

MATHEMATICAL ASPECTS OF NON-FOURIER HEAT EQUATIONS

RÓBERT KOVÁCS

Department of Energy Engineering, Budapest University of Technology and Economics
Műegyetem rkp. 3., H-1111, Budapest, Hungary

Department of Theoretical Physics, Wigner Research Centre for Physics, Hungary
kovacsrobert@energia.bme.hu

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Abstract. Due to technological advancement, as materials with complex structures (e.g., metamaterials and foams) appear in practice there is a need to develop advanced thermal models. These are called non-Fourier equations, and all have particular mathematical properties differing from the conventional attributes of Fourier's law. The present paper discusses the thermodynamic origin of non-Fourier equations and their consequences. The second law of thermodynamics influences the relations among the material parameters, and therefore, it restricts how the temperature-dependent properties can be included in the model. Furthermore, we present the properties of initial and boundary conditions, since these are crucial in solving any practical problems and are different from the usual interpretation used for the Fourier equation.

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1. INTRODUCTION

In engineering practice, continuum models are used to describe the behaviour of fluids and solids in space and time, usually utilising a finite element method. These software consist of knowledge about all the classical equations for fluid flow, solid mechanics and heat transfer. While this is suitable in numerous situations, there are cases in which these conventional methods are not applicable, such as the thermal modelling of thin layers [1, 2] and heterogeneous materials [3, 4, 5]. These, in general, can be described with advanced models in which the classical Fourier equation is extended with new space and time derivatives, forming the so-called non-Fourier models [6, 7].

Fourier's law prescribes a proportionality between the heat flux and the temperature gradient. That relation eases the initial and boundary conditions definitions as showing a straightforward connection between the field variables. However, this is not the case for non-Fourier equations. The Fourier constitutive equation is exchanged with a (partial) differential equation, thus modelling a significantly more complex relationship between the heat flux and temperature gradient. This generalisation has far-reaching consequences in the mathematical treatment of heat equations.

Therefore, this paper aims to present the aforementioned essential consequences related to initial and boundary conditions. Furthermore, we also present a less-known attribute that becomes crucial for nonlinearities: the functional dependence of the coefficients. These together are the most common aspects needed for engineers in the problem-solving procedure. It is challenging to obtain physically sound and reliable solutions without clarifying these properties.

In what follows, we begin with the thermodynamic background, from which it becomes visible how the coefficients in the equations (interpreted as material parameters) are connected. After that, we place our focus on the initial and boundary conditions by presenting the critical steps in the solution method.

2. THERMODYNAMICS OF HEAT EQUATIONS

While the approach of Classical Irreversible Thermodynamics (CIT) [8] was successful, it turned out that its basic hypothesis about local equilibrium is a substantial restriction, and therefore other ways must be discovered for the description of non-equilibrium phenomena. Thus numerous thermodynamic approaches have been developed in recent decades, such as Extended Irreversible Thermodynamics (EIT) [9, 10], Rational Extended Thermodynamics (RET) [11], GENERIC [12, 13] and the framework of internal variables [14, 15, 16, 17, 18]. Each approach has its specific advantages and disadvantages, depending on the particular problem. For instance, RET is better for rarefied gaseous materials but cannot be used for macroscale solids at room temperature. GENERIC is helpful in constructing numerical methods, and EIT fits best for low-temperature (< 20 K) problems.

For our purpose, the approach of internal variables is the best option as this theory does not restrict the model either to rarefied or low-temperature states. In that sense, it is more general than the other thermodynamic theories, since this approach does not necessarily introduce variables with strict physical interpretation. It restricts the tensorial order of the variable and fixes how that variable contributes to the potential functions entropy and internal energy, but leaves open its exact physical meaning, being understood as an ‘internal degree of freedom’. For our purpose, that freedom is not necessary, and to obtain compatibility with EIT, that internal variable can be identified as the heat flux, thus it is a non-equilibrium contribution to the heat conduction process. We focus on two non-Fourier heat equations in the following. These are the Maxwell-Cattaneo-Vernotte (MCV) [19, 20] and Guyer-Krumhansl (GK) [21] equations. These are the most common models in the non-Fourier literature. The GK equation seems to be the next reasonable and practically important extension of Fourier’s law due to its advantageous properties [22]. For the detailed derivation, we refer to the work of Fülöp and Ván [23, 24]; here we show only the essential steps and outcomes.

