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Inverse method for the simultaneous estimation of the thermophysical properties of foods at freezing temperatures

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ABSTRACT

Because the quality and shelf life of a frozen food greatly depend on the freezing processing time, its accurate estimation is highly relevant. In addition, the estimation of the freezing time is an enormous task due to the difficulty in developing a robust and accurate mathematical model and the need for appropriate thermophysical properties for an immense variety of foods.

The objective of this study was to explore, via simulation, the capability of an inverse method to simultaneously determine the thermal conductivity (*k(T)*) and apparent volumetric specific heat (*C(T)*) of foods in the freezing temperature range (i.e., initial freezing point to −40 °C).

Experiments and validation experiments were designed with the purpose of a systematic analysis and assessment of the potential capability of an inverse procedure for simultaneously determining the thermophysical properties of foods in the freezing temperature range. Assuming a one-dimensional freezing process and known thermophysical properties of the food material, temperatures were generated at different locations of the food sample by numerically solving the partial differential equation for heat conduction. The inverse method was designed to obtain the unknown parameters for the equations of the thermophysical properties *C(T)* and *k(T)*.

The ability of the inverse method to simultaneously determine *C(T)* and *k(T)* in the freezing temperature range was investigated, and it was determined that the technique is accurate, rapid and robust to typical measurement errors. This fact was supported by a sensitivity coefficient analysis, which compared the direct-adjustment to the inverse method.

1. Introduction

The refrigeration and freezing of both fresh (unprocessed) and processed foods are one of the most commonly used technologies in food preservation. Because the quality and shelf life of a frozen food depends greatly on the processing time, its accurate estimation is highly relevant. In addition, the estimation of the freezing time is an enormous task (Martins and Silva, 2003). First, difficulties include developing a robust and accurate mathematical model as well as obtaining the appropriate thermophysical properties. According to Succar and Hayakawa, 1984, the reliability of freezing time predictions is directly related to the accuracy with which the researcher is able to obtain or predict the thermophysical properties of the food system in the freezing temperature range. For this reason, it is necessary to obtain accurate thermophysical properties (density (ρ), specific heat (C_P), thermal conductivity (k), and initial freezing point (T_{sh})). If the aim is to study the freezing process, three aspects are critical. First, the determination of thermophysical properties is critical in the thermal processing of many foods because accurate calculations depend greatly on the estimated thermal properties. This fact is particularly true for calculations of the freezing time. Second, there is an immense variety of foods in a wide temperature range (normally from −40 °C upto +40 °C). According to the literature, the main sources of information regarding the thermophysical properties in the freezing temperature range are as follows: a) experimental data from the literature, b) prediction equations, and c) experimental determination. As was previously mentioned, the literature data on thermophysical properties in the freezing temperature range is available but scarce. Third, the

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Nomenclature

A	empirical constant (J/m^3 °C)
B	empirical constant (J/m^3 °C)
$C(T)$	apparent volumetric specific heat as a function of temperature (J/m^3 °C)
C_1	empirical constant (J/m^3 °C)
C_2	empirical constant (J-°C^{n-1}/m^3)
C_3	empirical constant
C_p	apparent specific heat (J/kg °C)
e_i	bootstrap total temperature error
h	heat transfer coefficient (W/m^2 °C)
$k(T)$	thermal conductivity as a function of temperature (W/m °C)
k_1	thermal conductivity above the initial freezing point (W/m °C)
k_f	empirical constant (W/m °C)
L	thickness of food material for heat transfer experiments (m)
P	analyzed cell
P_m	bootstrap parameter
S_k	empirical constant (W/m)
t	time (s)
T	temperature (°C)
T_a	ambient temperature (°C)
T_o	initial temperature (°C)
T_B	temperature of cell below analyzed volume (P cell) (°C)
T_P	temperature of analyzed cell (°C)
Ts	temperature at the food surface
T_T	temperature of cell above analyzed volume (P cell) (°C)
$\overline{T}_b$	: average temperature between P and B cell
$\overline{T}_t$	: average temperature between P and T cell
T_{sh}	initial freezing point of food material (°C)
T_{sw}	normal freezing temperature for pure water (°C)
x	position in x-axis (m)

