Heat and Mass Transfer in Partially Frozen Food

B. Watzke, H.Deyber and H-J. Limbach
Nestlé Research Centre, Lausanne, Switzerland

*Corresponding author: brigitte.watzke@rdls.nestle.com

Abstract: The freezing curve of food material was extracted from Differential Scanning Calorimetry experiments. A heat conductive model was generated in Comsol, including the thermo-physical characteristics and the phase transition behavior. The resulting temperature-time evolutions at different positions in space were in excellent agreement with our experimental data.

Keywords: Food, modeling, Heat transfer, Phase transition

1. Introduction

During storage frozen food can experience heat shocks variations. These temperature changes induce successive melting and freezing which at the end lead to ice crystal coarsening in the frozen food and cryo-concentration of the other components. One of the consequences is the lowering of the food structure quality perception (e.g. for ice cream). Understanding the process would help to resolve the issue. A first approach consists of considering the system as a bulk of foamy material which experiences phase transition (water-ice) during a heat conductive freeze-thawing process.

2. Model definition

The model for conductive heat transfer is based on Fourier heat transfer equations.

$$\rho Cp \frac{\partial T}{\partial t} = \nabla(k \nabla T) + S$$

In our case where we go forth and back through the phase transition, Cp the specific heat capacity [J/(kg K)] is not anymore temperature independent and its expression from enthalpy should be used.

$$\rho \frac{dH}{dT}\frac{\partial T}{\partial t} = \nabla(k \nabla T) + S$$

ρ, the density [kg/m^3] and k the thermal conductivity [W/(m K)] are expressed as combinations of the i main ingredients composition (typically Water, Ice, Protein, Carbohydrate, Lipid, Ash and Fibers).

$\rho = 1/(\Sigma (X_i^w / \rho_i))$

$\lambda_{parallel} = \Sigma\, \lambda_i X_i^v$, when components are arranged parallel to heat flux

$\lambda_{perpendicular} = 1/\Sigma\, (X_i^v / \lambda_i)$, when arranged perpendicular to heat flux

$\lambda_{mean} = (\lambda_{parallel} + \lambda_{perpendicular})/2$, when no special arrangement

With X_i^w and X_i^v being respectively the weight and the volume fraction of component i. ρ_i is the pure component density.

In order to account for the insulating effect of porosity, we employed the Maxwell model to estimate the resulting thermal conductivity. The equation describing the thermal conductivity was derived on the basis of randomly distributed discontinuous spheres in a continuous medium, and assumes that the discontinuous spheres are far enough apart that they do not interact.

$$\lambda = \frac{\left[2k_c + k_d - 2\varepsilon_d\left(k_c - k_d\right)\right]k_c}{2k_c + k_d + \varepsilon_d\left(k_c - k_d\right)}$$

Empirical equations were developed by Choi and Okos (1) relating experimental values (density, measured by volumetric pycnometry; specific heat, extracted from differential scanning calorimetry; thermal conductivity, measured by a modified probe) with the weight fractions of the major food components.

Model temperature function [T in °C]:
Thermal conductivity λ [W/(m K)]
Density ρ [kg/m^3]
Specific heat Cp [J/ (kg K)]
Water:
λ=$0.57109 + 1.7625\ 10^{-3}\ T - 6.7036\ 10^{-6}\ T^2$
ρ=$997.18 + 3.1439\ 10^{-3}\ T - 3.7574\ 10^{-3}\ T^2$
Cp=$4176.2 - 0.0909\ T + 5.4731\ 10^{-3}\ T^2$
Ice:
λ=$2.21960 - 6.2489\ 10^{-3}\ T + 1.0154\ 10^{-4}\ T^2$
ρ=$916.89 - 1.3071\ 10^{-1}\ T$
Cp=$2062.3 + 6.0769\ T$
Protein:
λ=$0.17881 + 1.1958\ 10^{-3}\ T - 2.7178\ 10^{-6}\ T^2$
ρ=$1329.9 - 5.1840\ 10^{-1}\ T$

