CFD-based Approach For Prediction Of Headspace Pressure In Can During Thermal Sterilization Of Foods

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Abstract

Thermal sterilization is a critical process in the food industry which ensures food safety and longer shelf life. However, understanding internal pressure during thermal sterilization is crucial for designing suitable packaging for both conventional and non-conventional sterilization processes. This study focuses on predicting internal headspace pressure due to vapour generation and dry air pressure in food packaging such as cans using Computational Fluid Dynamics (CFD). A 2D-axisymmetric model of a can containing a model food (mashed potato) was developed in COMSOL® Multiphysics 6.2 to simulate temperature and pressure fields. The model calculates the pressure due to dry air which reached a maximum of 1.35 bar, and experimental data showed a total internal headspace pressure of 3.45 bar. This indicated the significant role of water vapour pressure in a food packaging during the sterilization process. This study is one of the few to investigate the headspace pressure inside a can during a thermal sterilization process and highlights the importance of water vapour in headspace pressure evolution.

Keywords: Thermal sterilization, headspace pressure, computational fluid dynamics (CFD), food packaging

Introduction

External counter-pressure to tackle the inner pressure in food packaging is essential to maintain the packaging structure during a high-temperature thermal sterilization process in the food industry. However, an effective external counter-pressure can be applied only with a more accurate and precise understanding of the generated inner headspace pressure in the food packaging during the thermal sterilization process [1].

Thermal sterilization is a critical process in the food industry as it ensures the safety and shelf life of food products for long-term preservation by eliminating all microorganisms and their spores from a food product [2]. During this process, the temperature rises to 121°C for a certain period to eliminate one particular spore-forming microorganism, *Clostridium botulinum*. As the temperature inside the packaging rises above the boiling point of water, water vapour is generated inside the packaging due to water evaporation to the headspace from the food product. This significantly increases the internal pressure on the packaging. This internal pressure rise is primarily due to two factors: water vapour generation due to evaporation from the food product to the headspace, and dry air expansion in the headspace.

A good alignment between the external counter-pressure and the internally generated pressure is essential for preventing packaging failures [3]–[5]. If the external counter-pressure is higher than the internal pressure, the packaging may be crushed. On the other hand, if the internal pressure is higher than the external counter-pressure, the packaging is likely to have an explosion. For this purpose, as a standard practice in the food industry for food packaging in metal cans, the pressure difference between the external counter-pressure and internal pressure is kept at around 0.5 bar. Hence, in this work, we propose to develop a numerical model using Computational Fluid Dynamics (CFD) with COMSOL Multiphysics 6.2 to predict internal headspace pressure in cans during thermal sterilization process.

Experimental Setup

Thermal sterilization experiments were conducted using a STERITECH® retort in Oniris, Nantes, France. Mashed potato samples (76% moisture content in w.b%) were used as model food in metal cans with a headspace of 25 mm for the experiments. The primary aim of these experiments was to measure the experimental temperature profile at 4 locations inside the model food sample: top (T), center (C), bottom (B), and headspace (H) using temperature probes (SSR Type T, Ellab SARL, France). Another objective of the experiments was also to measure the total absolute pressure inside the container using pressure sensors (NanoVACQ PT, TMI Orion, France). Heat was supplied to the cans using pressurized steam in a retort. Heat is transferred by convection/conduction through the walls of the metal can with a height of 107 mm and diameter of 72 mm from all directions thereby heating the model food and the headspace air (Figure 1).

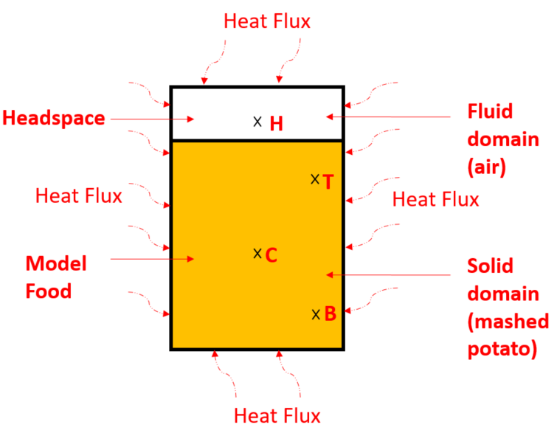

Figure 1: 2D geometry of metal can with model food with various locations of temperature measurement.

