined, and the solution is sought of the type

$$\theta^*(y^*,t^*)=\Theta^*\left(\xi^*\right)\ \ ,\ \ S^*(t^*)=\sqrt{2\gamma^*t^*}\,, \tag{25}$$

then, we get that $(19)-(22)$ yields

$$\frac{d^2\Theta^*}{d\xi^{*2}}+\gamma^*\xi^*\frac{d\Theta^*}{d\xi^*}=0\ ,\ -bq_0^*\sqrt{\tfrac{2}{\gamma^*}}<\xi^*<1 \tag{26}$$

$$\frac{d\Theta^*}{d\xi^*}\left(-bq_0^*\sqrt{\tfrac{2}{\gamma^*}}\right)=\sqrt{2\gamma^*}q_0^*b\ \Theta^*\left(-bq_0^*\sqrt{\tfrac{2}{\gamma^*}}\right) \tag{27}$$

$$\frac{d\Theta^*}{d\xi^*}\left(1\right)=\alpha^*\gamma^* \tag{28}$$

$$\Theta^*\left(1\right)=\theta_f^*. \tag{29}$$

The solution of the differential equation (26) is given by

$$\Theta^*\left(\xi^*\right)=A\,\mathrm{erf}\left(\sqrt{\tfrac{\gamma^*}{2}}\xi^*\right)+B \tag{30}$$

where A and B are two unknown coefficients to be determined. From (28) and (29) we get

$$A=\sqrt{\pi}\sqrt{\tfrac{\gamma^*}{2}}\alpha^*\exp\left(\tfrac{\gamma^*}{2}\right) \tag{31}$$

$$B = \tfrac{1}{a} - \sqrt{\pi}\sqrt{\tfrac{\gamma^*}{2}}\alpha^* \exp\left(\tfrac{\gamma^*}{2}\right) \operatorname{erf}\left(\sqrt{\tfrac{\gamma^*}{2}}\right). \tag{32}$$

where

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp\left(-u^2\right) du \ . \tag{33}$$

The unknown constant γ^* is determined by the remaining boundary condition (28) which yields the following equation

$$\alpha^*\sqrt{\gamma^*} = \sqrt{\tfrac{2}{\pi}} \frac{\theta_f^*}{g\left(bq_0^*, \frac{1}{\sqrt{\pi}}\right) + \operatorname{erf}\left(\sqrt{\frac{\gamma^*}{2}}\right)} \exp\left(-\tfrac{\gamma^*}{2}\right) \ , \ \gamma^* > 0, \tag{34}$$

where

$$\begin{aligned} &g(x,p) = \operatorname{erf}(x) + pR(x) \ , \ x > 0 \ , \ p \in \mathbb{R} \\ &R(x) = \frac{\exp(-x^2)}{x} = \frac{1}{P(x)} \ , \ P(x) = x\exp(x^2) \ , \ x > 0 \\ &E(x) = x\exp(x^2)\operatorname{erf}(x) = P(x)\operatorname{erf}(x) \ , \ x > 0. \end{aligned} \tag{35}$$

By defining the new unknown

$$\delta = \sqrt{\frac{\gamma^*}{2}} \tag{36}$$

the equation (34) is equivalent to the equation

$$g(bq_0^*, \tfrac{1}{\sqrt{\pi}})P(\delta) = \frac{\frac{ac}{bl} - 1}{\sqrt{\pi}} - E(\delta) \quad , \quad \delta > 0 \quad , \tag{37}$$

that is

$$g\left(\delta, \tfrac{1}{\sqrt{\pi}}(1 - \tfrac{a}{\alpha b})\right) = -g\left(bq_0^*, \tfrac{1}{\sqrt{\pi}}\right) \quad , \quad \delta > 0 \ . \tag{38}$$

Theorem 1.- If $b > 0$ and $a > \frac{bl}{c}$, or $b < 0$, then the free boundary problem $(1) - (4)$ has a unique solution of the similarity type which is given by

$$\begin{aligned} \theta(\xi) &= \frac{1}{b}\left[\frac{1}{A\operatorname{erf}\left(\sqrt{\frac{\gamma^*}{2}}\xi^*\right) + B} - a\right] \\ \xi = \tfrac{y}{\sqrt{2\gamma t}} &= \frac{\frac{2}{d}\left[(1+dx)^{\frac{1}{2}} - 1\right]}{\sqrt{2\gamma t}} \\ s(t) &= \frac{1}{d}\left[\left(1 + \frac{d}{2}\sqrt{2\gamma t}\right)^2 - 1\right] \end{aligned} \tag{39}$$

where

$$\xi = (-\alpha b + a) \int_{-\sqrt{\frac{2}{\gamma^*}} b q_0^*}^{\xi^*} \left[A \operatorname{erf}\left(\sqrt{\tfrac{\gamma^*}{2}} \sigma \right) + B \right] d\sigma \tag{40}$$

and A, B and γ are given by (31) , (32) and (43) respectively.

Proof. First, we have to study the existence and uniqueness of the equation (34) or (38) . It's easy to see that $g(0,p) = -\infty$, $g(+\infty, p) = 1$ and $\frac{\partial g}{\partial x}(x,p) > 0$, $\forall x > 0$, $\forall\, p < 0$ [4]. Therefore if we have $b > 0$ and

$$1 - \frac{a}{\alpha b} < 0 \text{ (that is } a > \alpha b = \tfrac{bl}{c}) \tag{41}$$

and taking into account that $g\left(b q_0^*, \frac{1}{\sqrt{\pi}} \right) > 1$, the equation (38) has a unique solution $\delta > 0$. From (25) we obtain the expression of $S(t)$ given by

$$S(t) = \sqrt{2\gamma t} \tag{42}$$

where γ is given by

$$\gamma = \frac{\gamma^*}{(-\alpha b + a)^2} \quad . \tag{43}$$

From (24) , (25) and (30) we can obtain the parametric solution of the problem $(1)-(4)$ given by (39) and (40) . Note that $\xi^* \mid_{\xi=0} = \frac{-2bq_0^*\sqrt{t^*}}{\sqrt{2\gamma^* t^*}} = -\sqrt{\frac{2}{\gamma^*}} b q_0^* = -\frac{bq_0^*}{\delta}$.

If we have now $b < 0$ then the equation (38) for δ is given by

$$g(\delta, \alpha_0) = -g\left(-b q_0^*, \tfrac{1}{\sqrt{\pi}} \right) \quad , \quad \delta > 0 \quad . \tag{44}$$

which has a unique solution $\delta > 0$ taking into account that

$$\alpha_0 = \tfrac{1}{\sqrt{\pi}}(1 - \tfrac{a}{\alpha b}) > 0 \quad , \quad g\left(-b q_0^*, \tfrac{1}{\sqrt{\pi}} \right) > 1 \quad , \quad \forall b < 0 \ . \tag{45}$$

Remark 1. There does not exist any solution to the free boundary problem $(1) - (4)$ if $b > 0$ and $0 < a < \frac{bl}{c}$ because the non existence of a real solution of the Eq.(38) .

In order to obtain the explicit solution for the cases $b > 0$ and $a > \frac{bl}{c}$, or $b < 0$ we have:

(i) There exists a unique $\delta > 0$ solution of the Eq. (38) .

(ii) We have

$$\gamma^* = 2\delta^2, A = \alpha^* \sqrt{\pi} P(\delta) \ , \ B = \theta_f^* - \alpha^* \sqrt{\pi} E(\delta) \tag{46}$$

where

$$\alpha^* = \tfrac{\alpha b}{a(a - \alpha b)} \ , \ \theta_f^* = \tfrac{1}{a} \ , \ \alpha = l/c. \tag{47}$$

(iii) We have

$$\theta^*(y^*,t^*)=\Theta^*\left(\xi^*\right)=A\,\mathrm{erf}\left(\sqrt{\tfrac{\gamma^*}{2}}\xi^*\right)+B=B+A\,\mathrm{erf}\left(\delta\xi^*\right) \tag{48}$$

with $\xi^*=\frac{y^*}{2\delta\sqrt{t}}$ and

$$S^*(t)=\sqrt{2\gamma^* t}=2\delta\sqrt{t}\,. \tag{49}$$

(iv) We have

$$y^*(y,t)=\int_0^y\left(a+b\overline{\theta}\left(\sigma,t\right)\right)d\sigma-2bq_0^*\sqrt{t}\ ,\ q_0^*=q_0/\rho c. \tag{50}$$

(v) We have

$$\overline{S}(t)=\tfrac{S^*(t)}{a-\alpha b}=\tfrac{2\delta}{a-\alpha b}\sqrt{t}\ , \tag{51}$$

$$\begin{aligned}\tfrac{1}{a+b\overline{\theta}(y,t)} &= \theta^*(y^*,t)=\Theta^*\left(\xi^*\right)=A\,\mathrm{erf}\left(\tfrac{y^*}{2\sqrt{t}}\right)+B=\\ &= B+A\,\mathrm{erf}\left[\tfrac{1}{2\sqrt{t}}\int_0^y\left(a+b\overline{\theta}\left(\sigma,t\right)\right)d\sigma-bq_0^*\right]\end{aligned}$$

which is an integral equation for $\overline{\theta}=\overline{\theta}(y,t)$ where $t>0$ is a parameter.

(vi) The free boundary $s=s(t)$ is given by:

$$\begin{aligned}s(t) &= \tfrac{1}{d}\left[\left(1+\tfrac{d}{2}\overline{S}(t)\right)^2-1\right]=\tfrac{1}{d}\left[\left(1+\tfrac{d\delta}{a-\alpha b}\sqrt{t}\right)^2-1\right]= \\ &= \tfrac{2\delta}{a-\alpha b}\sqrt{t}+\tfrac{d\delta^2}{(a-\alpha b)^2}t=\tfrac{\delta}{a-\alpha b}\left[2\sqrt{t}+\tfrac{d\delta}{a-\alpha b}t\right]\end{aligned} \tag{52}$$

(vii) If we define

$$Y(y,t)=-bq_0^*=\tfrac{1}{2\sqrt{t}}\int_0^y\left(a+b\overline{\theta}\left(\sigma,t\right)\right)d\sigma \tag{53}$$

then we obtain

$$\frac{\partial Y}{\partial y}(y,t)=\frac{a+b\overline{\theta}\left(y,t\right)}{2\sqrt{t}} \tag{54}$$

that is $Y=Y(y,t)$ satisfies the following Cauchy problem in variable y :

$$\tfrac{\partial Y}{\partial y}(y,t)=\tfrac{1}{2\sqrt{t}}\left(\tfrac{1}{B+A\,\mathrm{erf}(Y(y,t))}\right),0<y<\overline{S}(t),t>0 \tag{55}$$

$$Y(0,t)=-bq_0^*\,, \tag{56}$$

where $t>0$ is a parameter.

(*viii*) The temperature $\overline{\theta} = \overline{\theta}(y,t)$ is given by:

$$\overline{\theta}(y,t) = \frac{1}{b}\left[\frac{1}{B+A\,\mathrm{erf}(Y(y,t))} - a\right] \ , \ 0 < y < \overline{S}(t) \ , \ t > 0 \tag{57}$$

as a function of Y.

(*ix*) The temperature $\theta = \theta(x,t)$ is given by:

$$\theta(x,t) = \overline{\theta}\left(\tfrac{2}{d}\left(\sqrt{1+dx}-1\right),t\right) = \tag{58}$$

$$= \frac{1}{b}\left[\frac{1}{B+A\,\mathrm{erf}(Y(\frac{2}{d}(\sqrt{1+dx}-1),t))} - a\right], 0 < x < s(t), t > 0$$

as a function of Y where $s(t)$ as defined in (52).

Theorem 2 Let us consider the hypothesis $b > 0$ and $a > bl/c$, or $b < 0$. Let $\delta > 0$ be the unique solution of the Eq. (38) and A and B the coefficients defined by (31) and (32) respectively or by (46).

(*i*) There exists a unique solution $Y = Y(y,t)$ of the Cauchy problem $(55)-(56)$ for all $t \geqslant t_0 > 0$ where t_0 is an arbitrary positive time.

(*ii*) There exists a unique solution $\theta = \theta(x,t)$ and $s = s(t)$ given by (58) and (52) respectively of the free boundary problem $(1)-(4)$ for $t \geqslant t_0 > 0$ where t_0 is an arbitrary positive time.

Proof:

It is sufficient to prove that the Cauchy problem has a unique solution for $t \geqslant t_0 > 0$. The ordinary differential equation, with parameter $t > 0$, can be written as

$$\frac{\partial Y}{\partial y}(y,t) = G(y,t,Y(y,t))) \tag{59}$$

where

$$G(y,t,Y) = \frac{1}{2\sqrt{t}}\left(\frac{1}{B+A\,\mathrm{erf}(Y)}\right) \tag{60}$$

satisfies the condition

$$\left|\frac{\partial G}{\partial Y}(y,t,Y)\right| \leq Const \quad , \quad \forall t \geqslant t_0 > 0 \tag{61}$$

with $t_0 > 0$ an arbitrary positive time.

Remark 2. The existence of a solution for $t \geqslant t_0 > 0$ with t_0 an arbitrary positive time for the cases $b > 0$ and $a > bl/c$, or $b < 0$ is similar to the one obtained in the free boundary problem studied in [20].

Remark 3:

The particular case $b > 0$ and $a = bl/c$ can not be studied through a similar method developed for the case $b > 0$ and $a > bl/c$ because the transformation (15) is not useful due to the definition of the free boundary $S^*(t^*)$ as a function of the $\overline{S}(t)$.

Remark 4:

For the cases $b > 0$ and $a > bl/c$, or $b < 0$ we can obtain the explicit solution $\theta = \theta(x,t)$ and $s = s(t)$ of the free boundary problem $(1)-(4)$ by the following process:

(i) Compute $\delta > 0$ as the unique solution of the Eq. (38).

(ii) Compute

$$A = \alpha^* \sqrt{\pi} P(\delta) \quad , \quad B = \theta_f^* - \alpha^* \sqrt{\pi} E(\delta)$$

where α^*, θ_f^* and α are defined in (47).

(iii) Fix t_0 as an arbitrary positive time and compute $Y = Y(y,t)$ as the unique solution of the Cauchy problem $(55) - (56)$ for $t \geqslant t_0 > 0$.

(iv) Compute the free boundary $s = s(t)$ by the explicit expression (52)

(v) Compute the temperature $\theta = \theta(x,t)$ by the explicit expression (58).

