

Mathematical Modelling in Food Engineering

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Abstract

Nowadays, in industrialized countries, food products that are frequently consumed are processed in order to prolong their shelf life, to avoid as much as possible their decomposition, and to maintain or even improve their natural qualities such as flavor and color. Decomposition of food is mainly due to microorganisms and enzymes, since they are involved in the physical and chemical processes of transformation of food substances. At present, consumers look for minimally processed, additive-free food products that maintain their organoleptic properties. This has promoted the development of new technologies for food processing. One of these new emerging technologies is high hydrostatic pressure, as it has turned out to be very effective in prolonging the shelf life of foods without losing its properties.

This work deals with the modelling and simulation of the effect of the combination of Thermal and High Pressure Processes, focusing on the inactivation that occurs during the process of certain enzymes and microorganisms that are harmful to food. We propose various mathematical models that study the behavior of these enzymes and microorganisms during and after the process, and study some related inverse problems.

1 INTRODUCTION

Food Engineering has been studied in the past decades, specially from mid-twentieth century to now on. Obviously, humans have been interested in food conservation since ancient times, using traditional techniques such as desiccation, conservation in oil, salting, smoking, cooling, etc. Due to the massive movement of the population to the city, a great supply of food in adequate conditions was necessary. Therefore, the food industry was

developed in order to guarantee large-scale food techniques, to prolong its shelf life, and to make logistic aspects such as transport, distribution and storage, easier.

Classical industrial processes are based on thermal treatments. For example, pasteurization, sterilization and freezing. The disadvantages of freezing are non-homogeneous crystallization, that produces big crystals that may damage the food. For classical heat application processes, temperature is in a range of 60 to 120°C, and the processing time can vary from a few seconds to several minutes. The main aim of these processes is to inactivate microorganisms and enzymes that are harmful to food, in order to prolong its shelf life, to maintain or even to improve its natural qualities, and mainly to provide consumers with products in good conditions. The problem of processing food via thermal treatments is that it may lose a significant part of its nutritional and organoleptic properties. At present, consumers look for minimally processed, additive-free food products that maintain such properties. Therefore the development of new technologies with lower processing temperatures has increased notoriously in the past years.

One of the new emerging technologies in this field is the combination of thermal treatments (at moderate temperatures) with high hydrostatic pressure, thereby reducing the problems described above. Many companies are using this technology and it is being increasingly used in countries such as Japan, USA and UK. Recent studies [2, 13] have proven that high pressure causes inactivation of enzymes and microorganisms in food, while leaving small molecules (such as flavor and vitamins) intact, and therefore it does not modify significantly the organoleptic properties of the food. High pressure can also be used for freezing, resulting in uniform nucleation and crystallization. Our aim is to model mathematically these high pressure processes, in order to simulate and optimize them.

Two principles underlie the effect of high pressure. Firstly, Le Chatelier Principle, according to which any phenomenon (phase transition, chemical reaction, chemical reactivity, change in molecular configuration) accompanied by a decrease in volume will be enhanced by pressure. Secondly, pressure is instantaneously and uniformly transmitted independently of the size and the geometry of the food (isostatic pressure).

2 MATHEMATICAL MODELLING OF MICROBIAL AND ENZYMATIC INACTIVATION

Kinetic models are used for the development of food preservation processes to ensure safety. They also provide tools to compare the impact of different process technologies on the reduction of microbial populations or enzymatic activity. In this section we present mathematical models and the parameters that describe Microbial and Enzymatical Inactivation¹ due to the combination of thermal and high pressure treatments.

In order to describe changes in microbial populations as a function of time, when the food sample is processed at temperature T and pressure P we can use the first-order kinetic model²:

$$\left\{ \begin{array}{l} \frac{dN(t; T, P)}{dt} = -\kappa(T, P)N(t; T, P), \\ N(0; T, P) = N_0, \\ \textbf{Solution: } N(t; T, P) = N_0 \exp\left(-\int_0^t \kappa(T(s), P(s)) ds\right), \end{array} \right. \quad t \geq 0, \tag{2.1}$$

where $N(t; T, P)$ is the microbial population at time t , when the food sample is processed at temperature T and pressure P , N_0 is the initial microbial population and $\kappa(T, P)$ is the *inactivation rate constant* [min^{-1}], also called *death velocity constant* in the case of microorganisms. Therefore, we have encountered a first inverse problem: to identify $\kappa(T, P)$ for adequate ranges of temperature and pressure. The same model can be used to estimate the changes in the enzymatic activity as a function of time by changing $N(t; T, P)$ for $A(t; T, P)$, and N_0 for A_0 .

Another equation used very often (e.g. [14]) to calculate changes of microbial population as a function of time is the following:

$$\left\{ \begin{array}{l} \log\left(\frac{N(t; T, P)}{N_0}\right) = \frac{-t}{D(T, P)}, \\ N(0; T, P) = N_0, \\ \textbf{Solution: } N(t; T, P) = N_0 10^{-\int_0^t \frac{1}{D(T(s), P(s))} ds}, \end{array} \right. \quad t \geq 0, \tag{2.2}$$

¹**Inactivation** may be defined as the reduction of undesired biological activity, such as enzymatic catalysis and microbial contamination.

