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Unphysical effects of the dual-phase-lag model of heat conduction

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ABSTRACT

We consider the model of heat conduction, based on the first-order approximation to the dual-phase-lag (DPL) constitutive relation. This model is described by the Jeffreys-type equation. We study an initial value problem for the three-dimensional Jeffreys-type equation with a positive localized source of short duration. We demonstrate that solutions to the problem manifest unphysical behavior with negative values of temperature. We conclude that the DPL model in the form of the Jeffreys-type equation is not in general an appropriate model of heat conduction.

1. Introduction

The heat equation, based on Fourier's law, is commonly used for description of heat conduction. However, Fourier's law is valid under the assumption of local thermodynamic equilibrium, which is violated in very small dimensions and short timescales [1].

The simplest modification of Fourier's law, taking into account thermal "inertia", is Cattaneo's equation [1–5]

$$\tau\frac{\partial \boldsymbol{q}}{\partial t}+\boldsymbol{q}=-k\nabla T, \tag{1.1}$$

where $T\equiv T(\boldsymbol{x},t)$ is temperature, $\boldsymbol{q}\equiv\boldsymbol{q}(\boldsymbol{x},t)$ is heat flux, k is the thermal conductivity, τ is a relaxation time. Eq. (1.1) is also the first-order approximation to the single-phase-lag constitutive relation [6,7]

$$\boldsymbol{q}(\boldsymbol{x},t+\tau)=-k\nabla T(\boldsymbol{x},t). \tag{1.2}$$

Combined with the energy equation for heat conduction, Cattaneo's equation leads to the hyperbolic model of heat conduction described by the telegraph (or damped wave) equation, which provides the finite speed of heat propagation [1–4,8]. However, this model meets formal obstacles since the telegraph equation does not preserve the nonnegativity of its solutions [9–11]. Besides, the applicability of the telegraph equation to the description of heat conduction is doubtful [12,13].

The dual-phase-lag (DPL) model of heat conduction, based on the constitutive relation

$$\boldsymbol{q}(\boldsymbol{x},t+\tau_q)=-k\nabla T(\boldsymbol{x},t+\tau_T), \tag{1.3}$$

where τ_q and τ_T are positive time (or phase) lags, was proposed in Refs. [6,14], see also [1,5]. In Refs. [7,15,16] this constitutive relation was derived from the Boltzmann equation. The relation (1.3) is equivalent to the relation (1.2) with $\tau=\tau_q-\tau_T$. Both relations are sensible only if $\tau\geqslant 0$.

Eq. (1.2) and the energy equation

$$C\frac{\partial T}{\partial t}+\operatorname{div}\boldsymbol{q}=0,$$

where C is the volumetric heat capacity, yield the delay heat equation

$$\frac{\partial T(\boldsymbol{x},t)}{\partial t}-\alpha\Delta T(\boldsymbol{x},t-\tau)=0, \tag{1.4}$$

where $\alpha=k/C$ is the thermal diffusivity. However, initial value problems for Eq. (1.4) are ill-posed (with unstable solutions) [17–19]. Therefore, the phase-lag constitutive relations (1.2) and (1.3) cannot be considered as sensible physical ones.

The first-order approximation to Eq. (1.3) is given by the Jeffreys-type constitutive relation [2]

$$\tau_q\frac{\partial \boldsymbol{q}}{\partial t}+\boldsymbol{q}=-k\left[\tau_T\frac{\partial\nabla T}{\partial t}+\nabla T\right]. \tag{1.5}$$

This relation and the energy equation

$$C\frac{\partial T}{\partial t}+\operatorname{div}\boldsymbol{q}=Q,$$

where $Q\equiv Q(\boldsymbol{x},t)$ is the heat source term, yield the Jeffreys-type equation [1,2]

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$$\tau_q \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} - \alpha\left[\tau_T \frac{\partial \Delta T}{\partial t} + \Delta T\right] = \frac{1}{C}\left(Q + \tau_q \frac{\partial Q}{\partial t}\right).$$

Initial value problems for this equation are well-posed, therefore, the Jeffreys-type constitutive relation (1.5) cannot be considered as a real approximation of the DPL relation (1.3) leading to ill-posed problems [18].

The DPL model is often identified with the Jeffreys-type equation. Strictly speaking, this is not correct, since higher-order approximations to Eq. (1.3) were also considered in literature, see [5,7,18,20–24]. Nevertheless, in this paper we interpret the DPL model mainly as a model of heat conduction described by the Jeffreys-type equation.

The Jeffreys-type equation was used for simulation of bioheat transfer in Refs. [22,23,25–32]. To simulate the propagation of heat waves in a finite one- and two-dimensional medium under pulse surface heating in the framework of the DPL model, the method of space–time conservation element and solution element was used in Refs. [33,34]. The DPL model was used in Ref. [35] for simulation of transient heat transfer in a two-dimensional nanoscale metal–oxide–semiconductor field-effect transistor. A higher-order unconditionally stable compact finite difference scheme for solving the one-dimensional Jeffreys-type equation was proposed in Ref. [36]. The one-dimensional DPL model was used in Ref. [37] to investigate heat transfer in a gas-saturated porous medium heated by a short laser pulse. In Ref. [38] the Jeffreys-type constitutive relation was derived (among Fourier's, Cattaneo's, and others) in the framework of weakly nonlocal thermodynamics.

