Arch. Mech., 49, 2, pp. 285–291, Warszawa 1997

On hyperbolic heat conduction

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IN A PREVIOUS PAPER [5], numerical solutions of initial-boundary value problems for the *semi-empirical* model of heat conduction were compared with available experimental results. In [6] the model was modified by introducing more realistic approximations of the constitutive functions, basing on measured specific heat, heat conductivities and second sound speeds for NaF at low temperatures (10 ... 20° K). In the present paper we suggest a method to choose the free parameters entering the constitutive functions by minimizing an *error functional*, measuring the differences between the theoretical and experimental heat pulses.

1. Introduction

IN A SERIES OF PAPERS [1, 2, 3], KOSIŃSKI and co-workers introduced a model based on thermodynamics with internal state variables, describing heat conduction at low temperatures. Such a hyperbolic model avoids the paradox of infinite thermal wave speed. According to Kosiński's point of view the absolute temperature, as a concept of thermodynamical equilibrium, is not appropriate to describe the thermal evolution of systems far from equilibrium, such as dielectric crystals at low temperatures (bismuth and sodium fluoride) in which thermal waves, called second sound, can be detected. The introduction of a non-equilibrium temperature as an internal state variable is the main idea of his approach. A kinetic equation describes the evolution of that non-equilibrium temperature with time. CIMMELLI and KOSIŃSKI call such a variable *semi-empirical temperature scale*, [1].

The new model contains three physical material functions: heat conductivity, specific heat and thermal relaxation time, which can be determined by experiments. The mentioned parameter functions enter the constitutive equations for the heat flux, internal energy and the right-hand side of the kinetic equation.

On the background of the existing experimental data it is reasonable to restrict our considerations to the 1D case. For certain choices of physical parameters, length of the specimen, initial temperatures and initial thermal increments at one side of the specimen, the model equations have been solved numerically, cf. FRISCHMUTH and CIMMELLI, [5], and the results are in good accordance with the experimental data. However, some of the parameters used in the model were choosen by hand. Hence it seems to be of some interest to try to find an objective procedure for the choice of all unknown parameters which minimizes the difference between theoretical and experimental results. To this end we define a functional, called *error functional*, measuring the degree of deviation between theoretical and experimental heat pulses.

Finally, we minimize the above error functional by an appropriate choice of the free constitutive parameters. Note that the evaluation of the error functional for a given set of parameters requires the solution of an initial boundary value problem for a hyperbolic system of balance laws. Previously, [6], the comparison between theoretical results and measured heat pulses was based only on the wave speed which was taken as the characteristic speed for the theoretical solutions.

2. The direct problem

In order to keep the paper possibly self–contained, let us shortly outline the assumptions of the semi-empirical theory of heat conduction. First we have the basic equation of energy balance for a rigid heat conductor([1])

$$\dot{\varepsilon} + \operatorname{div} q = r\,. \tag{1}$$

By r we denoted heat sources and by q the heat flux vector. We assume the energy to depend only on temperature: $\varepsilon = \varepsilon(\theta)$ and thus $c_v = c_v(\theta) := \varepsilon'(\theta)$([2]). Especially for NaF, we have

$$\varepsilon = \varepsilon_0\theta^4/4 + \varepsilon_1\theta^5/5\,, \tag{2}$$

which is a generalization of the classical Debye's law, and which has been proposed on the basis of data obtained by HARDY and JASWAL [7].

We postulate the existence of a scalar field β, the semi-empirical temperature, whose evolution is governed by the kinetic equation

$$\dot{\beta} = f(\theta, \beta), \tag{3}$$

and define the heat flux via a Fourier-like law of the type

$$q(x,t) = -\alpha\nabla_x\beta(x,t), \tag{4}$$

where α means the heat conductivity.

We assume further that ε, respectively the specific heat c_v, can be measured directly [7], and that these functions should be independent of the considered theory of heat conduction.

The functions $\alpha : \mathbb{R}^+ \to \mathbb{R}^+$ and $f : \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}$ can be approximately determined by measuring the heat flux and the equilibrium wave speed [6], i.e. the speed of a wave travelling into a medium where $q = 0$. As far as that last

([1]) A more realistic model should include the effects due to the anisotropy together with those related to the elastic behaviour of the materials. Actually, bismuth and sodium fluoride possess both properties. However, as a first approximation we will limit ourselves to consider a one-dimensional rigid heat conductor.

([2]) For convenience, we refer all quantities to volume measures and not to mass, following the experimental papers [8, 7]. Specifically, in the 1-D case, all quantities are referred to the unit of length.

function is concerned, satisfactory numerical fits of experimental data were given by COLEMANN and NEUMANN [4] and by CIMMELLI and FRISCHMUTH [6](3).

For practical purposes it is necessary to replace $\mathbb{R}^+$ by a small temperature range $\mathcal{R} = [\theta_{\min}, \theta_{\max}]$ which is covered by experiments and where the hyperbolic effects are relevant. We choose $\theta_{\min} = 10$ and $\theta_{\max} = 20$(4), bearing in mind the available data for NaF.

