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THE EFFECT OF TEMPERATURE-DEPENDENT THERMAL CONDUCTIVITY IN HEAT TRANSFER SIMULATIONS OF FROZEN BIOMATERIALS

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Summary

The thermal conductivity value of pure water ice is inversely proportional to the temperature and decreases about 5-fold as the temperature increases from the liquid nitrogen boiling temperature (77K) to the freezing point of pure water. The temperature dependency of the thermal conductivity is typically overlooked in bioheat transfer simulations. A closed-form solution of the one-dimensional temperature distribution in frozen water and blood is presented in this study, based on a new thermal conductivity model. Results indicate that temperatures are overestimated by up to 38K, and heat fluxes through the frozen region boundaries are underestimated by a factor of 2, when the temperature dependency of the thermal conductivity is neglected.

Keywords: Thermal Conductivity, Temperature Dependency, Cryogenic Temperatures, Frozen Biomaterial, Thermal Analysis

INTRODUCTION

Heat transfer simulations of bioprocesses at cryogenic temperatures have been extensively applied in the study of cryopreservation and cryosurgery in the past four decades. Due to the high water content of biological tissues and mixtures, the thermophysical properties of water and ice are typically assumed for first order analyses of bioheat transfer. The thermophysical properties of ice are highly temperature-dependent (6,7), a functional behavior which is typically overlooked in mathematical simulations. Instead of tracing the actual temperature-dependency, certain constant representative values are usually chosen for the unfrozen region, the frozen region, and, in some mathematical models, the phase-transition subregion.

Phase-change problems can be categorized with regard to the Stephan number, which represents the ratio of sensible heat release during cooling of the frozen region to latent heat release of phase transition. It is well established that a quasi-steady solution is a good approximation for the temperature distribution in the frozen region in cases of low Stephan number, where the freezing front velocity is mainly affected by the magnitude of the latent heat release (4). Alternatively, an integral method can be applied for cases of high Stephan

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number (10).

The effect of the rate dependency and the magnitude of the latent heat on the thermal history of freezing in biological tissues has recently been presented by Smith et al. (13). In their analysis, they assumed linear temperature dependency for the thermal conductivity in the frozen region, as suggested by Alexiades and Solomon (1). By contrast to the linear correlation suggested in (1), this report suggests that the thermal conductivity of biomaterials behaves like an inverse function of temperature, which can significantly affect heat transfer calculations.

The current study arises from efforts to quantify the effect of the temperature-dependent thermal conductivity in the entire cryogenic temperature range applicable for bioheat transfer simulations. This general objective is achieved by focusing on the characteristics of the temperature distribution within the frozen region. A closed-form solution for the temperature distribution within the frozen region is developed for the purpose of this study, and results are presented in terms of temperature differences between the newly developed solution and the commonly assumed one, and in terms of heat fluxes through the frozen region boundaries. The mathematical treatment presented in this study is superior to the mathematical treatment presented previously (13) due to the applied mathematical tools. The previous study (13) relies on numerical simulations, which give insight only on specific cases and, therefore, requires tremendous efforts when attempting to study the entire cryogenic temperature range. By contrast, the current study relies on a closed-form solution, which enables the analysis of a wide spectrum of cases with relatively minor effort, as shown below. Furthermore, the effect of the temperature dependency of the thermal conductivity is isolated in this study, which enables a careful investigation of its influence on the freezing process, while it is one of many linked parameters in the previous study (13).

The current study is also relevant to real-time temperature simulations during cryosurgery. One practical example of solving only the temperature distribution in the frozen region can be found in the report of Hong et al. (8). In their work, Hong et al. applied a quasi-steady solution to calculate the temperature distribution within the frozen region during MRI-monitored cryosurgery, while the freezing front location was interpolated from MRI images. This technique of evaluating the temperature distribution could be performed in combination with other imaging techniques, such as ultrasound and CT. In these cases, the sole parameter affecting the temperature solution is the thermal conductivity.

