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FOOD THERMOPHYSICAL PROPERTY MODELS

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ABSTRACT

The design engineer must predict the thermophysical properties of foods in order to design food storage and refrigeration equipment and estimate process times for refrigerating, freezing, heating or drying of foods. Since the thermophysical properties of foods are strongly dependent upon chemical composition and temperature, composition based models provide a means of estimating these properties. Numerous models of this type have been proposed and the designer of food processing equipment is thus faced with the challenge of selecting appropriate models from the plethora of those available. This paper describes selected food thermophysical property models and evaluates their performance by comparing their results to experimental thermophysical property data. The results given in this paper will be of value to the design engineer in the selection of appropriate food thermophysical property models. © 1999 Elsevier Science Ltd

Introduction

Knowledge of the thermophysical properties of foods is required to perform the various heat transfer calculations which are involved in the design of food storage and refrigeration equipment. The estimation of process times for refrigerating, freezing, heating or drying of foods also requires knowledge of food thermal properties. Due to the multitude of food items available, it is nearly impossible to experimentally determine and tabulate the thermal properties of foods for all possible conditions and compositions. Because the thermal properties of foods are strongly dependent upon chemical composition and temperature, the most viable option is to predict the thermophysical properties of foods using mathematical models which account for the effects of chemical composition and temperature.

Composition data for foods are readily available in the literature [1-3]. This data consists of the mass fractions of the major components found in food items. Such components include water, protein, fat, carbohydrate, fiber and ash. Food thermal properties can be predicted by using this composition data in conjunction with temperature dependent mathematical models of the thermal properties of the individual components. Choi and Okos [4] have developed mathematical models for predicting the thermal properties of food components as functions of temperature in the range of -40°C to 150°C. In addition, Choi and Okos developed models for predicting the thermal properties of water and ice.

Thermophysical properties of foods which are often required for heat transfer calculations include ice fraction, specific heat and thermal conductivity. This paper provides a summary of prediction methods for estimating these thermophysical properties. In addition, the performance of the various thermophysical property models is evaluated by comparing their calculated results with experimentally determined thermophysical property data available from the literature.

Ice Fraction

In general, food items consist of water, dissolved solids and undissolved solids. During the freezing process, as some of the liquid water crystallizes, the solids dissolved in the remaining liquid water become increasingly more concentrated, thus lowering the freezing temperature. This unfrozen solution can be assumed to obey the freezing point depression equation given by Raoult's law [5]. Thus, based upon Raoult's law, Chen [6] proposed the following model for predicting the mass fraction of ice, x_{ice}, in a food item:

$$x_{ice} = \frac{x_s R T_o^2}{M_s L_o} \cdot \frac{(t_f - t)}{t_f t} \tag{1}$$

If the molecular weight of the soluble solids, M_s, is unknown, then the following simple method may be used to estimate the ice fraction of a food item [7]:

$$x_{ice} = (x_{wo} - x_b)\left[1 - \frac{t_f}{t}\right] \tag{2}$$

Because Equation (2) underestimates the ice fraction at temperatures near the initial freezing point and overestimates the ice fraction at lower temperatures, Tchigeov [8] proposed an empirical relationship to estimate the mass fraction of ice:

$$x_{ice} = x_{wo}\left[\frac{1.105}{1 + \dfrac{0.7138}{\ln(t_f - t + 1)}}\right] \tag{3}$$

Specific Heat

Unfrozen

The specific heat of a food item, at temperatures above its initial freezing point, can be obtained from the mass average of the specific heats of the food components. Thus, the specific heat of an unfrozen food item, c_u, may be determined as follows:

$$c_u = \sum c_i x_i \tag{4}$$

If detailed composition data is not available, a simpler model for the specific heat of an unfrozen food item can be used [9]:

$$c_u = 4.19 - 2.30x_s - 0.628x_s^3 \tag{5}$$

Frozen

Below the freezing point of the food item, the sensible heat due to temperature change and the latent heat due to the fusion of water must be considered. Because latent heat is not released at a constant temperature, but rather over a range of temperatures, an apparent specific heat can be used to account for both the sensible and latent heat effects. A common method to predict the apparent specific heat of food items is that of Schwartzberg [10]:

$$c_a = c_u + (x_b - x_{wo})\Delta c + Ex_s\left[\frac{RT_o^2}{M_w t^2} - 0.8\Delta c\right] \tag{6}$$

The specific heat of the food item above its initial freezing point may be estimated with Equation (4) or Equation (5).

