

ON THE ESTIMATION OF THERMOPHYSICAL PROPERTIES IN NONLINEAR HEAT-CONDUCTION PROBLEMS

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Abstract—The influence of thermophysical property variations on the resulting temperature fields is investigated with reference to quasilinear heat-conduction problems. Both theoretical and experimental evidence is produced to show that errors in the calculation of temperature distributions, brought about by an inaccurate estimate of thermal properties, are small if approximate heat capacities, even exhibiting large local differences with respect to the actual ones in a small range of temperatures, retain enthalpy variations and if the integral across the whole working temperature interval of the absolute value of the difference between approximate and actual thermal conductivities is small. Then the practical relevance of these results is pointed out with reference to freezing and thawing processes of biological materials whose thermal coefficients vary sharply over the phase change zone, where only mean values of thermophysical properties can be easily measured.

NOMENCLATURE

A, measure of the region (defined in the text) [m · s];
c, specific heat [J/kg.K];
C, volumetric heat capacity [J/m³K];
e, temperature error [K];
f, g, surface temperatures [°C];
h, initial temperature distribution [°C];
k, thermal conductivity [W/m.K];
R, slab thickness [m];
t, temperature [°C];
t.p., thermophysical properties;
x, position coordinate [m].

m, minimum;
M, maximum;
 1, exact;
 2, approximate.

INTRODUCTION

TEMPERATURE dependence of physical properties must be taken into account in many heat-conduction problems associated with thermal design and/or process control of industrial and scientific applications such as freezing and thawing of foodstuffs [3], high-rate heat-transfer processes [11] and heat transfer at cryogenic temperatures [7]. The resulting nonlinear heat-conduction equations can be easily dealt with by numerical methods whenever the values of thermophysical properties in the temperature range under consideration are available [4]. Unfortunately, compared to the increasing need of this kind of information, very few source data can be found in literature. Perhaps this trend is justified by the great difficulties involved in the determination of heat capacity and thermal conductivity vs. temperature curves in the phase change zone or in correspondence with extreme temperature levels. However, for biological substances in particular, the lack of knowledge is so serious that no less than three different international projects, aiming at retrieving and assembling data on a number of thermophysical properties, have been launched in the last four years [1, 10, 13].

In this paper, using the concept of "weak solutions", it is shown that the computation of thermal fields is rather insensitive to the shape of heat capacity and

Greek letters

$\Delta\gamma$, quantity defined by equation (13) [J/m³];
 $\Delta\lambda$, quantity defined by equation (15) [J/m³];
 Δt , quantity defined by equation (17) [K];
 $\Delta\kappa$, quantity defined by equation (16) [W/m];
 λ , enthalpy difference per unit volume across the phase change interval [J/m³];
 λ_i , quantity defined by equation (14) [J/m³];
 τ , time [s].

Subscripts

l, u, lower and upper limit to the phase change interval;

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thermal conductivity vs. temperature curves in the phase change zone provided that enthalpy variations are retained and that the integral across the whole working temperature interval of the absolute value of the difference between approximate and actual thermal conductivities is small. Experiments with several biological materials performed in the phase-change zone where thermophysical properties vary sharply over a small temperature range, have confirmed the above mentioned theoretical results. As it is outlined in the following sections, this should lead to a considerable simplification of apparatuses and techniques connected with the determination of thermophysical properties needed for the prediction of temperature fields.

FORMULATION OF THE PROBLEM

For the sake of simplicity reference is made to a one-dimensional nonlinear heat-conduction problem, while boundary conditions of the first kind are chosen because of experimental convenience.

Denoting by $t_1(x, \tau)$ and $t_2(x, \tau)$ the temperature distributions in the domain $\Omega: 0 \leq x \leq R; 0 < \tau \leq \theta$, corresponding to the same initial and boundary conditions and to thermal coefficients $C_1(t_1), k_1(t_1)$ and $C_2(t_2), k_2(t_2)$ respectively, the following heat-conduction problems can be considered:

$$C_i(t_i) \frac{\partial t_i}{\partial \tau} = \frac{\partial}{\partial x} \left[k_i(t_i) \frac{\partial t_i}{\partial x} \right], \text{ in } \Omega; \tag{1}$$

$$t_i(x, 0) = h(x), \quad 0 \leq x \leq R; \tag{2}$$

$$t_i(0, \tau) = f(\tau), \quad 0 < \tau \leq \theta; \tag{3}$$

$$t_i(R, \tau) = g(\tau), \quad 0 < \tau \leq \theta; \tag{4}$$

where: $i = 1, 2$ and f, g, h, C_i, k_i are assigned functions of their respective arguments.