THERMAL CONDUCTIVITY MODEL

From the theory of physics, the thermal conductivity of ice is expected to vary proportionally to T^{-1} above some cryogenic temperature threshold (6), where T is the absolute temperature. This has prompted the author of this report to seek a thermal conductivity correlation of the form:

$$k = \frac{k_0}{T^m} \tag{1}$$

where k_0 and m are thermal conductivity parameters found from the best-fit curve with experimental data.

From parametric estimation based on experimental data published by Jakob and Erk (9), Ratcliffe (12), and Dean and Timmerhous (5), the best-fit parameters for ice above 80K are: m=1.235 and k_0=2153 W/m-K^{1+m}. Similarly, the best-fit parameters for blood above 173K (3) are: m=1.15 and k_0=1005 W/m-K^{1+m}. Figure 1 shows the thermal conductivity calculated with these values, as well as the theoretical curve, in which m=1 and k_0 are chosen to give a thermal conductivity value of 2 W/m-K at 273K.

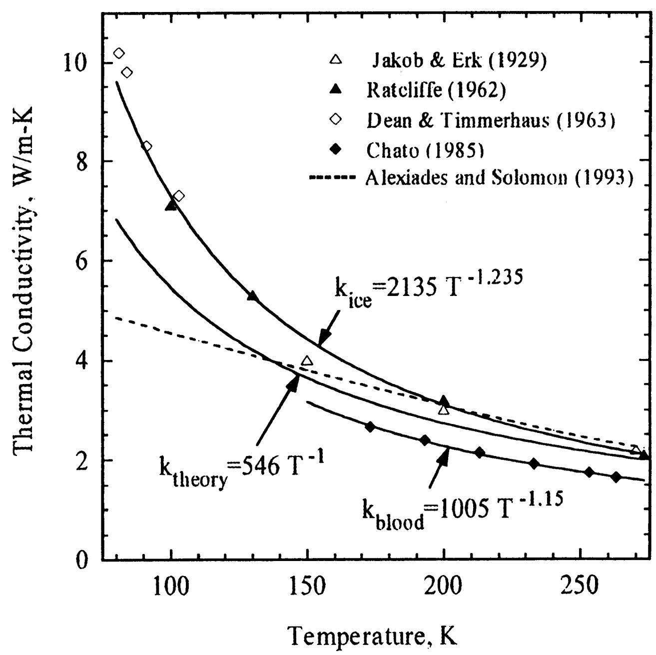

Figure 1: Thermal conductivity model

Figure 1 also shows a linear dependency of the thermal conductivity in temperature, as suggested by Alexiades and Solomon (1). Clearly, the functional behavior presented by Eq. (1) can be fitted very well to the experimental data, while the correlation suggested by Alexiades and Solomon (1) does not represent the experimental data adequately. For example, the thermal conductivity at 80K according to Alexiades and Solomon (1) is less than one half of the experimental data.

The thermal conductivity model presented in Eq. (1), is suggested for the first time in the context of frozen biological materials. Its simple functional behavior allows for the generation of an explicit closed-form solution as is presented below. Note that for the general problem of temperature dependent thermal conductivity, a closed-form solution is available for a limited number of cases only.

MATHEMATICAL FORMULATION

The underlying assumption in this study is that the effect of the temperature-dependent thermal conductivity can be studied from a quasi-steady analysis of the frozen region, which is also applicable for transient processes characterized by low Stephan number, as is often the case in cryosurgery (4). A quasi-steady assumption allows generation of a closed-form solution, which allows analysis in a wide range of parameters, while avoiding an expensive and intensive numerical work, and without losing the overall picture.

The one-dimensional governing equation in steady-state is:

$$\frac{1}{\xi^n}\frac{d}{d\xi}\left(\frac{k_0}{T^m}\xi^n\frac{dT}{d\xi}\right)=0 \qquad n=\begin{cases}0: & Cartesian \quad \xi=x\\ 1: & Cylindrical \quad \xi=r\\ 2: & Spherical \quad \xi=r\end{cases} \tag{2}$$

where ξ, x, and r are coordinates, and n is a coordinate system index.

