Modelling and Simulation of Heat and Mass Transfer for Liquid Type Foods under High Pressure Processes

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Abstract: High Pressure (HP) Processing has turned out to be very effective in order to prolong the shelf life of some foods. This paper deals with the modelling and simulation of the effect of the combination of high pressure with thermal treatments on food. The behaviour and stability of this model are checked by various numerical examples. Furthermore, a simplified version of the model is presented and compared with the full model in terms of accuracy and computational time. The models developed provide a useful tool to design suitable industrial equipments and optimize the processes.

Keywords: Modelling; Food Technology; High Pressure; Heat and Mass Transfer.

1. Introduction

At present, the demand of safe and minimally processed food, prepared for immediate consumption (ready–to–use and ready–to–eat) has increased significantly, in order to give service to the needs of restaurants, collective dining rooms (colleges, companies, hospitals, residences, etc.) as well as to domestic consumption.

One of the technologies that can be used for the preparation of these products is High Pressure (HP) Processing, which has turned out to be very effective in order to prolong the shelf life of some foods (cooked ham, juices, guacamole, oysters, etc.) being already a reality at industrial level. These treatments have the great advantage of not being based on the incorporation of additives, which consumers prefer to elude. Furthermore, they allow to avoid treatments with high temperatures (as Pasteurization), which have adverse effects on some nutritional properties of the food, its flavor, etc. (see, e.g., [4] and [5]).

This paper deals with the modelling and simulation of the effect of the combination of high pressure with thermal treatments on food. Due to the high computational complexity needed for solving the full model (which include heat and mass transfer and nonconstant thermophysical properties), we also consider and study a simplified version of it. These models may be very important in order to be able to design suitable industrial equipments and optimize the processes.

2. Heat and Mass Transfer Modelling

When HP is applied in Food Technology, it is necessary to consider thermal effects produced by variations of temperature due to the work of compression/expansion in both the food and the pressurizing fluid.

After compression, heat exchange appears between the pressure chamber, the pressure medium and the food sample giving a time–dependent distribution of temperatures. In the fluid media (the pressurizing fluid and also the food when it is in liquid state) changes in temperatures imply changes in fluid density leading to free convection during the high pressure process. Therefore, conduction and convection have been considered in the models, taking into account heat and mass transfer (see [1, 8]).

Often, HP experiments are carried out in a cylindrical pressure vessel (typically a hollow steel cylinder) previously filled with the food and the pressure medium. The sample is located in the inner chamber at a temperature that can be the same or different to the one in the pressure medium and/or the solid domain surrounding it, which may cool or warm the food following user's criteria.

The axial symmetry of the model allows us to consider cylindrical coordinates and the domain given by half a cross section (intersection of the cylinder with a plane containing the axis). Let us consider four bidimensional sub–domains (see Figure 1):

- Ω_{F}: domain where the sample of food is located.
- Ω_{C}: cap of the sample holder (typically a rubber cap).
- Ω_{P}: domain occupied by the pressurizing medium.

•$\Omega_{\rm S}$: domain of the steel surrounding the above domains.

Our domain in the (r,z)–coordinates is the rectangle $\Omega = [0,L]\times[0,H]$ defined by $\overline{\Omega} = \overline{\Omega_{\rm F}\cup\Omega_{\rm C}\cup\Omega_{\rm P}\cup\Omega_{\rm S}}$, where $\{0\}\times(0,H)$ generates the axis of symmetry. In the boundary of Ω, which is denoted by Γ, we distinguish:

• $\Gamma_{\rm r}\subset\{L\}\times(0,H)$, where the temperature will be known.

• $\Gamma_{\rm up}=[0,L]\times\{H\}$, where heat transfer with the room where the equipment is located could take place.

• $\Gamma\backslash\{\Gamma_{\rm r}\cup\Gamma_{\rm up}\}$, with zero heat flux, either by axial symmetry or by isolation of the equipment.