If $C_1(t)$ and $k_1(t)$ are referred to as exact determinations of heat capacity and thermal conductivity vs. temperature curves, while $C_2(t)$ and $k_2(t)$ indicate approximate estimates of the same functions, the difference:

$$e(x, \tau) = t_2(x, \tau) - t_1(x, \tau) \tag{5}$$

represents the "temperature error" which will be analysed in the following sections.

ERROR ANALYSIS

The aim of this section is to estimate $e(x, \tau)$ in order to investigate the effect of thermophysical property variations upon temperature distributions.

In so far as classical solutions of equations (1)–(4) are considered, self suggesting ways of tackling the problem are the application of the maximum principle or the use of bounds on Green's function to evaluate

the upper limit to the solution of the parabolic problem solved by $e(x, \tau)$. Unfortunately, by employing these methods, temperature errors can only be shown to be proportional to the maximum differences between corresponding exact and approximate values of C_2 and C_1, k_2 and k_1 and even between dk_2/dt and dk_1/dt . Moreover, proportionality factors depend critically on quantities, such as the maximum of $C(t)$, which can be expected to be very large in many practical situations [8]. Therefore this information, while interesting from a theoretical point of view, is not of great help in practice. Thus a different approach, based on a generalized formulation of the heat-conduction problem and on the definition of "weak solutions", has been considered here since this procedure provides very effective analytical tools and yields most significant results which are of immediate use for practical applications. In fact, an uniqueness theorem ensures that a weak solution coincides with the classical one whenever the latter exists.*

For the sake of concreteness, reference is made throughout this paper to biological substances which exhibit sharp variations of thermophysical properties over the phase change zone [3], but it would not have been difficult to take into consideration other quasi-linear heat-conduction problems.

In order to state the main results concisely it is convenient to introduce the following notations. First suppose that f, g and h are bounded, piecewise continuous functions, so that:

$$t_m = \min[\inf h(x), \inf f(\tau), \inf g(\tau)]; \tag{6}$$

$$t_M = \text{Max}[\sup h(x), \sup f(\tau), \sup g(\tau)]. \tag{7}$$

Next assume that C_i and k_i are positive bounded, piecewise continuous functions and set:

$$C_m = \min[\inf C_1(t), \inf C_2(t)] > 0; \tag{8}$$

$$C_M = \text{Max}[\sup C_1(t), \sup C_2(t)]; \tag{9}$$

$$k_m = \min[\inf k_1(t), \inf k_2(t)] > 0; \tag{10}$$

and

$$k_M = \text{Max}[\sup k_1(t), \sup k_2(t)]. \tag{11}$$

Let then t_l and t_u represent respectively the lower and the upper bound to the interval where thermal properties undergo the sharpest variations; if, in addition, it is assumed, according to the physical situations to be dealt with, that the inequality:

$$t_m < t_l < t_u < t_M \tag{12}$$

*This theorem will be a consequence of the stability result stated below [see (19)].

holds good, the quantities:

$$\Delta\gamma = \text{Max} \left[\int_{t_m}^{t_l} |C_2(t) - C_1(t)| dt, \int_{t_u}^{t_M} |C_2(t) - C_1(t)| dt \right]; \quad (13)$$

$$\lambda_i = \int_{t_i}^{t_u} C_i(t) dt, \quad i = 1, 2; \quad (14)$$

$$\Delta\lambda = |\lambda_2 - \lambda_1|; \quad (15)$$

$$\Delta\kappa = \int_{t_m}^{t_M} |k_2(t) - k_1(t)| dt; \quad (16)$$

and:

$$\Delta t = t_M - t_m \quad (17)$$

have a well defined physical meaning. The same is true for A which is the measure of the region of the plane (x, τ) where approximate and actual thermophysical properties differ significantly:

