TEMPERATURE EFFECTS OF THERMOPHYSICAL PROPERTY VARIATIONS IN NONLINEAR CONDUCTIVE HEAT TRANSFER

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Abstract: This study provides a simple and economic procedure for the computation of thermal fields, avoiding lengthy and difficult measurements of the thermophysical properties within the "phase change zone", where such coefficients have been approximated according to very simple rules. The method carries out to be satisfactory on the basis of comparison of experimental and numerical determinations of the thermal fields in a number of substances with particular specifications.

Introduction: Heat conduction in substances exhibiting sharp variations of thermal coefficients—and in particular a large peak of the heat capacity over a relatively small temperature interval—has been considered by the Authors in a previous paper (Bonacina 1974); change of phase of impure substances was particularly focused.

The aim was to provide a simple and economic procedure for the computation of thermal fields, avoiding lengthy and difficult measurements of the thermophysical properties within the "phase change zone", where such coefficients have been approximated according to very simple rules. The method carries out to be satisfactory on the basis of comparison of experimental and numerical determinations of the thermal field in a number of substances behaving in the way described above.

The approach of (Bonacina 1974) is theoretically grounded on the following result. Let \( t_1(x, \tau), t_2(x, \tau), (x, \tau) \in \Omega = (0, R) \times (0, T) \), denote the temperatures due to the one-dimensional heat flow in media having heat capacity and thermal conductivity \( c_1(t_1), k_1(t_1), c_2(t_2), k_2(t_2) \) respectively, with the initial and boundary conditions: \( t_i(x, 0) = h(x), t_i(0, \tau) = f(\tau), t_i(R, \tau) = g(\tau), i = 1, 2. \)

Assume the functions \( k_i, c_i \), are positive bounded and integrable \( 0 < C_m \leq C_i \leq C_M \) and the functions \( f, g, h \) are bounded and piecewise continuous (accordingly, \( t_i(x, \tau) \) will be bounded in terms of the data: \( t_m \leq t_i \leq t_M \)). If \( t_i \) and \( t_u \) represent the lower and upper bounds of the interval where thermal properties undergo the sharpest variations \( (t_m \leq t_i \leq t_u \leq t_M) \), we have:
where $\phi$ is a known function of its arguments which tends to zero when $\Delta y$, $\Delta \lambda$, $\Delta x$, $A$ all tend to zero and

$$
\Delta y = \text{Max} \left[ \int_{t_m}^{t_1} |C_1(t) - C_1(t)| dt, \int_{t_u}^{t_M} |C_2(t) - C_2(t)| dt \right] ;
$$

(2)

$$
\lambda_1 = \int_{t_i}^{t_u} C_1(t) dt, i=1, 2 ; \quad \Delta \lambda = |\lambda_2 - \lambda_1| ;
$$

(3)

$$
\Delta x = \int_{t_m}^{t_M} |k_3(t) - k_1(t)| dt ;
$$

(4)

and $A$ is the measure of the subset of $\Omega$ where $t_1 \leq t_2 \leq t_u$. The most relevant features of estimate (1) are pointed out in (Bonacina 1974). Here $t_1$, $t_2$ are meant to be weak solutions of the respective equations $C_i(t) \frac{\partial t_i}{\partial t} = \partial_t \left[ k_i(t) \frac{\partial t_i}{\partial x} \right], i=1, 2$ with the same initial and boundary data $h, f$ and $g$, defined as bounded measurable functions such that, for any sufficiently smooth test function $F(x, \tau), F(0, \tau) = F(R, \tau) = F(x, 0) = 0$, the following equality holds (omitting subscripts):

$$
\int_0^R \int_0^R \left[ \mathcal{H}(K) \frac{\partial F}{\partial \tau} + K \frac{\partial^2 F}{\partial x^2} \right] dx \, dt = - \int_0^R H[h(x)] F(x, 0) dx
$$

$$
- \int_0^R \left[ K(f) \frac{\partial F}{\partial x} \bigg|_{x=0} - K(g) \frac{\partial F}{\partial x} \bigg|_{x=R} \right] dt
$$

(5)

where

$$
H(t) = \int_{t_M}^t C(y) dy, \quad K(t) = \int_{t_m}^t k(y) dy
$$

and since $\frac{\partial K}{\partial t} > k_m > 0$ the inverse function $t = t(K)$ exists and the definition $\mathcal{H}(K) = H(t(K))$ makes sense.