Numerical Model

A numerical model was developed using COMSOL® Multiphysics 6.2 software by utilizing the heat transfer and CFD modules. The "Heat Transfer in Solids and Fluids" interface was applied to simulate heat transfer through conduction and convection in both solid (metal can and model food) and fluid (air) domains. The "Laminar Flow" interface was employed to solve the pressure and velocity fields within the headspace air domain.

Governing equations

Heat transfer equation:

The heat transfer is calculated using the general heat transfer equation for both the solids and fluid domain:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \boldsymbol{u}.\nabla T + \nabla.\boldsymbol{q} = 0 \quad (1)$$

where the heat flux vector $\boldsymbol{q}$ is defined as:

$$\boldsymbol{q} = -k\nabla T \quad (2)$$

where ρ is the density (kg/m^3), C_p is the heat capacity at constant pressure $(J/kg/K)$, k is the thermal conductivity $(W/m/K)$, **u** is the velocity field (m/s) which is solved only for the air domain.

Heat flux calculation:

The heat flux at the boundary is calculated as:

$$-n.q = q_0 \quad (3)$$

$$q_0 = h_{global}(T_{retort} - T) \quad (4)$$

where the temperature of the retort is defined in Figure 2.

And, the global heat transfer coefficient is defined as [6], [7]:

$$h_{global} = \begin{cases} 90\ W/(m^2.K) & T < 100°C \\ 124.5\ W/(m^2.K) & T > 100°C \end{cases}$$

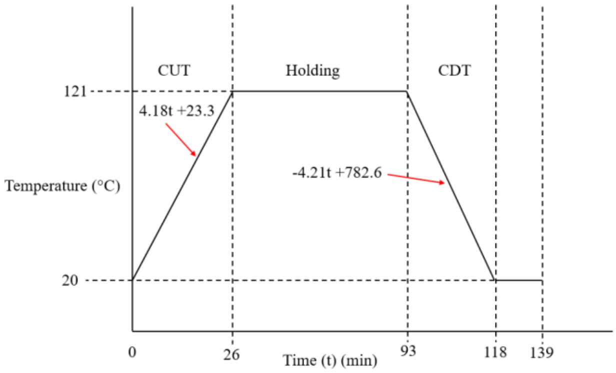

Figure 2: Temperature profile of retort (T_{retort})

Navier-stokes, and continuity equations:

The Laminar Flow interface solves the Navier-Stokes, and continuity equations within air domain:

- Momentum equation:

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} = -\nabla p + \mu \nabla^2 \boldsymbol{u} + F \quad (5)$$

where F is external forces due to gravity defined as:

$$F = \rho g \quad (6)$$

- Continuity equation:

$$\frac{D\rho}{Dt} + \rho \nabla.\boldsymbol{u} = 0 \quad (7)$$

where, $\frac{D}{Dt} = \frac{\partial}{\partial t} + \boldsymbol{u}.\nabla$ (8)

A no-slip boundary condition was applied to the walls.

$$\boldsymbol{u} = 0 \ on\ the\ wall\ surface$$

Model description

A 2D-axisymmetric geometry of a metal can with radius 36 mm and height 107 mm containing model food (mashed potato) was constructed in COMSOL® Multiphysics. The geometry had two domains: the solid domain containing the model food, and the fluid domain containing the air. The Finite Element model was used for a thorough examination of the temperature distribution and pressure distribution within the can during thermal sterilization process. A compressible flow (Ma<0.3) was assumed as air density changes due to temperature and pressure. Thermophysical properties linked with temperatures were incorporated as input parameters (Table 1). Material properties such as dry air were imported from the application library and mashed potato material properties were imported from experimental measurements. A physics-controlled mesh with "fine" element size was used for the numerical modelling. The study was computed from 0 s to 8340 s with mesh size of 1681 elements (Figure 3). Inbuilt operators from COMSOL® were used to calculate the average of variables (pressure and temperature).

