

Modified Fourier law — comparison of two approaches

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THE OBJECTIVE of this note is to compare two different models leading to modified Fourier laws. The first model uses the concept of semi-empirical temperature, the second one is built in the framework of extended thermodynamics. For both approaches three experimental curves, namely the specific heat, heat conduction coefficient and second sound speed, all given in terms of the absolute temperature, determine the models. Conditions under which both models lead to similar results are formulated.

1. Introduction

VARIOUS TYPES of hyperbolic heat conduction equations leading to finite speed of thermal wave propagation were postulated for rigid and deformable heat conductors in the last three decades. After MAXWELL [1], CATTANEO [2, 3] and VERNOTTE [4] one can find dozens of papers in which different approaches have been used to model second sound effect observed in solids [5, 6].

It is well known that the simple dependence of energy ψ^* on the thermodynamic (absolute) temperature and the classical Fourier law combined with the first and second laws of thermodynamics lead to the heat conduction equation of the parabolic (nonlinear) type. Unfortunately, the same result will be obtained if under the function symbol ψ^* the temperature gradient appears.

To modify the heat conduction equation and to get a finite speed of propagation of any thermal disturbances, the constitutive equation for the energy must be changed by adding at least one extra variable under the function symbol ψ^* , different from the temperature gradient. This extra variable can be regarded as an additional state variable.

In this paper two approaches are compared: the first phenomenological⁽¹⁾ one developed by the present authors in the series of papers [7–13] and based on the concept of semi-empirical temperature scale, different from the absolute one⁽²⁾, and the second model developed by Morro and Ruggeri in the framework of the extended thermodynamics [14, 15] and further applied to shock wave propagation in crystals at low temperature [16, 17]. The first model has a statistical background; in both the approaches, however, three experimental curves, namely the specific heat, heat conduction coefficient and second sound speed, all given in terms of the absolute temperature, determine the models.

⁽¹⁾A kinetic theory approach was developed, for example, in [18, 19], while a generalized thermoelasticity with one relaxation time in [20, 21].

⁽²⁾In [22] the concept of inertial systems was used to derive a second order equation of heat for the integrated history of the absolute temperature.

2. Model with semi-empirical temperature

Recently in a series of papers [7–9, 11–13] a thermodynamic, phenomenological theory of heat conduction with finite wave speed has been developed and applied to thermal wave propagation problems; the well-posedness of a Cauchy problem has been demonstrated as well (cf. [10]). The theory is based on the concept of the semi-empirical temperature β that at a typical particle X of a medium under consideration is a solution of an initial value problem

$$(1) \quad \dot{\beta} = F(\vartheta, \beta), \quad \beta(t_0) = \beta_0,$$

where ϑ is the absolute (thermodynamic) temperature at X and the superposed dot denotes the differentiation with respect to time t . The material function F depends on thermal properties of the medium at hand, e.g. conductivity, and on some time interval τ characteristic for the thermal inertia.

In further constitutive modelling of the theory one assumes, after CATTANEO [2–3], that both relations: the classical Fourier law of heat conduction

$$(2) \quad \mathbf{q} = -k \text{ grad } \vartheta,$$

(with $k(\vartheta)$ as a thermal conductivity coefficient) as well as the differential relation derived for the heat flux \mathbf{q} from Eq. (1) and a set of constitutive equations for remaining quantities (and based on the semi-empirical temperature), play the role of balance equations, however, with different approximations of the mean kinetic energy of molecules of the medium. This point of view, together with the statistical arguments given in [9], imply that instead of the temperature gradient the spatial gradient of the semi-empirical temperature, i.e. $\text{grad } \beta$, appears in the following constitutive relations for the Helmholtz free energy ψ , specific entropy η and heat flux \mathbf{q}

$$(3) \quad \begin{aligned} \psi &= \psi^*(\vartheta, \text{grad } \beta), \\ \eta &= \eta^*(\vartheta, \text{grad } \beta), \\ \mathbf{q} &= \mathbf{q}^*(\vartheta, \text{grad } \beta). \end{aligned}$$

Moreover, it is assumed that the Fourier law is obtained when the thermal relaxation time τ vanishes; then β becomes a function of ϑ . This assumption will be used in the derivation of the relations between material functions and the heat conduction coefficient $k(\vartheta)$ measured in classical experiments on heat conduction⁽³⁾.

Since τ represents the time dimension parameter in F , and both variables β and ϑ have the dimension of temperature (kelvin), the dimensional analysis implies the existence of a function f (of β and ϑ) of the dimension of temperature, such that

$$(4) \quad F(\vartheta, \beta) \equiv \tau^{-1} f(\vartheta, \beta).$$

Then the kinetic equation (1) takes the form

$$(5) \quad \tau \dot{\beta} = f(\vartheta, \beta)$$

and the limit case of vanishing τ corresponds to $f(\vartheta, \beta) = 0$, identically in ϑ and β . Hence the sought relation between the both scales follows, provided the derivative $(\partial f / \partial \beta)$ is different from zero. (Note that stability of solutions of Eq. (5) is guaranteed if that derivative is negative, exactly non-positive, for positive τ [9]).