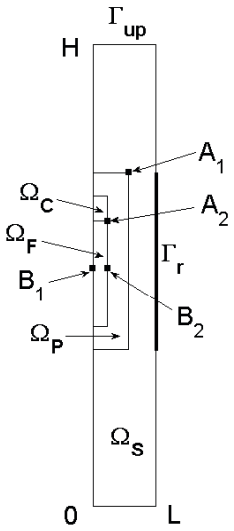

Figure 1. Computational domain.

We denote by Ω^*, $\Omega^*_{\rm F}$, $\Omega^*_{\rm C}$, $\Omega^*_{\rm P}$, $\Omega^*_{\rm S}$, Γ^*, $\Gamma^*_{\rm r}$ and $\Gamma^*_{\rm up}$ the domains generated when rotating Ω, $\Omega_{\rm F}$, $\Omega_{\rm C}$, $\Omega_{\rm P}$, $\Omega_{\rm S}$, $\Gamma\backslash(\{0\}\times(0,H))$, $\Gamma_{\rm r}$ and $\Gamma_{\rm up}$ along the axis of symmetry (in the 3D space), respectively.

2.1 Liquid food modelling

For the mathematical model we will consider a liquid type food. We propose a model considering convection both in the pressurizing medium and the region Ω_F. We distinguish two separated velocity fields $\mathbf{u_F}$ and $\mathbf{u_P}$ for the food and the pressurizing fluid, respectively. We point out that the pressure medium and the food are separated by the sample holder and do not mix.

The governing equations are

$$\begin{cases} \rho C_p\dfrac{\partial T}{\partial t}-\nabla\cdot(k\nabla T)+\rho C_p\mathbf{u}\cdot\nabla T \\ \qquad =\alpha\dfrac{dP}{dt}T \ \text{ in } \Omega^*\times(0,t_{\rm f}), \\ \rho\dfrac{\partial\mathbf{u_F}}{\partial t}-\nabla\cdot\eta(\nabla\mathbf{u_F}+\nabla\mathbf{u_F^t}) \\ \qquad +\rho(\mathbf{u_F}\cdot\nabla)\mathbf{u_F} \\ \qquad =-\nabla p-\nabla\cdot\left(\dfrac{2\eta}{3}(\nabla\cdot\mathbf{u})I\right) \\ \qquad -\rho\mathbf{g} \ \text{ in } \Omega^*_{\rm F}\times(0,t_{\rm f}), \\ \rho\dfrac{\partial\mathbf{u_P}}{\partial t}-\nabla\cdot\eta(\nabla\mathbf{u_P}+\nabla\mathbf{u_P^t}) \\ \qquad +\rho(\mathbf{u_P}\cdot\nabla)\mathbf{u_P} \\ \qquad =-\nabla p-\nabla\cdot\left(\dfrac{2\eta}{3}(\nabla\cdot\mathbf{u})I\right) \\ \qquad -\rho\mathbf{g} \ \text{ in } \Omega^*_{\rm P}\times(0,t_{\rm f}), \\ \dfrac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u_F})=0 \ \text{ in } \Omega^*_{\rm F}\times(0,t_{\rm f}), \\ \dfrac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u_P})=0 \ \text{ in } \Omega^*_{\rm P}\times(0,t_{\rm f}), \end{cases} \tag{1}$$

where P is the pressure (Pa) applied by the equipment, p is the pressure (Pa) generated by the mass transfer inside the fluid, T is the temperature (K), ρ is the density (kg m^{-3}), C_p is the heat capacity (J kg^{-1} K^{-1}), k is the thermal conductivity (W m^{-1}K^{-1}), $t_{\rm f}$ (s) is the final time, η is the dynamic viscosity (Pa s), $\mathbf{g}$ is the gravity vector (m s^{-2}) and α is given by

$$\alpha=\begin{cases} \text{thermal expansion coefficient (K}^{-1}\text{)} \\ \text{of the food in } \Omega^*_{\rm F}, \\ \text{thermal expansion coefficient (K}^{-1}\text{)} \\ \text{of the pressure fluid in } \Omega^*_{\rm P}, \\ 0, \text{ elsewhere.} \end{cases}$$

Right hand term of first equation in (1) results from the following law:

$$\frac{\Delta T}{\Delta P}=\frac{\alpha TV}{MC_p}=\frac{\alpha T}{\rho C_p},$$

where ΔT is the change of temperature due to a change of pressure ΔP, V (m^3) is the volume and M (kg) is the mass.