²Higher-order models that describe changes in microbial populations as a function of time can also be found in the literature [15].

where $D(T, P)$ is the *decimal reduction time* [min], or time required for a 1-log-cycle³ reduction in the microbial population. We have encountered another inverse problem: to identify $D(T, P)$ for adequate ranges of temperature and pressure.

2.1 Identification of kinetic parameters

For isostatic processes, $\kappa(T)$ can be given by Arrhenius' equation:

$$\kappa(T) = \kappa_{T_{\text{ref}}} \exp\left(\left(\frac{-E_a}{R}\right)\left(\frac{1}{T} - \frac{1}{T_{\text{ref}}}\right)\right), \quad (2.3)$$

where $\kappa(T)$ [min^{-1}] is the inactivation rate for an arbitrary temperature T [K], $\kappa_{T_{\text{ref}}}$ [min^{-1}] is the inactivation rate at reference temperature T_{ref} [K], E_a [J/mol] is the activation energy⁴ and $R = 8,314$ [J/(mol K)] is the universal gas constant. And for isothermal processes, $\kappa(P)$ can be given by the following equation (based on Eyring's equation):

$$\kappa(P) = \kappa_{P_{\text{ref}}} \exp\left(\frac{-\Delta V^*(P - P_{\text{ref}})}{RT}\right), \quad (2.4)$$

where $\kappa(P)$ [min^{-1}] is the inactivation rate for an arbitrary pressure P [MPa], $\kappa_{P_{\text{ref}}}$ [min^{-1}] is the inactivation rate at reference pressure P_{ref} [MPa] and ΔV^* [cm^3/mol] is the volume of activation⁵.

For temperature and pressure dependent processes, $\kappa(T, P)$ may be calculated by:

$$\begin{aligned} \kappa(P, T) = & \kappa_{\text{ref}} \exp\left(\frac{-\Delta V_{\text{ref}}}{RT}(P - P_{\text{ref}})\right) \exp\left(\frac{\Delta S_{\text{ref}}}{RT}(T - T_{\text{ref}})\right) \exp\left(\frac{-\Delta \kappa}{2RT}(P - P_{\text{ref}})^2\right) \\ & \exp\left(\frac{-2\Delta \zeta}{RT}(P - P_{\text{ref}})(T - T_{\text{ref}})\right) \exp\left(\frac{\Delta C_p}{RT}\left(T\left(\ln\frac{T}{T_{\text{ref}}}\right) - 1\right) + T_{\text{ref}}\right), \end{aligned} \quad (2.5)$$

where there are several kinetic constants that express the dependence of $\kappa(T, P)$ on temperature and pressure.

By construction $\kappa(T, P)$ and $D(T, P)$ are related by $\kappa = \frac{\ln(10)}{D}$, thereby it is possible to move from one model to the other. However, we may also calculate $D(T, P)$ directly by

³A 1-log-cycle reduction is equivalent to reducing the population dividing it by ten. In the same way, a n log-cycle is equivalent to reducing the population dividing it by 10^n .

⁴Activation energy (chemistry): the minimum amount of energy that is required to activate atoms or molecules to a condition in which they can undergo chemical transformation or physical transport.

⁵The volume of activation is interpreted, according to transition state theory, as the difference between the partial molar volumes of the transition state (V) and the sums of the partial volumes of the reactants at the same temperature and pressure.

using suitable equations. For $D(T)$ and $D(P)$, we have, resp. [14]:

$$\log \left(\frac{D(T)}{D_{T_{\text{ref}}}} \right) = - \frac{T - T_{\text{ref}}}{z_T} \quad (2.6)$$

$$\log \left(\frac{D(P)}{D_{P_{\text{ref}}}} \right) = - \frac{P - P_{\text{ref}}}{z_P} \quad (2.7)$$

where z_T [K] (resp., z_P [MPa]) is the thermal (resp., pressure) resistance constant that can be defined as the temperature (resp., pressure) increase needed to accomplish a 1-log-cycle reduction in the decimal reduction time value D [min]; $D_{T_{\text{ref}}}$ (resp., $D_{P_{\text{ref}}}$) [min] is the reference decimal reduction time at reference temperature T_{ref} [K] (resp., reference pressure P_{ref} [MPa]) within the range of temperatures (resp., pressures) used to generate experimental data.

Therefore, the inverse problems consisting of identifying functions $\kappa(T, P)$ and/or $D(T, P)$ are converted into parameter estimation problems (we have to identify E_a , ΔV^* , z_T , z_P , etc...).

This parameter identification may be done using linear regression. For example, if we have experimental data of the concentration of a certain microorganism in food after being processed for different times and at different pressures and constant temperatures, we could proceed as follows: Firstly we consider the measurements done at the same pressure, therefore we would follow model (2.1) and model (2.2). Using linear regression we identify the kinetic parameters κ and D . Secondly, as we have data measured at different pressure values, we follow equations (2.4) and (2.7) in order to find a formula to express the pressure dependence of $\kappa(P)$ and $D(P)$. The parameters we identify are ΔV^* , P_{ref} and $\kappa_{P_{\text{ref}}}$ for $\kappa(P)$; z_P , P_{ref} and $D_{P_{\text{ref}}}$ for $D(P)$. We do this again using linear regression. For general processes we could use, for instance, equation (2.5) with non-linear regression techniques.