3. Heat pulse experiments

We consider a 1-D NaF specimen, occupying the domain $W = [0, L] \subset \mathbb{R}$. Typical values of L are about 1 cm. Moreover, we suppose that on the left-hand boundary of W, a heat pulse of the form

$$\theta_L(t) = \theta_0 + \Delta\theta(H(t - t_0) - H(t - t_0 - \Delta t)), \tag{5}$$

with H some appropriate Heaviside-like function, is applied. Inside the specimen, the following equations hold

$$c_v\dot{\theta} + \operatorname{div} q = r, \tag{6}$$

$$q = -\alpha\nabla\beta, \tag{7}$$

$$\dot{\beta} = f(\theta, \beta). \tag{8}$$

On the right-hand side, Neumann or mixed type boundary conditions of the type

$$q_n = -\alpha(\theta)\beta_{,x} = -p(\theta - \theta_0) \tag{9}$$

are assumed to hold. Their meaning is rather clear: $p = 0$ represents thermal insulation, i.e. pure Neumann conditions, while $p > 0$ corresponds to a more realistic interface condition.

We assume that either the heat source r vanishes uniformly – which corresponds to an ideally insulated lateral surface of the specimen – or rather impose an analogous interface condition of the type(5)

$$r = r(\theta) = -\pi(\theta - \theta_0), \tag{10}$$

with $\pi > 0$. By solving the initial value-boundary problem given by (5)–(10), we can define a transition functional such that

$$\theta_L \mapsto \theta_r =: \theta(L, \cdot) \tag{11}$$

(3) In our opinion the experimental calculation of α, the most crucial physical parameter, is not completely satisfactory since often the equations of the underlying theory are already used in the experiment for transforming the measured electrical quantities into the caloric ones.

(4) Through this paper, all temperatures are in K, all lengths in cm, times in μs and masses in g.

(5) Note that here we are neglecting the dependence on x in the constitutive functions. Furthermore, a realistic r should contain a term representing the mechanical work due to velocity and stress fields. Of course, in our simplification to a rigid heat conductor, these effects are disregarded in our considerations.

i.e. giving the measured pulse on the right-hand side as a result of the transmitted impulse applied on the left-hand side. Obviously, the transition causes a delay and a change in shape and amplitude of the wave. Further, it depends on the physical setup which is determined by the parameters: θ_0 – temperature of the environment, L – length of the specimen, π – energy losses under way, p – right boundary condition, together with the constitutive functions c_v, α and f. Now we want to compare the theoretical transition functional with the experimental results. Some additional difficulties arise from the scaling of the experimental data. Indeed, in [7, 8] only the arrival time of the pulse was of interest so that the electrical signals have been measured but not calibrated. As a consequence, we cannot give the experimental transition operator absolutely but only up to an affine transformation. In what follows we consider a theoretical result θ_r to be in accordance with a measured output pulse $\bar{\theta}_r$ if there exist two coefficients λ_0 and λ_1 such that

$$\lambda_0 + \lambda_1 \bar{\theta}_r = \theta_r \,. \tag{12}$$

Otherwise we consider the term

$$\psi = \min_{\lambda_0, \lambda_1} \int [\lambda_0 + \lambda_1 \bar{\theta}_r(t) - \theta_r(t)]\, dt \tag{13}$$

as a measure of the deviation between theory and experimental data.

4. The error functional

In the previous section we have described a mathematical method to compare numerical solutions of the model equations with the experimental data, for given fixed conditions of the conductor and the experimental setup. These conditions are described by three different types of quantities:

(a) some constants, which are well known (e.g. L, ε_0, ε_1);

(b) some parameters, varying in a certain range but which are well documented in the experiments (e.g. the temperature θ_0 of the environment, coinciding with the temperature of the unperturbed initial state);

(c) some physical quantities to be determined under minimization of the error (e.g. α, f, p, π, $\Delta\theta$, Δt).

After fixing all the well known quantities let us introduce two denotations:
u, representing the collection of all unknown quantities;
v, representing the collection of the variable quantities.
Then, according to he previous section, we have the quantity

$$\psi = \psi(u, v) \tag{14}$$

as a measure of the model error. Finally, we introduce the functional

$$\Psi = \Psi(u) = \int_V \psi(u, v)\, dv \tag{15}$$

as a measure of the global performance of the considered model over the range V of the variable experimental conditions. For practical purposes we can choose V to be finite and calculate the integral with respect to a discrete measure, i.e. a weighted sum. Analogously, the integral definition of the local error will be replaced by a sum of the squared errors on the time steps of the numerical solution. According to the previous considerations we can state the following identification problem:

Choose the unknown parameters u of the model in such a way that the global error functional

$$\Psi = \Psi(u) = \int_V \psi(u, v)\, dv = \int_V \min_{\lambda_0, \lambda_1} \int [\lambda_0 + \lambda_1 \theta_m r(t) - \theta_r(t)]\, dt\, dv \tag{16}$$

attains a minimum over the domain of all feasable parameters u.