We also consider the following point, boundary

and initial conditions:

$$\begin{cases} k\dfrac{\partial T}{\partial \mathbf{n}} = 0 \ \text{ on } \ \Gamma^* \backslash (\Gamma_r^* \cup \Gamma_{\text{up}}^*) \times (0, t_{\text{f}}), \\ k\dfrac{\partial T}{\partial \mathbf{n}} = h(T_{\text{amb}} - T) \ \text{ on } \ \Gamma_{\text{up}}^* \times (0, t_{\text{f}}), \\ T = T_{\text{ref}} \ \text{ on } \ \Gamma_r^* \times (0, t_{\text{f}}), \\ \mathbf{u_F} = 0 \ \text{ on } \ \Gamma_{\text{F}}^* \times (0, t_{\text{f}}), \\ \mathbf{u_P} = 0 \ \text{ on } \ \Gamma_{\text{P}}^* \times (0, t_{\text{f}}), \\ T = T_0 \ \text{ in } \ \Omega^*, \\ p = 10^5 \ \text{ in } \ A_1 \times (0, t_{\text{f}}), \\ p = 10^5 \ \text{ in } \ A_2 \times (0, t_{\text{f}}), \end{cases} \tag{2}$$

where Γ_{F}^* denotes the boundary of Ω_{F}^*, Γ_{P}^* is the boundary of Ω_{P}^*, $A_1,\ A_2$ are corner points of Γ_{P}^* and Γ_{F}^*, respectively (see Figure 1), $\mathbf{n}$ is the outward normal vector on the boundary of the domain, T_0 us the initial temperature, T_{ref} is the temperature that is kept constant in Γ_r^* (cooling or warming the food sample), T_{amb} is the (constant) temperature at the external environment and h ($\text{Wm}^{-2}\text{K}^{-1}$) is the heat transfer coefficient.

2.2 Model sensitivity

In practice, the coefficients used in equations (1)–(2) are usually approximated using experimental data with a standard deviation inferior to $\pm 5\%$ of the value (see [17]). Furthermore, due to equipment limitations, some experimental discrepancies could occur during the process (for instance, the pressure curve is not strictly respected). In order to study the impact of those errors on the temperature, we perform a sensitivity study on the considered model.

More precisely, we generate $N \in \mathbb{N}$ perturbed models considering the original one where ρ, C_p, k, α, η, T_0, T_{ref}, P are perturbed randomly by $\pm 5\%$. Then, we compute the mean temperature error T_{err} as follows:

$$T_{\text{err}} = \frac{1}{N} \sum_{i=1}^{N} ||T - T_i||^2_{L^2(\Omega \times (0,t_f))}, \tag{3}$$

where T is the temperature distribution obtained using the original model and $\{T_i\}_{i=1}^N$ are the solutions corresponding to the N perturbed models.

2.3 Simplified model

Due to the high computational complexity needed to solve the "full" model (1)–(2), it may be interesting to consider some simplified versions (called "simplified models"), cheaper to evaluate and with results close enough to the full model. Indeed, simplified models are useful when they are used, for example, during optimization processes needing a lot of model evaluations (see [6, 7, 16]). A description of this methodology can be found in [10, 11].

Thus, we carry out the study of the numerical characteristics of one simplified version of the liquid food model (1)–(2) described previously.

More precisely, we consider a version with constant coefficients (except the density ρ which we consider always depending on temperature and pressure in order to keep the effect of the heat transfer by convection in the liquid domains) setting C_p, k, α and η to their mean value in the range of temperature and pressure considered in the process (other simplifications, as the Boussinesq approximation, could be also considered). This model is denoted by **T–CC**.