3 MODELLING THE TEMPERATURE PROFILES

As can be seen in Section 2, kinetic equation (2.1) describing the enzymatic activity evolution, as a function of time t , depends on the pressure and temperature evolution, $P(t)$ and $T(t)$, respectively.

In practice, the pressure evolution, $P(t)$, is known as it is imposed by the user and the limits of the equipment. In the case of the temperature evolution $T(t)$, it is necessary

to consider the adiabatic heating effects due to the work of compression/expansion in the considered High Pressure device. The temperature of the processed food may change with time and with space, therefore we need a heat transfer model capable of predicting the temperature for the processed food. In this work, firstly a heat transfer model taking into account only conduction effects is presented, and secondly a model also including the convection effect. As these models are time and spatial dependent, we also introduce a brief description of the domain describing the High Pressure device considered in our simulations.

3.1 Spatial domain description

High Pressure experiments are often carried out in a cylindrical pressure vessel (typically a hollow steel cylinder, see Figure 1) previously filled with the food and the pressurizing medium [9, 12]. The sample is located in the inner chamber at a temperature that can be the same or different to the one in the pressurizing medium and/or the solid domain surrounding it, which may cool or warm the food following user criteria.

Let us consider three domains: the whole domain Ω^* of the High Pressure device; the domain Ω_f^* where the food sample is located; and the domain Ω_p^* occupied by the pressurizing medium. Due to the characteristics of this kind of processes, we assume that thermally induced flow instabilities are negligible. Therefore, axial symmetry allows us to use cylindrical coordinates and the corresponding domain is given by half of a cross section (intersection of the cylinder with a plane containing the axis) and are denoted by Ω , Ω_f and Ω_p , respectively (see Figure 1).

3.2 Heat transfer by conduction

We consider the heat conduction equation

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = \alpha \frac{dP}{dt} T \quad \text{in } \Omega^* \times (0, t_f), \quad (3.1)$$

where T [K] is the temperature, $\rho = \rho(T, P)$ the density [Kg m^{-3}], $C_p = C_p(T, P)$ the heat capacity [$\text{J Kg}^{-1}\text{K}$], $k = k(T, P)$ [$\text{W m}^{-1}\text{K}^{-1}$] the thermal conductivity, t_f [s] the final time

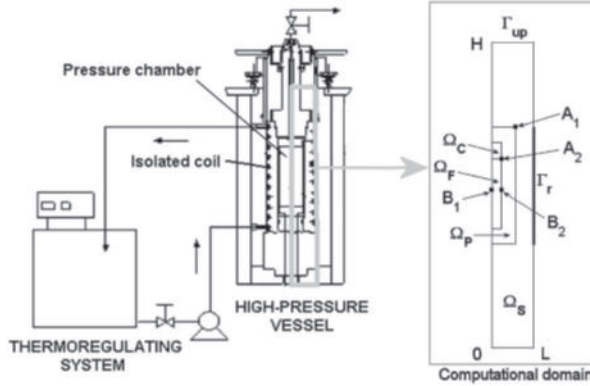


Figure 1: Scheme of the High Pressure device (**Left**) and its corresponding 2D computational domain (**Right**). More details about the notations can be found in [9].

and $\alpha = \alpha(T, P)$ is given by

$$\alpha = \begin{cases} \text{thermal expansion coefficient [K}^{-1}\text{] of the food in } \Omega_F^*, \\ \text{thermal expansion coefficient [K}^{-1}\text{] of the pressurizing fluid in } \Omega_P^*, \\ 0, \text{ elsewhere.} \end{cases}$$

The conductive heat transfer equation (3.1) is completed with appropriate initial and boundary conditions depending on the High Pressure machine, in order to determine the solution that we are looking for (see [9]).

As previously, the coefficients in (3.1) can be evaluated considering inverse problems. For instance, in Section 5 the thermal conductivity k is estimated as a function of pressure P [5, 6, 8].

This model is suitable when the filling ratio of the food sample inside the vessel is much higher than the one of the pressurizing medium. But when this does not occur, the solution of this model is very different from the experimental measurements [12]. One way to solve this problem is to include the convection phenomenon that takes place in the pressurizing medium. The resulting model is more expensive from a computational point of view but the results are more accurate.

