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Journal of Food Engineering

journal homepage: www.elsevier.com/locate/jfoodeng



Adiabatic compression heating coefficients for high-pressure processing of water, propylene-glycol and mixtures – A combined experimental and numerical approach

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ARTICLE INFO

Article history: Received 5 January 2009 Received in revised form 22 July 2009 Accepted 23 July 2009 Available online 28 July 2009

Keywords:
High-pressure processing
High pressure thermal sterilisation
Compression heating
Adiabatic heating
Thermophysical properties

ABSTRACT

The compression heating of water and water/propylene-glycol mixtures during high-pressure processing was studied using a purpose-designed experimental setup allowing for near-adiabatic conditions. The fluids were pressurised in a Stansted ISO-LAB FPG11501 HPP 3 L unit up to 750 MPa. Pressure/temperature profiles at varying initial temperatures (5–90 °C) were recorded and numerically evaluated to obtain pressure and temperature dependent compression heating properties of water/glycol mixtures at 0%, 25%, 50%, 75% and 100% glycol concentration. A further step was implemented in the numerical routine to derive the compression heating properties as function of pressure, temperature and glycol concentration.

Similarly, the proposed method also can be used to determine compression heating properties of any other liquid or semi-solid material, allowing for accurate prediction of adiabatic temperature increases upon pressurisation in high-pressure processing.

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1. Introduction

The key to a successful food process is the production of safe and palatable food that is attractive to the consumer. Increasingly, the consumer is also seeking health benefits from foods (Norton et al., 2006). Thermal processing is still the most commonly used method for reducing microbial load and enhancing shelf-life. Often a problem is to avoid the over-processing associated with local excess heating, which typically lowers product quality. For pasteurisation it is necessary to lower only the concentration of viable microbial cells. For sterilisation of low-acid foods, however, it is necessary to inactivate microbial spores as well or at least the spores of *Clostridium botulinum*, typically requiring temperatures above 115 °C (Holdsworth, 1997).

High-pressure processing (HPP) is a relatively new food preservation technology, which aims to satisfy the increasing consumer demand for fresh-like products with minimal degradation of nutritional properties.

High pressure is becoming a widely accepted method for pasteurisation of foods because of its ability to inactivate vegetative cells of microorganisms and enzymes near room temperature (Hernando Saiz et al., 2008). Moreover, this technology in combination with elevated temperatures is also a potential candidate for

high-temperature short-time sterilisation of low-acid food products. It involves combining pressures of 600–800 MPa, and moderate initial product and pressure chamber temperatures of 60–90 °C. During pressurisation, the process temperature increases to a point where spores are inactivated (Matser et al., 2004; Margosch, 2005).

The phenomenon of temperature increase during pressurisation is induced by compressive work against intermolecular forces and commonly known as adiabatic heating. Assuming no thermal losses, the temperature reached during pressurisation can be readily derived assuming that there are no thermal losses. If the variation in entropy dS in the system is a function of both temperature T and pressure P, i.e. S = f(T, P), then:

$$dS = \left(\frac{\partial S}{\partial T}\right)_{P} dT + \left(\frac{\partial S}{\partial P}\right)_{T} dP \tag{1}$$

If the process is assumed to be completely reversible, then the total entropy change is zero. Rearranging, the compression heating rate can be expressed as:

$$\frac{dT}{dP} = -\frac{\left(\frac{\partial S}{\partial P}\right)_T}{\left(\frac{\partial S}{\partial T}\right)_P} = \frac{V\left(\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p\right)}{\frac{1}{T}\left(T\left(\frac{\partial S}{\partial T}\right)_p\right)} = \frac{T\alpha_p}{\rho C_p}$$
(2)

Or:

$$\frac{dT}{dP} = k_C \cdot T, \quad \text{with} : k_C = f(P, T) = \frac{\alpha_p}{\rho C_p}$$
 (3)