III. Solution of the free boundary problem with temperature boundary condition on the fixed face.

Now, we consider the problem $(1) - (4)$ with $a, d \in \mathbb{R}^+$ and $b < 0$ but the heat flux boundary condition (2) will be replaced by the following temperature boundary condition ($\theta_0 > 0$) given by

$$\theta(0,t) = \theta_0 \ , \ t > 0 \ , \ \text{with } a + b\theta_0 > 0. \tag{62}$$

We can define the same transformations (10) and (15) as were done for the previous Section but now we get

$$\begin{aligned} \frac{\partial y^*}{\partial t} &= b \int_{S(t)}^{y} \frac{\partial \overline{\theta}}{\partial t}(\sigma,t) d\sigma + \frac{b}{\left(a + b\overline{\theta}(0,t)\right)^2} \frac{\partial \overline{\theta}}{\partial y}(0,t) = \\ &= b \int_0^y \frac{\partial \overline{\theta}}{\partial t}(\sigma,t) d\sigma + \frac{b}{(a+b\theta_0)^2} \frac{\partial \overline{\theta}}{\partial y}(0,t) \ . \end{aligned}$$

Then

$$y^*(y,t) = \int_0^t \left(\int_0^y \frac{\partial}{\partial \tau} \left(a + b\overline{\theta}(\sigma,\tau)\right) d\sigma + \frac{b}{(a+b\theta_0)^2} \frac{\partial \overline{\theta}}{\partial y}(0,\tau) \right) d\tau + \int_0^y \left(a + b\overline{\theta}(\sigma,0)\right) d\sigma =$$

$$= \int_0^y \left(a + b\overline{\theta}(\sigma,t)\right) d\sigma + \frac{b}{(a+b\theta_0)^2} \int_0^t \frac{\partial \overline{\theta}}{\partial y}(0,\tau) d\tau. \tag{63}$$

Therefore our free boundary problem becomes (21) − (22) and

$$\frac{\partial \theta^*}{\partial t} = \frac{\partial^2 \theta^*}{\partial y^{*}} \ , \ b\theta_0^{*2} \int_0^{t^*} \frac{\partial \overline{\theta}}{\partial y}(0,\tau) d\tau < y^* < S^*(t^*) \ , \ t^* > 0 \tag{64}$$

$$\theta^* \left(b\theta_0^{*2} \int_0^{t^*} \frac{\partial \overline{\theta}}{\partial y}(0,\tau) d\tau, t^* \right) = \theta_0^* \tag{65}$$

where θ_f^* and α^* are given by (23) and

$$\theta_0^* = \tfrac{1}{a+b\overline{\theta}(0,t)} = \tfrac{1}{a+b\theta(0,t)} = \tfrac{1}{a+b\theta_0} \quad . \tag{66}$$

It is easy to see that we have a classical Stefan problem so that the free boundary must be of the type

$$S^*(t^*) = \sqrt{2\gamma^* t^*} \qquad \left(\overline{S}(t) = \sqrt{2\gamma t} \quad , \quad \gamma^* = \gamma\,(a-\alpha b)^2\right) \tag{67}$$

where γ^* (i.e. γ) is a dimensionless constant to be determined.

If we introduce the similarity variable (24) and we propose the solution of the type (25) then the problem (21) − (22) and (64) − (65) yields (28) , (29) and

$$\frac{d^2\Theta^*}{d\xi^{*2}} + \gamma^*\xi^*\frac{d\Theta^*}{d\xi^*} = 0\ ,\ \frac{b\theta_0^{*2}}{\sqrt{2\gamma^* t^*}}\int_0^{t^*}\frac{\partial\overline{\theta}}{\partial y}(0,\tau)d\tau < \xi^* < 1\ ,\ t^* > 0 \tag{68}$$

$$\Theta^*\left(\tfrac{b\theta_0^{*2}}{\sqrt{2\gamma^* t^*}}\int_0^{t^*}\frac{\partial\overline{\theta}}{\partial y}(0,\tau)d\tau\right) = \theta_0^*\ ,\ t^* > 0 \tag{69}$$

From (69) we must necessarily have that there exists a constant ξ_0^* such that

$$\int_0^{t^*}\frac{\partial\overline{\theta}}{\partial y}(0,\tau)d\tau = \xi_0^*\tfrac{1}{b\theta_0^{*2}}\sqrt{2\gamma^* t^*}\ . \tag{70}$$

Therefore (68) and (69) can be written as

$$\frac{d^2\Theta^*}{d\xi^{*2}} + \gamma^*\xi^*\frac{d\Theta^*}{d\xi^*} = 0\ ,\ \xi_0^* < \xi^* < 1 \tag{71}$$

$$\Theta^*\left(\xi_0^*\right) = \theta_0^*\ . \tag{72}$$

The solution of the problem (28) , (29) , (71) and (72) is given by

$$\Theta^*\left(\xi^*\right) = A'\,\mathrm{erf}\left(\sqrt{\tfrac{\gamma^*}{2}}\xi^*\right) + B' \qquad , \qquad \xi_0^* < \xi^* < 1 \tag{73}$$

where the unknown coefficients ξ_0^*, A', B' and γ^* must satisfy the following equations

$$A'\,\mathrm{erf}\left(\xi_0^*\sqrt{\tfrac{\gamma^*}{2}}\right) + B' = \theta_0^* \quad , \quad \sqrt{\tfrac{2}{\pi\gamma^*}}\exp\left(-\tfrac{\gamma^*}{2}\right) = \tfrac{\alpha^*}{A'}, \tag{74}$$

$$A'\,\mathrm{erf}\left(\sqrt{\tfrac{\gamma^*}{2}}\right) + B' = \theta_f^* \ \text{ and } \ \theta_0^*\sqrt{\tfrac{\gamma^*}{2}}\xi_0^* = -\tfrac{A'}{\sqrt{\pi}}\exp\left(-\tfrac{\gamma^*}{2}\xi_0^{*2}\right) \tag{75}$$

If we define

$$\beta = \sqrt{\tfrac{\gamma^*}{2}} \ , \ \ z = \xi_0^* \sqrt{\tfrac{\gamma^*}{2}} \ \ (\beta > z) \tag{76}$$

we have to solve the following system of equations:

$$A' \operatorname{erf}(z) + B' = \theta_0^* \ \ , \ \ A' \operatorname{erf}(\beta) + B' = \theta_f^* \tag{77}$$

$$\frac{\exp(-\beta^2)}{\beta} = \frac{\alpha^*}{A'}\sqrt{\pi} \ \ , \ \ \theta_0^* \, z = -\frac{A'}{\sqrt{\pi}} \exp(-z^2) \tag{78}$$

From (77) we get

$$A' = \frac{\theta_f^* - \theta_0^*}{\operatorname{erf}(\beta) - \operatorname{erf}(z)} \tag{79}$$

$$B' = \frac{\theta_0^* \operatorname{erf}(\beta) - \theta_f^* \operatorname{erf}(z)}{\operatorname{erf}(\beta) - \operatorname{erf}(z)} \tag{80}$$

and from (78) we obtain

$$\frac{\exp(-\beta^2)}{\beta} = \delta_1 \left[\operatorname{erf}(\beta) - \operatorname{erf}(z)\right] \tag{81}$$

$$\frac{\exp(-z^2)}{z} = \delta_2 \left[\operatorname{erf}(\beta) - \operatorname{erf}(z)\right] \tag{82}$$

with

$$\delta_1 = \frac{\alpha^*\sqrt{\pi}}{\theta_f^* - \theta_0^*} = \frac{\alpha\sqrt{\pi}\,(a + b\theta_0)}{(a - \alpha b)\,\theta_0} \ \ , \ \ \delta_2 = -\frac{\sqrt{\pi} a}{b\theta_0}. \tag{83}$$

Taking into account that $\xi_0^* < 1, b < 0$ and $a + b\theta_0 > 0$, we have $[\operatorname{erf}(\beta) - \operatorname{erf}(z)] > 0$, $\delta_1 > 0$ and $\delta_2 > 0$.

Taking into account the properties of the real function $g = g(x, p)$, defined in (35), for $p < 0$, from (81) we have

$$z = \operatorname{erf}^{\ -1}\left[\operatorname{erf}(\beta) - \frac{1}{\delta_1}\frac{\exp(-\beta^2)}{\beta}\right] \tag{84}$$

if $\beta > x_0$ where $x_0 > 0$ is the unique positive zero of $g(x, -\frac{1}{\delta_1}) = 0$ which is given by $x_0 = E^{-1}(1/\delta_1)$.

Moreover, for β we have the following equation:

$$\frac{\delta_2}{\delta_1}\frac{F(\beta)}{\beta \exp(\beta^2)} = 1 \ \ , \ \ \beta > x_0 = E^{-1}(1/\delta_1) \tag{85}$$

where the real function F is defined by

$$F(x) = \exp\left[\left(\operatorname{erf}^{\ -1}\left(g(x, \tfrac{-1}{\delta_1})\right)\right)^2\right] \operatorname{erf}^{\ -1}\left(g(x, \tfrac{-1}{\delta_1})\right) \ , \ x > 0. \tag{86}$$

If we define the real function:

$$G(x) = \frac{\delta_2}{\delta_1} \frac{F(x)}{x \exp(x^2)} \quad , \quad x > 0 \tag{87}$$

and following [20] we have the following properties:

$$G(x_0^+) = 0, \quad \lim_{x \to +\infty} G(x) = \frac{\delta_2}{\delta_1 + \sqrt{\pi}}. \tag{88}$$

Then there exists a unique solution $\beta > x_0$ of the Eq. (85) if and only if $\frac{\delta_2}{\delta_1+\sqrt{\pi}} > 1$ if and only if $a + b\theta_0 > 0$ which is our hypothesis.

Moreover, we have

$$\overline{S}(t) = \frac{2\beta}{a - \alpha b} \sqrt{t} \, , \tag{89}$$

and for $0 < y < \overline{S}(t) \ , \ t > 0$, we obtain

$$\begin{aligned} \frac{1}{a + b\overline{\theta}(y,t)} &= \theta^*(y^*,t) = \Theta^*(\xi^*) = A' \operatorname{erf}(\beta \xi^*) + B' = \\ &= B' + A' \operatorname{erf}\left(\frac{y^*}{2\sqrt{t}}\right) = \\ &= B' + A' \operatorname{erf}\left[z + \frac{1}{2\sqrt{t}} \int_0^y \left(a + b\overline{\theta}(\sigma,t)\right) d\sigma \right] \end{aligned} \tag{90}$$

which represents an integral equation for $\overline{\theta}$ in variable y with t a parameter.

In order to solve this integral equation we define

$$Y(y,t) = z + \frac{1}{2\sqrt{t}} \int_0^y \left(a + b\overline{\theta}(\sigma,t)\right) d\sigma, \tag{91}$$

which must satisfy the following Cauchy problem

$$\frac{\partial Y}{\partial y}(y,t) = \frac{1}{2\sqrt{t}} \left(\frac{1}{B' + A' \operatorname{erf}(Y(y,t))} \right), \ 0 < y < \overline{S}(t) \ , \ t > 0 \tag{92}$$

$$Y(0,t) = z \tag{93}$$

Therefore we obtain the following theorem.

Theorem 3. Let us consider the hypothesis $a > 0, d > 0, b < 0$ and $a + b\theta_0 > 0$. Let $\beta > 0$ be the unique solution of the Eq. (85) , and A' and B' the coefficients defined by (79) and (80) respectively.

(i) There exists a unique solution $Y = Y(y,t)$ of the Cauchy problem (92) − (93) for all $t \geqslant t_0 > 0$ where $t_0 > 0$ is an arbitrary positive time.

(*ii*) There exists a unique solution $\theta = \theta(x,t)$ and $s = s(t)$ given by (95) and (96) respectively of the free boundary problem $(1), (3)-(4)$ and (62).

Proof.

(*i*) The Cauchy problem $(92)-(93)$ has a unique solution $Y = Y(y,t)$ for all $t \geqslant t_0 > 0$ with $t_0 > 0$ is an arbitrary positive time following a similar method given in Theorem 2.

(*ii*) From (90) and (91) we get

$$\overline{\theta}(y,t) = \frac{1}{b}\left[\frac{1}{B' + A'\operatorname{erf}(Y(y,t))} - a\right] \tag{94}$$

that is

$$\theta(x,t) = \overline{\theta}(y,t) = \overline{\theta}\left(\frac{2}{d}\left(\sqrt{1+dx}-1\right), t\right) = \tag{95}$$

$$= \frac{1}{b}\left[\frac{1}{B' + A'\operatorname{erf}(Y(\frac{2}{d}\left(\sqrt{1+dx}-1\right), t))} - a\right]$$

and

$$s(t) = \frac{1}{d}\left[\left(1 + \frac{d}{2}\overline{S}(t)\right)^2 - 1\right] = \frac{1}{d}\left[\left(1 + \frac{d\beta}{a-\alpha b}\sqrt{t}\right)^2 - 1\right] = \tag{96}$$

$$= \frac{\beta}{a-\alpha b}\left[2\sqrt{t} + \frac{d\beta}{a-\alpha b}t\right]$$

Remark 5 For the case $a > 0, d > 0, b < 0$ and $a + b\theta_0 > 0$ we can obtain the explicit solution $\theta = \theta(x,t)$ and $s = s(t)$ of the free boundary $(1), (3)-(4)$ and (62) by the following process:

(*i*) Compute the positive parameters δ_1 and δ_2 given by (83).

(*ii*) Compute $\beta > 0$ as the unique solution of the Eq. (85)

(*iii*) Compute the coefficients

$$\begin{aligned} z &= \operatorname{erf}^{-1}\left[\operatorname{erf}(\beta) - \frac{1}{\delta_1}\frac{\exp(-\beta^2)}{\beta}\right] \\ \gamma^* &= 2\beta^2 \quad , \quad \gamma = \frac{\gamma^*}{(a-\alpha b)^2} = 2\left(\frac{\beta}{a-\alpha b}\right)^2 \\ \xi_0^* &= \frac{z}{\beta} \end{aligned}$$

(*iv*) Compute the coefficients $A' < 0$ and $B' > 0$ given by (79) and (80) respectively.

(*v*) Fix t_0 as an arbitrary positive time and compute $Y = Y(y,t)$ as the unique solution of the Cauchy problem $(92)-(93)$.

(*vi*) Compute the free boundary $s = s(t)$ by the explicit expression (96)

(*vi*) Compute the temperature $\theta = \theta(x,t)$ by the explicit expression (95).

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NON-LOCAL DIFFUSION

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1. Introduction.

Let $K : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$ be a nonnegative, smooth function such that $\int_{\mathbb{R}^N} K(x,y)dy = 1$ for all $x \in \mathbb{R}^N$.

Equations of the form

$$u_t(x,t) = \int_{\mathbb{R}^N} K(y,x)u(y,t)dy - u(x,t) \text{ in } \mathbb{R}^N \times [0,\infty) \tag{1.1}$$

have been widely used to model diffusion processes, see [1], [2], [8], [9], [10]. As stated in [8] if $u(x,t)$ is thought of as a density at the point x at time t and $K(y,x)$ is thought of as the probability distribution of jumping from location y to location x, then $\int_{\mathbb{R}^N} K(y,x)u(y,t)dy$ is the rate at which individuals are arriving to position x from all other places. On the other hand $-u(x,t) = -\int_{\mathbb{R}^N} K(x,y)u(x,t)dy$ is the rate at which they are leaving location x to travel to all other sites. This consideration, in the absence of external sources, leads immediately to the fact that the density u satisfies equation (1.1).

In this note we will describe some of the results obtained recently by the authors, in collaboration with J. Coville, S. Martinez, J. Rossi and N. Wolanski, in the topic of non local diffusion. We have decided to describe the results in a rather informal fashion since detailed statements and proofs can be found in the corresponding references.

2. An homogeneous model.

The Cauchy problem in $\mathbb{R}^N$.

A type of kernels that have been widely used in modeling diffusion are kernels of the form

$$K(y,x) = J(x-y)$$

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where $J : \mathbb{R}^N \to \mathbb{R}$ is a smooth non negative function such that $\int_{\mathbb{R}^N} J(x)dx = 1$ and that we will assume symmetric with respect to the origin. Moreover, throughout this note, we will assume that J is supported in the unit ball centered at the origin $B(0,1)$. In this case equation (1.1) takes the form

$$u_t = J * u - u \tag{2.1}$$

where $J*u$ denotes the convolution of J and u. Since J is supported in $B(0,1)$ individuals at location x are not allowed to jump, up to probability zero, off the ball $B(x,1)$. By this reason we refer to this dispersion process as an homogeneous random walk, continuous in time, of step of size one.