This note is concerned with the proof of (1). A similar result has been demonstrated in (Pasano 1973), where heat flux is specified on the boundary. Nevertheless, the methods of
(Fasano 1973) cannot be used in order to achieve the estimate (1), since quite different arguments are needed throughout the proof: only the main differences will be dealt with.

**Proof of the (1):** From (5) setting \( K_s = K_s(t_s) \), we have

\[
\frac{\partial}{\partial \tau} \int_0^\theta \int_0^R [\mathcal{H}_s(K_s) - \mathcal{H}_s(K_s')] \left( \frac{\partial F}{\partial \tau} + \frac{\partial^2 F}{\partial x^2} \right) \, dx \, d\tau
\]

\[-\int_0^\theta \int_0^R [\mathcal{H}_s(K_s) - \mathcal{H}_s(K_s')] \frac{\partial F}{\partial \tau} \, dx \, d\tau - \int_0^R [H_2(h) - H_1(h)]F(x, 0)\, dx
\]

\[-\int_0^\theta [K_s(f) - K_s(f')] \frac{\partial F}{\partial x|_{x=0}} \, d\tau + \int_0^\theta [K_s(g) - K_s(g')] \frac{\partial F}{\partial x|_{x=R}} \, d\tau \tag{6}
\]

where

\[
\zeta(x, \tau) = \begin{cases} 
(K_s - K_s')[(\mathcal{H}_s(K_s) - \mathcal{H}_s(K_s')), & K_s \neq K_s' \\
\zeta_0, & K_s = K_s'
\end{cases}
\tag{7}
\]

\( \zeta_0 \) being a positive constant which can be defined as

\[
\zeta_0 = \inf \left\{ \frac{(K_s - K_s')[(\mathcal{H}_s(K_s) - \mathcal{H}_s(K_s))]}{K_s + K_s'} \right\}
\tag{8}
\]

It is worth noting here that the actual knowledge of the constant \( \zeta_0 \), essentially involving the function \( C_s(t_s) \), is not needed in the final computation of \( \zeta_0 \). As it will be seen, in fact, the function \( \zeta(x, \tau) \) enters the error estimates only through its upper bound:

\[
\zeta(x, \tau) \leq k_M/C_M
\tag{9}
\]

which is easily derived from the definitions.

Following the procedures of (Fasano 1973) smooth approximations \( \zeta_n(x, \tau), \ n = 1, 2, ... \) are now introduced which converge to \( \zeta(x, \tau) \), in the sense of the \( L_2(\Omega) \) norm, and are such that:

\[
0 < \zeta_n < \sup (\zeta) \leq k_M/C_m
\tag{10}
\]

Then a sequence of "test functions" \( F_n(x, \tau), \ n = 1, 2, ... \) can be found by solving the parabolic problems:

\[
\frac{\partial F_n}{\partial \tau} + \zeta_n \frac{\partial^2 F_n}{\partial x^2} = \zeta_n \varepsilon_n, \text{ in } \Omega
\tag{11}
\]
where \( e_n(x, \tau), n = 1, 2, \ldots \) is a sequence of smooth functions converging towards the error \( e(x, \tau) \), in the \( L_2(\Omega) \) norm, and such that

\[
\max |e_n| \leq \text{ess sup} |e| \leq t_{M} - t_{m} = \triangle t
\]

By substituting \( F_n \) for \( F \) into (6) and letting \( n \) tend to infinity, it is possible to obtain an estimate of \( \|l\| \).

