Original Article

Mathematical Modeling the simulation effect of the combination of Thermal and High Pressure in food Process

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Abstract

Introduction: Food Science has been studied in the past decades, especially 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.

In this paper, we study the modeling and simulation of the effect of the combination of Thermal and High Pressure food Processes, focusing on the inactivation that occurs during the process of certain enzymes and microorganisms that are harmful to food. Also, 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.

Materials and methods: The parameters of the selected equation have been estimated using regression techniques on the data provided by experimental measurements of the activity

Results: The models developed in this paper provide a useful tool to design suitable industrial equipments and optimize the processes.

Conclusion: The mathematical models described provide a useful tool to design and optimize processes based on the combination of thermal and high pressure processes in Food Technology. They take into account the

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INTRODUCTION

In these days, in advanced 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 flavour and colour. 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.

Classical industrial processes are based on thermal treatments. 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 loose 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

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temperatures have increased notoriously in the past years.
One of the new emerging technologies in this field is the combination of thermal treatments 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 L. Otero et.al [3] Smelt [13] have proven that high pressure causes inactivation of enzymes and microorganisms in food. while leaving stall molecules intact, and therefore it does not modify significantly the organoleptic properties of the food. High pressure can also be 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 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.
Throughout this paper, we follow the notation, terminology and their SI units

$A(t;T;P)$	Enzymatic activity at time *t*, for a process at constant pressure *P* and temperature *T*.	
$A0$	Enzymatic activity time 0	
D	Decimal reduction time	$[min^{-1}]$
$DTref, DPref$	Decimal reduction time at *T*ref / *P*ref	$[min^{-1}]$
Ea	Activation energy	$[kJ/mol]$
k	Inactivation rate	$[min^{-1}]$
$kTref; Pref$	Inactivation rate at *T*ref and *P*ref	$[min^{-1}]$
$N(t;T;P)$	Microbial population at time *t*, for a process at constant pressure *P* and temperature *T*	$[cfu/g]$
N_0	Initial microbial population	$[cfu/g]$
$P; Pref$	Pressure / Reference pressure	$[MPa]$
t	Time	$[min]$
$T;\ Tref$	Temperature / Reference temperature	$[K]$
ΔV^*	Volume of activation	$[cm^3/mol]$
z_T	Temperature resistant coefficient	$[K]$
z_P	Pressure resistant coefficient	$[MPa]$
Φ^*	Whole domain of the device	
Φ^*_F	Sample food domain	
Φ^*_P	Pressurizing medium domain	
H	Heat transfer coefficient	$[W/\ m^2 K_1]$
α	Thermal expansion coefficient	$[K_1]$
η	Dynamic viscosity	$[Pa\ s]$
ρ	Density	$[Kg/\ m^3]$
$\boldsymbol{g}$	Gravity vector	$[m/\ s^2]$
S	Surface area of the heat being transferred	$[m^2]$
V	Heated volume	$[m^3]$
Cp	Heat capacity	$[J/Kg\ K]$
P	Mass transfer pressure	$[Pa]$

MATHEMATICAL MODELLING OF 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 induction of microbial populations or enzymatic activity. In this section we present mathematical models and the parameters that describe Microbial and Enzymatical Inactivation 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 sample is processed at temperature T and pressure P we can use the first-order kinetic model":

$$\frac{dN(t;\ T;\ P)}{dt} = -k(T;\ P)N(t;\ T;\ P); \quad t \tag{1}$$

With initial conditions $N(0; T; P) = N_0$ (2)

For isobaric/isothermal processes the solution of above equation is $N(t;\ T;\ P) = N_0 e^{(-k(T,\ P),\ t)}$.For dynamic processes$N(t;\ T;\ P) = N_0 e^{\left(\int_0^t -k(T(s),\ P(s))ds\right)}$.*N(t: T, P)* is the microbial population at time, when the food sample is processed at temperature *T* and pressure *P*. N_o is the initial microbial population and *(T. P)* is the inactivation rate constant fruin, also called death velocity constant in the case of microorganisms. Therefore, we have encountered a first inverse problem: to identify (TP) 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. P)* for *A(t: T. P),* and N_o for A_0