⁽³⁾ In the classical heat conduction experiment no concept of thermal relaxation time appears.

In the case of an isotropic medium the second law of thermodynamics is satisfied (cf. [8, 9, 13]) if

$$(6) \quad \mathbf{q} = -\tilde{\alpha} \text{grad } \beta, \quad \eta = -\partial\psi^*/\partial\vartheta, \quad \text{and} \quad \frac{\tilde{\alpha}(\partial f/\partial\beta)}{(\partial f/\partial\vartheta)} \leq 0,$$

where $\tilde{\alpha}(\vartheta) = \rho\vartheta\tau^{-1}(\partial f/\partial\vartheta)\frac{\partial\psi^*}{\partial|\text{grad } \beta|} \frac{1}{|\text{grad } \beta|}$ has the dimension of a thermal conductivity coefficient (say k_0). Let us first notice that the coefficient $\tilde{\alpha}$ cannot depend on β for the form of Eq. (3) to be valid, and consequently the function f is governed by the equation $\partial^2 f/\partial\vartheta\partial\beta = 0$. Thus the general form of f is

$$(7) \quad f(\vartheta, \beta) = f_1(\vartheta) + f_2(\beta).$$

If one assumes that $\tilde{\alpha}$ is independent of $|\text{grad } \beta|$ then the last expression for $\tilde{\alpha}$ can be regarded as a differential equation for ψ^* ; integrating it one gets

$$(8) \quad \psi = \psi_1^*(\vartheta) + 0.5\tilde{\psi}_2(\vartheta)|\text{grad } \beta|^2,$$

where $\psi_1^*(\vartheta)$ plays the role of the classical free energy function, and

$$(9) \quad \tilde{\psi}_2(\vartheta) := \tau\tilde{\alpha}(\rho\vartheta\partial f/\partial\vartheta)^{-1}.$$

The last relation can be regarded as a compatibility condition. From Eqs. (6) the form of the entropy function η^* follows. However, to compare the present model with that developed by MORRO and RUGGERI [14] in the framework of extended thermodynamics (cf. [15–17]), we assume after them that the internal energy ε is a function of ϑ only (i.e. independent of $\text{grad } \beta$); this assumption is compatible with the Debye theory in which at low temperatures the specific heat is a cubic function of the absolute temperature only. Then necessarily $\tilde{\psi}_2(\vartheta)$ is a linear function of temperature, for $\varepsilon = \psi + \eta\vartheta$; this together with Eq. (6)₂ leads to two expressions

$$(10) \quad \tilde{\psi}_2(\vartheta) = \psi_{20}\vartheta \quad \text{and} \quad \eta^*(\vartheta, |\text{grad } \beta|) = \eta_E(\vartheta) - 0.5\psi_{20}|\text{grad } \beta|^2,$$

where $\eta_E(\vartheta) = -d\psi_1^*/d\vartheta$, and the dimensional analysis (cf. [7]) requires

$$(11) \quad \psi_{20} = \tau k_0/\rho\vartheta_0^2$$

with some reference temperature ϑ_0 and positive⁽⁴⁾ constant k_0 of the dimension of a thermal conductivity coefficient. The term η_E represents the classical equilibrium entropy. Hence the compatibility condition (9) will take the form

$$(12) \quad \tau k_0/\rho\vartheta_0^2 = \tau\tilde{\alpha}(\vartheta)(\rho\vartheta^2 f_1'(\vartheta))^{-1},$$

where $f_1'(\vartheta) := df_1(\vartheta)/d\vartheta$. Now, if Eq. (6)₁ is used then the RHS of Eq. (10)₂ can be expressed in terms of ϑ and \mathbf{q} as

$$(13) \quad \eta = \eta_E(\vartheta) - 0.5\frac{\psi_{20}}{\tilde{\alpha}(\vartheta)^2}|\mathbf{q}|^2.$$

Speeds of propagation of weak discontinuities, i.e. discontinuities in the first (time and spatial) derivatives of the energy and the heat flux, are given as solutions of the so-called

⁽⁴⁾ Here the principle of maximum for entropy at equilibrium holds.