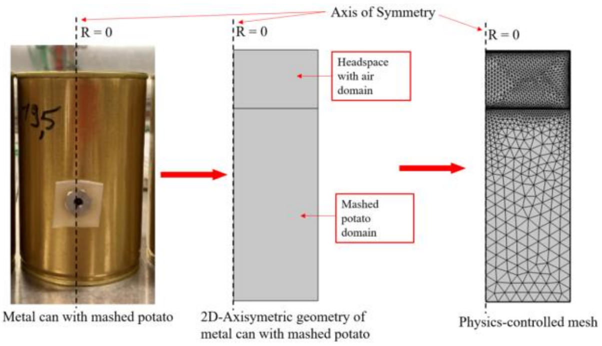

Figure 3: Metal can geometry and meshing in COMSOL® Multiphysics.

The ideal gas law was used to model the behaviour of the dry air and water vapour in the headspace:

$$P_{air}V_{headspace} = n_{air}RT \quad (9)$$

$$P_{vapour}V_{headspace} = n_{vapour}RT \quad (10)$$

where, P_{air} and P_{vapour} are dry air and vapour pressures, $V_{headspace}$ is headspace volume, n_{air} is number of moles of air, n_{vapour} is number of moles of vapour, R is ideal gas constant (8.3145 $J/mol/K$), T is temperature (K).

Dalton's law of partial pressure was used to account for the presence of both dry air and water vapour:

$$P_{total} = P_{air} + P_{vapour} \quad (11)$$

The vapour pressure values as a function of time was estimated from the knowledge of the total pressure in the headspace (from experiments) and the dry air pressure (from the model).

Table 1: Input Model Parameters

Parameters		Values
Density of model food (mashed potato)	ρ_{mp}	1052.96 kg/m^3
Thermal conductivity of model food (mashed potato)	k_{mp}	0.55 $W/m/K$
Specific heat capacity model food (mashed potato)	Cp_{mp}	0.0576 T^2 – 33.551 T + 8445.2 $J/kg/K$
Density of metal can	ρ_{can}	7900 kg/m^3
Thermal conductivity of metal can	k_{can}	45 $W/m/K$
Specific heat capacity of metal can	Cp_{can}	213 $J/kg/K)$

Simulation Results

The numerical model was computed in a Dell® Precision™ Workstation computer equipped with 2 × Intel® Xeon processors (8 cores), at 2.5 GHz, with 256 GB RAM, running on Windows® 10 Professional, 64 bits. The computation time was 3 min 29 s with 4350 degrees of freedom. The results obtained from the simulations were compared with experimental data collected from the experiments conducted with the retort sterilization system to assess the accuracy and reliability of the numerical model.

Temperature modelling

The experimental temperature profiles were compared with the simulated temperature profiles in four different locations: headspace (0 mm, 85.77mm), top (34 mm, 69.7 mm), center (0 mm, 41 mm), and bottom (34 mm, 15 mm). Figure 4 displays both experimental and simulated temperature profiles at various locations. The presented figures confirms the consistency between the experimental temperature profile and the simulated temperature profile, thus validating the accuracy of the numerical model. However, slight discrepancies between experimental and simulated results have been observed in Figure 4(b) and 4(d) for center and headspace location respectively due to non-consideration of moisture in the solid domain. The evolution of temperature within the can is displayed in Figure 5 at 10 s (beginning of the sterilization process), 4821 s (at the middle of the sterilization process), and 7968 s (at the end of the sterilization process).