5. A reduced problem and its numerical realization

The minimization problem, such as stated in the previous section, is still too general and difficult to solve, so that some further simplifications seem to be necessary.

Till now, the unknown parameters in the above "least squares" problem contain still the functional parameters α and f, i.e. scalar functions on $\mathcal{R}$, resp. $\mathcal{R} \times \mathcal{R}$. Bearing in mind that our experimental evidence is rather very limited ($|V| = 10$), a reduction of the problem is imperative.

To this end we use – as the first attempt – a very restrictive approach – hoping that a more refined version will be prepared in the near future. First, we use a thermodynamical argument in order to replace one function on $\mathcal{R} \times \mathcal{R}$ by two functions on $\mathcal{R}$. Then we postulate a certain compatibility to the classical case, assuming $\beta = \theta$ at relaxed states, and $\alpha = \kappa$. Finally, we need hence just to identify one scalar function f_1 (because $f_2 = f_1$, $f(\theta, \beta) = f_1(\theta) - f_1(\beta)$) which in turn is approximated by a linear spline f_1^s with the coefficients $s = (s_1, \ldots, s_d) \in \mathbb{R}$.

Hence, for the numerical realization, the unknown parameter u is substituted by the spline coefficients s. In order to avoid more notations, we still denote the functionals by Ψ and Φ:

$$\Psi(s) = \sum_{v \in V} \psi(s, v). \tag{17}$$

In this case the variable parameter is identified with the temperature θ_0. So we have

$$\Psi(s) = \sum_{\theta_0=\theta_{\min}}^{\theta_{\max}} \psi(s, \theta_0). \tag{18}$$

The results of our optimization are shown in Fig. 1 in form of a comparison between theoretical and measured pulses at 15 K.

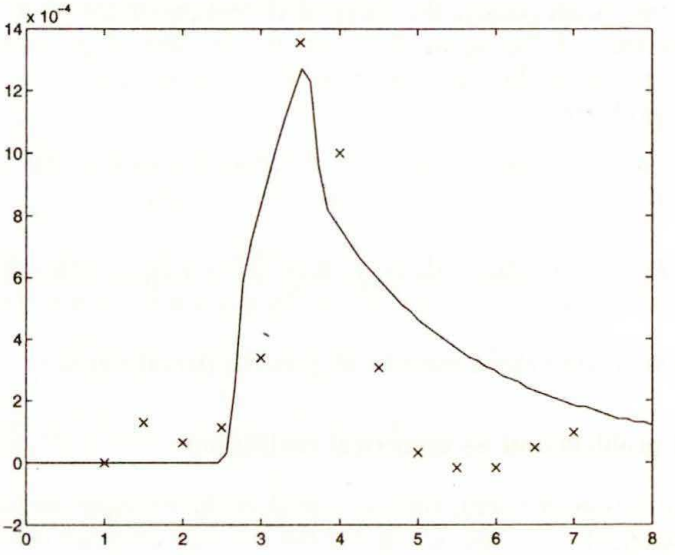

FIG. 1. Theoretical and measured pulses at 15 K.

6. Conclusions

We solved an inverse problem arising in semi-empirical heat conduction theory, in order to find the optimal values of physical parameters characterizing the model. The first results, obtained in this paper, seem to be encouraging. However, it is obvious that there is still some considerable model error. More refined numerical techniques should allow us to avoid some of the additional simplifications of Sec. 5, and thus to reduce the remaining error. This will be the subject of a forthcoming paper.

References

1. V.A. CIMMELLI and W. KOSIŃSKI, *Nonequilibrium semi-empirical temperature in materials with thermal relaxation*, Arch. Mech., **43**, 6, 753, 1991.
2. V.A. CIMMELLI and W. KOSIŃSKI, *Heat waves in dielectric crystals at low temperatures*, University of Basilicata, Quaderni del Dipartimento di Matematica, Report n.6/1992.

3. V.A. CIMMELLI, W. KOSIŃSKI and K. SAXTON, *A new approach to the theory of heat conduction with finite wave speeds*, [in:] Proc. VI International Conference on Waves and Stability in Continuous Media, S. RIONERO, G. MULONE, F. SALEMI [Eds.], Acireale, Italy 1991.
4. B.D. COLEMAN and D.C. NEUMANN, *Implications of a nonlinearity in the theory of second sound in solids*, Phys. Rev. B, **32**, 1492, 1988.
5. K. FRISCHMUTH and V.A. CIMMELLI, *Numerical reconstruction of heat pulse experiments*, Int. J. Engng. Sci., **33**, 2, 215, 1995.
6. V.A. CIMMELLI and K. FRISCHMUTH, *Determination of material functions through second sound measurements in a hyperbolic heat conduction theory*, Mathematical and Computer Modelling, 1996 [in press].
7. R.J. HARDY and S.S. JASWAL, *Velocity of second sound in NaF*, Phys. Rev. B, **3**, 4385, 1971.
8. H.E. JACKSON and C.T. WALKER, *Thermal conductivity, second sound, and phonon-phonon interactions in NaF*, Phys. Rev. Letters, **3**, 4, 1428, 1971.

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Received November 8, 1996.