Equation (2.1) can be written in integral form

$$u(x,t) = e^{-t}u(x,0) + \int_0^t e^{-(t-s)} \int_{\mathbb{R}^N} J(x-y)u(y,s)dyds. \tag{2.2}$$

It follows that existence and uniqueness of solutions of (2.1) can be obtained by an application of Banach's fixed point theorem to the right hand side operator of (2.2) in a suitable space of functions. It is also a consequence of the proof that if $u(x,0) \geq 0$, then $u(x,t) \geq 0$ for all $t \geq 0$. This plus the fact that the problem is linear imply the following comparison principle for two solutions u_1 and u_2 of (2.1):

$$u_1(x,0) \leq u_2(x,0) \Rightarrow u_1(x,t) \leq u_2(x,t) \text{ for all } t \geq 0.$$

An important aspect of equation (2.1) is its relation, the so called Brownian Motion, with the classic heat equation

$$v_t = \Delta v \text{ in } \mathbb{R}^N \times [0,\infty) \tag{2.3}$$

described in the following theorem which is classical. We give its proof to illustrate the techniques that can be used.

Theorem 2.1 *Let $\varepsilon > 0$ and let u^ε be a solution of the re-scaled problem*

$$u_t^\varepsilon(x,t) = \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}^N} J(\frac{x-y}{\varepsilon})\frac{u^\varepsilon(y,t)}{\varepsilon^N}dy - u^\varepsilon(x,t)\right].$$

Let v be a solution of

$$v_t = A\Delta v$$

where A is a suitable constant that will be apparent in the proof.

Assume that $u^\varepsilon(x,0) \equiv v(x,0)$ and that $v(\cdot,0)$ is smooth enough. Then

$$\lim_{\varepsilon \to 0} u^\varepsilon = v \text{ uniformly in } \mathbb{R}^{\mathbb{N}} \times [\nVdash, \mathbb{T}]$$

for any $T > 0$.

Proof:

To simplify the notation set $u = u^\varepsilon$ and define

$$L_\varepsilon u = \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}^N} J(\frac{x-y}{\varepsilon})\frac{u(y,t)}{\varepsilon^N}dy - u(x,t)\right],$$

Set $w = u - v$ and note that$w$ satisfies

$$w_t = L_\varepsilon w + F$$

where

$$F(x,t) = L_\varepsilon v(x,t) - A\Delta v(x,t).$$

Making the change of variables

$$z = \frac{x-y}{\varepsilon}$$

in the integral, noting that $\int_{\mathbb{R}^N} J(z)dz = 1$ and choosing properly the constant A we have

$$F(x,t) = \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}^N} J(z)\left(v(x+\varepsilon z,t) - v(x,t) - \varepsilon^2|z|^2\Delta v(x,t)\right)dz\right].$$

Using the symmetry of J we obtain

$$F(x,t) =$$

$$\frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}^N} J(z)\left(v(x+\varepsilon z,t) - v(x,t) - \varepsilon\sum_{i=1}^{N}\frac{\partial v}{\partial z_i}(x,t)z_i - \varepsilon^2\sum_{i,j=1}^{N}\frac{\partial^2 v}{\partial z_i\partial z_j}(x,t)z_iz_j\right)dz\right].$$

Finally using Taylor's expansion for the regular function v we get

$$F(x,t) = \varepsilon B(x,t)$$

where B is a function which is bounded independently of ε.

So w satisfies

$$w_t \leq L_\varepsilon w + \varepsilon M$$

and

$$w(x,0) = 0.$$

Since the function $h(t) = t\varepsilon M$ satisfies

$$h_t = L_\varepsilon h + \varepsilon M$$

and

$$h(x,0) = 0$$

by comparison we have

$$|u^\varepsilon(x,t) - v(x,t)| \leq t\varepsilon M$$

and the proof is finished. □

Remark 2.1 *The kernel in the re-scaled problem has been modified in such a way that the size of the step now is ε. The shortening of the step size is compensated by the multiplication by $\frac{1}{\varepsilon^2}$ of the right hand side. This factor represents an speed up of the walk necessary to compensate reduction of the size of the step.*

The Neumann problem.

The following model for the Neumann problem has been proposed in [6] and [7]. Let Ω be a domain in $\mathbb{R}^{\mathbb{N}}$ and $g : \overline{\mathbb{R}^{\mathbb{N}} \setminus \Omega} \to \mathbb{R}$ smooth. Consider the problem

$$u_t(x,t) = \int_\Omega J(x-y)(u(y,t)-u(x,t))dy + \int_{\mathbb{R}^{\mathbb{N}}\setminus\Omega} J(x-y)g(y,t). \tag{2.4}$$

In this model we have that the first integral takes into account the diffusion inside Ω. In fact, the integral $\int_\Omega J(x-y)(u(y,t)-u(x,t))dy$ takes into account the individuals arriving or leaving position x from or to other places. Since we are integrating in Ω, we are imposing that diffusion takes place only inside Ω. The last term takes into account the prescribed flux (given by the data $g(x,t)$) of individuals from outside (that is individuals that enter or leave the domain according to the sign of g). This is what is called Neumann boundary conditions.

Existence, uniqueness and some qualitative properties, such as the asymptotic behavior, of the solutions of problem (2.4) with suitable initial conditions have been studied in [6].

With respect to its relation with the classical Neumann problem the following result has been obtained in [7]: Let u^ε be a solution of the re-scaled problem

$$u_t^\varepsilon(x,t) = \frac{1}{\varepsilon^{N+2}} \int_\Omega J(\frac{x-y}{\varepsilon})(u^\varepsilon(y,t)-u^\varepsilon(x,t))dy$$

$$+\frac{1}{\varepsilon^{N+1}} \int_{\mathbb{R}^{\mathbb{N}}\setminus\Omega} J(\frac{x-y}{\varepsilon})g(y,t).$$

and let v be the solution of

$$v_t = A\Delta v \text{ in } \Omega \times [0,\infty),$$
$$v = g \text{ on } \partial\Omega \times [0,\infty).$$

Assume that for all ε one has

$$u^\varepsilon(x,0) = v(x,0) \text{ on } \Omega.$$

Then u^ε converges to v as $\varepsilon \to 0$. The convergence is uniform on compact subsets in the case that $g \equiv 0$ and takes place weakly in $C([0,T], L^1(\Omega))$ in the general case.

The Dirichlet problem.

A non local Dirichlet problem has been proposed in [5] as follows: Let $\Omega \subset \mathbb{R}^N$ and $h; \mathbb{R}^N \to \mathbb{R}$. Consider the problem

$$\begin{aligned} u_t(x,t) &= \int_{\mathbb{R}^N} J(x-y)u(y,t)dy - u(x,t) \text{ for } x \in \Omega, \\ u(x,t) &= h(x) \text{ for } x \in \mathbb{R}^N \setminus \Omega \text{ and } t \geq 0 \end{aligned} \tag{2.5}$$

with initial condition $u(x,0)$.

Existence, uniqueness and some properties of the solutions of problem (2.5) have been proved in [5]. Moreover it is proved there that if u^ε is the solution of the corresponding, to this case, re-scaled problem with $u^\varepsilon(x,0) = v(x,0)$ where v is the solution of

$$v_t = A\Delta v \text{ in } \Omega \times [0,\infty),$$

$$v = h \text{ on } \partial\Omega \times [0,\infty).$$

Then u^ε converges to v uniformly on compact subsets of $\Omega \times [0,\infty)$.

3. A non homogeneous model.

In [3] a non homogeneous dispersal model in the real line was studied. Kernels of the form

$$K(x,y) = J\left(\frac{x-y}{g(y)}\right)\frac{1}{g(y)}$$

were considered where $g : \mathbb{R} \to \mathbb{R}$ is a continuous bounded function that satisfies: The set $\{x \in \mathbb{R} \mid g(x) = 0\} \cap [-K, K]$ is finite for any $K > 0$. If $g(\bar{x}) = 0$, then there exist $r > 0$, $C > 0$ and $0 < \alpha < 1$ such that $g(x) \geq C|x - \bar{x}|^\alpha$ for all $x \in [\bar{x} - r, \bar{x} + r]$.

The evolution equation considered in this case is

$$u_t(x,t) = \int_{\mathbb{R}} J\left(\frac{x-y}{g(y)}\right)\frac{u(y,t)}{g(y)}dy - u(x,t). \tag{3.1}$$

Under the above mentioned hypotheses it is proved that (3.1) has a globally defined mass preserving solution for any given $u(\cdot,0) \in L^1(\mathbb{R})$. Moreover even though g can vanish at some points, these solutions have an infinite speed of propagation in the sense that if $u(x,0) \geq 0$ and $u(x,0) \neq 0$, then $u(x,0) > 0$ for all x and all $t > 0$.

In order to study the asymptotic behavior of solutions of (3.1) we are lead to the analysis stationary solutions, namely solutions of the equation

$$p(x) = \int_{\mathbb{R}} J\left(\frac{x-y}{g(y)}\right)\frac{p(y)}{g(y)}dy. \tag{3.2}$$

It is proved the existence of bounded positive solutions of (3.2) and that solutions of (3.1) converge to solutions of (3.2) as $t \to \infty$.

An important role in the study of problem (3.2) is played by the following lemma that can be of independent interest.

Lemma 3.1 *A continuous function p is a solution of* (3.2) *if and only if there exist constants P and Q such that*

$$\int_0^1 \int_{x-w}^{x+w} p(s) \int_{\frac{w}{g(s)}}^1 J(z)dzdsdw \equiv Px + Q.$$

Proof: Differentiate twice the left hand side to obtain 0 if and only if p is a solution of (3.2). □

The hypothesis that if $g(\bar{x}) = 0$, then there exist $r > 0$, $C > 0$ and $0 < \alpha < 1$ such that $g(x) \geq C|x - \bar{x}|^\alpha$ for all $x \in [\bar{x} - r, \bar{x} + r]$ is important in our arguments. Nothing is known, to the best of our knowledge, if it does not hold.

4. A non linear model.

In this section we will deal with a non linear model that was introduced in [4]. We propose to use a kernel where the size of the step depends on the density at the point. The simplest model, with $N = 1$, is

$$K(y,x) = J\left(\frac{x-y}{u(y,t)}\right)\frac{1}{u(y,t)}.$$

The equation that governs the dispersal becomes in this case

$$u_t(x,t) = \int_{\mathbb{R}} J\left(\frac{x-y}{u(y,t)}\right)\frac{1}{u(y,t)}dy - u(x,t). \tag{4.1}$$

One of the main features of solutions of (4.1) is that if the support of the initial condition $u(\cdot,0)$ is compact, then the support of $u(\cdot,t)$ remains compact for all $t > 0$. This gives rise to a free boundary like in the case of the porous medium equation $u_t = (u^m)_{xx}$ with $m > 1$.

With the additional hypothesis that J is decreasing in the interval $[0,1]$ one can prove existence, uniqueness and a comparison principle for solutions of (4.1). Moreover it is trivial to check that the constant functions are solutions of (4.1) and hence if $u(x,0) \geq 0$, then $u(x,t) \geq 0$ for all $t > 0$.

We state now as a theorem the fact that the compactness of the support is preserved and provide a proof.

Theorem 4.2 *If $u(\cdot,0) \geq 0$ is compactly supported and bounded then $u(\cdot,t)$ is also compactly supported for all $t \geq 0$.*

Proof: Due to the scaling invariance of the equation, namely if $u(x,t)$ is a solution then for any $\lambda > 0$ the function $v_\lambda(x,t) = \lambda u(\frac{x}{\lambda},t)$ is also a solution, we can restrict ourselves to initial data supported in $[-1,1]$ and such that $\sup_{x\in\mathbb{R}} u(x,0) \leq 1$.

We note first that

$$u_t(x,t) \leq \int_{\mathbb{R}} J\left(\frac{x-y}{u(y,t)}\right)dy. \tag{4.2}$$

Therefore, since $0 \leq u \leq 1$, we get by (4.2) that

$$u(x,t) \leq \frac{1}{2} \text{ for all } t \leq \frac{1}{2} \text{ and all } x \text{ such that } |x| \geq 1.$$

Now if $|x| \geq 2$ and $t \leq \frac{1}{2}$ we have that $|x-y| \leq u(y,t)$ implies that $|y| \geq 1$ and hence $u(y,t) \leq \frac{1}{2}$. Therefore, again by (4.2), we have

$$u(x,t) \leq \frac{1}{4} \text{ for all } t \leq \frac{1}{2} \text{ and all } x \text{ such that } |x| \geq 2.$$

We look now at the case $|x| \geq 2 + \frac{1}{2}$ and $t \leq \frac{1}{2}$. In this case $|x-y| \leq u(y,t)$ implies that $|y| \geq 2$ and hence $u(y,t) \leq \frac{1}{4}$. Again by (4.2), we have

$$u(x,t) \leq \frac{1}{8} \text{ for all } t \leq \frac{1}{2} \text{ and all } x \text{ such that } |x| \geq 2 + \frac{1}{2}.$$

Repeating this procedure we obtain by induction that for any integer $n \geq 1$ one has

$$u(x,t) \leq \frac{1}{2^{n+2}} \text{ for all } t \leq \frac{1}{2} \text{ and all } x \text{ such that } |x| \geq 2 + \sum_{k=1}^{n} \frac{1}{2^k}.$$

It follows that the support of $u(\cdot,t)$ is contained in the interval $[-3,3]$ for all $t \leq \frac{1}{2}$ as we wanted to prove. □

We will give now a formal argument that suggest what relation is expected to exist between these non linear random walks and the porous medium equation.

Consider the re-scaled problem

$$u_t(x,t) = \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}} J\left(\frac{|x-y|}{\varepsilon u(y,t)}\right)\frac{dy}{\varepsilon} - u(x,t)\right]$$

and assume that their solutions u^ε converge to a function v as $\varepsilon \to 0$. In order to do not overload the notation we set $u^\varepsilon = u$.

We take the Fourier transform

$$\hat{u}_t(\xi,t) = \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}}\int_{\mathbb{R}} J\left(\frac{x-y}{\varepsilon u(y,t)}\right)e^{-ix\xi}\frac{dydx}{\varepsilon} - \hat{u}(\xi,t)\right].$$

Setting

$$z = \frac{x-y}{\varepsilon u(y,t)}$$

we have

$$\hat{u}_t(x,t) = \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}}\int_{\mathbb{R}} J(z)\, e^{-i\xi\varepsilon u(y,t)z}e^{-iy\xi}u(y,t)dzdy - \hat{u}(\xi,t)\right].$$

Or

$$\hat{u}_t(\xi,t) = \frac{1}{\varepsilon^2}\int_{\mathbb{R}}\left[\hat{J}\left(\xi\varepsilon u(y,t)\right) - 1\right]e^{-iy\xi}u(y,t)dy.$$

Taking the Taylor expansion of $\hat{J}$ about zero we get

$$\hat{u}_t(\xi,t) = \frac{1}{\varepsilon^2}\int_{\mathbb{R}}\left[\hat{J}''(0)\xi^2\varepsilon^2u^2(y,t)\right)\right]e^{-iy\xi}u(y,t)dy + \frac{O(\varepsilon^3)}{\varepsilon^2}.$$

Or

$$\hat{u}_t(\xi,t) = C\int_{\mathbb{R}}(-\xi^2)u^3(y,t)e^{-iy\xi}dy + O(\varepsilon).$$

As $\varepsilon \to 0$

$$\hat{v}_t(x,t) = C\int_{\mathbb{R}}(-\xi^2)v^3(y,t)e^{-iy\xi}dy$$

which means

$$\hat{v}_t(x,t) = C\widehat{(v^3)_{xx}}.$$

Hence the solutions of the re-scaled problems should converge, as $\varepsilon \to 0$, to a solution of the porous medium equation

$$v_t = (v^3)_{xx}.$$

There are several questions that can be raised and for which we do not have an answer. For example: Do the free boundaries converge to the free boundary?