characteristic equations. In the semi-empirical temperature model this equation is of the form

$$(15) \quad \tau \rho c_v(\vartheta) \lambda^2 + \tau \tilde{\alpha}'(\vartheta) \text{grad } \beta \cdot \mathbf{n} \lambda - \tilde{\alpha}(\vartheta) f_1'(\vartheta) = 0,$$

where λ denotes the speed and \mathbf{n} the direction of propagation, and $c_v(\vartheta) = -\vartheta d^2 \psi_1^*(\vartheta)/(d\vartheta^2)$ represents the specific heat. Let us notice that the constraint (6)₃ together with the assumed stability of solutions of Eq. (5) assert real solutions to Eq. (15), provided the product of τ and the specific heat is positive. In the case of the so-called equilibrium case, i.e. when $\text{grad } \beta = \mathbf{0}$, we get the equilibrium characteristic speed U_E being a function of ϑ only

$$(16) \quad U_E(\vartheta) = \lambda|_{\text{grad } \beta = \mathbf{0}} = \pm \{ \tilde{\alpha}(\vartheta) f_1'(\vartheta) (\tau \rho c_v(\vartheta))^{-1} \}^{0.5}.$$

Hence, knowing the specific heat and the (positive) second sound speed $U_E(\vartheta)$ one can express two material functions f_1 and $\tilde{\alpha}$ as follows

$$(17) \quad \begin{aligned} f_1(\vartheta) \sqrt{\psi_{20}/\tau^2} &= \int \vartheta^{-1} U_E(\vartheta) \sqrt{c_v(\vartheta)} d\vartheta, \\ \tilde{\alpha}(\vartheta) / \sqrt{\psi_{20}} &= \rho \vartheta U_E(\vartheta) \sqrt{c_v(\vartheta)}. \end{aligned}$$

Now our assumption following Eqs. (3) is used to identify the second material function $f_2(\beta)$. Since the Fourier law is the zero-order approximation of the both modified approaches of [7] and [14], let us pass to the limit with τ tending to zero in Eq. (5). Then from the RHS of Eq. (5) we obtain a functional equation

$$(18) \quad f_1(\vartheta) + f_2(\beta) = 0.$$

Its solution given by the inverse function $f_2^{-1}(-f_1(\vartheta))$ (which expresses β in terms of ϑ) we denote by $B(\vartheta)$; this is a differentiable function which satisfies Eq. (18) as an identity, i.e. $f(\vartheta, B(\vartheta)) \equiv 0$. This means, that in the limit of vanishing τ the semi-empirical scale β is equal to $B(\vartheta)$. From Eq. (6)₁ we obtain — as required — the classical Fourier law

$$(19) \quad \mathbf{q} = -k(\vartheta) \text{grad } \vartheta \quad \text{with} \quad k(\vartheta) = \tilde{\alpha}(\vartheta) B'(\vartheta).$$

In that way the last material function $f_2(\beta)$ can be determined in terms of the observed quantities $U_E(\vartheta)$, $c_v(\vartheta)$ and $k(\vartheta)$.

Now we show the prolongation of the kinetic equation (5); taking the spatial derivative of it, we obtain an evolution equation for heat flux

$$(20) \quad \frac{\dot{\tau}}{\tilde{\alpha}(\vartheta)} \mathbf{q} + \text{grad } f_1(\vartheta) = \frac{f_2'(\beta)}{\tilde{\alpha}(\vartheta)} \mathbf{q},$$

where Eq. (6)₁ has been used. Let us notice that only in the case of linear material function f_2 the RHS of Eq. (20) does not depend on β . Since then $f_2'(\beta)$ is equal to a constant c_1 and consequently $B'(\vartheta)$ is equal to $-c_1^{-1} f_1'(\vartheta)$, in view of Eq. (19)₂ we obtain the term $-c_1^{-1} f_1'(\vartheta)/k(\vartheta)$ in front of \mathbf{q} .

We shall close this section with the final remark concerning the structure of the system of differential equations of the model in the case when the RHS of Eq. (5) can be inverted with respect to ϑ . If one introduces two additional variables: $w = \dot{\beta}$ and $\mathbf{p} = \text{grad } \beta$, then ϑ becomes a function of β and w , say $\vartheta = \theta(\beta, w)$, and the governing system becomes

of the first order⁽⁵⁾

$$(21) \quad \begin{aligned} \dot{\beta} &= w, \quad \rho \dot{\epsilon} + \operatorname{div} \mathbf{q} = \mathbf{0}, \\ \dot{\tau} \mathbf{p} - \operatorname{grad} f_1(\vartheta) &= f_2'(\beta) \mathbf{p}, \end{aligned}$$

where, due to Eqs. (6)–(9), $\mathbf{q} = -\tilde{\alpha}(\vartheta) \mathbf{p}$ with $\tilde{\alpha}(\vartheta) = \rho \psi_{20} \vartheta^2 f_1'(\vartheta) / \tau$ and the last equation (21)₃ is a prolonged kinetic equation (cf. Eq. (20)). Note, that if f_2 is linear the first equation decouples from the remaining two, and the problem can be solved in terms of ϑ and \mathbf{q} .