2.1. Fourier equation. The derivation of constitutive equations - such as Fourier’s law - is based on the balance of entropy density s . In CIT, s depends only on the specific internal energy e . Together with the entropy density current $\mathbf{J}_s = \mathbf{q}/T$ (with T is the temperature and \mathbf{q} is the heat flux), it is possible to determine the entropy

production (σ_s) using the balance equation,

$$\rho \dot{s} + \nabla \cdot \mathbf{J}_s = \sigma_s \geq 0, \quad (2.1)$$

where the upper dot represents the time derivative and $\nabla \cdot$ stands for the divergence. Eq. (2.1) mathematically forms the second law of thermodynamics for continuum systems [25]. It is a balance equation for entropy density, which is a concave potential function of e , thus having a maxima at the equilibrium. The entropy production σ_s appears as a source term, and that must be positive semi-definite, $\sigma_s = 0$ only in equilibrium for dissipative phenomena. Mathematically, the solution of $\sigma_s \geq 0$ results in the constitutive relations. Interestingly, while infinitely many solutions are possible [28], mostly the linear solutions are investigated as they are simple enough to understand, interpret and implement in practice. To obtain Fourier's law, after substitution, (2.1) leads to the Onsagerian equation [26, 27],

$$\sigma_s = \mathbf{q} \cdot \nabla \frac{1}{T} \geq 0, \quad (2.2)$$

for which we choose a linear solution,

$$\mathbf{q} = \frac{l}{T^2} \nabla T = -\lambda \nabla T = -\lambda \text{grad} T. \quad (2.3)$$

This is called Fourier's law, and the thermal conductivity λ is naturally formed by a positive coefficient $l > 0$ to satisfy the inequality's positive semi-definiteness. The calculation of entropy production requires the balance of internal energy e ,

$$\rho \dot{e} + \nabla \cdot \mathbf{q} = 0, \quad (2.4)$$

in which we neglected the volumetric heat sources, and $e = cT$ is considered with c being the isochoric specific heat. Here, we restrict ourselves to rigid materials in order to clearly reveal the difficulties and the limits of the theory. The derivation of non-Fourier equations with internal variables repeats this procedure.

2.2. Models beyond Fourier. In any of the generalised thermodynamic theories, the variable space is extended with a new type of non-equilibrium variable. In the internal variable approach, that non-equilibrium variable is not necessarily interpreted or connected to a known physical quantity, merely its existence and its tensorial order are restricted. In other words, one can suppose that $s = s(e, \xi)$, where ξ is a vectorial quantity. This is a general approach indeed. However, we do not need to keep this level of generality to derive the MCV and GK equations. Instead, it is possible to identify ξ with the heat flux \mathbf{q} at that step, achieving compatibility with EIT and RET [29], i.e., having $s = s(e, \mathbf{q})$, which must be a concave function. The concavity is ensured by using

$$s(e, \mathbf{q}) = s_{eq}(e) - \frac{m}{2} \mathbf{q}^2, \quad (2.5)$$

where the first term $s_{eq}(e)$ expresses the classical local equilibrium assumption and $\frac{m}{2} \mathbf{q}^2$ represents a deviation from this local equilibrium with $m \geq 0$. The derivation also requires \mathbf{J}_s . According to the paper [24], \mathbf{J}_s can be formulated using a so-called Nyíri multiplier (\mathbf{B}), as $\mathbf{J}_s = \mathbf{B} \mathbf{q}$ [30]. In EIT, $\mathbf{J}_s = \frac{\mathbf{q}}{T} + \mu \nabla \mathbf{q} \cdot \mathbf{q}$ is used. These approaches are equivalent, as the inequality (2.1) automatically restricts \mathbf{B} so that