3.3 Heat transfer by conduction and convection

The non-homogeneous temperature distribution induces a non-homogeneous density distribution in the pressurizing medium and consequently a buoyancy fluid motion (i.e., free convection). This fluid motion may strongly influence the temperature distribution. In order to take into account this fact, a non-isothermal flow model is considered. Therefore, we suppose that the fluid velocity field, \mathbf{u} [m s^{-1}], satisfies Navier-Stokes' equations for compressible Newtonian fluid under Stokes' assumption (see, for instance, [1]). The resulting system of equations is:

$$\begin{cases} \rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) + \rho C_p \mathbf{u} \cdot \nabla T = \alpha \frac{dP}{dt} T & \text{in } \Omega^* \times (0, t_f), \\ \rho \frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \eta (\nabla \mathbf{u} + \nabla \mathbf{u}^t) + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p - \frac{2}{3} \nabla (\eta \nabla \cdot \mathbf{u}) + \rho \mathbf{g} & \text{in } \Omega_p^* \times (0, t_f), \\ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 & \text{in } \Omega_p^* \times (0, t_f), \end{cases} \quad (3.2)$$

where \mathbf{g} is the gravity vector [m s^{-2}], $\eta = \eta(T, P)$ the dynamic viscosity [Pa s], $p = p(x, t)$ the pressure [Pa] generated by the mass transfer inside the fluid, and $P + p$ is the total pressure [Pa] in the pressurizing medium Ω_p^* . System (3.2) is completed with appropriate point, boundary and initial conditions. If the food sample is liquid two more equations for its velocity and density should be added (see [8, 9]).

The coefficients in (3.2) can be determined by considering various inverse problems (see [5, 8]).

4 COUPLING OF INACTIVATION AND HEAT-MASS TRANSFER MODELS

Figure 2 shows an example of final temperature and food sample enzymatic activity distributions obtained using a numerical version of models (2.1) and (3.2) (see [9] for more details). We have considered the following treatment:

The initial temperature is $T_0 = 40^\circ \text{C}$ in Ω_S and $T_0 = 22^\circ \text{C}$ in $\Omega \setminus \Omega_S$, and the pressure is linearly increased during the first 305 seconds until it reaches 600 MPa. Thus, the

pressure generated by the equipment satisfies $P(0) = 0$ and

$$\frac{dP}{dt} = \begin{cases} \frac{120}{61} 10^6 \text{ Pa s}^{-1}, & 0 < t \leq 305, \\ 0 \text{ Pa s}^{-1}, & t > 305. \end{cases}$$

The considered enzyme is Lipoxygenase (LOX): this enzyme is present in various plants and vegetables such as green beans and green peas. It is responsible for the appearance of undesirable aromas in those products.

Equation (2.5) is used to describe κ with $P_{\text{ref}} = 500 \text{ MPa}$, $T_{\text{ref}} = 298 \text{ K}$, $\kappa_{\text{ref}} = 1.34 \times 10^{-2} \text{ min}^{-1}$, $\Delta V_{\text{ref}} = -308.14 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta S_{\text{ref}} = 90.63 \text{ J mol}^{-1} \text{ K}^{-1}$, $\Delta C_p = 2466.71 \text{ J mol}^{-1} \text{ K}^{-1}$, $\Delta \zeta = 2.22 \text{ cm}^3 \text{ mol}^{-1} \text{ K}^{-1}$, $\Delta \nu = -0.54 \text{ cm}^6 \text{ J}^{-1} \text{ mol}^{-1}$ (see Ref. [10] for more details).

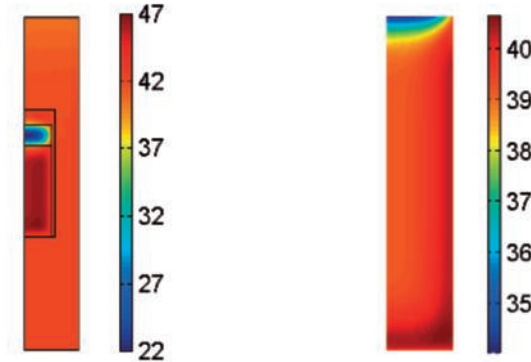


Figure 2: Temperature distributions in Ω (**Left**) and LOX enzymatic distributions in Ω_s (**Right**) at time $t = 15 \text{ min}$ after the considered process.

5 IDENTIFICATION OF A THERMAL CONDUCTIVITY COEFFICIENT

We assume that the thermal conductivity depends only on pressure: $k = k(P)$; this is a reasonable assumption, for example, in processes where the temperature range is moderate and there is no phase change. The problem of identifying the function $k(P)$ from

certain experimental measurements of the temperature is considered. If the experiment is performed with an injective curve of pressure P (e.g. if it is a strictly increasing function) the problem of identifying $k(P)$ is equivalent to identify $k(t) = k(P(t))$.

We consider a simplified model in which the sample of solid food is assumed to be contained in a cylindrical pressurized chamber, with a very high filling ratio, so convection phenomena is not taken into account. Moreover, we assume there is heat transfer between the food sample and the walls of the equipment, and its temperature is given by a known function $T^e(t)$. Also, the only heat source is due to the pressure increase and the heat transfer coefficient h is assumed known. Finally, we consider that the heat conduction in the vertical direction is negligible and, therefore, our interest lies in knowing what happens in a certain height of the sample where the thermocouples are placed.