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CONSIDERACIONES SOBRE EL BUEN PLANTEO DE UN MODELO DE FRONTERA LIBRE – MOVIL DESCRIPTIVO DE UN PROCESO DE FREÍDO POR INMERSIÓN

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Resumen
El objetivo del presente trabajo consiste en abordar un análisis concerniente a la cuestión básica del buen planteo de la solución de un problema de frontera libre–móvil, unidimensional a dos fases para la ecuación del calor y difusión de materia, emergente del modelado de la etapa principal de un proceso de freído de papa natural por inmersión en aceite comestible caliente. Se provee un resultado para la unicidad de la solución del modelo analizado. También se obtiene un resultado de dependencia monótona del avance de la frontera libre con la temperatura del baño de aceite, y con la temperatura inicial de la porción a freir.

Abstract
The goal of the present work concern to the basic question of well-posedness of the solution of a one dimensional two phase initial free–moving boundary value problem for the heat–diffusion equation. Such problem arise from the corresponding mathematical modeling of the so called principal stage (bubbling stage) during a immersion frying process, applied to natural potato. A result regarding the uniqueness of the solution is provided. Also, a result on monotone dependence for the progress of the free boundary with the oil bath temperature, and with the initial temperature of the potato sample are consigned.

Nomenclatura

x, t : Variables independientes, espacial y tiempo respectivamente (m), (seg).

A : Constante positiva, área superficial principal de la porción de papa (m^2).

$C = C(x,t)$: Perfil de concentración de agua líquida $\left(kg/m_t^3\right)$.

$\overline{C} = \overline{C}(x,t)$: Función concentración adimensional de agua líquida definida por (22).

$F(t)$, $f(t)$: Funciones del tiempo t, definidas por (20) y (21) respectivamente.

L, ℓ : Semiespesor de la porción prismática de papa (m) y parámetro definido por (18), respectivamente.

m, p_o, p_1, q, r : Parámetros definidos por (18), (15), (16) y (25) respectivamente.

$S(t)$: Función frontera libre o coordenada móvil que ubica la interfase Corteza-Corazón en la región sólido papa (m).

t_2: Tiempo conllevado por la etapa del freído previa a la etapa principal (seg).

$T = T(x,t)$, $U = U(x,t)$: Perfiles de temperatura en las zonas Corazón y Corteza de la papa respectivamente (ºC).

$\overline{T} = \overline{T}(x,t), \overline{U} = \overline{U}(x,t)$: Perfiles de temperatura en las zonas Corazón y Corteza, definidas por (22) (ºC).

T_b , T_e , T_0: Temperaturas de: baño de aceite, ebullición del agua, inicial de la porción de papa, respectivamente (ºC).

G, V : Funciones definidas por (42) y (43) respectivamente.

Z : Variable espacial independiente adimensional definida por (22).

Subíndices:

t : Total

Propiedades del sólido papa o Termodinámicas:

C_c , C_s , C_v: Calores específicos de las zonas Corteza, Corazón y vapor de agua a 100ºC, respectivamente $\left(J/kg^{\circ}C\right)$.

D : Difusividad efectiva del agua líquida $\left(m^2/seg\right)$.

h : Coeficiente global de transferencia de calor $\left(W/m^{2\,\circ}C\right)$.

h_c , h_s : Entalpías de las zonas Corteza y Corazón respectivamente $\left(J/kg\right)$.

h_a , H_v : Entalpías del agua y vapor a 100ºC, respectivamente $\left(J/kg\right)$.

ΔH_v : Calor latente de vaporización del agua $\left(J/mol\right)$.

k_c , k_s : Conductividades térmicas de las zonas Corteza y Corazón respectivamente $\left(W/m\ ^{\circ}C\right)$.

K_v : Permeabilidad (Conductividad hidráulica) $\left(m^2\right)$.

V_a , V_v : Volúmenes molares específicos del agua y vapor a 100º C $\left(m^3/mol\right)$.

Símbolos Griegos

$\varepsilon_c, \varepsilon_s, \varepsilon_v$: Fracción de volumen $\left(m^3/m_t^3\right)$ de las zonas Corteza, Corazón y vapor de agua respectivamente.

ρ_c , ρ_s , ρ_v : Densidades $\left(kg/m^3\right)$ de las zonas Corteza, Corazón y vapor de agua a 100ºC, respectivamente.

μ_v : Viscosidad del vapor de agua a 100ºC.

$\alpha, \beta, \gamma, \delta, \mu, \lambda, \nu, \Lambda$: Parámetros definidos por (23) y (24).

$\omega = \omega(t)$, $\Omega = \Omega(t)$: Funciones definidas por (37) y (38) respectivamente.

Ω_1, Ω_2 : Regiones definidas por (41) y (42) respectivamente.

τ : Variable tiempo desplazada definida por (22).

Introducción:

En el presente nos abocaremos a realizar un análisis básico desde el punto de vista matemático, cual es el atinente a cuestiones relativas al buen planteo (comenzando por la unicidad de solución) de un problema de valor inicial y frontera libre–móvil, como modelo matemático descriptivo de un proceso de freído de papa natural por inmersión en aceite comestible caliente.

Tal proceso, puede caracterizarse fenomenológicamente como ocurriendo según tres etapas consecutivas temporalmente, a saber:

Etapa 0 (de precalentamiento del sólido).
Etapa 1 (Vaporización de humedad "libre" o "agua capilar").
Etapa 2 (la denominamos etapa principal en el presente. También se denomina de burbujeo. Es la más larga del proceso) (Para detalles ver [1], [2]).
En el presente, específicamente centramos el análisis en la **etapa principal**.
En las figuras 1, 2 y 3 se ilustran el dominio sólido (papa en porción prismática) considerado, las dos zonas caracterizantes del sólido durante la evolución dinámica de la etapa y los correspondientes perfiles de temperatura y humedad, de ocurrencia esperada en el sólido, respectivamente.

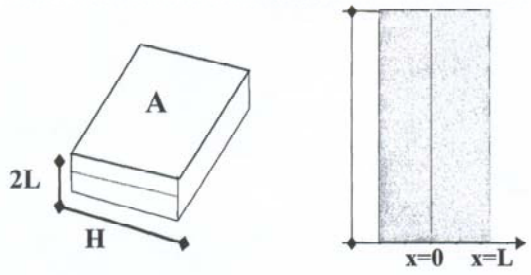

Fig 1: Esquema de la geometría de muestra de papa usada

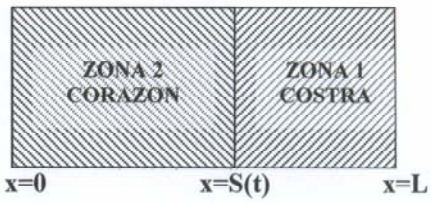

Fig 2

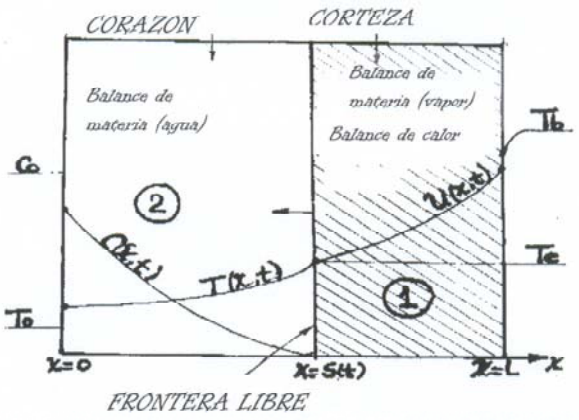

Fig 3: Diagrama esquemático de perfiles de temperatura y concentración de agua en la papa durante la Etapa principal

Como puede apreciarse, en el modelo asumido la vaporización del agua contenida en la papa se postula ocurriendo esencialmente sobre un frente o superficie móvil cuya coordenada viene justamente proporcionada por la función frontera libre $S= S(t)$, esperándose ser una función monótona decreciente desde su valor inicial $S(0) = L$ coincidente con la superficie de contacto papa- baño de aceite, moviéndose hacia el centro de simetría de la porción sólida al transcurrir el proceso.
Entonces, durante la etapa en análisis, el dominio sólido viene caracterizado por las dos zonas esquemáticamente ilustradas en la Fig. 2:
Zona 1: Corteza ó Costra, $S(t)<x<L$
Zona 2: Corazón, $0<x<S(t)$

Con la ocurrencia de los siguientes fenómenos de transporte de calor y materia:
Zona Corazón: Conducción de calor y transporte de agua líquida por difusión molecular, para vaporizarse sobre el frente x=S(t).
Zona Corteza: Conducción de calor y transporte de vapor de agua por gradiente de presión (se asume un flujo sin resistencia prácticamente a través de un medio poroso).

En la Fig. 4 se ilustra esquemáticamente los dominios y condiciones de contorno correspondientes a cada función incógnita ocurrentes en el proceso

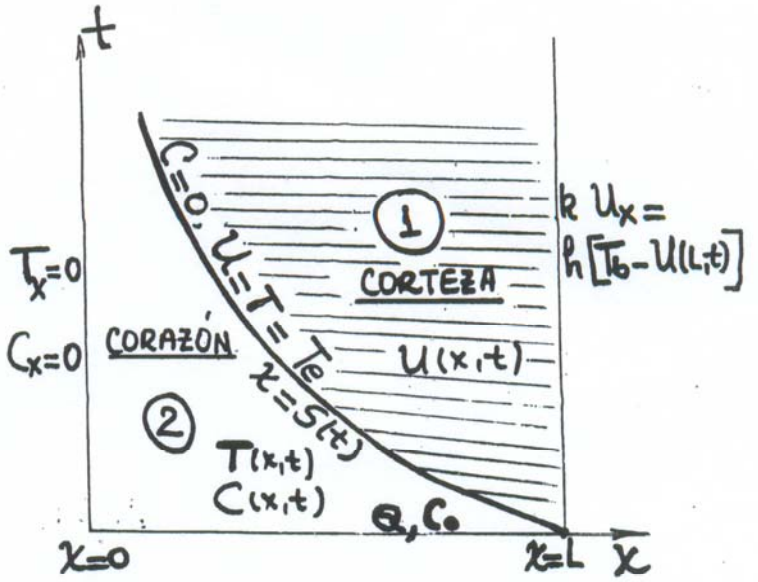

Fig 4: Esquema de dominios y condiciones de contorno correspondientes a cada función incógnita

Modelo Matemático Descriptivo

Bajo el supuesto del cumplimiento de un cierto conjunto de hipótesis y restricciones oportunamente contempladas y respetando la notación consignada en la nomenclatura referente a variables, parámetros y funciones, emerge el siguiente modelo matemático descriptivo de la evolución del proceso de freído durante la etapa considerada:

$$\varepsilon_s \rho_s C_s \frac{\partial T}{\partial t} = k_s \frac{\partial^2 T}{\partial x^2}, \qquad 0 < x < S(t), \qquad t > t_2, \tag{1}$$

$$\frac{\partial T}{\partial x}(0,t) = 0, \qquad t > t_2, \tag{2}$$

$$T\left(S(t),t\right) = T_e \quad , \qquad t > t_2, \tag{3}$$

$$T = Q(x) \quad , \quad 0 \le x \le L, \qquad t = t_2, \tag{4}$$

$$Q(x) = 1.52\exp(0.8)x^3 - 9.13\exp(0.5)x^2 + 2.05\exp(0.3)x + 20, \tag{5}$$

$$(\varepsilon_v \rho_v C_v + \varepsilon_c \rho_c C_c)\frac{\partial U}{\partial t} = k_c \frac{\partial^2 U}{\partial x^2}, \qquad S(t) < x < L, \quad t > t_2, \tag{6}$$

$$k_c \frac{\partial U}{\partial x}(L,t) = h\left[T_b - U\left(L,t\right)\right], \qquad t > t_2, \tag{7}$$

$$U\left(S(t),t\right) = T_e, \qquad t > t_2, \tag{8}$$

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}, \quad 0 < x < S(t), \qquad t > t_2, \tag{9}$$

$$\frac{\partial C}{\partial x}(0,t)=0, \qquad t>t_2, \tag{10}$$

$$C(S(t),t)=0, \qquad t>t_{2,} \tag{11}$$

$$C=C_0, \qquad 0\le x\le L, \qquad t=t_2, \tag{12}$$

$$S\left(t_2\right)=L\,. \tag{13}$$

Balance de Energía sobre la Frontera Libre *S(t)*

$$p_0\frac{dS}{\partial t}=p_1\frac{\partial U}{\partial X}\left(S(t),t\right)+k_s\frac{\partial T}{\partial x}\left(S(t),t\right)\ , \quad \mathrm{t}>\mathrm{t}_2 \tag{14}$$

donde los parámetros p_0 y p_1 vienen dados como

$$p_0=\mathcal{E}_s\rho_s\ (h_c-h_s)+\mathcal{E}_v\rho_v(H_v-\rho_d)\,, \tag{15}$$

$$p_1=\frac{(H_v-h_a)\rho_v K_v\Delta H_v}{T_e\mu_v(V_v-V_a)}-k_c\,. \tag{16}$$

Balance de Materia sobre la Frontera Libre *S(t)*

$$m\frac{dS}{dt}=D\frac{\partial C}{\partial x}(S(t),t)-\ell\frac{\partial U}{\partial x}(S(t),t) \qquad ,t>t_2, \tag{17}$$

con los parámetros m y ℓ dados como

$$m=\varepsilon_a\rho_a-\varepsilon_v\rho_v \quad , \quad \ell=\frac{\rho_v K_v}{\mu_v T_e}\frac{\Delta H_v}{(V_v-V_a)}. \tag{18}$$

Observación 1

En adelante la condición de contorno dada por la ecuación (7), para el perfil de temperatura U, se reemplazará por la siguiente:

$$k_c\frac{\partial U}{\partial x}\left(L,t\right)=F(t), \qquad t>t_2, \tag{19}$$

con *F = F(t)* dada como:

$$F\left(t\right)=h\left[T_b-f\left(t\right)\right], \qquad t>t_2, \tag{20}$$

donde

$$f\left(t\right)=1\exp(-10)t^4-3\exp(-0.7)t^3+0.0003t^2-0.0037t+108.82\,. \tag{21}$$

Observación 2

Se debe tener presente en adelante que la condición de contorno sustitutiva consignada por la ecuación (19) proviene de datos experimentales de la historia térmica del proceso medida en un punto muy cercano a la superficie externa de contacto papa - aceite. En efecto, $f=f(t)$ dado por la ecuación (21) es una función de ajuste de los citados datos .