By means of techniques which are similar, in some aspects, to those of [8], the following inequality can be shown to hold true:*

$$\|e(x, \tau)\|_{L_2(\Omega)} \leq \Phi(\Delta\gamma, \Delta\lambda, \Delta\kappa, A; \Delta t, \lambda_1, \lambda_2, C_m, k_m, k_M, R, \theta) \quad (19)$$

where Φ is a known function of its arguments which tends to zero when $\Delta\gamma, \Delta\lambda, \Delta\kappa$ and A all tend to zero. The quantities $\Delta\gamma, \Delta\lambda, \Delta\kappa$ can be determined *a priori* as errors in the estimation of thermophysical properties. The measure A instead can be evaluated only *a posteriori* once $t_2(x, \tau)$ has been computed, since it depends also on the actual freezing or thawing processes followed. While at this point it can be said solely that an upper bound for A is the measure of the region Ω_u where:

$$t_l \leq t_2(x, \tau) \leq t_u, \quad (20)$$

much numerical evidence, in addition to the examples of applications reported here, might be produced to suggest that this estimate is rather conservative. Moreover, temperature gradients are usually quite large in practical processes, so that the influence of A on temperature errors can be expected to be negligible in most cases of technical interest.

Another noteworthy feature of formula (19) is that the function Φ does not retain any dependence on C_M nor on the shape of the approximate heat capacity vs. temperature curve in the phase change zone.

*The analytical details of the proof, however, are considerably different from those reported in [8]. A complete analysis of the present problem has been thus written in order to save the interested readers unnecessary efforts [5].

ESTIMATION OF THERMOPHYSICAL PROPERTIES

In most biological substances water is the major component. Thus when these materials are cooled below 0°C ice formation occurs, starting at a temperature t_u usually between -1 and -3°C —the initial freezing point—which depends on the molar concentration of the soluble cell components [9]. As the temperature is progressively reduced, more and more water is turned into ice and the latent heat of ice formation adds to the sensible heat involved in cooling both ice and the unfrozen part. This leads to large variations in heat capacities, while thermal conductivities too change considerably, mainly because the thermal conductivity coefficient of ice is four times greater than that of water [3, 9]. For most biological materials the largest part of the freezing process takes place in a temperature interval of $4-8^\circ\text{K}$ below the initial freezing point, but only at temperatures ranging from -20 to -40°C and even less there is no more measurable change with temperature in the amount of ice present and the remaining water can be considered as non-freezable [9]. However, for practical purposes, a lower limit t_l to the phase-change interval can be conveniently defined on the basis of a ratio of ice to residual freezable water content of, say, about 90 per cent, thus identifying the phase change zone with the zone of maximum crystallization. This choice, in addition to providing an easily applicable criterion, allows all the same, as it will be seen later, to approximate the actual $C_1(t)$ and $k_1(t)$ curves below t_l by means of constant average values.

Therefore, according to the above reported considerations and to the results obtained in the previous section, only the following source data are really needed for the approximate computation of thermal fields in biological substances undergoing phase changes:

1. The values of heat capacities and thermal conductivities outside the phase change interval;
2. The enthalpy variations λ across the same interval.

Once these data are known and reasonable estimates have been made of the values of t_l and t_u , the $k_2(t)$ curve can be completed by means of a simple linear interpolation between t_l and t_u while any arbitrary function will do for $C_2(t)$ in the same range, provided that enthalpy changes are retained. A triangular curve has been used in this research because of its simplicity and likeness to the actual curve but, when tested, also different shapes, like for example rectangular and bell shaped functions, have proved to be almost equally satisfactory choices.

Obviously, accurate values of t_u and t_l or the exact location and the value of the maximum of $C(t)$ can be used if available. However, several numerical experiments confirm that only the values of the thermal

properties listed at points 1 and 2 have a critical influence on the computation of freezing and thawing times.

As a consequence it can be deduced that only as few as four local measurements, i.e. thermal conductivities and heat capacities above and below the phase change interval, and a calorimetric determination of the enthalpy variation across the same interval are strictly requested to compute thermal fields in most materials dealt with in food technology, bio-engineering and bio-medicine.