Thus, the simplified model for which we address the problem of identification of thermal conductivity is

$$\begin{cases} \rho C_p \frac{\partial T}{\partial t} - k(t)\Delta T = \alpha P'(t)T & \text{in } B_R \times (0, t_f), \\ k(t) \frac{\partial T}{\partial \vec{n}} = h(T^e(t) - T) & \text{on } \partial B_R \times (0, t_f), \\ T = T_0 & \text{in } B_R \times \{0\}, \end{cases} \quad (5.1)$$

where $R > 0$ and $t_f > 0$. $B_R \subset \mathbb{R}^2$ denotes the ball of center 0 and radius R ; $P \in \mathcal{C}^1([0, t_f])$; $k \in \mathcal{C}([0, t_f])$, with $k(t) \geq k_0 > 0$, is the unknown heat conductivity coefficient; $T^e \in \mathcal{C}([0, t_f])$ denotes the chamber walls temperature; \vec{n} is the outward normal to the boundary of B_R unitary vector; $h > 0$ denotes the heat transfer coefficient and T_0 is the sample initial temperature, assumed constant. Our goal is to identify function k from temperature measurements done at points of B_R . Since the values of the coefficients at atmospheric pressure are known, we take the initial pressure to be the atmospheric one, hence, $k(0)$ is known.

5.1 Expression of the solution in terms of their values on the boundary.

Denoting as $X = \mathcal{C}^{2,1}(B_R \times (0, t_f)) \cap \mathcal{C}^{1,0}(\overline{B_R} \times [0, t_f])$, we have

Theorem 1: *If k is a Lipschitz function in $[0, t_f]$, P' is a Hölder continuous function in*

the same interval and the compatibility condition

$$T^e(0) = T_0$$

holds, then problem (5.1) has a unique (classical) solution $T \in X$. Moreover, T is a radial function. \square

Now, we find an integral representation of the solution of the problem (5.1) in terms of its values on the boundary:

Theorem 2: Denoting by

$$m(t) = \bar{T}(R, t), \quad \gamma(r, \theta) = R^2 - 2Rr \cos \theta + r^2, \quad K(s) = \int_s^{t_f} k(z) dz,$$

$$g(t, \tau) = \frac{1}{K(\tau) - K(t)} \quad \text{and} \quad Q(t, \tau) = e^{-\frac{\alpha}{\rho C_p}(P(t)-P(\tau))},$$

for $r \in [0, R)$ and $t \in [0, t_f]$ the solution of problem (5.1) can be written as

$$\begin{aligned} \bar{T}(r, t) = & T_0 Q(t, 0) + \frac{Rh}{4\pi} \int_0^t (T^e(\tau) - m(\tau)) Q(t, \tau) g(t, \tau) \int_0^{2\pi} e^{-\frac{\rho C_p}{4} \gamma(r, \theta) g(t, \tau)} d\theta d\tau \\ & + \frac{R}{2\pi} \int_0^t \left(m'(\tau) - \frac{\alpha}{\rho C_p} m(\tau) P'(\tau) \right) Q(t, \tau) \int_0^{2\pi} \frac{R - r \cos \theta}{\gamma(r, \theta)} e^{-\frac{\rho C_p}{4} \gamma(r, \theta) g(t, \tau)} d\theta d\tau. \end{aligned}$$

5.2 Uniqueness of solution of the inverse problem

Here we deal with the uniqueness of solution of the inverse problem, meaning that function $k(t)$ is uniquely determined in some interval $[0, t_f]$ by the values of function $\bar{T}(r, t)$ at $r = R$ and at another point $r_0 \in [0, R)$, for every $t \in [0, t_f]$.

We point out that this is not true in general. For example, if the external temperature evolves as

$$T^e(t) = T_0 e^{\frac{\alpha}{\rho C_p}(P(t)-P(0))}$$

the function $T(t) = T^e(t)$ is the solution of direct problem (5.1), regardless of function k .

To ensure the uniqueness of solution of the problem of identifying the coefficient of conductivity, we restrict the context in which the problem is posed assuming the following hypotheses:

(H1) $T^e(t) \equiv T_0$ for all $t \in [0, t_f]$.

(H2) P is a linear increasing function. Thus, $P' \equiv \beta > 0$.

If there are different functions k_1 and k_2 that produce the same measurements $m(t)$ at the right end, R , and also at some other point $r_0 \in [0, R)$, the following result proves that such functions must be equal.

Theorem 3: *Let T_1 and T_2 be the solutions of the following problems, respectively*

$$\begin{cases} \varrho C_p \frac{\partial T}{\partial t} - k_1(t)\Delta T = \alpha P'(t)T & \text{in } B_R \times (0, t_f), \\ k_1(t) \frac{\partial T}{\partial \vec{n}} = h(T^e(t) - T) & \text{on } \partial B_R \times (0, t_f), \\ T = T_0 & \text{in } B_R \times \{0\}, \end{cases}$$

and

$$\begin{cases} \varrho C_p \frac{\partial T}{\partial t} - k_2(t)\Delta T = \alpha P'(t)T & \text{in } B_R \times (0, t_f), \\ k_2(t) \frac{\partial T}{\partial \vec{n}} = h(T^e(t) - T) & \text{on } \partial B_R \times (0, t_f), \\ T = T_0 & \text{in } B_R \times \{0\}, \end{cases}$$

where $k_i \in C^1([0, t_f])$, with $k_i \geq k_0 > 0, i = 1, 2$. Assuming **(H1)**, **(H2)** and that for all $t \in [0, t_f]$ it holds that

$$\bar{T}_1(R, t) = \bar{T}_2(R, t) \text{ and } \bar{T}_1(r_0, t) = \bar{T}_2(r_0, t) \text{ for some } r_0 \in [0, R).$$