Observación 3

Con vista a efectuar el tratamiento del Modelo descriptivo consignado por la ecuaciones (1) a (21) explicitadas precedentemente, conviene trabajar sobre una versión equivalente a la dada por tales ecuaciones. A tal efecto, se introducen las siguientes transformaciones de variables y funciones a saber:

$$\begin{aligned} &Z = 1 - \frac{x}{L}, \qquad \tau = t - t_2, \qquad \sigma(t) = \frac{L - S(t)}{L}, \\ &\bar{C}(x,t) = \frac{C(x,t)}{C_0}, \quad \bar{T}(x,t) = T_e - T(x,t), \\ &\bar{U}(x,t) = U(x,t) - T_e \end{aligned} \tag{22}$$

y además los siguientes parámetros nuevos, definidos en términos de los básicos:

$$\alpha = \frac{k_s}{\rho_s C_s \varepsilon_s L^2}, \quad \beta = \frac{k_c}{L^2(\varepsilon_v \rho_v C_v + \rho_c \varepsilon_c C_c)}, \quad \Lambda = \frac{D}{L^2}, \tag{23}$$

$$\lambda = \frac{k_s}{p_0 L^2}, \quad \upsilon = \frac{p_1}{p_0 L^2}, \quad \gamma = \frac{\upsilon}{\beta}, \delta = \frac{\lambda}{\alpha}, \mu = \frac{\upsilon L}{k_c}, \tag{24}$$

$$q = \frac{DC_0}{mL^2}, \quad r = \frac{\ell}{L^2 m} \quad . \tag{25}$$

Entonces, teniendo presente la Observación 1, las transformaciones dadas por (22) y (23) a (25), trabajando sobre las ecuaciones (1) a (21) se obtiene la siguiente versión equivalente, donde en pro de facilitar la escritura y no complicarse con tanta nueva simbología, las funciones $\bar{U}, \bar{T}, \bar{C}$ se volvieron a denotar con U, T, C y a la variable tiempo τ como t

$$(I) \begin{cases} \dfrac{\partial U}{\partial t} = \beta \dfrac{\partial^2 U}{\partial Z^2}, \quad 0 < Z < \sigma(t), \quad t > 0, \\ -\dfrac{k_c}{L} \dfrac{\partial U}{\partial Z} = F(t) \quad , \qquad Z = 0 \ , \quad t > 0, \\ U = 0, \qquad Z = \sigma(t), \quad t > 0, \end{cases} \tag{26}$$

$$(II) \begin{cases} \dfrac{\partial T}{\partial t} = \alpha \dfrac{\partial^2 T}{\partial Z^2}, \quad \sigma(t) < Z < 1, \qquad t > 0, \\ \dfrac{\partial T}{\partial Z} = 0, \qquad Z = 1, \qquad t > 0, \\ T = 0 \qquad Z = \sigma(t), \qquad t > 0, \\ T = W(Z) = T_e - Q(L - LZ), \quad 0 \le Z \le 1, \qquad t = 0, \end{cases} \tag{27}$$

$$(III) \begin{cases} \dfrac{d\sigma}{dt} = \upsilon \dfrac{\partial U}{\partial Z}(\sigma(t), t) - \lambda \dfrac{\partial T}{\partial Z}(\sigma(t), t), \qquad t > 0, \\ \sigma(0) = 0 \end{cases} \tag{28}$$

$$(IV)\begin{cases} \dfrac{\partial C}{\partial t} = \Lambda \dfrac{\partial^2 C}{\partial Z^2}, \quad \sigma(t) < Z < 1, \qquad t > 0, \\ \dfrac{\partial C}{\partial Z} = 0, \quad Z = 1, \qquad t > 0, \\ C = 0, \qquad Z = \sigma(t), \qquad t > 0, \\ C = 1, \qquad 0 \le Z \le 1, \qquad t = 0, \end{cases} \tag{29}$$

$$(V)\begin{cases} \dfrac{d\sigma}{dt} = q\dfrac{\partial C}{\partial Z}(\sigma(t),t) - r\dfrac{\partial U}{\partial Z}(\sigma(t),t), \end{cases} \tag{30}$$

Observación 4

Desde el punto de vista conceptual, es importante puntualizar que los sistemas agrupados como (I), (II) y (III), partes del modelo descriptivo (26) a (38), constituyen un problema de frontera libre unidimensional a dos fases. En tanto que, los sistemas (IV) y (V) relacionados con (I), (II), (III) a través de la función $\sigma = \sigma(t)$, constituyen un problema de frontera móvil para la función incógnita *C = C(x,t).*

El flujo de información es el siguiente:

- Se resuelve (I), (II), (III) para las incógnitas U, T, σ.
- Se resuelve (IV) usando la σ del paso precedente.
- De (V) se calcula $\dfrac{\partial C}{\partial Z}(\sigma(t),t)$

Unicidad de la solución del Submodelo de Frontera Libre (I), (II), (III).

Supongamos que fuera posible la ocurrencia de dos soluciones distintas σ_1, T_1, U_1 y σ_2, T_2, U_2 para el problema de frontera libre consignado por (I), (II), (III). Por consiguiente, en virtud de las ecs. (26) a (33) ((I), (II), (III)), se deberá verificar

$$(I)'\begin{cases} \dfrac{\partial U_1}{\partial t} = \beta \dfrac{\partial^2 U_1}{\partial Z^2}, \ 0 < Z < \sigma_1(t), \qquad t > 0, \\ -\dfrac{kc}{L}\dfrac{\partial U_1}{\partial Z} = F(t), \ \ Z = 0, \qquad\qquad t > 0, \\ U_1 = 0, \quad \mathrm{Z} = \sigma_1(t), \qquad\qquad t > 0, \end{cases} \tag{31}$$

$$(II)'\begin{cases} \dfrac{\partial T_1}{\partial Z} = \alpha \dfrac{\partial^2 T_1}{\partial Z^2}, \quad \sigma_1(t) < z < 1, \qquad t > 0, \\ \dfrac{\partial T_1}{\partial Z} = 0, \qquad Z = 1, \qquad t > 0, \\ T_1 = 0, \qquad Z = \sigma_1(t), \qquad t > 0, \\ T_1 = W(z), \qquad 0 \le Z \le 1, \qquad t = 0, \end{cases} \tag{32}$$

$$(III)'\begin{cases} \dfrac{d\sigma_1}{dt} = \upsilon \dfrac{\partial U_1}{\partial Z}(\sigma_1(t),t) - \lambda \dfrac{\partial T_1}{\partial Z}(\sigma_1(t),t) \\ \sigma_1(0) = 0 \end{cases} \tag{33}$$

$$(I)''\begin{cases} \dfrac{\partial U_2}{\partial t} = \beta \dfrac{\partial^2 U_2}{\partial Z^2}, \quad 0 < Z < \sigma_2(t), \qquad t > 0, \\ -\dfrac{kc}{L}\dfrac{\partial U_2}{\partial Z} = F(t), \qquad Z = 0, \qquad t > 0, \\ \mathrm{U}_2 = 0, \qquad Z = \sigma_2(t), \qquad t > 0, \end{cases} \tag{34}$$

$$(II)''\begin{cases} \dfrac{\partial T_2}{\partial Z} = \alpha \dfrac{\partial^2 T_2}{\partial Z^2}, \quad \sigma_2(t) < Z < 1, \quad t > 0, \\ \dfrac{\partial T_2}{\partial Z} = 0, \qquad Z = 1, \qquad t > 0, \\ T_2 = 0 \quad Z = \sigma_2(t), \qquad t > 0, \\ T_2 = W(Z), \quad 0 \le Z \le 1, \qquad t = 0, \end{cases} \tag{35}$$

$$(III)''\begin{cases} \dfrac{d\sigma_2}{dt} = \upsilon \dfrac{\partial U_2}{\partial Z}(\sigma_2(t)) - \lambda \dfrac{\partial T_2}{\partial Z}(\sigma_2(t),t) \\ \sigma_2(0) = 0 \end{cases} \tag{36}$$

Definimos ahora a las funciones $\omega = \omega(t)$, $\Omega = \Omega(t)$ y a las regiones Ω_1, Ω_2 como:

$$\omega(t) = Min\{\sigma_1(t), \sigma_2(t)\}, \tag{37}$$

$$\Omega(t) = Max\{\sigma_1(t), \sigma_2(t)\}, \tag{38}$$

$$\Omega_1 \equiv \{(Z,t)/0 < Z < \omega(t), t > 0\}, \tag{39}$$

$$\Omega_2 \equiv \{(Z,t)/\Omega(t) < Z < 1, t > 0\}, \tag{40}$$

Para tomar una de las alternativas posibles, supóngase que

$$\sigma_1(t) > \sigma_2(t), \qquad t > 0 \qquad . \tag{41}$$

Entonces, se pueden formular los siguientes problemas auxiliares emergentes de (I)' a (II)' y (I)'' a (II)'', teniendo presente (37) a (41):

$$(a)\begin{cases} \dfrac{\partial U_1}{\partial t}=\beta\dfrac{\partial^2 U_1}{\partial Z^2},(Z,t)\in\Omega_1\equiv\left\{(Z,t)/0<Z<\sigma_2(t),\ t>0\right\} \\ -\dfrac{k_c}{L}\dfrac{\partial U_1}{\partial Z}=F(t),\ Z=0, \quad t>0, \\ U_1(\sigma_2(t),t)>0, \quad t>0, \end{cases}$$

$$(b)\begin{cases} \dfrac{\partial U_2}{\partial t}=\beta\dfrac{\partial^2 U}{\partial Z^2},\ (Z,t)\in\Omega_1 \\ -\dfrac{k_c}{L}\dfrac{\partial U_2}{\partial Z}=F(t),\ Z=0, \quad t>0, \\ U_2(\sigma_2(t),t)=0, \quad t>0, \end{cases}$$

$$(c)\begin{cases} \dfrac{\partial T_1}{\partial t}=\alpha\dfrac{\partial\ T_1}{\partial Z^2},(Z,t)\in\Omega_2\equiv\left\{(Z,t)/\sigma_1(t)<Z<1,\ t>0\right\} \\ \dfrac{\partial T_1}{\partial Z}=0,\ Z=1, \quad t>0, \\ T_1(\sigma_1(t),t)=0, \quad t>0, \\ T_1(Z,0)=W(Z), \quad 0\le Z\le 1, \quad t=0, \end{cases}$$

$$(d)\begin{cases} \dfrac{\partial T_2}{\partial t}=\alpha\dfrac{\partial\ T_2}{\partial Z^2},(Z,t)\in\Omega_2 \\ \dfrac{\partial T_2}{\partial Z}=0,\ Z=1, \quad t>0, \\ T_2(\sigma_1(t),t)>0, \quad t>0, \\ T_2(Z,0)=W(Z), \quad 0\le Z\le 1 \end{cases}$$

Definimos ahora las funciones G=*G(z,t)* y *V=V(z,t)* como:

$$G(z,t)=U_1(z,t)-U_2(z,t), \quad (z,t)\in\Omega_1 \tag{42}$$

$$V(z,t)=T_2(z,t)-T_1(z,t), \quad (z,t)\in\Omega_2 \tag{43}$$

que resultan satisfacer los siguientes problemas:

$$(e)\begin{cases} \dfrac{\partial G}{\partial t}=\beta\dfrac{\partial^2 G}{\partial Z^2}, \quad (\mathrm{Z,t})\in\Omega_1 \\ \dfrac{\partial G}{\partial Z}=0, \quad z=0, \qquad t>0, \\ \mathrm{G}(\sigma_2(\mathrm{t}),\mathrm{t})>0 \qquad \mathrm{t}>0, \end{cases}$$

$$(f)\begin{cases} \dfrac{\partial V}{\partial t}=\alpha\dfrac{\partial^2 V}{\partial Z^2}, \quad (\mathrm{Z,t})\in\Omega_2 \\ \dfrac{\partial V}{\partial Z}=0, \quad z=1, \quad t>0, \\ V\left(\sigma_1(t),t\right)>0, \quad \mathrm{t}>0, \\ \mathrm{V}(\mathrm{Z},0)=0, \quad 0\le \mathrm{Z}\le 1 \end{cases}$$

Teniendo presente (7), (20) y (22), en virtud del Principio del máximo aplicado a los problemas (e) y (f) se infiere la siguiente propiedad de comparación para las funciones U_1, U_2, T_1, T_2:

$$U_1(Z,t)>U_2(Z,t),\forall(Z,t)\in\Omega_1, \tag{44}$$

$$T_2(Z,t)>T_1(Z,t),\forall(Z,t)\in\Omega_2. \tag{45}$$

En la Fig. 5 se ilustra esquemáticamente los comportamientos emergentes para las citadas funciones.

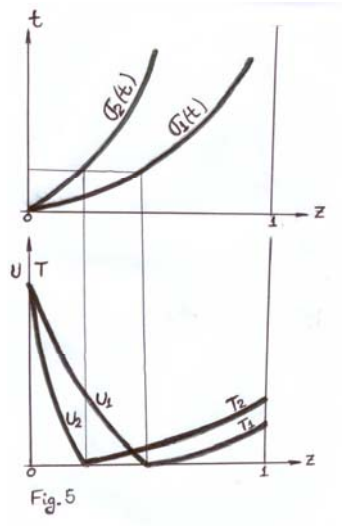

Fig. 5

Formulación Integral a partir de (I), (II), (III) para la Frontera Libre $\sigma(t)$.

Integrando en los respectivos dominios las ecuaciones diferenciales de (I) y (II), se obtienen expresiones para $\int_0^t \frac{\partial U}{\partial Z}(\sigma(\eta),\eta)d\eta$, $\int_0^t \frac{\partial T}{\partial Z}(\sigma(\eta),\eta)d\eta$, lo que usado en (III) permite obtener la siguiente expresión para $\sigma(t)$:

$$\sigma(t)=\gamma\int_0^{\sigma(t)}U(z,t)dz+\delta\int_{\sigma(t)}^1 T(z,t)dz+\mu\int_0^t F(\eta)d\eta-\delta\int_0^1 W(z)dz, \tag{46}$$

Teniendo presente (41), a partir de (46) se puede escribir:

$$\begin{aligned}&\sigma_1(t)-\sigma_2(t)=\gamma\left[\int_0^{\sigma_1(t)}U_1(Z,t)\,dZ-\int_0^{\sigma_2(t)}U_2(Z,t)\,dZ\right]+\\&\delta\left[\int_{\sigma_1(t)}^1 T_1(Z,t)\,dZ-\int_{\sigma_2(t)}^1 T_2(Z,t)\,dZ\right],\end{aligned} \tag{47}$$

donde cabe consignar que los parámetros γ y δ verifican

$$\gamma<0\,,\ \delta>0\,, \tag{48}$$

Entonces, teniendo presente lo establecido por las desigualdades (44), (45) y (48), de (47) se sigue que el segundo miembro de tal igualdad resulta negativo, debiendo ser el primer miembro positivo por lo supuesto explicitado por (41).

Obviamente, a la misma conclusión se arribará, si se hubiese supuesto la desigualdad contraria a la dada por (41), es decir $\sigma_1(t)<\sigma_2(t)$.

Se concluye entonces de que no pueden existir dos soluciones distintas (ternas distintas: $(\sigma_1,T_1,U_1),(\sigma_2,T_2,U_2)$) correspondientes a los mismos datos iniciales y de contorno para los sistemas (I), (II), (III).

Dependencia del avance de la frontera libre con la temperatura Tb del baño de aceite.