RESULTS

When thermophysical properties change with varying temperatures, no analytical solutions of the resulting nonlinear heat-conduction equations are available. Instead finite difference techniques can be used to deal with such problems [4] but the accuracy of the solutions thus obtained can only be evaluated experimentally.

Therefore, several heating and cooling tests have been carried out on samples of different biological materials having a circular cross-section and thermally insulated at the lateral surface in order to prevent radial heat conduction. Care has also been taken to ensure uniform temperatures at the ends, so that one-dimensional thermal fields are believed to have been realized in the axial region of the specimens. The experimental apparatus and procedures used are described in detail in [5].

The centre and the end surface temperatures of the samples have been recorded during each test and the centre temperatures have been assumed as $t_1(x, \tau)$. Then, with reference to the known initial and boundary conditions and to the sample thicknesses, temperature-time curves have been computed using approximate

and, when available, experimentally determined-values of the thermophysical properties.

Experimental values of density have been used in all the computations since density can always be accurately measured at room temperatures, while the volume increase as a result of ice formation is about 6 per cent for most biological materials [9].

The numerical method used in the calculations has been discussed elsewhere [4] and will not be treated again here.

Only homogeneous and commercially available products have been chosen for the experiments, in order not to introduce difficulties connected with handling and preparation of most biological materials. The first substance considered has been "Tylose", a water and methylcellulose (77 per cent and 23 per cent in weight) mixture whose thermal properties are about the same as those of lean beef [15]. Thermal conductivity and specific heat of "Tylose", which are plotted as unbroken lines in Fig. 1, are well known and, therefore, allow a comparison with the results obtained using approximate data. The approximations of the experimental curves represented as dotted lines in Fig. 1 follow the fundamental rules previously reported and have proved to be satisfactory. However, different locations of the peak of heat capacity as well as different values of the width of the phase change interval have also been tried and have not led to significant changes in freezing and thawing times.

Experimental and computed curves, typical of freezing tests on "Tylose", are plotted in Fig. 2. As it can be seen, the agreement between measured and computed values is about 1 per cent of the total temperature change during the run if experimental values of thermal parameters are employed, while it is of the order of 2 per cent if approximate values are used.

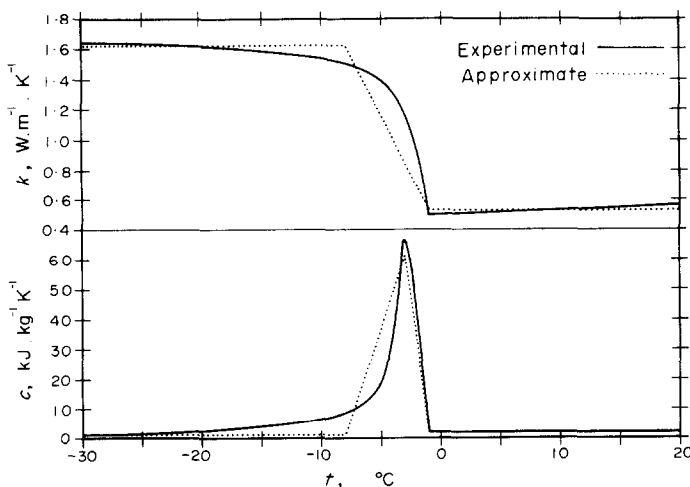


FIG. 1. Thermophysical properties of "Tylose".

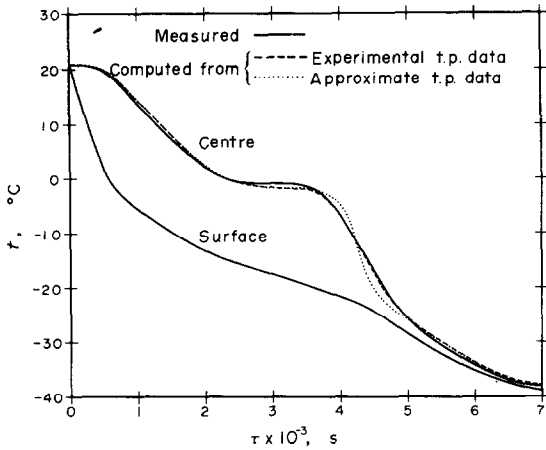


FIG. 2. Freezing curve of a "Tylose" sample;
 $\rho_{20^\circ\text{C}} = 1006 \text{ kg/m}^3$, $R = 0.0425 \text{ m}$.