$\mathbf{B} = \frac{1}{T}\mathbf{I} + \mu\nabla\mathbf{q}$ holds. Recently, Szűcs et al. showed [31] that $\mathbf{J}_s = \frac{\mathbf{q}}{T} + \mathbf{B}\mathbf{q}$ is a more natural introduction of a current multiplier \mathbf{B} as it is $\mathbf{B} = \nabla\mathbf{q}$, thus having a more direct and clear physical interpretation. The entropy production becomes

$$\sigma_s = \nabla\mathbf{q} : \left(\mathbf{B} - \frac{1}{T}\mathbf{I} \right) + \mathbf{q} \cdot (\nabla \cdot \mathbf{B} - \rho m \dot{\mathbf{q}}) \geq 0, \quad (2.6)$$

and its solution, the Onsagerian relations are

$$\begin{aligned} \mathbf{B} - \frac{1}{T}\mathbf{I} &= l_1 \nabla\mathbf{q}, \\ \nabla \cdot \mathbf{B} - \rho m \dot{\mathbf{q}} &= l_2 \mathbf{q}, \end{aligned} \quad (2.7)$$

with $l_1, l_2, m \geq 0$, furthermore

$$\tau = \frac{\rho m}{l_2}, \quad \lambda = \frac{1}{l_2 T^2}, \quad \kappa^2 = \frac{l_1}{l_2}, \quad (2.8)$$

forming the coefficients of the GK equation, which reads

$$\tau \partial_t q + q = -\lambda \partial_x T + \kappa^2 \partial_{xx} q \quad (2.9)$$

in one spatial dimension for simplicity. If $l_1 = 0$, the model reduces to the MCV equation, i.e., $\kappa^2 = 0$ and

$$\tau \partial_t q + q = -\lambda \partial_x T. \quad (2.10)$$

The MCV and GK constitutive equations (2.9)-(2.10) are coupled to the internal energy balance (2.4), and thus form a mathematically and physically complete system of equations, describing the time evolution of temperature and heat flux in space and time.

Initially, the GK equation is derived on the basis of kinetic theory and therefore the coefficients (2.8) are strictly restricted to a particular heat transfer mechanism. That original approach would not be applicable for engineering problems in general. However, the present continuum model does not require assumptions about the heat conduction mechanism prior to the derivation. Therefore the coefficients (2.8) can be freely adjusted and fitted to experiments, as is usual with the thermal conductivity λ in the Fourier equation. Consequently, while the form of the GK equation remains the same, the coefficients differ from the original case. Therefore, in this sense, the internal variable approach extends the range of validity.

3. NONLINEAR MODELS

It is well-known that the behaviour of materials depends on numerous factors. Here, for demonstration, we consider only the temperature dependence of the coefficients defined by (2.8) and appearing in the GK equation (2.9). We want to emphasise that the new thermal parameters (τ and κ^2) are not independent of the thermal conductivity λ and are connected through the Onsagerian relations. This is demonstrated in the following.

Let us suppose that $\lambda(T) = \lambda_0 \exp(a(T - T_0))$, with λ_0 being thermal conductivity at a reference temperature T_0 . Consequently,

$$\frac{1}{l_2 T^2} = \lambda_0 e^{a(T-T_0)} \Rightarrow \frac{1}{l_2} = \lambda_0 T^2 e^{a(T-T_0)} \Rightarrow l_2 = \frac{1}{\lambda_0 T^2} e^{-a(T-T_0)} \quad (3.1)$$

restricts one Onsagerian coefficient l_2 . Moreover, as l_2 is also present in both coefficients τ and κ^2 , it influences their treatment. This follows from The second law of thermodynamics directly, and has an impact on the entire model, that is,

$$\tau = \frac{\rho m}{l_2} = \rho m \lambda_0 T^2 e^{a(T-T_0)}, \quad \kappa^2 = \frac{l_1}{l_2} = l_1 \lambda_0 T^2 e^{a(T-T_0)}. \quad (3.2)$$

Interestingly, κ^2 alone can depend on the temperature through l_1 .