Supóngase 2 procesos de freído que ocurren en idénticas condiciones excepto que un caso la temperatura del baño de aceite es T_b^2 y en el otro T_b^1, teniéndose por ejemplo que

$$T_b^2>T_b^1 \tag{49}$$

La condición dada por (49) implica la siguiente desigualdad para el término $\mu\int_0^t F(\eta)d\eta$ relacionado al flujo de calor F que ingresa hacia la porción de papa desde el baño de aceite durante el freído

$$\mu\int_0^t F_1(\eta)d\eta<\mu\int_0^t F_2(\eta)d\eta \tag{50}$$

donde con F_1 y F_2 se ha denotado a los flujos en correspondencia con T_b^1 y T_b^2 respectivamente. Supongamos que el orden de los datos establecidos por (49) conlleva al siguiente resultado de comparación para los avances de la frontera libre $\sigma(t)$

$$\sigma_2(t)<\sigma_1(t) \tag{51}$$

correspondiendo σ_2 al dato T_b^2 y σ_1 al T_b^1. En vista de (51), ahora se puede escribir:

$$\begin{aligned}&\sigma_1(t)-\sigma_2(t)=\gamma\left[\int_0^{\sigma_1(t)}U_1(Z,t)\,dZ-\int_0^{\sigma_2(t)}U_2(Z,t)\,dZ\right]+\\&\delta\left[\int_{\sigma_1(t)}^1 T_1(Z,t)\,dZ-\int_{\sigma_2(t)}^1 T_2(Z,t)\,dZ\right]+\mu\left[\int_0^t\left[F_1(\eta)-F_2(\eta)\right]d\eta\right]\end{aligned} \tag{52}$$

Teniendo presente de que seguirian valiendo las comparaciones establecidas por (44), (45), y en vista de que $\mu > 0$ y lo consignado por (50), de (52) se concluye que el segundo miembro resulta negativo, debiendo ser el primer miembro positivo.

Debe entonces darse lo contrario:

$$T_b^2 > T_b^1 \Rightarrow \sigma_2(t) \geq \sigma_1(t), \quad t > 0, \tag{53}$$

como se espera naturalmente.

Dependencia del avance de la frontera libre con la temperatura inicial de la porción de papa.

Ahora se tienen dos procesos de freído cuyas condiciones operativas difieren únicamente en la temperatura inicial T_0 de la porción de papa a freir. Para tomar un caso consideremos

$$T_0^1 > T_0^2 \tag{54}$$

Ahora, la desigualdad (55) implica la siguiente para el término relacionado a la condición inicial en (46):

$$\int_0^1 W_1(z)dz < \int_0^1 W_2(z)dz\,, \tag{55}$$

De aquí en más se procede con un argumento similar al aplicado para deducir el resultado expresado por (53) para la dependencia de $\sigma(t)$ con T_b. Así, se obtiene el resultado:

$$T_0^1 > T_0^2 \Rightarrow \sigma_1(t) \geq \sigma_2(t), \quad t > 0, \tag{56}$$

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SIMPLE, PRACTICAL, AND EFFICIENT ON-LINE CORRECTION OF PROCESS DEVIATIONS IN BATCH RETORT THROUGH SIMULATION

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ABSTRACT

This paper describes a practical and efficient (nearly precise, yet safe) strategy for on-line correction of thermal process deviations during retort sterilization of canned foods. Commercial systems currently in use for on-line correction of process deviations do so by extending process time to that which would be needed had the entire process been carried out at the lower retort temperature reached at the lowest point in the deviation ("commercial" correction). This method of correction often results in extensive unnecessary over-processing with concomitant deterioration in product quality, and costly interruption to the retort loading/unloading rotation schedules in retort cook room operations. These problems are addressed by a novel control strategy that takes into account the duration of the deviation in addition to the magnitude of the temperature drop. It calculates a "proportional" extended process time at the recovered retort temperature that will deliver the final specified target lethality with very little over processing in comparison to current industry practice. In addition, a strategy for online-correction without extending process time was developed and preliminarily validated. Results from an exhaustive "optimization" search routine using the complex method are also reported, that show the proposed strategy will always result in a corrected process that delivers no less than the final target lethality specified for the originally scheduled process.

KEY WORDS: On-line Control, Low Acid Foods, Batch Retort, Process Deviations.

INTRODUCTION

Thermal processing is an important method of food preservation in the manufacture of shelf stable canned foods. Most of the work done in thermal processes deal with the microbiological and biochemical aspects of the process and are rarely related to the engineering aspects or practical industrial operations of the process. The basic function of a thermal process is to inactivate pathogenic and food spoilage causing bacteria in sealed containers of food using heat treatments at temperatures well above ambient boiling point of water in pressurized steam retorts (autoclaves). Excessive heat treatment should be avoided because it is detrimental to food quality, wastes energy, and under utilizes plant capacity. Thermal process calculations, in which process times at specified retort temperatures are calculated in order to achieve safe levels of microbial inactivation (lethality), must be carried out carefully to assure public health safety (Bigelow and others, 1920; Ball, 1928; Stumbo, 1973; Pham, 1987; Teixeira, 1992; Holdsworth, 1997). However, over-processing must be avoided thermal processes also have a detrimental effect on the quality (nutritional and sensorial

factors) of foods. Therefore, the accuracy of the methods used for this purpose is of importance to food science and engineering professionals working in this field.

Control of thermal process operations in food canning factories has consisted of maintaining specified operating conditions that have been predetermined from product and process heat penetration tests, such as the process calculations for the time and temperature of a batch cook. Sometimes unexpected changes can occur during the course of the process operation such that the pre-specified processing conditions are no longer valid or appropriate. These types of situations are known as process deviations. Because of the important emphasis placed on the public safety of canned foods, processors must operate in strict compliance with the US Food and Drug Administration's Low-Acid Canned Food (FDA/LACF) regulations. A succinct summary and brief discussion of these regulations can be found in Teixeira (1992). Among other things, these regulations require strict documentation and record-keeping of all critical control points in the processing of each retort load or batch of canned product. Particular emphasis is placed on product batches that experience an unscheduled process deviation**,** such as when a drop in retort temperature occurs during the course of the process, which may result from loss of steam pressure. In such a case, the product will not have received the established scheduled process, and must be either fully reprocessed, destroyed, or set aside for evaluation by a competent processing authority. If the product is judged to be safe then batch records must contain documentation showing how that judgment was reached. If judged unsafe, then the product must be fully reprocessed or destroyed. Such practices are costly.

In one very traditional method, on-line correction is accomplished by extending process time to that which would be needed had the entire process been carried out at the retort temperature reached at the lowest point in the deviation (Larkin, 2002). This method of correction will always assure sufficient food safety (process lethality), but often results in significant unnecessary over-processing with concomitant deterioration in product quality. Alternative methods proposed initially by Teixeira and Manson (1982) and Datta, Teixeira and Manson (1986), and later summarized in Teixeira and Tucker (1997) and demonstrated and validated by Teixeira, Balaban, Germer, Sadahira, Teixeira-Neto, and Vitali (1999) make use of heat transfer simulation software to automatically extend process time at the recovered retort temperature to reach precisely the original target lethality required of the process. An alternative approach to on-line correction of process deviations was described in the work of Akterian (1996, 1999), who calculated correction factors using mathematical sensitivity functions.

The aim of this research study was the development of a safe, simple, efficient and easy to use procedure to manage on-line corrections of unexpected process deviations in any canning plant facility. Specific objectives were to:

1. Develop strategy to correct the process deviation by an alternative "proportional-corrected" process that delivers no less than final target lethality, but with near minimum extended process time at the recovered retort temperature.

2. Demonstrate strategy performance by comparing "proportional-corrected" with "commercial-corrected" and "exact-corrected" process times.

3. Demonstrate consistent safety of the strategy by exhaustive search over an extensive domain of product and process conditions to find a case in which safety is compromised.

4. Develop and preliminarily validate a strategy for online-correction without extending process time for any low acid canned food.

METHODOLOGY

Scope of Work

To reach the objectives stated above, the approach to this work was carried out in four tasks, one in support of each objective. Task 1 consisted of developing the strategy for on-line correction of process deviations with minimum extended process time using the method of "proportional correction". Task 2 consisted of choosing appropriate mathematical heat transfer models for construction of the equivalent lethality curves or "look-up tables" needed for use with each respective strategy, and for determining the final lethality and quality retention for each of the thousands of cases simulated in the study. Task 3 included the complex optimization search routine that was carried out to demonstrate validity and consistent safety of the strategy. Task 4 consisted of developing and validating the strategy for on-line correction of process deviations without extending process time.
Methodology employed in carrying out each of these tasks is described in greater detail below.

Task 1 - Proportional Correction Strategy Development

The objective for the strategy required in this task was to accomplish an on-line correction of an unexpected retort temperature deviation by an alternative process that delivers final target lethality, but with minimum extended process time at the recovered retort temperature. This would be accomplished with use of the same alternative process "look-up tables" that would normally be used with currently accepted methods of on-line correction of process deviations, but with a "proportional correction" applied to the alternative process time that would reduce it to a minimum without compromising safety. In order to fully understand this strategy, it will be helpful to first review the currently accepted method that is in common practice throughout the industry. Commercial systems currently in use for on-line correction of process deviations do so by extending process time to that which would be needed to deliver the same final lethality had the entire process been carried out with an alternative lower constant retort temperature equal to that reached at the lowest point in the deviation. These alternative retort temperature-time combinations that deliver the same final process lethality (F_o) are called equivalent lethality processes. When these equivalent time-temperature combinations are plotted on a graph of process time versus retort temperature, they fall along a smooth curve called an equivalent lethality curve. These curves are predetermined for each product from heat penetration tests and thermal process calculations carried out for different retort temperatures.

The strategy will calculate the corrected process time (t_D) as a function of the temperature drop experienced during the deviation, but also the time duration of the deviation. The following expression illustrates mathematically how this "proportional-corrected" process time would be calculated for any number (n) of deviations occurring throughout the course of a single process:

$$t_D = t_{TRT} + \sum_{i=1}^{n} (t_D - t_{TRT}) \left(\frac{\Delta t_i}{t_{TRT}} \right), t_D \geq t_{TRT} \quad (1)$$

If we considered the commercial correction as a valid correction, that is:

$$t_{D\,commercial} = t_{TRT} + (t_D - t_{TRT}) \frac{t_{TRTi}}{t_{TRT}} \quad (2)$$

then it is intuitive that a safe correction for a process deviated for a short time is a correction proportional to the time the deviation occurs:

$$t_{D\ proportional} = t_{TRT} + (t_D - t_{TRT})\frac{\Delta t_i}{t_{TRT}} \quad (3)$$

Task 2 - Performance Demonstration

This task consisted of demonstrating the performance of these strategies by simulating the occurrence of process deviations happening at different times during the process (early, late and randomly) to both solid and liquid canned food products, calculating the alternative corrected process times, and predicting the outcomes of each corrected process in terms of final lethality and quality retention. For each deviation, three different alternative corrected process times were calculated:

- "Exact correction", giving corrected process time to reach precisely the final target lethality specified for the scheduled process, using computer simulation with heat transfer models;
- "Proportional-correction", using the strategy described in this paper with look-up tables; and,
- "Commercial correction", using current industry practice with look-up tables (manually or computerized).

The heat transfer models were explicitly chosen to simulate the two extreme heat transfer cases encountered in thermal processing of canned foods. The rationale behind this decision was that canned foods possess heating characteristics between these two extreme situations. Conclusions extracted from these simulations will be extended to all canned foods.

The F value is calculated by:

$$F = \int_0^t 10^{\frac{T_{cp}(t)-T_{ref}}{z}} dt \quad (4)$$

First was the case of pure conduction heating of a solid product under a still-cook retort process (equation 5 is the differential equation for heat conduction, Biot>40). The second was the case of forced convection heating of a liquid product under mechanical agitation (equation 6 is the differential equation for heat convection, Biot<1). In both cases, the container shape of a finite cylinder was assumed, typical of a metal can or wide-mouthed glass jar. However, suitable models appropriate for a true container shapes can be used as required for this purpose. Examples of such models can be found in the literature (Teixeira and others, 1969; Manson and others, 1970; Manson and others, 1974; Datta and others, 1986; Simpson and others, 1989; Simpson and others, 2004). The product and process conditions chosen to carry out the demonstrated simulations for each case are given in Table 1.

$$\frac{\partial T}{\partial t} = \alpha\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial h^2}\right] \quad (5)$$

$$\frac{\partial T(t)}{\partial t} = \frac{U_{ht}\cdot A}{\rho \cdot Vol \cdot Cp}[TRT_corr(t) - T(t)] \quad (6)$$

Task 3 - Demonstration of Safety Assurance by Complex Optimization Search Routine

This on-line correction strategy was validated and tested for safety assurance by executing a strict and exhaustive search routine with the use of the heat transfer models selected in Task 2 on high-speed computer. The problem to be solved by the search routine was to determine if the

minimum final lethality delivered by all the corrected processes that could be found among all the various types of deviations and process conditions considered in the problem domain met the criterion that it had to be greater than or equal to the lethality specified for the original scheduled process. This criterion can be expressed mathematically:

$$\underset{U}{Mín} \left\lfloor F_{proportion\ al} - F_{Tol} \right\rfloor \geq 0 \qquad (7)$$

Table 2 identifies the various types of deviations and process conditions that were explored and evaluated in the search routine (problem domain). The search routine was designed as an attempt to find a set of conditions under which the required search constraint was not met. The table gives the symbol used to represent each variable and a description of that variable, along with the minimum and maximum values limiting the range over which the search was conducted.

Task 4 – On-line Correction without Extending Process Time

For the developing of this strategy, we assume the retort control system to include a computer that is running the software containing the appropriate mathematical heat transfer model, and it reads the actual retort temperature from a temperature-sensing probe through an analogue/digital (A/D) data acquisition system. This continual reading of retort temperature would be used as real-time input of dynamic boundary condition for the mathematical heat transfer model. The model, in turn, would be accurately predicting the internal product cold spot temperature profile as it develops in response to the actual dynamic boundary condition (retort temperature). As the predicted cold spot temperature profile develops over time, the accumulating lethality (F_o) would be calculated by the General method, and would be known at any time during the process. Should a deviation occur during the process a simulated search routine would be carried out on the computer to find the combination of process conditions for the remainder of the process that would result in meeting the final target lethality without over extending process time. The key in this strategy was to identify the retort temperature as the control variable to be manipulated during the remainder of the process (rather than process time). Therefore, upon recovery of the deviation, the search routine would find the new higher retort temperature to be used for the remainder of the process, and send the appropriate signals through the data acquisition system to readjust the retort temperature accordingly.

Increasing retort temperature cannot be accomplished without increasing steam pressure correspondingly, which dictates a practical upper limit to choice of higher retort temperature. This upper limit comes into play when the deviation occurs near the end of the process, when the little time remaining forces the simulation search routine to choose the upper limit for retort temperature. In these cases, the safety requirement for reaching the final target lethality (F_o) must take priority over compromising process time. This will inevitably require some extension in process time, but it will be an absolute minimum, that would not likely upset scheduling routines. Validation of this method was confirmed by demonstrating consistent safety of the strategy by exhaustive "optimization" search over an extensive domain of product and process conditions in an attempt to find a case in which safety was compromised. No such case could be found.