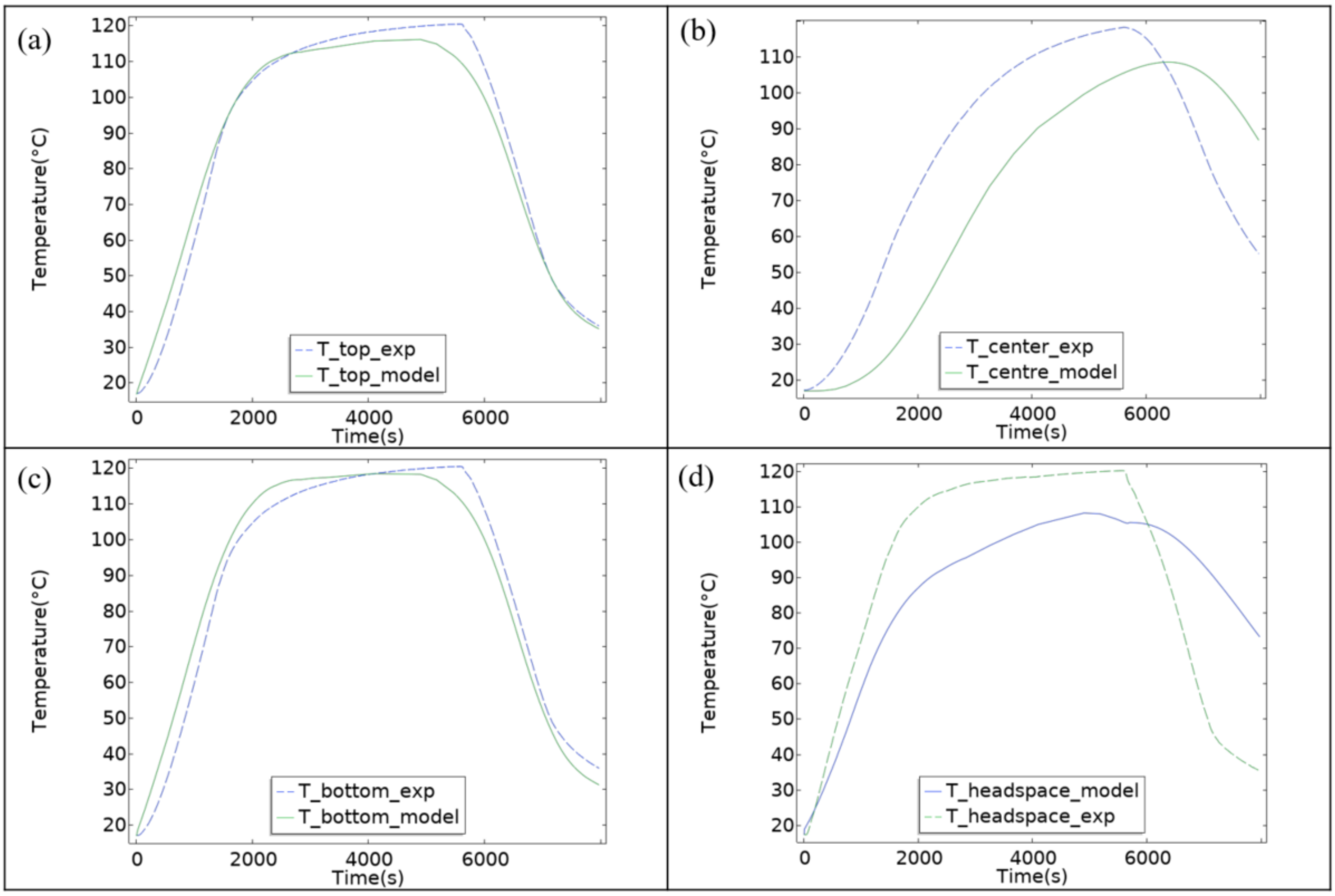

Figure 4: Experimental and simulated temperature profile at (a) Top location (b) Center location (c) Bottom location (d) Headspace location.