Now let us assume a more complex situation, i.e., both τ and λ possess a linear temperature dependence

$$\lambda(T) = \lambda_0 + a(T - T_0), \quad \text{and} \quad \tau(T) = \tau_0 + b(T - T_0), \quad (3.3)$$

from which

$$l_2 = \frac{1}{(\lambda_0 + a(T - T_0))T^2}, \quad \text{and} \quad \rho m = \frac{\tau_0 + b(T - T_0)}{(\lambda_0 + a(T - T_0))T^2} \quad (3.4)$$

follows [32]. This is a real, experimentally measured set of parameters. Interestingly, we have a choice about which coefficient is assigned to satisfy (3.4), either ρ , m or both can be temperature dependent. If m alone becomes a function of the temperature, then it introduces further terms into the constitutive equation being proportional with dm/dT . If ρ is considered to be a function of T , then the introduction of the mechanical field is essential in order to take account of thermal expansion with the corresponding balance equations and its contribution to the internal energy [33]. The temperature dependence of κ^2 , however, is still an open question, as experimental data are lacking. Although that parameter is experimentally determined for various heterogeneous materials at room temperature [34], the reference temperature is not yet varied. Either way, the derivation must be restarted in order to preserve the physical and mathematical consistency [32]. This is a notable difference compared to the Fourier equation.

Overall, even the simplest nonlinearity originating in the state dependence of the material coefficients can make the situation significantly more difficult. While this is common for Fourier's law, it is not straightforward for a non-Fourier equation. Without a proper thermodynamic background, one cannot discover the relationship of the coefficients. This is one reason, among many others, why the so-called dual phase lag (DPL) model is not recommended. This is an ad hoc model, based on the assumption that there is a time lag for both the heat flux and the temperature gradient [35],

$$q(x, t + \tau_q) = -\lambda \partial_x T(x, t + \tau_T). \quad (3.5)$$

Usually, Taylor series expansion is utilised on (3.5) up to an arbitrarily decided order. This manifests in ill-posed problems and instability [36, 37, 38, 39, 40, 41]. However, in a particular case, that model might be reduced to the MCV equation (2.10) and could

be viable for strictly restricted situations. However, as a thermodynamic background is missing, it is impossible to recover the connection between the two relaxation times τ_q and τ_T . Together with the mathematical issues, this is a severe limitation on the model, and thus it is not possible to reliably implement the DPL model for practical engineering tasks.

4. INITIAL AND BOUNDARY CONDITIONS

To be clear with the analogies among Fourier and non-Fourier models, we first briefly discuss the classical approach for one spatial dimension. For the Fourier equation, the usual initial condition is straightforward: the temperature distribution ($T(x, t = 0) = T_0(x)$) must be given at the initial time instant. For instance, $T_0(x)$ is also enough to calculate the initial heat flux $q_0(x)$. However, this is valid only for the T-representation of the Fourier heat equation (4.1). In case of q-representation (4.2), only q can be defined at the initial time instant since the temperature as a variable is completely missing in that situation. In other words, we have a choice of which field variable we eliminate using Eqs. (2.3) and (2.4):

$$\text{T-representation:} \quad \partial_t T = \alpha \partial_{xx} T, \quad (4.1)$$

$$\text{q-representation:} \quad \partial_t q = \alpha \partial_{xx} q, \quad (4.2)$$

where $\alpha = \lambda/(\rho c)$ is the thermal diffusivity with constant coefficients. While Eq. (4.1) is well-known in the literature, Eq. (4.2) is usually omitted. The q-representation could be useful for analytical solutions as here the heat flux q is treated as a first-type boundary condition. For certain situations, it could be more suitable, such as for time-dependent heat flux boundaries. After obtaining the time and space evolution of q , the temperature field can be recovered using the balance of internal energy (2.4). Furthermore, that form also reveals an interesting aspect. Eq. (4.2) also allows us to define the gradient of the heat flux as a second-type boundary condition: here it is $\partial_x q$. The unit of $\partial_x q$ is W/m^3 , although it is not a volumetric heat source. The unit can be rewritten as $\text{W/m}^3 = \text{J}/(\text{s m}^3) = \text{Pa/s}$. This is, interestingly, a pressure rate whose quantity appears in models for low-temperature phenomena, and therefore this type of boundary condition could be viable in such cases.