Cp$=2008.2 + 1.2089\ T - 1.3129\ 10^{-3}\ T^2$
Lipid:
$\lambda=0.18071 - 2.19\ 10^{-4}\ T$
$\rho=925.59 - 4.1757\ 10^{-1}\ T$
Cp$=1984.2 + 1.4373\ T - 4.8008\ 10^{-3}\ T^2$
Carbohydrate:
$\lambda=0.20141 + 1.3874\ 10^{-3}\ T - 4.3312\ 10^{-6}\ T^2$
$\rho=1599.1 - 3.1046\ 10^{-1}\ T$
Cp$=1548.8 + 1.9625\ T - 5.9399\ 10^{-3}\ T^2$
Fibre:
$\lambda=0.18331 + 1.2497\ 10^{-3}\ T - 3.1683\ 10^{-6}\ T^2$
$\rho=1311.5 - 3.6589\ 10^{-1}\ T$
Cp$=1845.9 + 1.8306\ T - 4.6509\ 10^{-3}\ T^2$
Ash:
$\lambda=0.32961 + 1.4011\ 10^{-3}\ T - 2.9069\ 10^{-6}\ T^2$
$\rho=2423.8 - 2.8063\ 10^{-1}\ T$
Cp$=1092.6 + 1.8896\ T - 3.6817\ 10^{-3}\ T^2$

It is known **(2)** that, under conditions of constant pressure, crystals of ice formed in the substance of the food are in equilibrium with the aqueous phase over a range of temperatures. The proportion of ice continuously declines as the temperature is raised, and reaches zero at the transition temperature, or the initial freezing point, T_f. Since the thermal properties of water and ice are very different, the proportion of ice has a profound influence on the thermal properties of frozen foods. For example, the enthalpy is markedly dependent on the temperature in regions where the ice content changes rapidly with temperature. This is caused by the large latent heat of fusion of ice (334kJ/kg at 0°C). The above model lacks one point: prediction of the ice content of the material with temperature. This prediction is based on an extension of Raoult's law which could be good enough for a very dilute food product, but is insufficient to reproduce the ice content behaviour of a solid food with temperature and to set the amount of freezable water. The ice content curve should present a plateau at a lower value than 100% frozen water, expressing the presence of unfreezable water (water bound to proteins, carbohydrates, etc.).
As mentioned previously, we cannot deal with specific heat only, but have to work with apparent specific heat which includes the phase change from ice to liquid water.
In order to obtain this missing information about apparent specific heat and ice content, we introduced Riedel's **(3)** empirical but logical formula fitting the enthalpy. From this equation, we also get the ice content versus temperature, which is necessary to estimate the thermal conductivity.

Riedel's formula for enthalpy H
H = V - Y - N in (kJ/kg)
$V = \{x_w\ T + T\ (\alpha + 0.0005\ T)(1- x_w)\}\ 4186.8$; specific heat capacity of the part of the food without ice.
$N = Q\ \{(1 - z + 0.06\ z^{25}) / (1 + z^{50})\}$; fusion enthalpy of the ice part of the food.
$z = (1 - x_w) / s = 1 - x_{ice}$
$Q = \{79.8 + 0.49\ T - 0.001\ T^2\}\ 4186.8;\ T < 0$; evolution of the ice fusion heat with T for pure ice.
$Q = 0;\ T > 0$
$s = T / \{a + b\ T + c\ T^2 + d\ T^3\}$; term for the freezing curve: fraction of dry matter versus temperature.
$Y = \{\beta\ T\ (1 - 0.09\ x_w\ T)\ \exp(-43\ x_w^{\ 2.3})\}\ 4186.8$; corrective term for low water fractions.
where **α, β, a, b, c, d are the food specific constants to be determined**.
X_w is the total water mass fraction and T is the temperature expressed in °C.

3. Results and discussion

The model was directly treated in a 3D geometry. Heat transfer by conduction was applied to the domain. The study concerned a time-dependant treatment. The thermal properties are evaluated in the Global definitions section following the previously described equations derived from Choi and Okos and from the Riedel formula applied to DSC experiments.