If functions k_1 and k_2 are two positive constants, or more generally, if the k_i functions are locally analytic on the right in $[0, t_f]$ and verify

$$\int_0^{t_f} k_i(s) ds \leq \frac{\varrho C_p (R - r_0)^2}{4}, \quad i = 1, 2 \tag{5.2}$$

and

$$k'_i(t) \leq k_i(t) \frac{\alpha\beta}{\varrho C_p e^{\frac{\alpha\beta}{\varrho C_p} t} - 1}, \quad t \in [0, t_f], \quad i = 1, 2, \tag{5.3}$$

then $k_1 = k_2$. \square

The previous result shows that if we assume that the measurements at r_0 and R agree with those done at a temperature that is modeled by (5.1), with k verifying the requested hypothesis, then function k is uniquely determined from such measurements.

Moreover, it is remarkable that the more separate the measurements are done (i.e., the more closer r_0 is to zero), less restrictive becomes condition (5.2), related to the a priori information about k . Therefore, we can assure the uniqueness of solution of the inverse problem for a wider set of functions.

Remark: Inequality (5.3) is actually only a restriction over time intervals where k is an increasing function (in fact, (5.3) holds for constant and non-increasing functions). Moreover, since

$$\lim_{t \rightarrow 0^+} \frac{1}{e^{\frac{\alpha\beta}{\rho C_p} t} - 1} = \infty,$$

every function k satisfies (5.3) for short time intervals.

The functions considered in the numerical tests verify (5.3), which is part of the a priori information needed to identify the coefficient of conductivity. This means that coefficient k cannot have abrupt changes, which is typical of processes that produce a phase change, which does not happen in the cases studied here. \square

6 NUMERICAL IDENTIFICATION WITHOUT REGULARIZATION. NUMERICAL EXAMPLES

We begin this section describing the methodology used to solve an inverse problem, based on a collocation method with piecewise linear continuous functions in a temporal partition. An approximation of this kind for function k will be used (i.e., the unknowns will be the values of k at each of the points of the partition).

We assume the experimental measurements have been done at the center and boundary of the ball, for each instant $t_i, i = 1, 2, \dots, n$, of the partition. Then, the equality of Theorem 2 is written with $r = 0$ and $t = t_i$, the value of $\bar{T}(0, t_i)$ is replaced by the measurement at the center of the sample at that instant, and function m is replaced by the piecewise linear interpolation of the measurements of the boundary. The derivative of m is approximated by a first order progressive formula. The approximation of the integrals in $(0, t_i)$ is done by the trapezoidal rule, considering the values of the integrands at t_i to be zero (right limit of the integrands). These approximations result in a system of n non-linear equations with n unknowns, corresponding to the n values of k at instants $t_i, i = 1, 2, \dots, n$. As already said, the value of k at the initial instant is assumed to be

known, as it corresponds to the value of k at atmospheric pressure.

The results obtained for the identification of the coefficient of conductivity are presented for three test cases in which the same linear pressure increase has been used (see (6.1)) and the same data perturbation (as will be explained subsequently). Three different types of functional dependences for function k have been considered: linear, as a radical and as a power. The domain and the parameters of the physical problem have been taken to be the same as in the solid type food case considered in [9] (i.e., those of tylose). A process like P2 described in that paper is considered, except for in this case the pressure increase is much slower (in 1800 seconds instead of 183), so that the conductivity effect can be much more notorious.

In particular, the pressure has been taken to be

$$P(t) = 0'2t + 0'1 \quad (6.1)$$

and the functions k that will be identified have been chosen as

$$1) k(t) = \frac{0'75t + 450}{1800} \quad 2) k(t) = \sqrt{\frac{0'75t + 450}{1800}} \quad 3) k(t) = \left(\frac{0'25t + 1350}{1800}\right)^3.$$

Increasing k functions have been considered, as it is physically reasonable to expect conductivity to increase as pressure increases (see, e.g., data for different materials in [11]). The size of these functions has been chosen so that they have the same order as the average conductivity of tylose in [9], that is 0'559. All of these functions satisfy inequalities (5.3) and (5.2), related to the a priori information about k .

The obtained results are shown in Figure 3. As can be seen, the error in identifying k is bigger at the end of the time interval. This is because the values of k at the final instants are only involved in the last equations, therefore their value is less determinant in the non-linear system, and so the numerical solution with the required degree of precision admits bigger errors at the end of the interval. This makes it more difficult to obtain values for k , at those instants, that change with respect to the initial proposed value of the iteration. Coherently, the biggest errors for the temperature calculated after the identification are achieved when the error for k is biggest, and they stay related as time evolves. However, the errors in the approximation for T are of less order than those of the measurements, i.e., the order of perturbation, what makes the results very satisfactory.