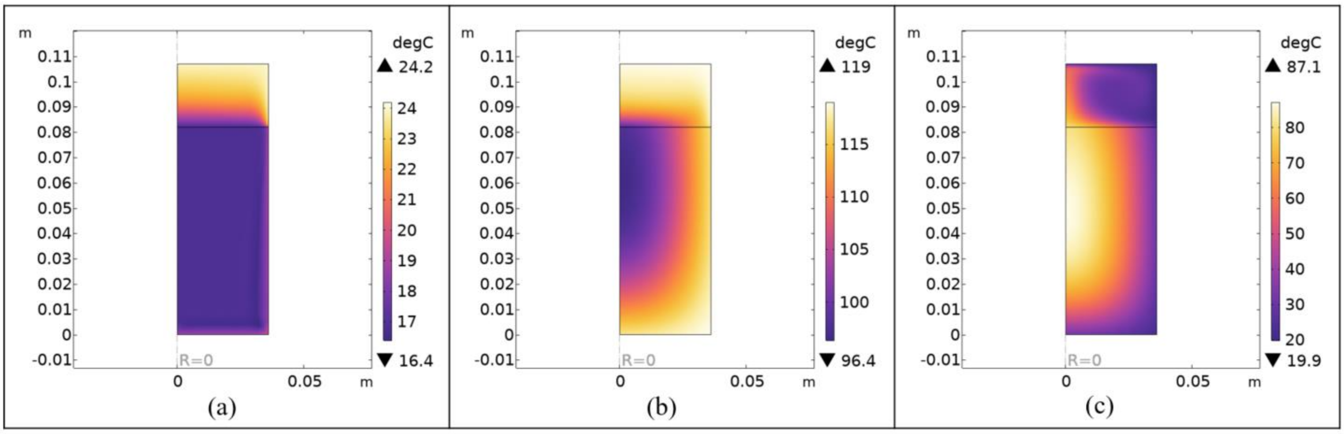

Figure 5: Temperature distribution at (a) 10 s (b) 4821 s (c) 7968 s

Pressure modelling

The experimental pressure profile of total pressure was compared with the simulated pressure profile of dry air in the headspace location and water vapour pressure was calculated from equation 9 and 10 (Figure 6 and Figure 7).

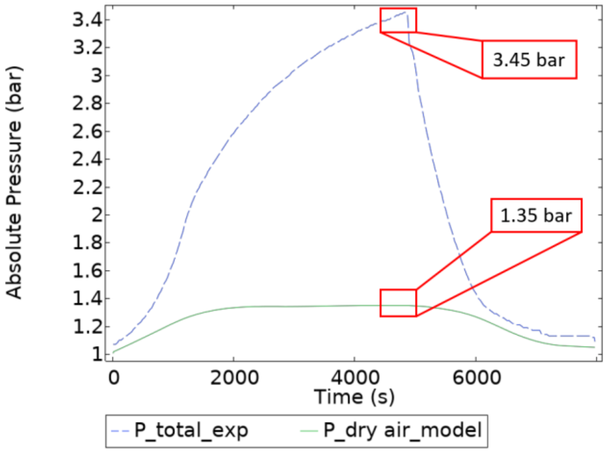

Figure 6:Experimental pressure profile of total pressure in comparison to simulated pressure profile of dry air.

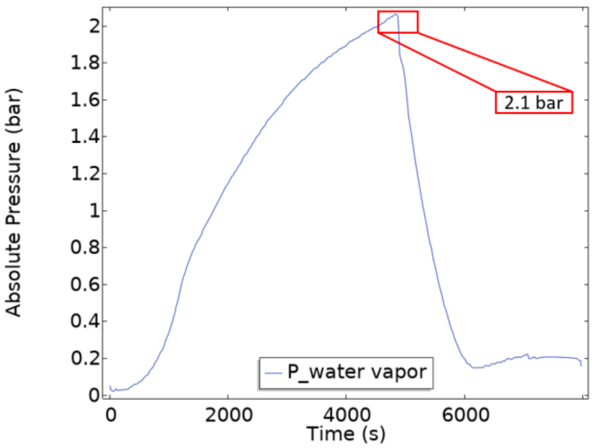

Figure 7: Estimated water vapour pressure profile.