Now, if the second equation multiplied by ϑ^{-1} is added to the third one multiplied by $-\rho \psi_{20} / \tau$ then one gets a balance law for the entropy density $\rho \eta = \rho \eta_E - 0.5 \rho \psi_{20} \mathbf{p} \cdot \mathbf{p}$ with the entropy flux $\mathbf{k} = \mathbf{q} / \vartheta$ and the production term $-\rho \psi_{20} f_2'(\beta) \mathbf{p} \cdot \mathbf{p} / \tau$.

3. Extended thermodynamics model

The rigid heat conductor model developed by Morro and Ruggeri [14] in the framework of extended thermodynamics and further applied to shock wave propagation in crystals [16, 17], is based on two balance laws:

$$(22) \quad \rho \dot{\epsilon} + \operatorname{div} \mathbf{q} = \mathbf{0},$$

$$(23) \quad \dot{\alpha} \mathbf{q} + \operatorname{grad} \nu(\vartheta) = -\frac{\nu'(\vartheta)}{k(\vartheta)} \mathbf{q},$$

where $\alpha(\vartheta)$ and $\nu(\vartheta)$ are two material scalar-valued functions, while $k(\vartheta)$ represents a heat conduction coefficient, dependent on temperature. The factor α plays the role of thermal inertia, and if one puts it equal to a constant then Eq. (23) coincides with the Maxwell-Cattaneo equation [2, 3, 7] $\tau \dot{\mathbf{q}} + \mathbf{q} = -k \operatorname{grad} \vartheta$, identifying

$$(24) \quad \tau = \alpha k / \nu'.$$

The second law of thermodynamics (the entropy principle) is satisfied if the specific entropy has the form

$$(25) \quad \hat{\eta}(\vartheta, \mathbf{q}) = \eta_E(\vartheta) - 0.5 \frac{\gamma}{\rho(\nu' \vartheta^2)^2} |\mathbf{q}|^2 \quad \text{with} \quad \alpha = \frac{\gamma}{\nu' \vartheta^2},$$

where γ is a constant to be determined; if it is positive then the entropy⁽⁶⁾ has a maximum at equilibrium, i.e. for $\mathbf{q} = \mathbf{0}$.

Let us notice that till now no assumption about the dimension of ν, α and γ has been made. The particular identification (24) says that dimensions of α and ν must be different. Choosing for α the dimension of τ / k means that ν' is dimensionless. Since in the first model in the limit of vanishing τ the coefficient $\tilde{\alpha}$ does not vary, the possible identification that is compatible with the chosen dimensions is

$$(26) \quad \alpha \equiv \tau / \tilde{\alpha}.$$

Hence both the entropy functions η^* and $\hat{\eta}$ will give the same values (for the same ϑ and \mathbf{q}) if

$$(27) \quad \gamma = \tau \vartheta_0^2 / k_0, \quad \text{i.e.} \quad \rho \gamma = \tau^2 / \psi_{20}.$$

⁽⁵⁾ In [12] such a system was derived for a particular form of f .

⁽⁶⁾ The entropy is concave if the specific heat and γ are positive [14].

Now due to the compatibility conditions (11), $(25)_2$ and (26) we get

$$(28) \quad \nu(\vartheta) \equiv f_1(\vartheta).$$

Now we can see that the last three equations (26)–(28) give the set of identification formulae for both models. Moreover, if f_2 is linear then both systems will lead to the same solutions, provided initial conditions $(\vartheta(0), \mathbf{q}(0))$ of the second model will be adjusted to initial conditions $(\beta(0), \vartheta(0))$ of the first model. In particular, at the initial time the equation $\mathbf{p} = \text{grad } \beta$ has to hold.

Let us notice that in the shock wave analysis performed in the second model (cf. [16]) the form of the function $k(\vartheta)$, and consequently of $f_2(\beta)$ — for the first model — does not influence the results.

It is worthwhile to mention that the second model has been already applied when investigating thermal hot and cold shocks propagating with finite speed in crystals at low absolute temperature. A structural temperature at which the physics of shock waves changes was observed by T. RUGGERI [17]. Moreover, in [16, 17] basing on experimental results of [5, 6] and analyzing quantitatively thermal shock wave propagation in crystals of NaF and Bi at low temperature, the obtained values of the critical structural temperatures were very closed to the values for which the second sound was clearly picked out in these crystals.

On the other hand in [11, 12] dealing with the first model weak discontinuity waves for rigid and elastic heat conductors were investigated; it was shown that the wave amplitude in both types of conductors can blow up in finite time which can lead to the formation of shocks. Description of the second sound effect in deformable conductors and within that model will be the subject of the next paper.

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