The exact solution, T_e, of Eqs. (1)-(2) for $m\neq 1$ is:

$$T_e=\left[F_n(\xi)\left(T_2^{1-m}-T_1^{1-m}\right)+T_1^{1-m}\right]^{1/(1-m)} \tag{3}$$

where T_1 and T_2 are the known boundary temperatures at x=0 and x=l for the Cartesian case, or at r=R_1 and r=R_2 for the radial cases, and where the function F is defined by:

$$F_n(\xi)\equiv\begin{cases}\dfrac{\xi}{l} & n=0\\[2ex] \dfrac{Log\left(\xi/R_1\right)}{Log\left(R_2/R_1\right)} & n=1\\[2ex] \dfrac{R_1/\xi-1}{R_1/R_2-1} & n=2\end{cases} \tag{4}$$

The solution of Eq. (2) for a temperature-independent thermal conductivity is given by:

$$T_a=F_n(\xi)\left(T_2-T_1\right)+T_1 \tag{5}$$

which is defined as the approximate solution, T_a, for the purpose of this study.

By comparing the first derivative of the difference between the exact solution, Eq. (3), and the approximate solution, Eq. (5), to zero, the maximal difference value is found at:

$$\xi=\begin{cases}A & n=0\\[2ex] R_1\left(\dfrac{R_2}{R_1}\right)^A & n=1\\[2ex] \dfrac{R_1}{1+A\left(R_1/R_2-1\right)} & n=2\end{cases} \tag{6}$$

where the location parameter A is defined by:

$$A \equiv \frac{1}{T_2^{1-m} - T_1^{1-m}} \left\{ \left[\frac{T_2 - T_1}{T_2^{1-m} - T_1^{1-m}} (1-m) \right]^{(1-m)/m} - T_1^{1-m} \right\} \tag{7}$$

RESULTS AND DISCUSSION

The exact and approximate solutions for representative cases in various coordinate systems, are shown in Fig. 2, where the boundaries are kept at 77K and 273K. The solutions for the radial cases are given for a hollow cylinder and sphere having a radii ratio of 0.15. This ratio was chosen to demonstrate an advanced stage of freezing in a minimally invasive cryoprocedure where, for example, the cryoprobe diameter is 3 mm and the frozen region diameter is 20 mm. It is clear that the difference between the exact and approximate solutions is significant in all of these cases. For example, the exact temperature distribution in the Cartesian case is by no means the commonly assumed linear temperature distribution.

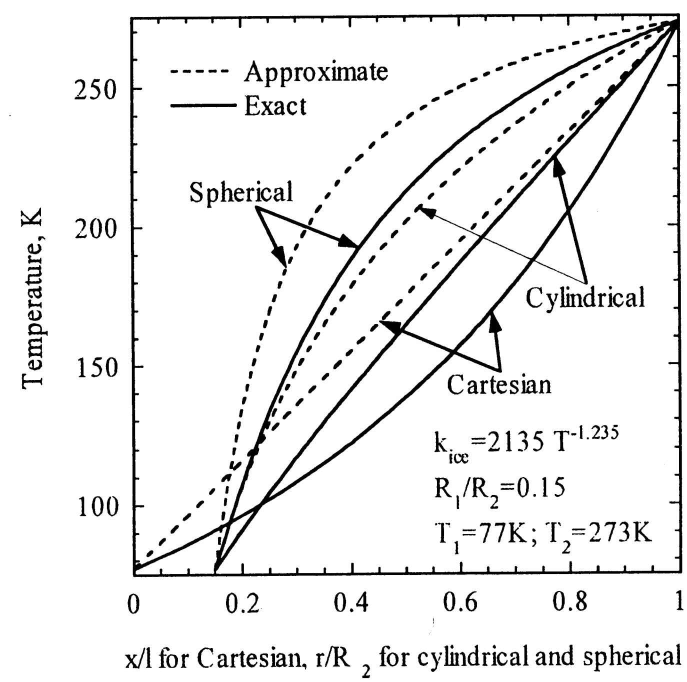

Figure 2: Exact temperature distributions based on a temperature-dependent thermal conductivity of ice, and approximated temperature distributions based on a temperature-independent thermal conductivity. The solutions for the radial cases are given for a hollow cylinder and sphere having a radii ratio of 0.15.