The T-representation of the Fourier heat equation (4.1) is commonly used due to practical reasons, such as that T is a measurable quantity. Moreover, as Fourier's law (2.3) is an equality, it becomes straightforward how to use the temperature in the definition of a boundary condition. Hence, it does not matter which variable we choose to use as a boundary condition, either T or q is adequate, even for temperature-dependent thermal conductivity. Unfortunately, following that thread is misleading for non-Fourier equations.

4.1. Linear case. For constant coefficients, it is straightforward to eliminate one of the field variables and obtain the representations, e.g., for the GK equation using

(2.4) and (2.9):

$$\text{T-representation:} \quad \tau \partial_{tt} T + \partial_t T = \alpha \partial_{xx} T + \kappa^2 \partial_{txx} T, \quad (4.3)$$

$$\text{q-representation:} \quad \tau \partial_{tt} q + \partial_t q = \alpha \partial_{xx} q + \kappa^2 \partial_{txx} q. \quad (4.4)$$

Let us recall that the definition of the second-type boundary condition depends on the field variable. Therefore, having the form of (4.3), it is not possible to explicitly prescribe the heat flux q on the boundary, only $\partial_x T$. However, these quantities are not proportional with each other; the partial differential equation (2.9) restricts their relationship. Consequently, one cannot solve the GK equation in the form of (4.3) for situations with prescribed q on the boundaries [28, 43]. This is the point where the q-representation becomes advantageous and can be used to determine the time (and space) evolution of q . The temperature can be recovered at the end by exploiting the energy balance (2.4). We also emphasise that both of these representations are the consequence of the system (2.4) and (2.9), which is more useful for analytical and numerical solutions [45, 43]. In the following, in Sec. 4.3, the discrete treatment of heat flux boundary conditions is presented. Overall, Eq. (4.3) is suggested only for T-type initial and boundary conditions. For any other situation, the most advantageous form is the system of equations (2.4) and (2.9), without eliminating any variables. For analytical solutions, however, Eq. (4.4) could be more suitable. Keeping in mind these properties, the usual boundary conditions remain valid, and the most suitable form can be chosen for the particular problem.

The treatment of initial conditions is also not evident. In many situations, the steady initial state is disturbed through the boundary (e.g., by a heat pulse), but non-equilibrium initial conditions are rarely investigated in regard to non-Fourier equations. As we mentioned, such a problem is straightforward in the Fourier model as it requires only the initial temperature distribution. However, for a non-Fourier equation, the initial time derivative is also necessary.

As the energy balance (2.4) suggests, the initial time derivative of temperature is determined by the initial heat flux field. It turned out recently [42] that the heat flux for the initial state can be determined using Fourier's law if the initial non-equilibrium state is close to equilibrium for both the MCV and GK equations. Moreover, as the energy balance is exploited in that step, a heat source could also contribute to the initial state. However, whether the initial state is close or far from equilibrium is still an open question. For such a non-equilibrium initial state, the initial time derivative can be found by exploiting the energy balance (2.4). The difficulty originates in the mathematical treatment of the initial conditions, where the differentiability stands as a crucial question. For further details, see [42].

4.2. Nonlinear case. With temperature-dependent parameters, such as (3.3) for the MCV equation, it is no longer possible to eliminate any of the variables, therefore pure T and q representations no longer exist. That difficulty does not affect the required number of boundary conditions, and the numerical treatment of the system of partial differential equations is still feasible with a staggered grid for the spatial domain [22]. The role of non-equilibrium initial conditions is still unclear as it has not yet been investigated with nonlinear non-Fourier models.