This control strategy finds the lowest process temperature, TRT_H, at which must be reestablishing the process temperature after the deviation i for the rest of the processing time, so the original process time remains the same and the required lethality value (F_{obj}) is reached.

$$TRT_H = Min\left\{TRT / F_p \geq F_{obj} \wedge t_p' = t_p\right\} \quad (8)$$

If TRT_H surpasses the practical limits, the final target lethality (F_o) is more important that the process time, that must be extended according to:

$$If \quad TRT_H > TRT_{\max} \Rightarrow \quad TRT_H = TRT_{\max} \wedge t_p' = Min\left\{t_p / F_p \geq F_{obj}\right\} \quad (9)$$

For a process that experiments more than one deviation, the temperature at which must be corrected the retort temperature after the deviation i, is:

$$TRT_{Hi} = Min\left\{TRT / F_p \geq F_{obj} \wedge t_p' = t_p\right\} \quad (10)$$

If TRT_{Hi} surpasses the practical limit, then:

$$If \quad TRT_{Hi} > TRT_{\max} \Rightarrow \quad TRT_{Hi} = TRT_{\max} \wedge t_p' = Min\left\{t_p / F_p \geq F_{obj}\right\} \quad (11)$$

This higher temperature, TRT_H, needs to be calculated using a look-up table or curve on a graph showing alternative retort temperature-time combinations that were predetermined to deliver the same target lethality (iso-lethality curves) for each product. Mathematically, this equivalent process time can be calculated from the anatomy of the recovered process deviation and original process conditions as follows:

$$t_H = \frac{t_{TRT}^{\ 2}}{t_{LDT}} \quad (12)$$

Equation 12 can be obtained as follows: consider a process in which two deviations occur in sequence. The normal retort temperature is TRT, the first deviation occurs over a time interval Δt at lower than normal retort temperature TRT_D and the second occurs later over an equal time interval Δt at a higher than normal retort temperature TRT_H. If a "proportional corrected process" is applied to each one of the deviations as described in the previous tasks, the mathematical expressions for each correction will be as follows:

$$Correction1 = \frac{t_{TRT} - t_H}{t_{TRT}} \Delta t \quad (13)$$

$$Correction2 = \frac{t_{LDT} - t_{TRT}}{t_{LDT}} \Delta t \quad (14)$$

If we supposed now that TRT_H is selected so both corrections are equivalent, we can equate both terms:

$$\frac{t_{TRT} - t_H}{t_{TRT}} \Delta t = \frac{t_{LDT} - t_{TRT}}{t_{LDT}} \Delta t \quad (15)$$

$$\Rightarrow t_H = \frac{t_{TRT}^{\ 2}}{t_{LDT}} \quad (16)$$

Equation (12) and equation (16) are identities.

Validation of Task 4.

The utility of this approach to on-line correction of process deviations was demonstrated experimentally as a means of preliminary validation. Cylindrical cans (0.075m diameter, 0.113m height) containing a commercially prepared food product (Centauri Ravioli, 350g) were thermally processed in a vertical still-cook retort under saturated steam with maximum working pressure of 40 psig at 140^{o}C (Loveless, Model 177). Both retort temperature and internal product cold spot temperature were monitored with K-type thermocouples, and recorded with an Omega 220 data logger and modem with COM1 connection port. Cans were processed under different combinations of retort temperature and process time, with the temperatures recorded every 2 seconds. Each normal process was defined with a come-up-time (CUT) of 7 minutes, during which the retort temperature increased linearly, followed by a period of constant retort temperature and a cooling cycle. Deviations during the process were deliberately perpetrated by manually shutting off the steam supply to the retort control system. Experiments were carried out in the Food Laboratory pilot plant of the Universidad Técnica Federico Santa Maria in Valparaiso, Chile.

RESULTS AND DISCUSSIONS

Equivalent Lethality Curves

Look-up tables are used to find the alternative process time for the corrected process, and can be presented graphically as "equivalent process lethality curves" for each scheduled product/process. Therefore, equivalent process lethality curves were constructed for each of the two simulated products used in this study, and are shown in Figures 1 and 2 for the case of solid (pure conduction) and liquid (forced convection), respectively.

Performance Demonstration

Figures 3-6 show results from the four product/process simulations carried out to demonstrate the performance of these strategies. The figures contain retort temperature profiles resulting from on-line correction of process deviations happening at different times during the process (early and late) to both solid and liquid canned food products. Each figure shows the "normal" constant retort temperature profile expected for the originally scheduled process, along with the occurrence of a deviation (sudden step-drop in retort temperature for short duration) either relatively early or late into the process. In addition, for each deviation (one in each figure), three different alternative corrected process times are shown resulting from different strategies: "exact correction", "proportional correction" and "commercial correction".

In all cases, the extended process time required by the "commercial correction" strategy, is far in excess of the extended times called for by the other two strategies. Moreover, the new "proportional correction" strategy results in extending process time only slightly beyond that required for an "exact correction", and will always do so. These results are summarized in Table 3, along with results from predicting the outcomes of each corrected process in terms of final process times required, and final lethality and quality retention achieved (using product/process data presented in Table 1). It is most interesting to note the dramatic improvement in nutrient (quality) retention between that resulting from the commercial correction (current industry practice) and that resulting from either of the other two strategies.

Demonstration of Safety Assurance by Complex Search Routine

This on-line correction strategy was validated and tested for safety assurance by executing an exhaustive search routine with the use of the heat transfer models. Recall, the problem to be solved by the search routine was to determine if the minimum final lethality delivered by all the corrected processes that could be found among all the various types of deviations and process conditions considered in the problem domain met the criterion that it had to be greater than or equal to the lethality specified for the original scheduled process. Table 2 (presented earlier) identifies the problem domain by specifying the various types of deviations and process conditions that were explored and evaluated in the search routine. The search routine was designed to find a set of conditions under which the required search constraint was not met. No such conditions could be found.

Correction strategy without extending process time and preliminary validation

Using data from the constant-temperature heat penetration tests carried out in this study, an equivalent process lethality curve (for a target lethality of F_o = 6 minutes) was constructed for the commercial ravioli product and can size used in this study, and is shown in Figure 7.

In order to validate the safety assurance of this new on-line control strategy, a number of heat penetration experiments were carried out in which process deviations were deliberately perpetrated by manual shut-off of the steam supply to the retort, causing the retort temperature and pressure to fall to a lower level for several minutes, after which the steam supply valve was reopened and the deviation quickly recovered. As soon as the complete anatomy of the deviation was known upon recovery, Equation (14) was used to calculate the high temperature equivalent process time (t_{Hi}), from which to obtain the higher retort temperature (TRT_H) needed to accomplish the correction, using the iso-lethality curve in Figure 7. The retort controller set point was immediately adjusted upward to the correction temperature (TRT_H), and brought back down to the originally scheduled retort temperature after an elapsed time equal to the duration of the initial perpetrated deviation. The process was then allowed to proceed normally for the duration of the remaining originally scheduled process time. During each test, retort and internal product cold spot temperatures were continually measured and recorded, and accumulated lethality was calculated as a function of cold spot temperature over time using the General method (assuming a z-value of 10 C). Results from a typical test run are presented in Figure 8, with the process conditions and parameters used for the test listed in Table 4.

Both temperature and lethality are shown as functions of time on Figure 8, with the temperature scale shown along the left side vertical axis, and the lethality scale shown along the right side vertical axis. In the case of this test, the target value for process lethality was 8 minutes and the normal scheduled retort temperature was intended to be 125^{o}C for a scheduled process time of 61 minutes. The perpetrated deviation was initiated after approximately 45 minutes into the process, and held for 5.5 minutes, during which time the retort temperature fell to 122 C. Upon recovery from the deviation, the retort temperature was elevated to approximately 128 ^{o}C (determined from the calculation procedure described above) for five more minutes, and returned to the originally scheduled 125 C for the remainder of the scheduled 61-minute process time.

The measured retort temperature profile (TRT) can be seen in Figure 8, clearly revealing the profile of the perpetrated deviation immediately followed by the high temperature correction process and return to normal, with the cooling cycle beginning right on schedule at the originally appointed process time of 61 minutes. The measured internal product cold spot temperature curve

(Tcp) in Figure 8 reflects the expected erratic response to the combined deviation and correction perturbations experienced by the dynamic retort temperature. Most importantly, in spite of the erratic profile of the internal product cold spot temperature, the final accumulated lethality, calculated as a function of this profile by the General Method, still reached the target value of 8 minutes specified for the process.

CONCLUSIONS

This paper has described a practical and efficient strategy for on-line correction of thermal process deviations during retort sterilization of canned foods. This strategy takes into account the duration of the deviation in addition to the magnitude of the temperature drop. It calculates a "proportional" extended process time at the recovered retort temperature that will deliver the final specified target lethality with very little over processing in comparison to current industry practice. In addition, it is described a strategy that can assure thermal sterilization during unexpected process deviations without extending scheduled process time, and with an absolute minimum of over-processing. They are applicable to all types of foods or containers (solids, liquids, mixtures) or mechanisms of heat transfer (conduction, convection, both combined)

Results from an exhaustive search routine using the complex method support the logic and rationale behind the strategy by showing that the proposed strategy will always result in a corrected process that delivers no less than the final target lethality specified for the originally scheduled process. Economic impact of adopting this strategy over that currently used in industry practice can be a significant increase in production capacity for a typical cannery. In addition, utilizing this novel strategy canned products will attain a much higher quality.

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Table 1. Product and process conditions used for on-line correction strategy simulations.

Product Simulated	**Dimensions (cm)**			**Properties**		**Normal Process**	
	Major	Intermedium	Minor	alfa (m^2/s)	f_h (min)	time (min)	TRT (°C)
Pure Conduction Can, Biot > 40	11.3	-	7.3	1.70E-07	44.4	64.1	120
Forced Convection Can, Biot < 1	11.3	-	7.3	-	4.4	15.6	120

Table 2. Problem domain for search routine

Process Variable	**Description of Process Variable**	**Minimum Value**	**Maximum Value**
TRT	Scheduled Retort Temperature	110 °C	135°C
TRT_i	Lowest retort temperature reached during deviation i	100 °C	TRT - 0.5°C
t_{CUT}	Initial come up time of retort to reach TRT.	5 [min]	15 [min]
t_{dev-i}	Time during the process at which the deviation i begins.	t_{cut}	t_{TRT}
t_i	Time duration of the deviation i	0.5 [min]	t_{TRT}-t_{dev-i}
T_{ini}	Initial product temperature.	20 °C	70 °C

Table 3. Outcomes of each corrected process deviation described in Figures 3-6 in terms of final process time, lethality and quality retention for the three different alternative correction methods.

	EARLY DEVIATION			**LATE DEVIATION**		
	time (min)	Fo (min)	Nutrient Retention	time (min)	Fo (min)	Nutrient Retention
PURE CONDUCTION						
Scheduled Process	64.1	6.0	72.7%	64.1	6.0	72.7%
Exact Correction	66.3	6.0	72.9%	66.8	6.0	72.7%
Proportional Correction	67.5	6.5	72.2%	67.5	6.2	72.3%
Comercial Correction	86.2	16.3	62.3%	86.2	14.4	62.8%
FORCED CONVECTION						
Scheduled Process	15.6	6.0	92.4%	15.6	6.0	92.4%
Exact Correction	18.4	6.1	91.5%	19.6	6.0	90.9%
Proportional Correction	20.8	8.0	89.7%	20.8	7.0	89.9%
Comercial Correction	25.6	11.8	86.2%	30.6	14.7	82.8%

Table 4. Process conditions and parameters used for heat penetration test with ravioli packed in cylindrical cans (0.075m diameter, 0.113m height) producing results shown in Figure 8.

Process Parameters (units)	**Value chosen for heat penetration test**
Reference Temperature (ºC)	121.1
Scheduled process time (min)	61
Low temperature at deviation (ºC)	122
Initial internal product temperature (ºC)	19
Time duration of deviation, Δ, (min)	5.5
Target process lethality, Fo, (min)	8
Microbial temperature factor, z, (ºC)	10
Scheduled retort temperature (ºC)	125

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Figure 2. Equivalent process lethality curve for simulated liquid product under forced convection heating, showing retort temperature / process time combinations that deliver the same final target lethality.

Figure 3. Pure conduction simulation for on-line correction of an unexpected retort temperature deviation occurring early into the scheduled process for a cylindrical can of solid food under still cook.

Figure 4. Pure conduction **s**imulation for on-line correction of an unexpected retort temperature deviation occurring late into the scheduled process for a cylindrical can of solid food under still cook.

Figure 5. Forced convection **s**imulation for on-line correction of an unexpected retort temperature deviation occurring early into the scheduled process for a cylindrical can of liquid food under agitated cook.

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Figure 7. Iso-lethality curve showing equivalent combinations of process time and retort temperature that achieve the same process lethality (F_o = 6 min) for ravioli packed in cylindrical cans (0.075m diameter, 0.113m height).

Figure 8. Profiles of retort (TRT) and internal product cold spot temperatures (Tcp) over time (scale on left), along with profile of accumulated lethality over time (scale on right) from heat penetration test with ravioli in cans (0.075m diameter, 0.113m height) experiencing perpetrated process deviation immediately followed by temporary high retort temperature correction (calculated on-line).

Figure 1. Equivalent process lethality curve for simulated solid product under pure conduction heating, showing retort temperature / process time combinations that deliver the same final target lethality.

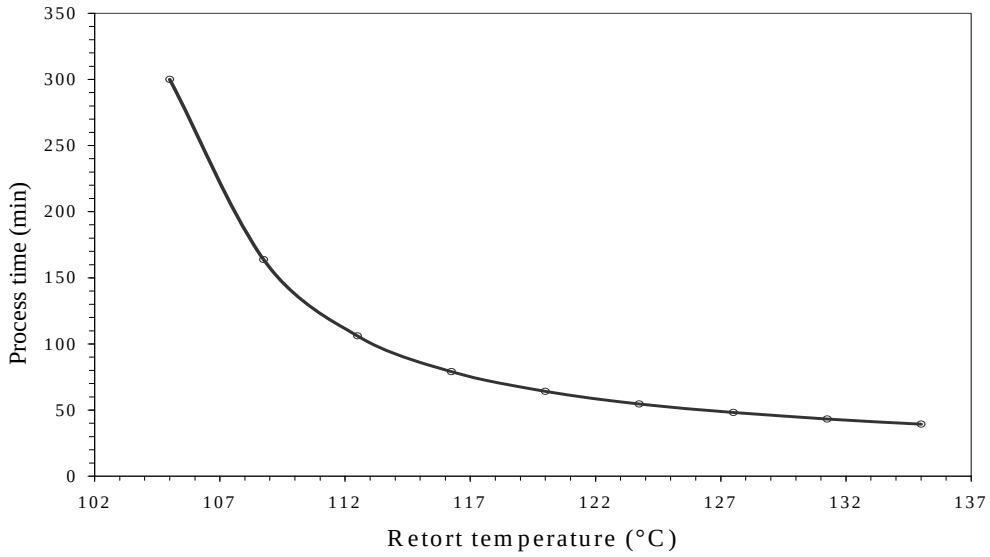


Figure 2. Equivalent process lethality curve for simulated liquid product under forced convection heating, showing retort temperature / process time combinations that deliver the same final target lethality.