When applying an integral method of solution to study the frozen region growth (2,10,11), the heat fluxes at the boundaries of the frozen region have to be carefully calculated (from Fourier law: the heat flux is the product of the thermal conductivity and the temperature gradient). For the Cartesian case shown in Fig. 2 for example, the temperature gradient of the exact solution at the lower temperature boundary is about one half of that of the approximate solution, while the thermal conductivity of the frozen material at this temperature is in the range of 3.5 to 5 times higher than that at the freezing temperature. It follows that the exact solution and the actual thermal conductivity at the lower temperature boundary yield up to 2.5-fold higher heat flux compared with the approximate solution. This means that the cooling power at the cryoprobe or at the cooling surface is underestimated by a factor of 2.5 in this case, when the temperature dependency of the thermal conductivity is ignored (the cooling power is the integral of the heat flux over the cooling surface).

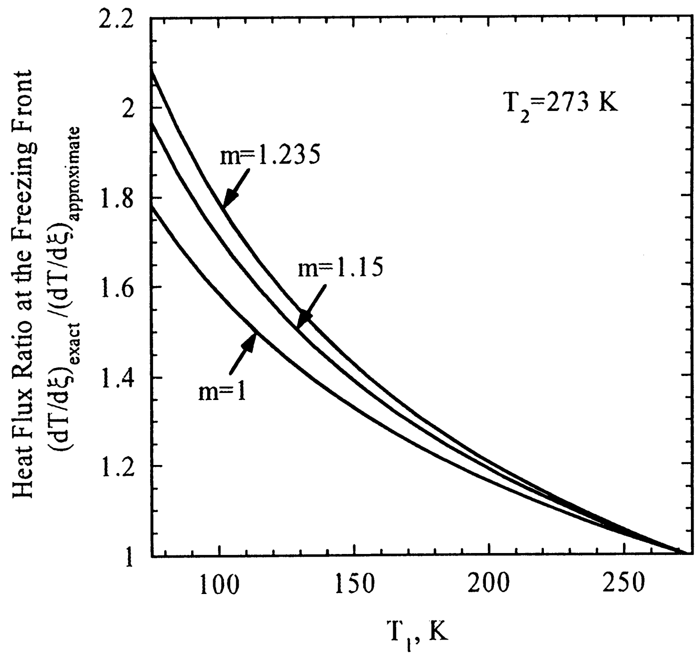

Figure 3: Ratio of the heat flux calculated by the exact solution to the heat flux calculated by the approximate solution, evaluated at the freezing front (the heat flux is the production of the thermal conductivity and the temperature gradient). The heat flux ratio is independent of the coordinate system.

Figure 3 shows the ratio of the heat flux calculated by the exact solution to the heat flux calculated by the approximate solution, when evaluating at the freezing front. For practical reasons, and in order to avoid further mathematical manipulations of Eqs. (1) and (2) for the case of m=1, an approximate value of m=1.00001 was taken for the relevant curve drawing. It can be seen that the exact solution yields up to a 2-fold higher heat flux than that calculated by the approximate solution. This ratio increases as the temperature at the cooled surface increases. It can further be seen that the heat flux ratio is affected by up to 15% by the value of m, and is independent of the coordinate system. When applying the integral method, the sum of the time integrals of the heat fluxes at the frozen region boundaries is proportional to the frozen region volumetric growth. Hence, applying the integral method based on the approximate solution is expected to produce fair results at the early stages of freezing only, a time period in which the approximate solution provides a fair approximation of the exact temperature distribution.

A higher heat flux value at the freezing front results in a faster freezing front velocity, which, in turn, results in a higher cooling rate at the freezing front. In a Cartesian geometry, following a step-like temperature change at the cooled surface, and under the assumptions of the current study, the heat flux at the freezing front is known to be proportional to the freezing front velocity. It follows that double the heat flux will result in a double freezing front velocity. The freezing front velocity should be less significantly affected in a cylindrical geometry, and even less in a spherical geometry, due to the expanding surface of the freezing front. Hence, the Cartesian case can always be taken as the upper boundary for freezing front velocities and cooling rates when compared with other geometries.

