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Numerical simulation of stress distribution in heterogeneous solids during high pressure processing

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ABSTRACT

It is generally assumed that the internal stress distribution in foods under high pressure processing (HPP) is uniform, which may not be true for solid foods with hard inclusions, like meats with bones or for particulate foods. Our objective was to simulate the internal stress distribution during HPP of a model heterogeneous solid food made with a gel and a wood inclusion and determine how mechanical properties affect the internal stress distribution. It was determined that hydrostatic pressure decreased and shear stress was generated at the interface between the soft solid and the hard inclusion. The differences in pressure and shear stresses increased as the shear modulus of the soft solid increased. Our studies suggest that a better understanding of the mechanical properties that affect the development of the internal stress field is needed, since they could affect the achieved microbial inactivation levels at different locations in HPP solid foods.

1. Introduction

The increasing demand for natural and less processed foods has triggered novel approaches to food preservation that aim at substituting thermal processing and the use of chemical preservatives with non-thermal processes that can extend the shelf life and improve microbial safety of high value-added products. In the last few years, high pressure processing (HPP) has gained acceptance because it can significantly reduce the microbial load without triggering extensive changes in the physical-chemical attributes of food products. Despite having a high initial capital investment, HPP technology can address the demands of consumers who prefer foods without preservatives while retaining most of the sensorial characteristic of freshness. Furthermore, since the pressure treatment is not dependent on size, shape or mass, unlike thermal treatments, the processing time can be greatly reduced for irregularly shaped large samples.

HPP of food products was firstly reported by Hite (1899), who was able to extend the shelf life of milk. Major HPP research programs were established in United States, Europe, and Japan in the late 1900s and they demonstrated that HPP is a useful technology in extending the shelf life of foods. Today HPP is a well-accepted technology in Europe and United States for products such as sliced ham, oysters, clams, guacamole, fruit juices, fruit purees, ready-to-eat meals, dips, salsas, etc. (Avure Technologies, 2015; Hiperbaric, 2012). Products treated by HPP do not need a specific label in the United States (Garriga & Aymerich, 2009). A high acceptability (67%) of HPP products by consumers was reported for France, Germany, and United Kingdom (Butz, Needs, Baron, Bayer, Geisel, Gupta, Oltersdorf & Tauscher, 2003). It has been shown that HPP is applicable to microbial inactivation in meat products at many stages of processing (Gola, Mutti, Manganelli, Squarcina, & Rovere, 2000; Yuste, Pla, & Mor-Mur, 2000). Numerous reviews have been published on the effects of HPP on microbial inactivation and chemical reactions in food products (Campus, 2010; Martinez-Monteagudo & Saldaña, 2014; Norton & Sun, 2008; Rastogi, Raghavarao, Balasubramaniam, Niranjan, & Knorr, 2007; Rendueles, Omer, Alvseike, Alonso-Calleja, Capita & Prieto, 2011).

One of the main advantages of HPP over thermal pasteurization, from the processing point of view, is that the pressure is considered or assumed to be transmitted uniformly and quasi-instantaneously throughout the sample, regardless of size, shape or packaging (Barbosa-Cánovas, Tapia, & Cano, 2005; Brennan, 2006; Doona & Feeherry, 2007; Rastogi, Raghavarao, Balasubramaniam, Niranjan & Knorr, 2007; Rendueles, Omer, Alvseike, Alonso-Calleja, Capita & Prieto, 2011; Sun, 2005). While this is clearly true for liquids and homogeneous solids, the published literature generally reports that there are no limitations to the validity of uniform pressure distribution. The only dissenting work is by Minerich and Labuza (2003) who did not offer any mechanistic explanation for their findings. They determined that the pressure at the center of a piece of ham during HPP was significantly lower, by 9 MPa, than the applied external hydrostatic pressure, between 400 MPa and 600 MPa. Even though the confidence interval of the individual pressure measurement by the sensor they used was ±16 MPa, as specified by the authors themselves, the fact

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that they used multiple sensors in their experiments allowed them to reach the conclusion.

There have been numerous experimental studies to quantify and correlate mechanical stress in the form of either pressure or shear, to cell mortality or physical damage. Perrier-Cornet, Marechal, and Gervais (1995); Perrier-Cornet, Hayert, and Gervais (1999) used experimental characterization to relate permeability of cell walls in yeast cells subjected to high hydrostatic pressure. Pagán and Mackey (2000) studied the effect of pressure on membrane damage in various strains of *Escherichia coli* bacteria. It was observed that the mechanism of inactivation is dependent on the level of pressure and the nature of cell membrane damage may differ between species and phases of growth. Shimada et al. (1993) observed mechanical damage to the mitochondria and nuclear membrane of *Saccharomyces cerevisiae* after HPP at 400 MPa–600 MPa for 10 min. Fernandes, Farina, and Kurtenbach (2001) observed large differences in the morphological changes after HPP between trehalose-6-phosphate synthase mutants and wild-type *S. cerevisiae*. Moussa, Espinasse, Perrier-Cornet, and Gervais (2013) studied the relationship of inactivation of *S. cerevisiae* and volume compression due to application of high hydrostatic pressure and found a critical volume compression of 10 μm^3 needed for cell inactivation. Bulut, Waites, and Mitchell (1999) observed a non-trivial effect of shear and thermal forces on the microbial inactivation of *Microbacterium lacticum*, and concluded that shear forces played a larger role in inactivation than heat.