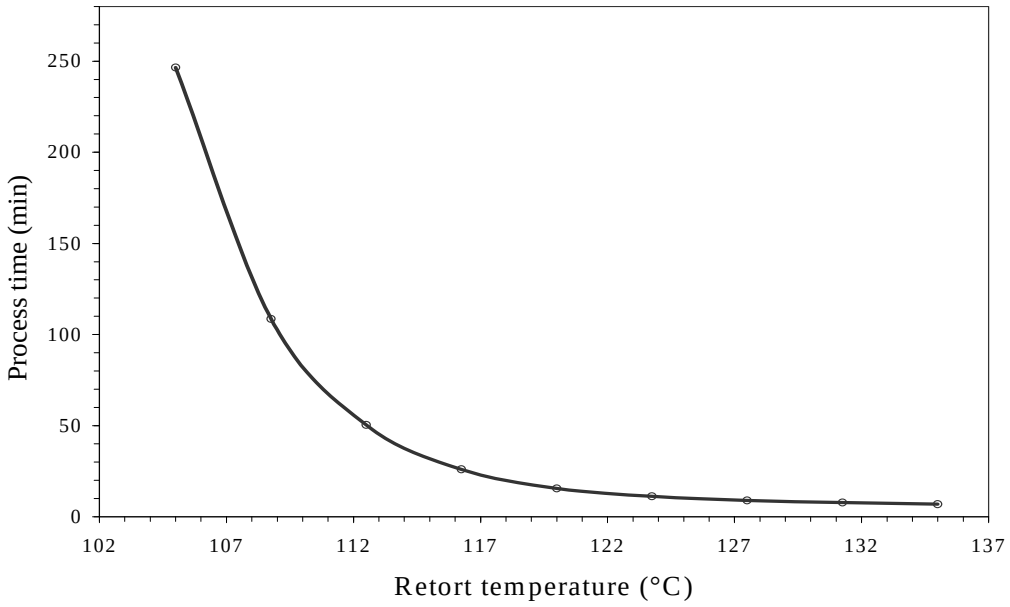


Figure 3. Pure conduction simulation for on-line correction of an unexpected retort temperature deviation occurring early into the scheduled process for a cylindrical can of solid food under still cook.

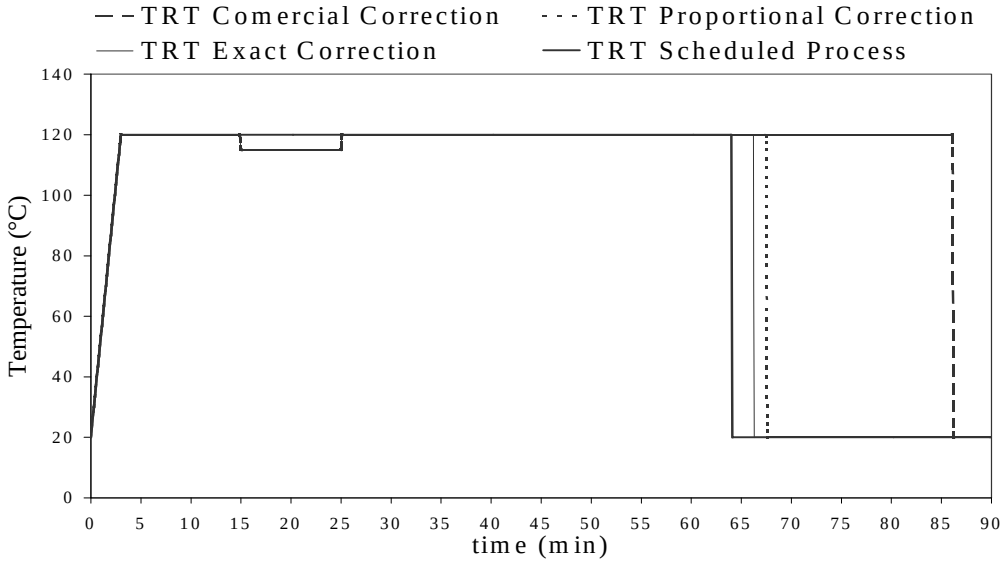


Figure 4. Pure conduction **s**imulation for on-line correction of an unexpected retort temperature deviation occurring late into the scheduled process for a cylindrical can of solid food under still cook.

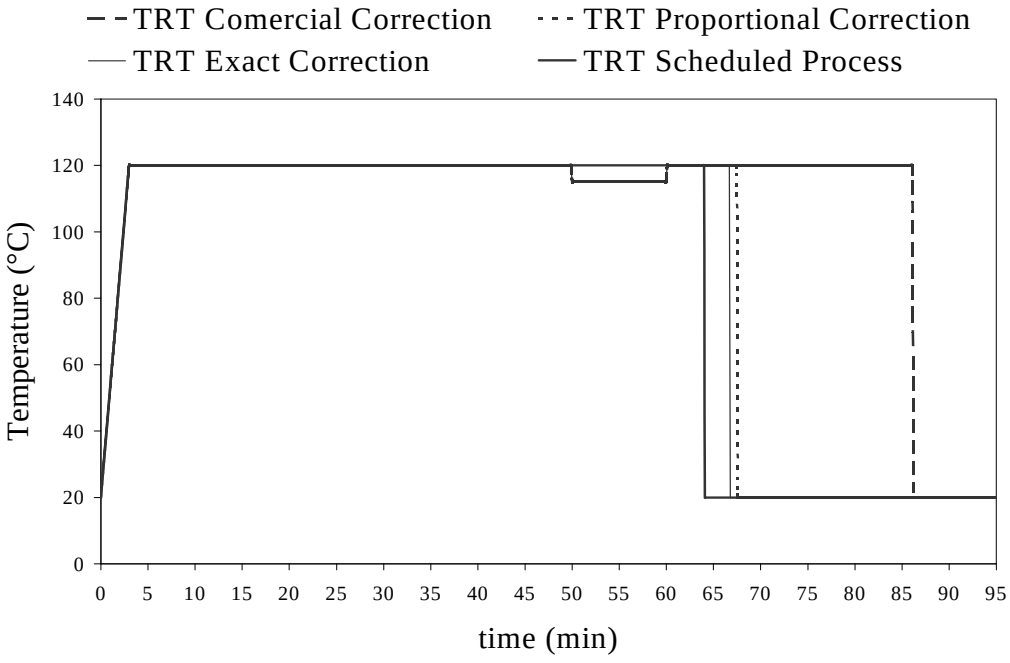
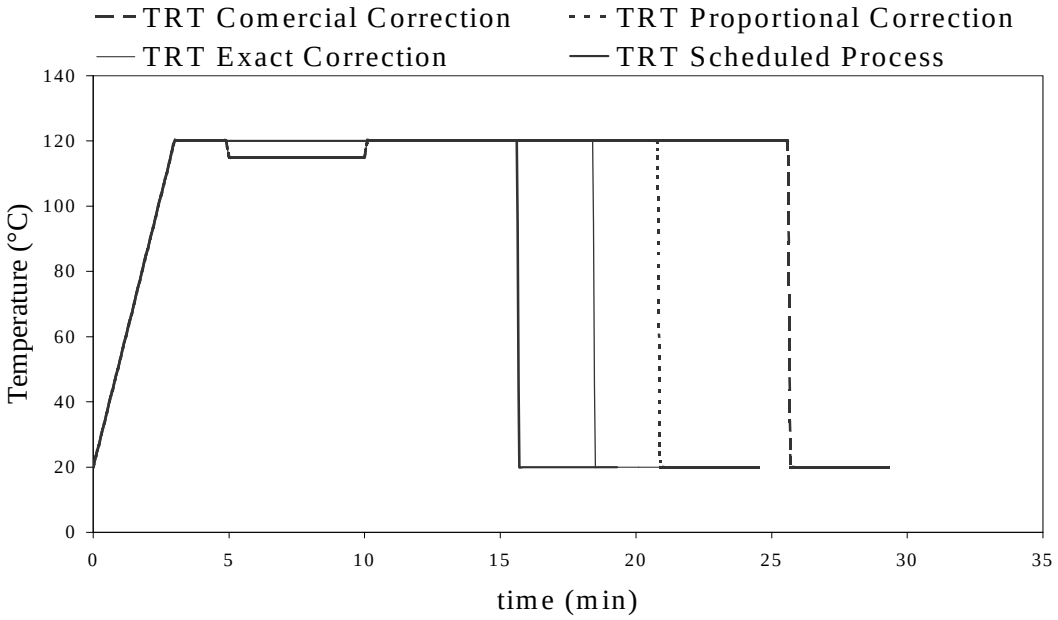


Figure 5. Forced convection **s**imulation for on-line correction of an unexpected retort temperature deviation occurring early into the scheduled process for a cylindrical can of liquid food under agitated cook.



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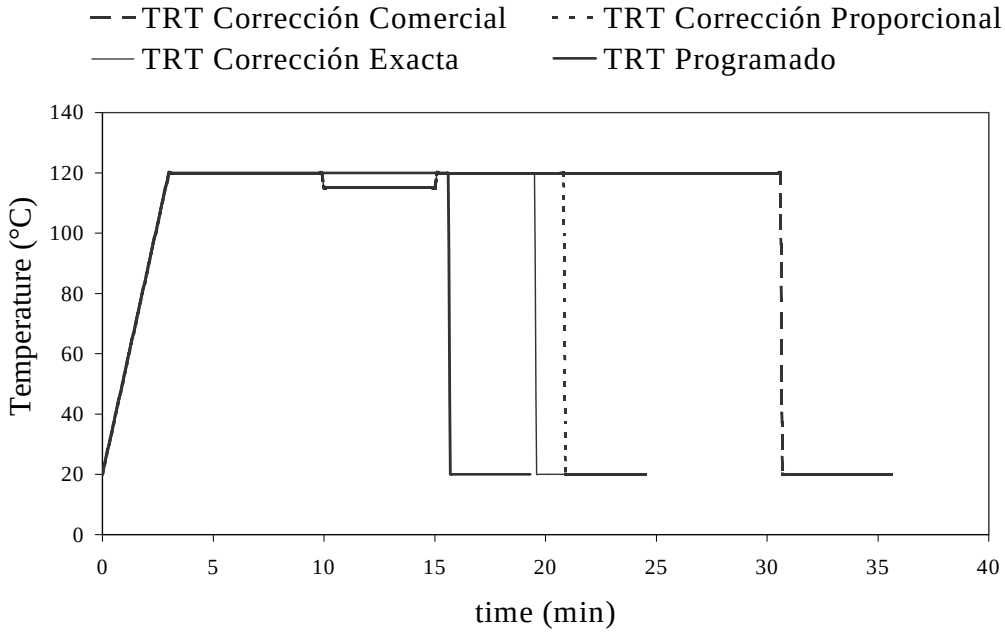

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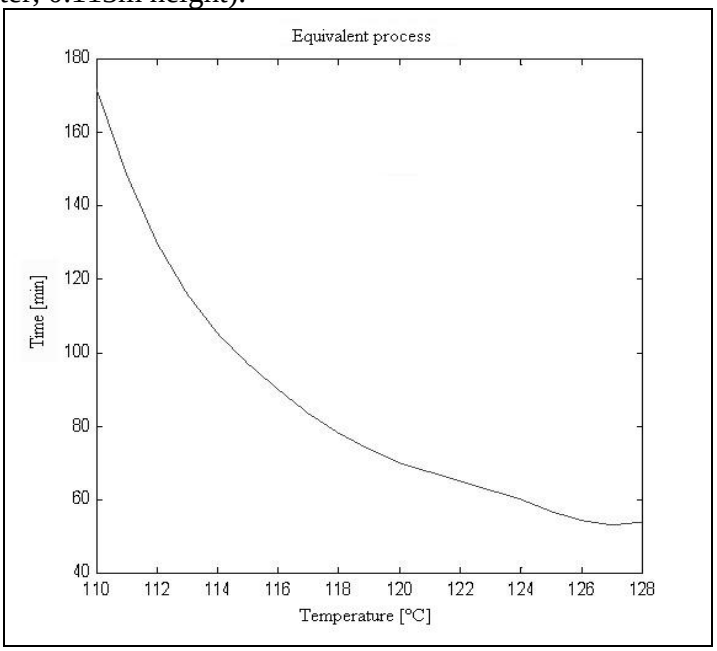

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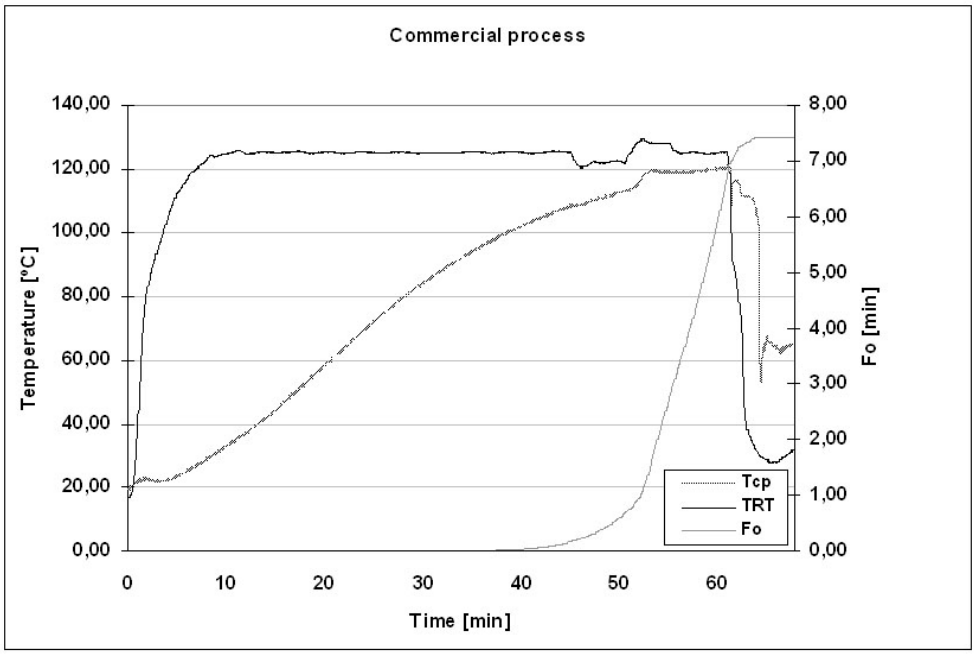

NOMENCLATURE

A : Heat transfer area
Cp : Heat capacity
F_{obj} : F-value established for the schedule process
F_p : F-value for the process with corrected deviations
$F_{proportional}$: F-value with the proportional correction
F_{TOL} : F-value specified for normal scheduled process
h : Vertical distance
H : Operating time of the plant during the season (h)
n : Number of deviations occurring during the process
N_{Bi} : Number of batches processed per retort **i** during the season
r : Radial distance
t : Time
t_{ci} : Time to load retort **i** with product **j** (h)
t_{di} : Time to download retort **i** with product **j** (h)
t_D : Corrected process time
$t_{D\ commercial}$: Corrected process time for commercial strategy
t_{Di} : Process time at the deviation temperature TRT_i
$t_{D\ proportional}$: Corrected process time for proportional strategy
t_H : Equivalent process time at required higher temperature
t_{LDT} : Equivalent process time at the lower deviation temperature
t_{oj} : Time to operate retort **i** (process cycle time) with product **j** (h)
t_p : Process time
t_{TRT} : Pre-established process time at retort temperature TRT
T : Temperature
Tcp : Temperature in the coldest point
T_{ref} : Reference temperature for microbial lethality
TRT : Retort temperature
TRT_H : Lowest temperature at which must be reestablished process temperature after deviation i
TRT_i : Lowest temperature during the deviation i
TRT_{max} : Temperature than cannot be surpassed (practical limit)
U : Universe of feasible process conditions in search routine
U_{ht} : Global heat transfer coefficient
Vol : Volume of can
z : Temperature change necessary to alter the TDT by one log-cycle
Δt : Duration time of the process deviation
Δt_i : Duration of deviation i
α : Thermal diffusivity
ρ : Liquid density

MAT
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[1] CAFFARELLI L. A. & VAZQUEZ J.L., *A free-boundary problem for the heat equation arising inflame propagation*, Trans. Amer. Math. Soc., 347 (1995), pp. 411-441.

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