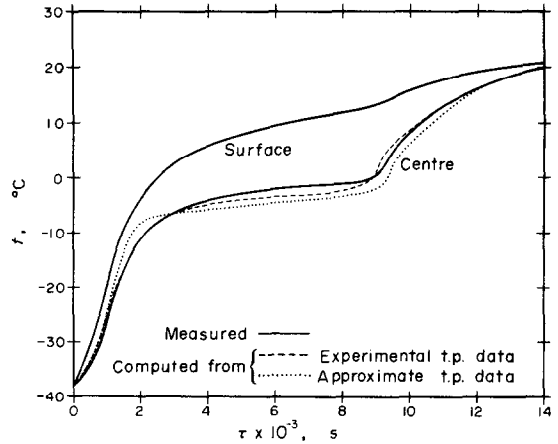


FIG. 3. Thawing curve of a "Tylose" sample;
 $\rho_{20^\circ\text{C}} = 1006 \text{ kg/m}^3$, $R = 0.0425 \text{ m}$.

Results that are typical of thawing tests on "Tylose" are reported in Fig. 3. The difference between experimental and computed centre temperature-time curves is of the order of 3 per cent, i.e. the temperature errors are larger than in freezing runs. This worsening can

be explained by allowing for the fact that thermo-physical property data at low temperatures are usually less accurate than at high temperatures, as it is certainly the case with approximate data, because of the uncertainties involved in the determination of t_l .

Table 1

Food product	Heat capacity (J/kg.K)		Thermal conductivity (W/m.K)		Density (kg/m ³)	Latent heat of phase change (J/kg)	t_l (°C)	$t(C_M)$ (°C)	t_u (°C)
	$t > t_u$	$t < t_l$	$t > t_u$	$t < t_l$					
Hamburger	3100	2100	0.43	1.2	990	199000	-6.5	-3.0	-1.0
Mashed potatoes	3517	1842	0.498	2.003	1000	267955	-7.0	-3.0	-1.0

Table 2

t (°C)	Hamburger			Mashed potatoes		
	Surface	Centre		Surface	Centre	
	Measured	Measured	Computed	Measured	Measured	Computed
$\tau \times 10^{-3}$ (s)						
0	19.3	19.3	19.3	20.1	20.1	20.1
0.24	10.1	18.8	19.3	10.2	19.8	20.0
0.72	-2.8	16.3	16.7	-1.9	16.1	16.9
1.20	-7.9	11.0	11.0	-5.3	10.0	10.9
1.68	-12.2	5.4	5.3	-8.6	4.9	5.3
2.16	-15.2	0.8	0.7	-11.4	1.0	0.8
2.64	-17.5	-2.1	-1.0	-13.8	-0.5	-1.3
3.12	-19.7	-2.4	-1.2	-15.9	-1.6	-1.8
3.60	-21.6	-3.7	-1.8	-18.1	-3.9	-2.6
4.08	-22.7	-9.5	-9.7	-20.3	-8.4	-4.2
4.56	-25.8	-19.7	-20.8	-24.8	-20.0	-21.7
5.04	-29.5	-26.9	-26.0	-29.9	-26.9	-27.5
5.52	-33.2	-31.1	-30.1	-32.8	-31.6	-31.6
6.00	-35.2	-33.6	-33.3	-35.3	-34.2	-34.3
6.48	-37.1	-36.2	-35.5	-37.2	-36.8	-36.4

Hamburger paste and mashed potatoes are the other substances used in the experiments. The available information on these materials is by no means complete. Thus, for the hamburger paste, a weighted mean has been utilized between data for lean beef [2, 12, 14] and those for fat [9], the fat content being about 15 per cent. For mashed potatoes instead, the formulae suggested in [2] for the evaluation of specific heat, thermal conductivity and latent heat when only the water percentage is known have been used, the water content being about 80 per cent in this case.