In Figure 3 the highest value of the percentage relative error is indicated (as “% máx. de error”), for each of the numerical tests. If the solution of the problem corresponding to the approximate identification of k is denoted by \tilde{T} , then the maximum value of such error is given by

$$\max_{k=1,2,\dots,n} \left(\frac{\|\tilde{T}(\cdot, t_k) - T(\cdot, t_k)\|_{C(B_R)}}{\|T(\cdot, t_k)\|_{C(B_R)}} \times 100 \right).$$

We calculate the “exact” solution of the direct problem using the Matlab tool `pdeTool`, on a partition of the time interval $[0, 1800]$ divided equally into 61 instants. Then the value at the center and boundary of the ball is calculated for such instants. The *measurements with error* are generated by perturbing the values of the temperatures at both points, and in the same way for all three cases. The perturbation is of order 1% of the temperature range.

7 REGULARIZATION ALGORITHM

In this section a regularization algorithm is presented for the problem under study. We consider the spaces $\mathcal{Z} = L_2(0, t_f)$ and $\mathcal{U} = L_2(0, t_f) \times L_2(0, t_f)$ and, for each $\varepsilon > 0$, the compact and convex subset $\mathcal{K}_\varepsilon \subset \mathcal{Z}$ defined by

$$\mathcal{K}_\varepsilon = \left\{ k \in H^1(0, t_f) : k(t) \geq k_0, t \in (0, t_f), k(t) \equiv k_0, t \in [0, \varepsilon], \int_0^{t_f} k(s) ds \leq \frac{\varrho C_p (R - r_0)^2}{4}, k'(t) \leq k(t) \frac{\alpha\beta}{\varrho C_p} \frac{1}{e^{\frac{\alpha\beta}{\varrho C_p} t} - 1} \text{ c.d. in } (0, t_f) \right\}.$$

Let $m(t) = \bar{T}(R, t)$, $m^0(t) = \bar{T}(r_0, t)$, be the exact temperatures measurements, that correspond to the solution of the model for a unique $k \in \mathcal{K}_\varepsilon$. Denoting by $m_\delta(t)$ and $m_\delta^0(t)$ the respective perturbed measurements with order δ , namely,

$$d \left(\begin{pmatrix} m_\delta \\ m_\delta^0 \end{pmatrix}, \begin{pmatrix} m \\ m^0 \end{pmatrix} \right) = \sqrt{\|m_\delta - m\|^2 + \|m_\delta^0 - m^0\|^2} \leq \delta,$$

and defining the operator

$$\begin{aligned} A : \mathcal{K}_\varepsilon &\longrightarrow \mathcal{U} \\ k &\mapsto (m(t), m^0(t)), \end{aligned}$$

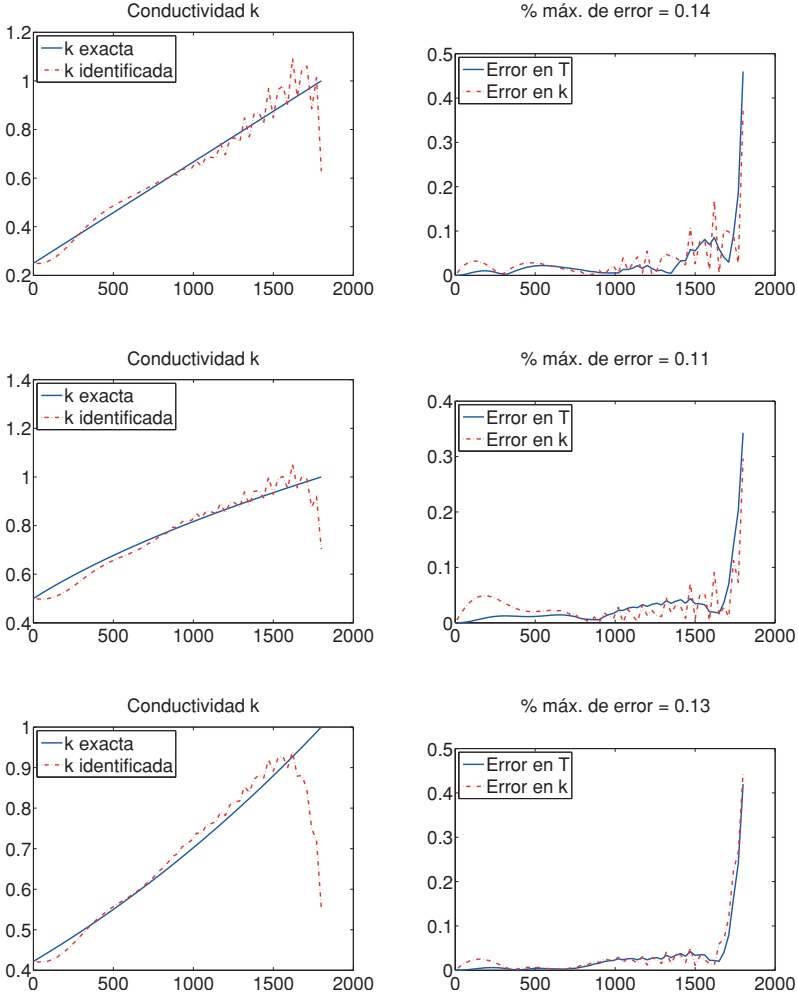


Figure 3: Thermal Conductivity (**Left**) and error in temperature (**Right**) corresponding to the case when k is a line (**Top**), a radical (**Center**) and a power (**Bottom**).