Figure 4 shows the maximal temperature difference between the approximate and the exact solutions, for an upper boundary temperature of 273K and a varying lower boundary temperature in the range of 77K to 273K. Figure 4 also shows the values of the location parameter A at which the maximal temperature difference between the exact and approximate solutions is found, Eq. (7). Interestingly, the maximal temperature difference between the exact and approximate solutions is also independent of the coordinate system.

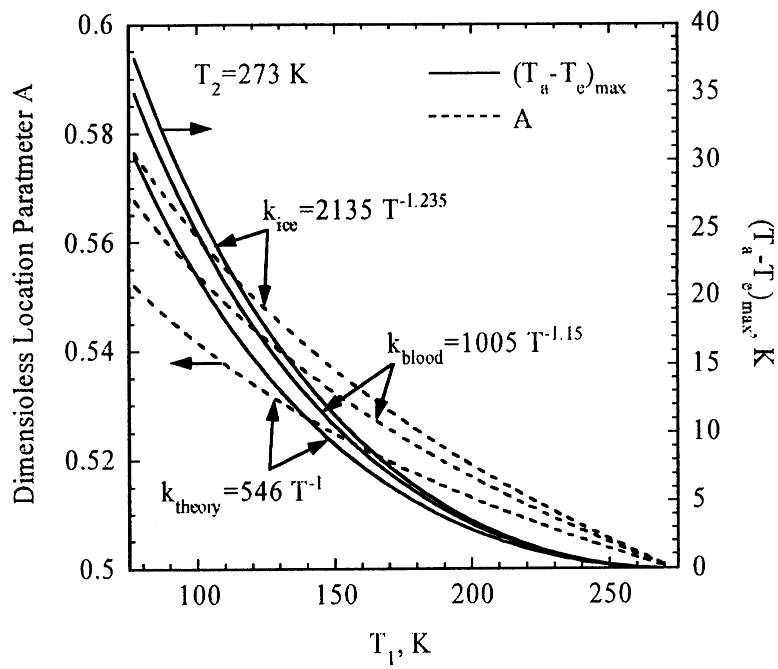

Figure 4: Maximal temperature difference between the approximate and the exact temperature distributions, $(T_a\text{-}T_e)_{max}$, and the location parameter A at which these extreme values are found, Eq. (7).

It can be seen from Fig. 4 that the maximal overestimation of the temperature distribution reaches 30K, 35K, and 38K, for thermal conductivity parameters of ice, blood, and theory, respectively, and for a lower temperature boundary of 77K. Similarly, maximal overestimation of 12K, 14K and 15K, are found for thermal conductivity parameters of ice, blood, and theory, respectively, and for a lower temperature boundary of 135K, which, for example, is typical for Joule-Thomson effect-based cryoprobes using Argon.

The location parameter A is shown to be only minimally affected by the lower boundary temperature. All in all, the parameter A decreases from 0.568 to 0.5, as the lower temperature boundary increases from 77K to 273K, respectively.

CONCLUSIONS

Results of this study indicate that the temperature dependency of the thermal conductivity has a major effect on cryogenic bioheat simulations. Although the analysis presented here is for a quasi-steady process only, there is no reason to believe that this effect will be less significant in a transient process. For numerical solutions, the implication is that the numerical scheme has to have the ability to deal with thermal conductivity gradients, as well as temperature gradients. One has to bear in mind that a temperature-dependent thermal diffusivity cannot be applied straightforwardly in such numerical solutions, as the solution of the heat balance equation is dependent upon the gradient of the thermal conductivity at any given spatial location.

This study shows that the thermal conductivity of biomaterials is inversely proportional to the temperature, and can not be treated as a linear function. It further shows that the correlation suggested by Alexiades and Solomon (1) underestimates the actual thermal conductivity by up to 100%, at the temperature range relevant to cryosurgery.

Results further indicate that temperature-dependent thermal conductivity results in higher heat fluxes at the frozen region boundaries, which indicate higher freezing front velocities. For integral solutions, the implication is that special attention must be paid to heat flux calculations along the frozen region boundaries. For thermal design, the implication is that the cooling power required from cryoprobes and cooling surfaces is significantly underestimated when the temperature dependency of the thermal conductivity is ignored.

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