Greek letters

ρ	density (kg/m^3)
σ	deviation between observed and predicted profiles (°C)
λ_i	parameter
ϕ	relative moisture content of the food material

wide temperature range includes a phase change within the food material. The phase change experienced by the food material during the process also makes it more difficult to have appropriate values for the thermophysical properties. Several models to estimate specific heat capacity (Cp) and thermal conductivity (k) have been developed. As an example, in the case of Cp, Fikiin and Fikiin (1999) proposed a unified formula for the specific heat capacity, which gets data at a wide range of temperatures with the only input being the relative moisture content (ϕ) and initial freezing point (T_{sh}) of the food material. On relation to k, also several models have been developed. Although, in the case of k, important aspects must be considered when choosing an adequate model, such as microstructure and the potential anisotropy of the food material. As detailed in the literature there are some models to estimate thermal conductivity (i.e., Series model, Parallel model, Kopelman isotropic model, Maxwell-Eucken model, Levy's model). However, the food must be classified into the following four class: 1) Unfrozen, non-porous food, 2) Frozen, non-porous foods, 3) Unfrozen, porous foods, and 4) Frozen, porous foods (Carson, 2006; Carson et al., 2016) to decide which model to use. Therefore, it is a difficult task to choose an adequate model for thermal conductivity during the freezing process.

Density, specific heat and thermal conductivity present a discontinuity or a large change around the freezing point (Pham, 2014). This drastic change and discontinuity of the thermal properties close to the initial freezing point is mainly due to the significant amount of water in most foods and the impact of the phase change on the properties of water, i.e., the thermal properties of the food change accordingly to ice crystal formation. Furthermore, as stated by Pham (2014), it will be necessary to put the experimental data of the thermal properties in a regression equation or interpolate the experimental data for the practical use of the referred properties in a mathematical model. In this sense, there are interesting works in which the data have been obtained experimentally. For example, Bantle et al., 2010 developed a novel method for simultaneous and continuous determination of the thermal properties during phase transition in the range of −40 to 20 °C using a prototype instrument. With this instrument it was possible to determine a continuous curve for each thermal property (thermal conductivity, specific heat, enthalpy and density) for a marine resource *Calanus finmarchicus.* Other example, Fasina, 2005 determined thermophysical properties of sweet potato puree at freezing temperatures range using DSC technique in the range of −40 °C to 20 °C, fitting a polynomial model to specific heat and enthalpy at temperatures lower the initial freezing point.

The main disadvantage of these and others experimental estimations of thermal properties is food heterogeneity. According to Bantle et al. (2010), “heat capacity can be determined by adiabatic or differential calorimetry. Food products are heterogeneous mixtures of different components and therefore require a large enough sample to determine heat capacity”. Furthermore, in terms of structure, the differences in thermal properties are significantly dependent on the kind of food. For example, Hamdami et al., 2004, studied the thermophysical properties evolution of French partly baked bread during freezing. It was noted that thermophysical properties were significantly different between crumb and crust. For instance, the initial freezing points were −5.7 °C and −15 °C for crumb and crust, respectively. Same trends were observed for specific heat and thermal conductivity.

In addition, the accuracy of experimental data for the thermophysical properties in the freezing temperature range must be examined due to assumptions in the procedures used to obtain such values (Cleland and Earle, 1984; Heldman, 1974; Simpson and Cortés, 2004)). As an example, most of the experimental procedures determined the thermophysical properties under steady state conditions; however, thermophysical properties change abruptly at temperatures close to the initial freezing point, and, thus, the experimental error introduced by temperature measurements is difficult to control. Wang and Kolbe (1991) applying dynamic correction techniques to DSC thermogram performed in surimi were able to determine, in the freezing range, its initial freezing point, unfreezable water, apparent specific heat, enthalpy and unfrozen water weight fraction. As recommended by Wang and Kolbe (1990), the determination of the thermophysical properties at temperatures close to the initial freezing point might be more accurately estimated by using an appropriate mathematical model