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

$$log\left(\frac{dN(t;\ T;\ P)}{N0}\right) = \frac{-t}{D(T,P)}, \tag{3}$$

With initial conditions $N(0; T; P) = N_0$ (4)

For isobaric or isothermal processes the solution of above equation is $N(t;\ T;\ P) = N_0 10^{-\left(\frac{t}{D(T,\ P)}\right)}$, for dynamic processes$N(t;\ T;\ P) = N_0 10^{\left(-\int_0^t -\frac{1}{D(T(s),\ P(s))}ds\right)}$. Where D(T. P) is the decimal redaction time (min), or time required for a 1-log-eyele reduction in the microbial population. We have encountered another inverse problem: to identity D(TP) for adequate ranges of temperature and pressure.

Identification of parameters of dynamic

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

$$k(T) = k_{T_{ref}} exp\left(\left(\frac{-E_a}{R}\right)\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right), \tag{5}$$

Where $k(T)[min^{-1}]$ is the inactivation rate for an arbitrary temperature $T[K]$, T_{ref} [K] min is a reference Temperature $k_{T_{ref}}[min^{-1}]$ is the inactivation rate at reference temperature .

$E_a[J/mol]$ is the activation energy. And for isothermal processes, by using Eyring's equations, $k(P)$ can be given by the following equation

$$k(P) = kP_{ref} exp\left(\frac{-\Delta V^*(P - P_{ref})}{RT}\right) \quad (6)$$

Where *k*(*P*) $[min^{-1}]$ is the inactivation rate for an arbitrary pressure *P* [MPa], *P*ref[MPa] is a reference pressure, *kP*ref [min-1] is the inactivation rate at reference pressure and $\Delta V*$[cm^3/mol] is the volume of activation.

For general temperature and pressure dependent processes, *k*(*T; P*) may be calculated by a combination of Arrehnius'and Eyring's equations

$$k(\mathrm{T;\ P}) = kT_{ref}; P_{ref} exp\left(-B\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) exp(-C(P - P_{ref})). \quad (7)$$

$$k(P;\ T) = krefexp\left(\frac{-\Delta Vref}{RT}\ (P - Pref)\right) exp\left(\frac{-\Delta Sref}{RT}(T - Tref)\right) \quad (8)$$

where *k*(*T; P*) $[min]^{-1}$is the inactivation rate for temperature *T* [K] and pressure *P* [MPa], and $kTref, Pref = k(Tref;\ Pref)\,[min]^{-1}$, *B*[K] and *C*[MPa] are kinetic constantsthat express the dependence of *k*(*T; P*) on temperature and pressure.

However, we may also calculate D(T. P) directly by using suitable equations. For D(T) and D(P), we have, resp. [14]:

$$log\left(\frac{D(T)}{D_{T_{ref}}}\right) = -\frac{T - T_{ref}}{z_T}, \quad (9)$$

$$log\left(\frac{D(P)}{D_{P_{ref}}}\right) = -\frac{P - P_{ref}}{z_P}, \quad (10)$$

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

Therefore, the inverse problems consisting of identifying functions $k(T, P)$ and/or $D(TP)$ are converted into parameter estimation problems

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 (1) and model (3). Using linear regression we identify the kinetic parameters k and D. Secondly, as we have data measured at different pressure values, we follow equations (6) and (10) in order to find a formula to express the pressure dependence of $k(P)$ and $D(P)$. The parameters we identify are ΔV^*, P_{ref} and $k_{P_{ref}}$ for $K(P)$; z_P, P_{ref} and $D_{P_{ref}}$ for $D(P)$. We do this again using linear regression. For general processes we could use, for instance, equation (7) with multiple linear regression or equation (8) withnon–linear regression techniques.

MODELLING THE TEMPERATURE OUTLINE

As can be seen in Section 2, kinetic equation (1) describing the enzymatic activity evolution, in a function of time t, needs to know the time evolution of 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 the adiabatic beating 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 order to determine *T*(*t*), we may consider various kinds of models based on ordinary differential equations, for the simplest ones, or partial differential equations, for the more complex ones.