In Table 2 the temperature values determined experimentally are compared with the results of computations made on the basis of the approximate values of thermal parameters obtained as previously outlined and reported in Table 1.

The accuracy reached in all the runs using the approximating technique proposed in this paper is surprisingly good.

CONCLUSIONS

The approximating technique described in this paper has enabled to compute temperature distributions in biological materials when only as few as four local thermophysical property values—heat capacities and thermal conductivities above and below the phase change interval—and the latent heat effect are known.

It has been shown that the method proposed here has a sound theoretical basis and it leads, in the calculations of thermal fields, to results which are well within the limits of accuracy usually imposed for thermal design.

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*References [5], [6] and [8] may be obtained from the first author.

SUR L'ESTIMATION DES PROPRIÉTÉS THERMOPHYSIQUES DANS LES PROBLÈMES NON LINÉAIRES DE CONDUCTION THERMIQUE

Résumé—On étudie l'influence des variations des propriétés thermophysiques sur les champs résultants de température en considérant les problèmes non linéaires de conduction thermique. Les calculs et les expériences montrent que dans les distributions de température, les erreurs apportées par une estimation inexacte des propriétés thermiques sont faibles si les chaleurs spécifiques approchées (même pour des différences locales grandes par rapport aux différences réelles dans un petit domaine de température), respectent les variations d'enthalpie et si est petite l'intégrale, étendue à l'intervalle de température concerné, de la valeur absolue de la différence entre les conductivités approchée et réelle. L'application pratique de ces résultats est faite au cas du gel ou du dégel des matériaux biologiques dont les coefficients thermiques varient très rapidement dans la zone de changement de phase, zone où l'on ne peut mesurer aisément que les valeurs moyennes des propriétés thermophysiques.

ZUR ABSCHÄTZUNG THERMOPHYSIKALISCHER EIGENSCHAFTEN BEI NICHTLINEAREN WÄRMELEITPROBLEMEN

Zusammenfassung—Der Einfluß von veränderlichen Stoffwerten auf das Temperaturfeld wird für quasi-lineare Wärmeleitprobleme untersucht. Sowohl theoretisch als auch experimentell wird nachgewiesen, daß die durch genaue Schätzung der thermischen Eigenschaften entstehenden Fehler bei der Berechnung

der Temperaturverteilung klein bleiben, wenn annähernd richtig geschätzte, spezifische Wärmen, die innerhalb eines kleinen Temperaturbereiches gegenüber den tatsächlichen Werten große Abweichungen aufweisen dürfen, eingesetzt, die Enthalpieänderungen niedrig gehalten und wenn das Integral des absoluten Fehlers der Wärmeleitfähigkeit über den gesamten Bereich des maßgebenden Temperaturgefälles klein bleibt. Die praktische Bedeutung dieser Ergebnisse für den Gefrier- und Auftauvorgang von biologischen Substanzen wird erläutert. Deren thermische Parameter ändern sich im Gebiet der Phasenumwandlung stark, und nur Mittelwerte können hier leicht gemessen werden.

ОБ ОЦЕНКЕ ТЕПЛОФИЗИЧЕСКИХ ХАРАКТЕРИСТИК В НЕЛИНЕЙНЫХ ЗАДАЧАХ ТЕПЛОПРОВОДНОСТИ

Аннотация — Исследуется влияние изменения теплофизических характеристик на результирующие температурные поля в применении к квазилинейным задачам теплопроводности. Теоретически и экспериментально подтверждается, что ошибки при расчете распределения температуры, вызванные неточной оценкой тепловых характеристик, незначительны, если приближенные значения теплоемкостей, даже в случае больших изменений локальных значений относительно точных значений теплоемкости в небольшом диапазоне температур, сохраняют изменения энтальпии, и если интеграл от абсолютного значения разности между приближенным и точным значением теплопроводности во всей области исследуемых температур невелик. Указано практическое применение этих результатов в приложении к процессам замерзания и оттаивания биологических материалов, тепловые коэффициенты которых резко изменяются за зоной фазовых превращений, где могут быть легко получены только средние значения теплофизических свойств.