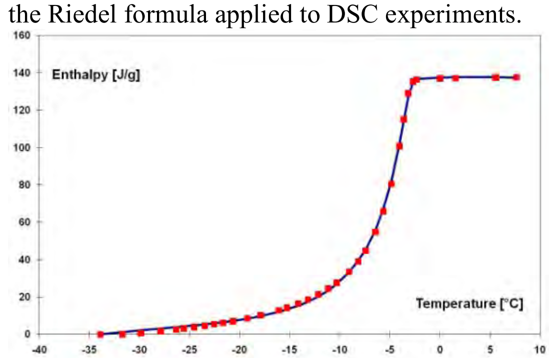

Figure1. Enthalpy curve obtained by DSC data integration (red squares), and Riedel fit (blue line)

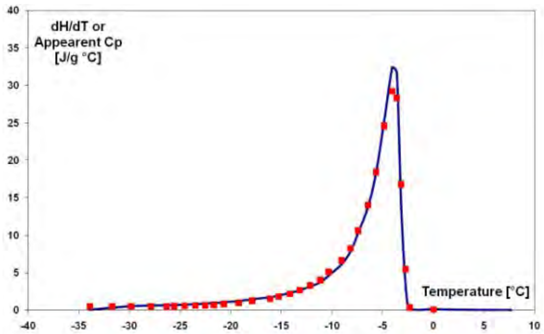

Figure2. Apparent Specific heat curve obtained by derivation of figure 1 curve. Data integration (red squares), and Riedel fit (blue line).

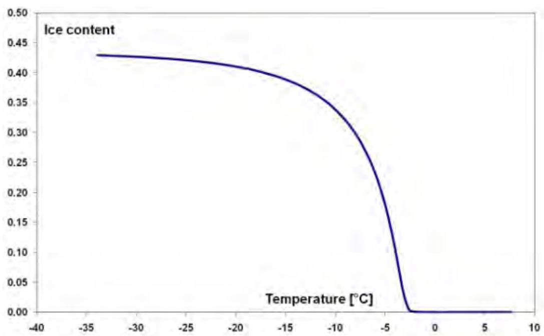

Figure 3. Freezing curve derived from Riedel formula.

For symmetry reasons a fourth of the ice cream block was considered delimited by 2 symmetry planes. The conductive heat transfer takes place equally from all other available surfaces. The inward heat flux follows an external temperature profile recorded with a thermo-couple. The heat transfer coefficient related to this flux is adapted after comparison between experimental and simulated results. Some 6 other thermo-couples are carefully inserted in precise locations into the ice cream allowing spatially different temperature evolution records.

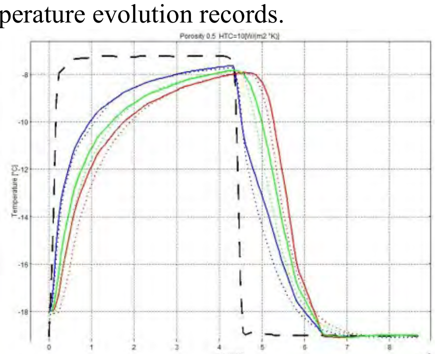

Figure 4. Combined results of temperature evolution at 3 different positions in an ice cream block subjected to step fluctuations of the external temperature (dashed black curve). Experimental data (dotted colored curves) and corresponding Comsol simulations (colored line curves).

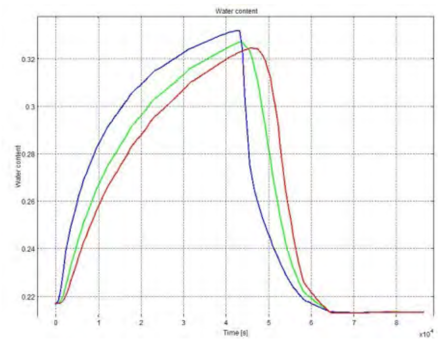

Figure5. Time evolution of the water content at the same 3 positions as shown on previous graph.

The model allows to nicely mimic the thermal behavior and to follow the ice content in a partially frozen food considered as a homogeneous bulk. By putting in perspective figure 4 and figure 5, it is interesting to visualize how much the water content influences the thermal behavior.

4. Conclusion

A simple heat transfer model incorporating the phase transition used for modeling the temperature behavior of a partially frozen food subjected to heat shocks, predicted the measured data very well using the fitted parameters derived from enthalpy measurements.

Taking care of single crystal growth will be the next step to model. By considering a single growing crystal and its semi-liquid surrounding domain we aim to follow the latent heat dissipation of the crystallization area and the diffusion of water towards the growing crystal.

5. References

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