First, note that the left member of (6) can be rewritten, after replacing \( F \) with \( F_n \), in the form:

\[
\int_0^R \int_0^1 \left[ \mathcal{H}_1(K_n) - \mathcal{H}_1(K_1) \right] e_n(x) dx dt
\]

\[
+ \int_0^R \int_0^1 \left[ \mathcal{H}_2(K_n) - \mathcal{H}_2(K_1) \right] \left( -\frac{\partial^2 F_n}{\partial x^2} \right) dx dt
\]

and, owing to the uniform boundedness of \( \frac{\partial^2 F_n}{\partial x^2} \) \( L_2(\Omega) \) \text{ Ladyzenskaja et al. } 1968, Thm. 9.1, p. 341 \) its limit for \( n \to \infty \) is:

\[
\int_0^R \int_0^1 (K_n - K_1)(t_n - t_1) dx dt
\]

In order to obtain estimates of the terms in the right member of equation (6), the following inequalities are to be proved:

\[
\left| \frac{\partial F_n}{\partial x} \right|_{x=0} \leq N_1, \quad \left| \frac{\partial F_n}{\partial x} \right|_{x=R} \leq N_1
\]

(14)

\[
\int_0^R \int_0^1 \left( \frac{\partial F_n}{\partial t} \right)^2 dx dt \leq N_2
\]

(15)

\[
\int_0^R \left[ F_n(x, 0) \right]^2 dx \leq N_2
\]

(16)

where \( N_1, N_2 \) and \( N_3 \) are computable constants, independent of \( n \). For the purpose of proving (14), consider the standard parabolic problem \( [\alpha(\xi, \eta) > 0] \).
TEMPERATURE EFFECTS OF THERMOPHYSICAL PROPERTY VARIATIONS ETC.

\[ \frac{\partial V}{\partial \eta} = a(\xi, \eta) \frac{\partial V}{\partial \xi} + a(\xi, \eta) \epsilon(\xi, \eta), \quad 0 < \xi < R, \quad 0 < \eta < \theta; \]

\[ V(0, \eta) = V(R, \eta) = V(\xi, 0) = 0. \]  

Each of problems (11), (12) can be put into the form (17), (18) by means of the following transformations:

\[ \xi = x; \]

\[ \eta = \theta - \tau; \]

\[ F_n(\xi, \theta - \eta) = V(\xi, \eta); \]

\[ \alpha_n(\xi, \theta - \eta) = a(\xi, \eta); \]

\[ \epsilon_n(\xi, \theta - \eta) = - \epsilon(\xi, \eta). \]

Since

\[ \frac{\partial F_n}{\partial x} = \frac{\partial V}{\partial x} \]

inequalities (14) will be proved if a bound for \( \frac{\partial V}{\partial \xi} \bigg|_{\xi=0} \) and \( \frac{\partial V}{\partial \xi} \bigg|_{\xi=R} \) is given in terms of quantities not depending on \( n \). Recalling that, by virtue of (13) and (23):

\[ \max |\epsilon| \leq \triangle t \]

the difference:

\[ \delta(\xi, \eta) = \triangle t (R - \xi) - V(\xi, \eta) \]

is such that:

\[ \frac{\partial \delta}{\partial \eta} - a \frac{\partial \delta}{\partial \xi} = a(\triangle t - \epsilon); \]

\[ \delta(0, \eta) = \Delta(\xi, \eta) = 0, \quad \delta(\xi, 0) \geq 0. \]

Therefore, the maximum principle leads to \( \delta \geq 0 \) and, consequently:

\[ \frac{\partial \delta}{\partial \xi} \bigg|_{\xi=0} \geq 0, \quad \frac{\partial \delta}{\partial \xi} \bigg|_{\xi=R} \leq 0 \]

and

\[ \frac{\partial V}{\partial \xi} \bigg|_{\xi=0} \leq \frac{R \Delta t}{2}, \quad \frac{\partial V}{\partial \xi} \bigg|_{\xi=R} \geq -\frac{R \Delta t}{2}. \]
In a similar way it can be shown that
\[
\frac{\partial V}{\partial \xi} \bigg|_{\xi = \infty} > \frac{R \Delta t}{2}, \quad \frac{\partial V}{\partial \xi} \bigg|_{\xi = -R} \leq \frac{R \Delta t}{2}
\]
thus concluding the proof of (14).