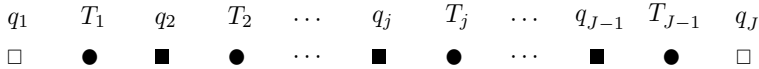


Figure 1. The staggered grid for the numerical solutions [43].

4.3. Time-delayed boundary. Fourier's law can be seen as the differential analogy of the Newton law for cooling, i.e., $q = h(T - T_\infty)$, where h stands for the heat transfer coefficient. In the following, let us suppose that this relationship changes together with the constitutive equation, i.e., for the MCV equation (2.10), it has a form of $\tau \text{d}_t q + q = h(T - T_\infty)$. It describes a time delay on the boundary as it is also a part of the same material for which the MCV equation is used. Here, for demonstration, we provide a particular example of a heat pulse experiment. In order to keep the temperature history and the parameters realistic for the MCV model, we chose a low-temperature experiment performed by McNelly et al. [46]. Therefore, let the parameters be $\lambda = 3000 \text{ W/(m K)}$, $\rho = 2800 \text{ kg/m}^3$, $c = 3.5 \text{ J/(kg K)}$, $\tau = 6 \text{ } \mu\text{s}$, with a heat pulse duration $t_p = 10 \text{ } \mu\text{s}$, on a 10 mm long NaF sample.

Initially, the sample is in a steady state. A short heat pulse is applied on the front side, and the temperature is recorded in time on the rear end. The heat pulse is modelled using $q(x = 0, t \leq t_p) = q_0(1 - \cos(2\pi t/t_p))$, then $q(x, t > t_p) = 0 \text{ W/m}^2$. We assume a cooling boundary on the rear side. The heat transfer coefficient is the same for both cases, $h = 10^4 \text{ W/(m}^2 \text{ K)}$. We solve this model utilising a finite difference method [43] on a staggered grid, illustrated in Figure 1. That staggering helps us to avoid problems on the boundary by allowing us to explicitly prescribe the heat flux on the boundary points. That structure can be realised for any other system with thermodynamic compatibility, even in a three-dimensional case [44]. Figure 2 presents the rear side temperature history, comparing the two cooling boundary conditions. Visibly, the vicinity of the wave shows significant differences; the temperature rises higher, which could be an essential part in the reproduction of such low-temperature heat pulse experiments [46, 47]. When the strong wave signal disappears, the temperature histories run together for both boundary conditions.

5. DISCUSSION

In the present paper, we discussed the thermodynamic origin of two non-Fourier equations, called Maxwell-Cattaneo-Vernotte and Guyer-Krumhansl equations. We took a closer look at the new material coefficients (τ and κ^2). Furthermore, it turned out that the thermal conductivity connects these parameters. That is, in the case of temperature-dependent thermal conductivity, the other coefficients inherit that dependence. Moreover, the mechanical field must be included as well through thermal expansion effects.

We investigated the analogies between the Fourier and non-Fourier equations related to the boundary conditions, showing that the usual approach does not work for advanced heat equations. This also holds for the initial conditions. Moreover, we performed a numerical analysis of how a possible time delay would modify the

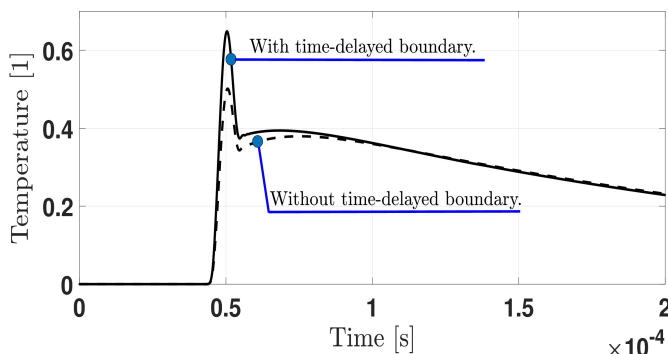


Figure 2. Rear side temperature history for both types of boundary conditions according to the MCV equation

temperature history. The time delay of the heat transfer causes significant differences in the vicinity of the wavefront. However, that difference disappears soon, and after a certain time instant, both boundaries predict the exact temperature history.

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