Ordinary differential equation based model

A first model, for studying the temperature evolution, equation obtained by combining Newton's law of cooling formula is

$$\frac{dQ}{dt} = k(T_2 - T_1) \quad (11)$$

Where Q = rate of heat transfer out of the body, T_2 be the temperature of a body of mass m with a specific heat potential s, and T_1 be the temperature of its environment.k – Proportionality constant

$$\frac{dT}{dt} = \frac{HS(T^e - T)}{\rho VCp} \quad (12)$$

Heating effect due to change of pressure is

$$\frac{\Delta T}{\Delta t} = \frac{\alpha T}{\rho Cp} \quad (13)$$

Where $\alpha$is the thermal expansion coefficient $[K^{-1}]$, $\rho = \rho(T;\ P)$ the density$[Kg/m^3]$, $S$the surface area where the heat is being transferred $[m^3]$, *V* the heated volume [*m*3], *H* the heat transfer coefficient $[W/m^2K1]$ and $Cp = Cp(T;\ P)$ the heat capacity [J/ Kg].

The Temperature $T(t)$ controlled by the equation

$$\frac{dT}{dt} = H(T^e - T) + \alpha T\frac{dP}{dt} \quad (14)$$

Partial Differential Equations based model

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.

Let us consider three domains: the whole domain Φ^* of the High Pressure device; the domain Φ^*_F; where the food sample is located; and the domain Φ^*_P occupied by the pressurizing medium. Due to the characteristics of this kind of processes, we assume that thermally induced flow instabilities are negligibles

Therefore, axial symmetry allows us to use cylindrical coordinates and the corresponding domain is given by half of a cross section

HEAT TRANSFER BY CONDUCTION

We consider the heat conduction equation

$$\rho C_p \frac{T}{\partial t} - \Delta \cdot (k\nabla T) = \alpha \frac{dP}{dt} T \qquad (15)$$

Where $T[K]$ is the temperature, $k = k(T, P)$ [W/mK] is the thermal conductivity, and $a = a(T; P)$ is given by

$$\alpha = \begin{cases} \text{Thermal expansion coefficient [K} - 1\text{]of} \\ \text{the food in } \Phi^*_F; \\ \text{Thermal expansion coefficient [K} - 1\text{]of} \\ \text{the pressurizing fluid in } \Phi^*_P; \\ 0, elsewhere \end{cases}$$

The conductive heat transfer equation (15) is completed with appropriate initial and boundary conditions depending on the High Pressure machine.

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. 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, satisfies Navier-Stokes equations for compressible Newtonian fluid under Stokes assumption.

The resulting system of equations is:

$$\rho C_p \frac{\partial T}{\partial t} - \Delta \cdot (k\nabla T) + \rho C_p u \cdot \nabla T = \alpha \frac{dP}{dt} T \qquad (16)$$

Where g is the gravity vector m/s^2], $\eta = \eta(T, P)$ the dynamic viscosity $[Pas]$, $p = p(x, t)$ the pressure [Pa] generated by the mass transfer inside the fluid, $[Pa]$ and $P + p$ is the total pressure $[Pa]$ in the pressurizing medium Φ^*_P. Equation (16) 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 (16) can be determined by considering various inverse problems (see [5], [8]).

CONCLUSION

The mathematical models that described our findings provide a useful tool to design and optimize processes based on the combination of thermal and high pressure processes in Food Technology. They take into account the heat and mass transfer phenomena and the enzymatic inactivation occurring during the process.

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Several simplified versions of the full models have been also proposed. When comparing them to the corresponding full model the results are quite similar. Therefore, since the simplified models need less computational time to be solved, they can be suitable for optimization procedures. All these numerical results show that there is not a general optimal treatment. For each particular kind of food and high pressure equipment we propose to carry out the following steps: (i) Identify the most important enzymes to be inactivated and get, for each one of them, a kinetic equation describing the evolution of their activity in terms of pressure and temperature. (ii) Choose a suitable model describing the distribution of temperature in the food and solve it numerically. (iii) Use this distribution of temperature as input data for the selected kinetic equations of the enzymes, in order to get their final activities after the thermal–HP process. Perform optimization techniques in order to reduce the enzymatic activities without using high temperatures

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Conflicts of interest

The authors declare that this research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflicts of interest

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