Schwartzberg [11] expanded upon his earlier work and developed an alternative method for determining the apparent specific heat of a food item below the initial freezing point as follows:

$$c_a = c_f + (x_{wo} - x_b)\left[\frac{L_o(T_o - T_f)}{(T_o - T)}\right] \tag{7}$$

A slightly simpler apparent specific heat model, which is similar in form to that of Schwartzberg [10], was developed by Chen [9]. Chen's model is an expansion of Siebel's equation [12] for specific heat and has the following form:

$$c_a = 1.55 + 1.26x_s + \frac{x_s R T_o^2}{M_s t^2} \tag{8}$$

Thermal Conductivity

Early work in the modeling of the thermal conductivity of foods includes Eucken's adaption of Maxwell's equation [13]. This model is based upon the thermal conductivity of dilute dispersions of small spheres in a continuous phase. In order to improve the performance of the Eucken-Maxwell equation, Levy [14] introduced a modified version of the Eucken-Maxwell equation as follows:

$$k = \frac{k_2[(2 + \Lambda) + 2(\Lambda - 1)F_1]}{(2 + \Lambda) - (\Lambda - 1)F_1} \tag{9}$$

The parameter, F_1, introduced by Levy is given as follows:

$$F_1 = 0.5\left[\left(\frac{2}{\sigma} - 1 + 2R_1\right) - \left[\left(\frac{2}{\sigma} - 1 + 2R_1\right)^2 - \frac{8R_1}{\sigma}\right]^{1/2}\right] \tag{10}$$

where

$$\sigma = \frac{(\Lambda - 1)^2}{(\Lambda + 1)^2 + \frac{\Lambda}{2}} \tag{11}$$

and R_1 is the volume fraction of component 1:

$$R_1 = \left[1 + \left(\frac{1}{x_1} - 1\right)\left(\frac{\rho_1}{\rho_2}\right)\right]^{-1} \tag{12}$$

In an effort to account for the different structural features of foods, Kopelman [15] developed thermal conductivity models for both homogeneous and fibrous food items. The differences in thermal conductivity parallel and perpendicular to the food fibers are taken into account in Kopelman's fibrous food thermal conductivity models.

For an isotropic, homogeneous two-component system composed of continuous and discontinuous phases, in which the thermal conductivity is independent of the direction of heat flow, Kopelman [15] developed the following expression for thermal conductivity, k:

$$k = k_c\left[\frac{1 - L^2}{1 - L^2(1 - L)}\right] \tag{13}$$

For an anisotropic, fibrous two-component system in which the thermal conductivity is dependent upon the direction of heat flow, Kopelman [15] developed two expressions for thermal conductivity. For heat flow which is parallel to the food fibers, Kopelman proposed the following expression for thermal conductivity, $k_{\parallel}$:

$$k_{\parallel} = k_c\left[1 - N^2\left(1 - \frac{k_d}{k_c}\right)\right] \tag{14}$$

If the heat flow is perpendicular to the food fibers, then the following expression for thermal conductivity, $k_{\perp}$, applies:

$$k_{\perp} = k_c\left[\frac{1 - P}{1 - P(1 - N)}\right] \tag{15}$$

Performance of Thermophysical Property Models

The performance of the previously discussed thermophysical property models was determined by comparing their results with empirical thermophysical property data available from the literature [16-22]. The data set contains 251 thermophysical property data points for the following food items: 1) Orange juice, 2) Lean beef, 3) Veal, 4) Lamb kidneys, 5) Lamb loin, 6) Cod, 7) Haddock, 8) Perch, and, 9) Poultry. The composition data for the food items were obtained from the USDA [3].