These figures highlight the capability of the numerical model to capture the pressure evolution process occurring inside a closed packaging system with model food during a conventional thermal sterilization process. The simulated model calculates the pressure of dry air during the process. The difference between this simulated pressure value of dry air and the experimental pressure value of the total pressure was used to calculate the pressure value of water vapour. Since the maximum total pressure was 3.45 bar absolute at 4821 s and the pressure of dry air was 1.35 bar, the maximum pressure exerted by water vapour was found to be 2.1 bar. The mass of water vapour generated was estimated using equation 9, 10 and 11 and was found to be 0.12 g during the sterilization process (Figure 8). This water vapour can be found as condensed water in the interior walls of the can at the end of the sterilization process.

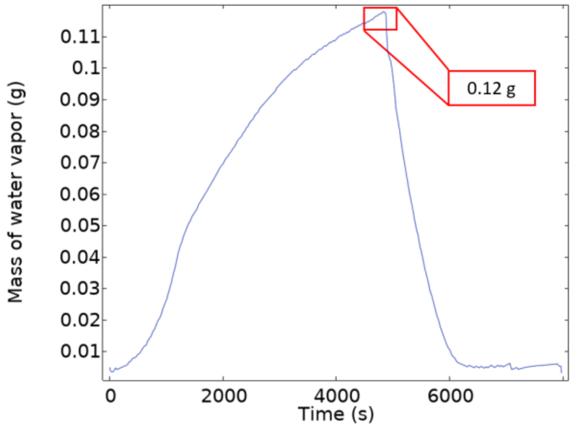

Figure 8: Estimated mass of water vapour generation..

Discussions

The numerical model effectively reproduces the process that takes place inside a closed food packaging system during a thermal sterilization process. The simulated temperature profiles at the three locations (top, center, and bottom) give values close to those of the experimental values. But, there has been a wider difference in the temperature profile for the headspace location. This is due to the influence of natural convection, which also contributes significantly towards heat transfer. As temperature increases, the rising vapour alters the temperature distribution in the headspace. This study does not take into account this rise of vapour due to evaporation. Therefore, this led to the variation of experimental and simulated headspace temperatures. Figure 6 which tells about the total pressure and average pressure due to dry air, shows the wide gap between simulated dry air pressure and the experimentally measured total pressure. The difference between this simulated dry air pressure and the experimental total pressure is the water vapour pressure which is very significant during the thermal sterilization process. Using this estimated water vapour pressure, the mass of water vapour generated during the thermal sterilization process was also estimated and was of the same order of magnitude of the one determined experimentally (less than 0.5 g). However, this value needs to be validated with accurate measurements in future experiments. This shows the importance of considering phase changes and water vapour generation due to evaporation during thermal treatments in future models.

Conclusions

A numerical model to study complex physical phenomena and predict the mass of vapour generation which leads to headspace pressure in food packaging such as cans during thermal sterilization has been developed using COMSOL® Multiphysics. The model accurately simulates the temperature distribution and dry air pressure within the can. It captures essential aspects of heat transfer and pressure evolution in the headspace. The model helps predict the dry air pressure during the thermal sterilization process in a can, which leads to the calculation of vapour pressure in the headspace from the knowledge of the total pressure. Using this estimated water vapour pressure, the mass of water vapour generated during the thermal sterilization process was also calculated. This highlights the significance of including water evaporation in future models. The model does not assume natural convection of vapour due to evaporation from the model food, which leads to slight differences between experimental and simulated headspace temperature profiles. Despite these limitations, this computational-experimental study using a CFD-based approach studies the headspace pressure in a can during thermal sterilization which is very essential to understand the structural integrity of a food packaging.

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