In order to evaluate the efficiency of the simplified model, we compute the error made on the temperature (**ET**) considering the simplified model instead of the full one. It is given by

$$\text{ET}(T_{\text{sim}}) = ||T - T_{\text{sim}}||^2_{L^2(\Omega \times (0,t_f)}, \tag{4}$$

where T_{sim} and T are the solution given by the simplified and full models, respectively.

2.4 Numerical tests

For the numerical experiments we have used the dimensions of the pilot unit (ACB GEC Alsthom, Nantes, France) that was used in [15]. Therefore, the 2D cylindrical domain has a radius of $L = 0.09$ m and a height of $H = 0.654$ m (see Figure 1).

We consider a representative example of sample food: a liquid type food with a small filling ratio. The dimensions and location of the sample is exactly the same as studied in [15] for solid type foods.

We present numerical tests computed in cylindrical coordinates using an iterative solver. We have considered the COMSOL Multiphysics 3.4 for solving the model. More precisely, velocity and pressure spacial discretization is based on P2–P1 Lagrange Finite Elements satisfying the Ladyzhenskaya, Babuska and Brezzi (LBB) stability condition. The convective diffusion equation is solved using a suitable direct method (UMFPACK: Unsymmetric MultiFrontal method for sparse linear

systems) combined with a stabilization technique (GLS: Galerkin Least Squares, see [18]).

The physical parameters of the pressurizing medium are supposed to be equal to those of the water and depending on temperature and pressure. For the liquid food sample, water physical parameters are considered too. In this case, ρ, C_p and k parameters are computed through a *shifting approach* (see [12, 14]) from atmospheric pressure, and using a suitable linear interpolation for other values of pressure. For parameter α we use the expression described in [13]. Finally, dynamic viscosity η is obtained also by interpolation of data obtained using [9].

For general cases where the thermophysical properties of a particular food are not known, identification of these parameters making use of mathematical tools for inverse problems may be needed. For example, in [3] the authors discuss how to identify the heat transfer coefficient for a particular prototype. Identification of coefficients depending on temperature is considered, in a rigorous mathematical way in [2] for a general abstract case.

The environmental temperature, the reference temperature and the heat transfer coefficient used in the test are $T_{\text{amb}} = 19.3$°C, $T_{\text{ref}} = 40$°C and $h = 28$ W m^{-2} K^{-1}, respectively. Initial temperature in the sample is chosen equal to 22 °C. Thermophysical properties of the steel and the rubber cap of the sample holder were considered to be constant ($\rho = 7833$ kg m^{-3}, $C_p = 465$ J kg^{-1} K^{-1} and $k = 55$ W m^{-1} K^{-1} for steel and $\rho = 1110$ kg m^{-3}, $C_p = 1884$ J kg^{-1} K^{-1} and $k = 0.173$ W m^{-1} K^{-1} for rubber).

We have performed several numerical experiments simulating the temperature evolution. For this sake, we consider a high pressure process as follows: for initial temperature

$$T_0 = \begin{cases} 40\text{°C in } \Omega_{\text{S}}, \\ 22\text{°C in } \Omega \backslash \Omega_{\text{S}}, \end{cases}$$

a constant pressure increase in the first 305 seconds until reaching 600 MPa is considered. Therefore, the derivative of pressure in the internal heat generation is

$$\frac{dP}{dt} = \begin{cases} \dfrac{600}{305}\, 10^6 \text{ Pa s}^{-1}, & 0 < t \leq 305, \\ 0 \text{ Pa s}^{-1}, & t > 305. \end{cases}$$

2.4.1 Full model analysis

Figure 2 shows the temperature distribution under the considered high pressure process at time $t = 15$ min.

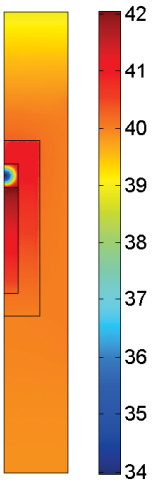

Figure 2. Temperature distribution (°C) in the whole domain at $t = 15$ after the considered process.