Numerical simulation has been used to study the stresses produced in microbial cells during HPP and shed light on the understanding of cell inactivation. Hartmann and Delgado (2004a, 2004b) used numerical simulation to quantify the stresses occurring within yeast cells during high pressure processing, and determined a critical Von Mises stress in the cell wall upon failure between 415 MPa and 460 MPa. Hartmann, Mathmann, and Delgado (2006) developed a nonlinear model of a yeast cell under high pressure and showed different type of stress conditions between the cell wall and the cytoplasm. Otero and Sanz (2003) provided reviews of numerical models for heat transfer in HPP products at sub-zero processing conditions. Guignon, Rey-Santos, and Sanz (2014) determined density, specific volume, isothermal compressibility and thermal expansion coefficient of whole and skim milk between 0 °C and 60 °C and up to 350 MPa to allow future process modeling.

We focus here on simulating the stress generated inside solid materials due to the application of high hydrostatic pressure on the surface using a neo-Hookean model, and how hard inclusions affect the internal stress distribution. Neo-Hookean models have been used previously to study large deformations of food materials (Rakesh & Datta, 2011) and polymeric materials (Chen & Lagoudas, 2008). The stress at any point can be split into effective pressure and shear, which cause volume change and deformation, respectively. Mechanistically, each of these components may play a role during microbial inactivation.

Preliminary experimental work was done with chicken and turkey drumsticks, raw and cooked, to take advantage of the system of meat wrapped around a bone. A bacterial inoculum in sodium alginate was injected at different positions in the meat and gelled with calcium chloride, high pressure processed, and enumerated. Unfortunately, there was high variability in the results since the inocula could not be fixed at consistent locations between experiments, even by gelling it. Moreover, each drumstick had a different meat and bone geometry, and the meat had layers of muscle and fat tissue which was reflected in Young's modulus measurement with over 28% variability (data not shown). Details of these experiments can be found in Maldonado (2016).

Since our work is aimed at exploring the pressure non-uniformity in heterogeneous systems and not in any particular food system, we used a model system to control for the natural variability of food materials. Our findings on the development of pressure gradients in soft materials with hard inclusion during high pressure processing still apply to a large extent to food materials.

2. Theory

In this section a review of the computational modeling aspects and the material model to simulate stress distribution are presented.

2.1. Pressure as a component of stress

The physical quantity known as stress is a representation of forces manifesting within the body in order to equilibrate with an externally applied load(s). The components of stress are arranged in a square matrix, called the stress matrix or stress tensor ($\boldsymbol{\sigma}$), which is used in mathematical modeling and numerical methods. The main diagonal of the matrix contains the normal stresses, and the remaining elements are the shear stresses.

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{bmatrix} \tag{1}$$

Since it is difficult to easily interpret the physical significance of the components of the stress-tensor, several invariant scalar measures of the stress-tensor have been defined in-order to quickly characterize the nature of the force distribution within a solid. The most significant of these measures are the hydrostatic pressure component (p), which is intimately related to volume change of a specimen, and the effective stress deviator also known as the Von Mises stress (σ_{VM}), responsible for shape changes (Bower, 2010; Solecki & Conant, 2003).

$$p = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) \tag{2}$$

$$\sigma_{VM} = \sqrt{\frac{(\sigma_{xx}-\sigma_{yy})^2 + (\sigma_{yy}-\sigma_{zz})^2 + (\sigma_{zz}-\sigma_{xx})^2 + 6({\tau_{xy}}^2 + {\tau_{yz}}^2 + {\tau_{zx}}^2)}{2}} \tag{3}$$

2.2. Mathematical model for stress distribution

The stress developed inside a material is a function of the material properties of the specimen and the strain that the material is subjected to. For a linearly elastic isotropic material the stress tensor "$\boldsymbol{\sigma}$" is written in terms of material constants (also known as Lamé constants) λ, μ, and the components of a strain tensor "$\boldsymbol{\varepsilon}$" as follows:

$$\boldsymbol{\sigma} = \lambda e \boldsymbol{I} + 2\mu\boldsymbol{\varepsilon} \tag{4}$$

where, the scalar quantity

$$e = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} \tag{5}$$

is also known as the volumetric strain measure in small deformation and $\boldsymbol{I}$ is the second-order identity tensor. All tensorial quantities are bold-faced to distinguish them from scalar valued functions and variables. The Lamé constants λ and μ can be written in terms of material properties, namely, the Young's modulus (E) and the Poisson's ratio (υ), which can be determined using standardized mechanical tests. The parameters λ and μ are given as follows:

$$\lambda = \frac{E\upsilon}{(1+\upsilon)(1-2\upsilon)} \tag{6}$$