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Nomenclature polynomial coefficients **Abbreviations** a, b, c polynomial coefficients 2D two-dimensional $a_{1}-a_{15}$ c_{Glycol} , c_G glycol concentration $(kg_{Glycol}/(kg_{Glycol} + kg_{Water}))$ 4D four-dimensional (in this particular case dimensions for specific heat capacity (J/(kg K)) pressure, initial temperature, glycol concentration and C_P D diameter (mm) temperature increase) estimated values in R^2 determination (Pa⁻¹) **ASME** American Society of Mechanical Engineers fi Н height (mm) CFD computational fluid dynamics compression heating coefficient (Pa⁻¹) k_C **CSV** comma-separated values Ρ pressure (Pa, MPa) HP high pressure $\frac{P_0}{R^2}$ mean pressure in sub-interval (Pa) HPP high-pressure processing coefficient of determination **MSE** mean squared error S **NIST** National Institute of Standards and Technology entropy (J/K) Т temperature (°C or K) PG. propylene-glycol T_0 temperature in sub-interval at P_0 (Pa) PΡ polypropylene initial temperature (°C or K) PΤ pressure/temperature sub-interval T_{init} V **PTFE** polytetrafluorethylene specific volume (m³) Χ index for different sub-intervals of pressure and temperature **Operators** mean of the measured values (Pa⁻¹) d differential ν measured values in R^2 determination (Pa⁻¹) y_i function difference Λ Greek symbols thermal expansion coefficient (K⁻¹) α_P density (kg/m³)

Using the appropriate Maxwell's relation:

$$\left(\frac{\partial S}{\partial P}\right)_{T} = -\left(\frac{\partial V}{\partial T}\right)_{P} \tag{4}$$

expressing the specific volume V as the inverse of the density ρ and defining the thermal expansion coefficient α_p and the isobaric heat capacity C_p as:

$$C_{P} = T \left(\frac{\partial s}{\partial T} \right)_{P} \quad \alpha_{P} = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_{P} \tag{5}$$

On decompression, the process is reversed and the temperature decreases. This method, with both rapid heating and cooling, offers the potential of producing high-quality shelf-stable products.

Due to differences of the thermophysical properties however, different materials undergo different temperature changes. This can result in non-uniform temperature distributions during processing. The different temperature profiles at different locations within a pressure vessel, hence, would likely impact on microbial, spore and enzyme inactivation (Denys et al., 2000; Knoerzer et al., 2007; Juliano et al., 2008).

Only very limited information is available on compression heating behaviour of any material except for water under combined pressure and temperature conditions. The compression heating of water under pressure has been extensively studied in the early 1900s by Bridgman (1912, 1923, 1935). After his pioneering work, the thermodynamic properties of water under pressure were well researched and documented. The data was made available by the International Association for the Properties of Water and Steam (IAPWS). A software implementation of the IAPWS work was published by the National Institute of Standards and Technology (NIST) (Harvey et al., 1996).

In recent times, studies related to compression heating of different pressure-transmitting fluids and food substances under high pressure are gaining strong interest (Ardia et al., 2004; Balasubramanian and Balasubramaniam, 2003; Patazca et al., 2007; Rasanayagam et al., 2003; Buzrul et al., 2008; Zhu et al., 2008; Shao et al., 2007).

Although that work extensively covers a wide range of process relevant materials, most of them only report the temperature rate as constants at different pressure and initial temperature combinations; hence, it lacks the determination of the compression heating properties as function of pressure and temperature. Ardia et al. (2004) based their work on the NIST database for water and mixture rules for water soluble components. They thus derived pressure and temperature dependent functions for the compression heating of various sugar solutions. However, this approach is only applicable to water-based solutions and potentially dispersions and not for the evaluation of compression heating of any compressible material. Furthermore, the validity of mixture rules under high pressure conditions is questionable as they had to incorporate correction factors in their equations to get an agreement with measurements.

2. Objectives

For accurate prediction of the maximum heating of any compressible substance during pressurisation according to Eqs. (2) and (3), and for CFD modelling of high pressure processes as described by Knoerzer et al. (2007) and Juliano et al. (2008), the knowledge of pressure and temperature dependent compression heating coefficients $k_C(P,T)=\frac{\alpha_p(P,T)}{\rho(P,T)\cdot C_p(P,T)}$ is essential.

The objectives of this research were to:

- (1) Develop an effective and relatively easy and widely applicable methodology to accurately determine compression heating coefficients as function of pressure and temperature,
- (2) validate the methodology with the compression heating properties of water as published by Harvey et al. (1996),
- (3) determine the compression heating coefficients k_C for water/ propylene-glycol mixtures covering the glycol concentration range from 0 to 100% $\frac{k_{\mathcal{B}Glycol}}{k_{\mathcal{B}Glycol}+k_{\mathcal{B}Water}}$ (0, 25, 50. 75 and 100%), and (4) develop an approach for determination of k_C at arbitrary gly-
- col concentrations, i.e. $k_C = f(P,T,c_{Glvcol})$.

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