Tables 1 through 3 summarize the statistical analyses which were performed on the thermophysical property models discussed in this paper. For each of the models, the following information is presented: the average absolute prediction error (%), the standard deviation (%), the 95% confidence range of the mean (%), the kurtosis and the skewness.

Performance of Ice Fraction Models

Of the three methods discussed for calculating ice fraction, that of Chen [6] produced the smallest average absolute prediction error, 4.04%, with a 95% confidence range of ±3.00%, as shown in Table 1. In addition, the distribution of prediction errors was sharply peaked around the average absolute prediction error as evidenced by the large, positive value for the kurtosis, 31.2. The ice fraction model of Tchigeov [8] also performed well. Tchiegeov's method produced an average absolute prediction error of 4.75% with a 95% confidence range of ±2.89% In addition, the distribution of prediction errors was sharply peaked around the average absolute prediction error as evidenced by the large, positive value for the kurtosis, 12.7. Tchigeov's model performed consistently for all the food types tested and this model produced its greatest average absolute prediction error of 7.07% for the orange juice data set. The ice fraction method reported by Miles [7] produced a large average absolute prediction error of 10.5% and a 95% confidence range of ±2.51%. The average absolute prediction errors for this model ranged from 4.5% for the beef data set to 20% for the orange juice data.

Both Chen's model and Tchigeov's model exhibited underestimation which tended to decrease as the temperature of the food item decreased. Thus, the maximum error for these two methods occurred near the initial freezing point of the food item. The model of Miles exhibited uniform error as a function of temperature.

TABLE 1
Statistical Analysis of Ice Fraction Models

Prediction Method	Average Absolute Prediction Error (%)	Standard Deviation (%)	95% Confidence Range (%)	Kurtosis	Skewness
Chen [6]	4.04	8.86	±3.00	31.2	5.44
Miles [7]	10.5	7.43	±2.51	-1.32	0.653
Tchigeov [8]	4.75	8.55	±2.89	12.7	3.60

Performance of Apparent Specific Heat Models

As shown in Table 2, the three apparent specific heat models, which were tested, produced large average absolute prediction errors along with large prediction variations. The two models of Schwartzberg [10, 11] performed similarly, both exhibiting average absolute prediction errors of approximately 20% with large standard deviations of approximately 25%. Their best performance was obtained with the fish data set, resulting in average absolute prediction errors of 10%, while their worst performance was obtained with the veal data set, producing average absolute prediction errors of 24%. The method of Chen [9] produced a slightly larger average absolute prediction error of 20.5% with a standard deviation of 25.6%. Chen's method performed best with the fish data set, producing an average absolute prediction error of 6.9% and performed worst with the veal data set, yielding an average absolute prediction error of 27%.

All of the apparent specific heat models exhibited large variations in prediction error. In addition, the absolute value of the prediction error for all three apparent specific heat models decreased as the temperature decreased. Thus, their maximum errors tended to occur near the initial freezing point of the food item.

TABLE 2
Statistical Analysis of Apparent Specific Heat Models

Estimation Method	Average Absolute Prediction Error (%)	Standard Deviation (%)	95% Confidence Range (%)	Kurtosis	Skewness
Chen [9]	20.5	25.6	±6.93	23.0	4.19
Schwartzberg [10]	19.3	25.4	±6.87	24.6	4.39
Schwartzberg [11]	19.7	25.1	±6.80	25.5	4.51

Performance of Thermal Conductivity Models

As shown in Table 3, the thermal conductivity model developed by Levy [14] produced both the lowest average absolute prediction error and the lowest standard deviation, 6.86% and 4.89%, respectively. The average absolute prediction errors for Levy's method ranged from 4.4% for the lamb data set to 9.5% for the poultry data set. The Kopelman [15] isotropic model performed well, producing an average absolute prediction error of 8.08% with a 95% confidence range of ±1.47%, and this model performed consistently for all data sets except for poultry. For the poultry data set, Kopelman's isotropic model exhibited an average absolute prediction error of 12.6% while for the rest of the data sets, the model produced average absolute prediction errors of 8.3% or less. The Kopelman perpendicular model produced good results, producing an average absolute prediction error of 8.96% with a 95% confidence range of ±1.42%. The Kopelman parallel model exhibited a large average absolute prediction error of 16.4% with a large standard deviation of 10.4%.