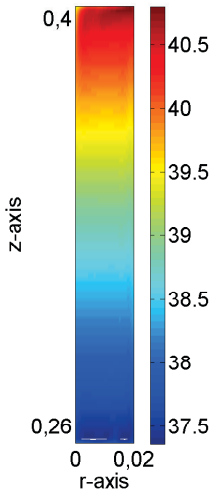

Figure 3. Time–averaged temperature distribution (°C) during 15 min in the food sample after the considered process.

Time–averaged temperature distribution for the considered case is represented in Figure 3. Both figures illustrate how the model captures the non-homogeneous temperature distribution in the domain.

Figure 4 plots the evolution of the temperature at two points: the first one, B_1, is located at the center of the sample (at the symmetry axis) and the second one, B_2, at the surface of the sample, located at the same height than B_1 (see Figure 1). Evolution of sample mean temperature is also plotted.

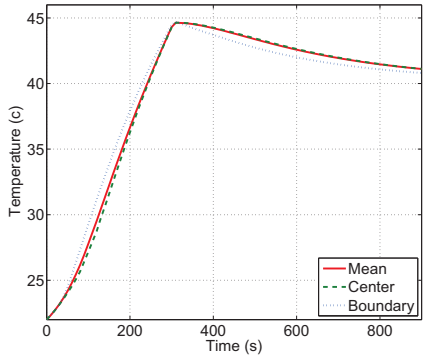

Figure 4. Evolution of the sample's mean temperature (—), temperature in the center point B_1 (- -) and in the boundary point B_2 (...) of the sample during the process.

Therefore, the model and the numerical approximation of its solution is consistent with what is physically expected.

As already remarked in [15] for solid type foods, these results show that for liquid foods it can be also interesting to use an initial temperature for the food smaller than T_{ref} in order to anticipate the temperature increase that results from compression, which allows to get a more uniform process avoiding big temperature gradients inside the food and temperatures much higher than T_{ref} (we remember that one of the goals of the high–pressure technology is to process the food without using high temperatures, which degrade some of the main qualities of the food).

2.4.2 Model sensitivity analysis

According to Section 2.2, in order to evaluate the sensitivity of our model, we have generated $N = 10$ perturbed versions of the model. The mean temperature error defined in (3) satisfies $T_{\text{err}} \leq 2$°C. This represents $\pm 8\%$ of the range of temperature $[21\text{°C}, 47\text{°C}]$ reached during the processes (see Table 1).

Minimun Temperature	21
Maximun Temperature	47
Mean Temperature	40

Table 1. Range of temperature (°C) obtained in the food sample.

Furthermore, as we can observe in Figure 5, which represents an example of the distribution of the error in the whole equipment, the average error committed in the food sample, that is close to 1.2°C ($\pm 5\%$), is less important than the error committed in the other parts of the device.

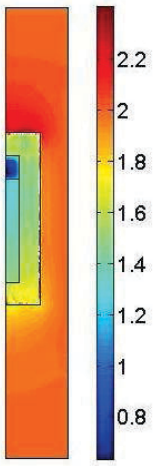

Figure 5. Example of temperature average error distribution (°C) between the full and the perturbed models.

2.4.3 Simplified model analysis

We report in Table 2 some results obtained when checking the efficiency of the simplified model introduced in Section 2.3. The **T–CC** model produces an error of $ET(T_{\text{T}-\text{CC}})$=0.15°C ($\pm 0.6\%$). This simplified model gives a good alternative to the full one for possible optimization procedures.

Model	ET	CT
Full model	—	35000
T–CC model	0.15	7500

Table 2. Results obtained in the food sample for the full and simplified models. **ET**: Error on the temperature (°C). **CT**: Computational time (s).

3. Concluding Remarks

The mathematical models described in this paper 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 occurring during the process. A sensitivity analysis has been developed in order to show the dependence of the solution with respect to the thermophysical parameters, showing the robustness of the model. In this paper a simplified version of the full model has been also proposed. When comparing with the full model the results are very close. Therefore, since the simplified model needs less computational time to be solved, it can be suitable for optimization procedures (which usually need to compute the solution of the corresponding model for different data).

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