we propose the problem of solving, in a stable way, equation: $Ak = (m_\delta(t), m_\delta^0(t))$, through the solution of the optimization problem

$$\min_{k \in \mathcal{K}_\varepsilon} d^2 \left(Ak, \begin{pmatrix} m_\delta \\ m_\delta^0 \end{pmatrix} \right).$$

The methodology we design to approximate such solution is based on the discretization of the set \mathcal{K}_ε and the functional A by means of piecewise linear continuous functions in the intervals $[t_{j-1}, t_j]$, where $t_j = \frac{j t_f}{n}$ are the instants when the n measurements are done. Parameter ε has to satisfy the restriction of being smaller than the time interval between two measuring instants, i.e., $0 < \varepsilon < \frac{t_f}{n}$. As shown by the approximate solution method (see [3]), the corresponding iterative process should stop at the first instant i verifying

$$d^2 \left(Ak_i, \begin{pmatrix} m_\delta \\ m_\delta^0 \end{pmatrix} \right) \leq \delta^2,$$

for which a regularized solution is obtained.

The difficulty of this algorithm is the need to project the descent direction at each iterative step of the optimization method being used, on the compact set \mathcal{K}_ε , that has an empty interior in \mathcal{Z} (see [7]).

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REFERENCES

- [1] R. Aris, *Vectors, Tensors, and the Basic Equations of Fluid Mechanics*, Dover Publications, Inc. New York, 1989.
- [2] J. C. Cheftel, *Review: high-pressure, microbial inactivation and food preservation*. Food Science Technology International **1** (1995), 75–90.
- [3] A. M. Denisov, *Elements of the Theory of Inverse Problems*. Inverse and Ill-Posed Problems Series. VSP. 1999.
- [4] A. Fraguera, J. A. Infante, B. Ivorra, Á. M. Ramos, J. M. Rey and N. Smith, *Inverse problems in High Pressure Processes and Food Engineering*. Proceedings of First Symposium on Inverse Problems and Applications, Ixtapa, México. January 6–8, 2010.

- [5] A. Fraguela, J. A. Infante, Á. M. Ramos and J. M. Rey, *Identificación de la conductividad de un material cuando depende de la presión a la que está sometido*. Proceedings of First Symposium on Inverse Problems and Applications, Ixtapa, México. January 6–8, 2010.
- [6] A. Fraguela, J. A. Infante, Á. M. Ramos and J. M. Rey, *Identification of a Heat Transfer Coefficient when it is a Function Depending on Temperature*. WSEAS Transactions on Mathematics, ISSN: 1109-2769, Issue 4, Vol. 7, 2008, 160–172.
- [7] S. F. Gilyazov, *Regularization of ill posed problems by Iteration Methods*, Mathematics and its Applications, Volume 499, Springer, 1999.
- [8] J. A. Infante, *Análisis numérico de modelos matemáticos y problemas inversos en tecnología de alimentos*. Ph. D. Thesis, Universidad Complutense de Madrid, November 24, 2009. http://www.mat.ucm.es/momat/Tesis_JA_infante.pdf
- [9] J. A. Infante, B. Ivorra, Á. M. Ramos and J. M. Rey, *On the Modelling and Simulation of High Pressure Processes and Inactivation of Enzymes in Food Engineering*. Mathematical Models and Methods in Applied Sciences (M3AS), 19 (12), 2203–2229.
- [10] I. Indrawati, L. R. Ludikhuyze, A. M. van Loey and M. E. Hendrickx, *Lipoxygenase Inactivation in Green Beans (Phaseolus vulgaris L.) Due to High Pressure Treatment at Subzero and Elevated Temperatures*, J. Agric. Food Chem. **48** (2000), 1850–1859.
- [11] E. W. Lemmon, M. O. McLinden and D. G. Friend, Thermophysical properties of fluid systems. En *NIST Chemistry Web Book*. NIST Standard Reference Database **69**, P.J. Linstrom y W.G. Mallard eds. National Institute of Standards and Technology. Recurso electrónico <http://webbook.nist.gov/chemistry/>
- [12] L. Otero, Á. M. Ramos, C. de Elvira and P. D. Sanz, *A Model to Design High-Pressure Processes Towards an Uniform Temperature Distribution*. J. of Food Engineering **78** (2007), 1463–1470.
- [13] J. P. P. M. Smelt, *Recent advances in the microbiology of high pressure processing*. Trends in Food Science and Technology **9** Elsevier (1998), 152–158.

- [14] U.S. Food and Drug Administration. Center for Food Safety and Applied Nutrition, *Kinetics of Microbial Inactivation for Alternative Food Processing Technologies*. 2000. (Web: <http://www.cfsan.fda.gov/~comm/ift-over.html>)
- [15] R. Xiong, G. Xie, A. E. Edmondson, M. A. Sheard, *A mathematical model for bacterial inactivation*. International Journal of Food Microbiology **46** Elsevier (1999), 45–55.