Levy's model and Kopelman's isotropic model both tended to predict the thermal conductivity of frozen foods with less error than that of unfrozen foods. The remaining models, however, predicted unfrozen food thermal conductivity with less error than that of frozen food thermal conductivity.

TABLE 3
Statistical Analysis of Thermal Conductivity Models

Prediction Method	Average Absolute Prediction Error (%)	Standard Deviation (%)	95% Confidence Range (%)	Kurtosis	Skewness
Kopelman Isotropic [15]	8.08	6.12	±1.47	-0.687	0.604
Kopelman Parallel [15]	16.4	10.4	±2.49	-0.690	0.516
Kopelman Perpendicular [15]	8.98	5.90	±1.42	-0.117	0.564
Levy [14]	6.86	4.98	±1.20	0.633	1.00

Conclusions

A review of several composition based, thermophysical property models for foods was presented in this paper. In addition, the performance of each of the models was evaluated by comparing their calculated results with empirical thermophysical property data available from the literature.

For ice fraction prediction, the model of Chen [6] performed the best. The model of Tchigeov [8] also performed well. This method also has the added benefit of being easy to implement. The ice fraction model of Miles [7], while being the simplest of the three models tested, produced large prediction errors.

All three apparent specific heat models [9-11] performed similarly, producing large average absolute prediction errors of approximately 20%. These models also exhibited large prediction variations. Of the three models tested, Schwartzberg's [10] model yielded the lowest average absolute prediction error. The implementation of Schwartzberg's [11] model could be difficult as it relies on values for the specific heat of a fully frozen food item, which may not be readily available. Of the three models tested, Chen's [9] model is the easiest to use.

The thermal conductivity model of Levy [14] exhibited the lowest average absolute prediction error. Kopelman's [15] isotropic and perpendicular thermal conductivity models also performed well, and these models are less cumbersome to implement than Levy's model. Kopelman's parallel model produced large average absolute prediction errors.

In summary, for ice fraction prediction, the model of Chen [6] performed the best while Tchigeov's [8] model also performed well. For apparent specific heat, the model of Schwartzberg [10] performed the best. Finally, for thermal conductivity, the model of Levy [14] gave the best results and Kopelman's [15] isotropic model also did well.

Nomenclature

c_a	apparent specific heat
c_f	specific heat of fully frozen food
c_i	specific heat of ith food component
c_u	specific heat of unfrozen food
E	ratio of molecular weights of water and solids; $E = M_w/M_s$
F_1	parameter given by Equation (10)
k	thermal conductivity
k_1	thermal conductivity of component 1
k_2	thermal conductivity of component 2
k_c	thermal conductivity of continuous phase
k_d	thermal conductivity of discontinuous phase
$k_\parallel$	thermal conductivity with heat flow parallel to food fibers
$k_\perp$	thermal conductivity with heat flow perpendicular to food fibers
L^3	volume fraction of discontinuous phase
L_o	latent heat of fusion of water at 0°C; L_o = 333.6 kJ/kg
M_s	molecular weight of soluble solids
M_w	molecular weight of water
N^2	volume fraction of discontinuous phase
P	parameter in Equation (15); $P = N(1 - k_d/k_c)$
R	ideal gas constant; R = 8.314 kJ/(kmol·K)
R_1	volume fraction of component 1
t	food temperature (°C)
t_f	initial freezing temperature of food (°C)
T_f	initial freezing point of food item (K)
T_o	freezing point of water; T_o = 273.2 K
x_1	mass fraction of component 1
x_b	mass fraction of bound water
x_i	mass fraction of ith food component
x_{ice}	mass fraction of ice
x_s	mass fraction of solids
x_{wo}	mass fraction of water in unfrozen food
Δc	difference in specific heats of water and ice; $\Delta c = c_{water} - c_{ice}$
Λ	thermal conductivity ratio; $\Lambda = k_1/k_2$

ρ_1	density of component 1	σ	parameter given by Equation (11)
ρ_2	density of component 2		

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