In order to prove (15) the already quoted result of (Ladyzenskaja et al. 1968) is not useful since it gives an estimate of \(\| \frac{\partial^2 F_n}{\partial x^2} \|_{L^1(\Omega)}\) critically dependent on \(C_M\); therefore a different approach is needed. Multiplying both sides of equations (11) by \(\frac{\partial^3 F_n}{\partial x^3}\) integrating by parts the first term at the left hand side, taking into account (12) and applying Schwartz inequality to the right hand side, it follows that:
\[
\frac{1}{2} \int_{-R}^{R} \left( \frac{\partial F_n}{\partial x} \right)_{\xi = \infty}^2 dx + \left( \frac{\partial^2 x^{\frac{1}{2}} \frac{\partial^3 F_n}{\partial x^3} \|_{L^1(\Omega)} \right) \leq \left( \frac{\partial x^{\frac{1}{2}}}{\partial x} \right)_{\xi = \infty}^2 \|_{L^1(\Omega)} \times \left( \frac{\partial x^{\frac{1}{2}}}{\partial x} \right)_{\xi = \infty}^2 \|_{L^1(\Omega)}.
\]
From (32) the inequality:
\[
\left( \frac{\partial^2 F_n}{\partial x^2} \right)_{\xi = \infty}^2 \leq \left( \frac{k_M}{C_M} \right)^{1/2} \left( \frac{\partial x^{1/2}}{\partial x} \right)_{\xi = \infty}^2 \|_{L^1(\Omega)} \leq \left( \frac{k_M}{C_M} \right)^{1/2} \|_{L^1(\Omega)} \Delta t \sqrt{R \theta}
\]
is obtained immediately, then (15) follows easily from (11), (13) and (10).

Inequality (16) is now an immediate consequence of (15) and of the identity
\[
F_n(x,0) = \int F_n(x,0) \delta x.
\]

Finally, applying essentially the same techniques of (Pasano 1973) (Section 5) the following inequality is obtained:
\[
k_m \| e(x,\tau) \|_\infty \leq N_\delta \| \Delta x \sqrt{R \theta} \| e(x,\tau) \| + \Psi,
\]
where \(\Psi\) is a known function which depends on the same arguments of \(\Phi\) in (1) and possesses the same properties. From (35) estimate (1) is then obtained immediately.

Some numerical examples: Although only a mean square value for error \(\epsilon = \theta\) is estimated by (1), it has been pointed out in (Bonacina 1974) on experimental grounds that in many cases even local differences between measured and calculated thermal fields do not exceed a few percent.
As a further support to this conjecture we have realized numerical simulations of usual experimental conditions in the freezing of a sample of a biological substance, using three different standard-type approximations for the heat capacity: the corresponding thermal fields during the freezing process described below and the total "freezing times" $\Delta t_f$, i.e. the times at which the centre of the sample reaches the temperature of $-20^\circ$C, have been compared.

The sample considered is a cylinder of thickness 0.08 m. Its lateral surface is insulated and the temperature of opposite faces is decreasing from the initial value of the temperature throughout the sample, $-20^\circ$C, linearly at the rate of $10^{-8}K.s^{-1}$. The "latent heat" of $\approx 128 \text{kJ}kg^{-1}$, is comparable to that of "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.

One rectangular and two triangular shapes for the heat capacity in the temperature interval $-20^\circ$C, as shown in Fig. 1, have been used in calculations.

Numerical procedures are described in (Bonacina 1974). The thermal fields are found to be very close to each other (obviously except for temperatures in the freezing zone). Table 1 contains comparisons between the corresponding freezing times: the maximum relative difference is about 2.5 per cent.

<table>
<thead>
<tr>
<th>$\Delta t_f(s)$</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
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<tr>
<td>5995</td>
<td>6165</td>
<td>6105</td>
<td></td>
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</tbody>
</table>

**Fig. 1.**

Standard-type approximations for thermophysical properties.
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