In Ref. [39] non-Fourier heat conduction in a quasi-one-dimensional single-walled carbon nanotube subjected to a local subpicosecond heat pulse was investigated by means of classical molecular dynamics simulations. It was demonstrated that the observed wavelike heat conduction was not described by the hyperbolic heat (or telegraph) equation, while the spatiotemporal behavior of the heat wave was well described by the Jeffreys-type equation. However, Ref. [39] did not provide results for shorter times, when a phenomenon of local immobilization, inherent in solutions of the Jeffreys-type equation, is significant. This phenomenon was found in Ref. [40], where models of mass transfer were considered, yet the solutions of the Jeffreys-type equation, describing heat conduction, are mathematically the same. Therefore the results, presented in Ref. [39], do not allow to assess whether the Jeffreys-type equation describes heat conduction in the single-walled carbon nanotube for shorter times.

Whereas the DPL model in the form of the Jeffreys-type equation received widespread attention, physical anomalies and unphysical effects of heat conduction in the framework of this model were reported in Refs. [41,42], where one-dimensional heat transfer was considered.

In Ref. [41] it was demonstrated that the temperature of a heat wave, reflected from a constant temperature boundary, may take negative values (as in the framework of the hyperbolic heat conduction model described by the telegraph equation).

In Ref. [42] it was shown that interference of two cold thermal waves may result in negative values of temperature. A similar effect was discussed in Ref. [43], where interference of two hot thermal waves led to overshooting. Although in the latter case temperature was positive, both effects are equivalent from the mathematical point of view and in both cases the maximum principle [44] is violated. This effect is similar to that described in Ref. [9,11] in the framework of the hyperbolic heat conduction model. Note that violation of the maximum principle was observed also in Ref. [31].

In this paper we consider an initial value problem for the three-dimensional Jeffreys-type equation with positive temporal localized source. A similar problem for the telegraph equation was considered in Ref. [11]. We demonstrate that solutions to the problem manifest unphysical behavior with negative values of temperature.

2. Initial value problem for the three-dimensional Jeffreys-type equation with a positive localized source of short duration

Consider the Jeffreys-type equation in the three-dimensional space

$$\tau_q \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} - \alpha\left(\tau_T \frac{\partial \Delta T}{\partial t} + \Delta T\right) = \frac{1}{C}\left(Q + \tau_q \frac{\partial Q}{\partial t}\right), \quad \boldsymbol{x} \in \mathbb{R}^3, \quad t > -\theta \tag{2.1}$$

with a positive Gaussian source of finite duration

$$Q(\boldsymbol{x}, t) = p_\sigma(\boldsymbol{x})\chi_{[-\theta,0]}(t),$$

where

$$p_\sigma(\boldsymbol{x}) = \frac{1}{\left(\sqrt{2\pi}\sigma\right)^3} \exp\left(-\frac{|\boldsymbol{x}|^2}{2\sigma^2}\right)$$

and

$$\chi_{[-\theta,0]}(t) = \begin{cases} \frac{1}{\theta}, & -\theta < t \leqslant 0, \\ 0, & t > 0. \end{cases}$$

Note that the initial time is $t = -\theta$, the source is equal to zero for $t > 0$ and normalized to unity. Initial conditions for Eq. (2.1) are

$$T|_{t=-\theta} = 0, \quad \left.\frac{\partial T}{\partial t}\right|_{t=-\theta} = 0. \tag{2.2}$$

The solution to the problem (2.1) and (2.2) is given by

$$T(\boldsymbol{x}, t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \mathcal{F}T(\xi, t) e^{-i\xi \boldsymbol{x}} d\xi,$$

where

$$\mathcal{F}T(\xi, \cdot) = \int_{\mathbb{R}^3} T(\boldsymbol{x}, \cdot) e^{i\xi \boldsymbol{x}} d\boldsymbol{x}$$

is the Fourier transform of the solution, which is given by (see Appendix A)

$$\mathcal{F}T(\xi, t) = \frac{e^{-\sigma^2|\xi|^2/2}}{C[\lambda_1(\xi) - \lambda_2(\xi)]} \times \left\{\left[\lambda_1(\xi) + \frac{1}{\tau_q}\right] e^{\lambda_1(\xi)t} \frac{e^{\lambda_1(\xi)\theta} - 1}{\lambda_1(\xi)\theta} - \left[\lambda_2(\xi) + \frac{1}{\tau_q}\right] e^{\lambda_2(\xi)t} \frac{e^{\lambda_2(\xi)\theta} - 1}{\lambda_2(\xi)\theta}\right\}, \quad t > 0 \tag{2.3}$$

and

$$\lambda_{1,2}(\xi) = \frac{1}{2\tau_q}\left[-\left(1 + \alpha\tau_T|\xi|^2\right) \pm \sqrt{\left(1 - \alpha\tau_T|\xi|^2\right)^2 + 4\alpha(\tau_T - \tau_q)|\xi|^2}\right] \tag{2.4}$$

are the characteristic values (the plus sign corresponds to λ_1). Note that, if $\tau_q \leqslant \tau_T$, the characteristic values are real, otherwise, if $\tau_q > \tau_T$, there are two intervals on the real line, symmetric with respect to the origin, where the characteristic values are complex conjugate.

The asymptotic behavior of the characteristic values is described by

$$\lambda_1(\xi) = -\frac{1}{\tau_T} + O\left(\frac{1}{|\xi|^2}\right) \quad \text{as} \quad \xi \to \infty,$$

$$\lambda_2(\xi) = -\frac{\alpha\tau_T}{\tau_q}|\xi|^2 + O(1) \quad \text{as} \quad \xi \to \infty.$$

Therefore, the asymptotic behavior of the Fourier transform of the solution with respect to ξ is described by