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High order accurate dual-phase-lag numerical model for microscopic heating in multiple domains☆

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ABSTRACT

In this article, a characteristic-based dual-phase-lag numerical model based on finite difference method has been developed to predict the microscopic heating response in time as well as consideration of the micro-structured effect. High-order TVD (Total Variation Diminishing) schemes being oscillation-free can yield high-order accurate solutions without introducing wiggles and therefore are utilised in this work. A multi-domain approach integrated within the dual-phase-lag numerical model allows the computation of microscopic conjugate heat transfer problems. Effects of different phase-lag values on the behaviour of heat transfer are investigated. The model is capable of predicting temperature patterns transiting from the wave nature of heat propagation to additional diffusion being experienced within different solid regions via phonon–electron interaction or phonon scattering.

1. Introduction

In many engineering applications, heat conduction can be aptly described by the classical diffusion theory, which generally assumes that any thermal disturbance will cause an instantaneous response throughout the object, and the propagation speed of heat is infinite. However, such an assumption becomes questionable where there are regimes where such a macroscopic consideration is no longer applicable in spatial and/or temporal development of the heat transfer in microscopic problems such as heat conduction in biological materials [1] and layered-film heating in superconductors, fins and reactor walls [2].

A range of modified heat conduction models have been proposed to resolve microscopic heating problems. Cattaneo [3] and Vernotte [4] proposed a macroscopic thermal wave model to predict the finite speed of thermal propagation. The limitation of this model is that it only contributes to a microscopic response in time without the consideration of the micro-structured effect. Pioneered by Anisimov et al. [5], and advanced by Qiu and Tien [6], the two-step model, which modifies the phenomenological of the thermal wave model, captures nonetheless the fast transient heating behaviour as two separate stages: radiation energy deposited on electrons and energy exchange between electrons and the lattice. Compared to the two-step model where its emphasis is on metal films, the phonon scattering model (pure phonon scattering model) as proposed by Guyer and Krumhansl [7] focuses on the heat transport by phonon scattering. Such a model has been used to evaluate the thermal behaviour of a dielectric solid. To better shed light on the mechanism of non-equilibrium thermodynamic transition and the energy exchange in describing the microscopic heat phenomenon both in time and space, i.e. both for metal and dielectric, Tzou [8] developed a dual-phase-lag (DPL) model to depict the transient thermal phenomenon. Through the introduction of two lumped time parameters, this model accounts for the lagging behaviour caused by phonon–electron interaction in metals and the phonon scattering in dielectric media.

Significant efforts have been concentrated on the development of an explicit mathematical solution of the DPL model. Tzou et al. [9] solved the one-dimensional initial-boundary value problem with the initiation of a surface temperature-jump and numerically computed the inverse Laplace transformation integral with Riemann sum approximation. Liu et al. [10] also addressed the transient phenomenon in pulsed-laser-induced heating for nanoshell-based hyperthermia through Laplace inversion and Riemann sum approximation. Tang and Araki [11] attained the temperature distribution in a finite slab with an energy source near the surface via the Green's function method and finite integral transformation technique. These analytical solutions to the DPL heat conduction have nonetheless been obtained through very simple initial-boundary value problems. Strictly speaking, the intrinsic complexity of the DPL heat conduction equation (high-order mixed derivative with respect to space and time) poses a major obstacle towards the attainment of a

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general solution. Also, whenever a complicated geometry or a variable physical property is involved, a numerical solution is deemed to be the most appropriate (and perhaps in some circumstances the only) option.

The present study employs a purely numerical explicit TVD (total-variation-diminishing) scheme which has been developed based on the proposed model by Shen and Zhang [12] for a single-domain analysis. In contrast to Shen and Zhang [12] who have formulated their governing equations using dimensionless characteristic variables, the present work presents an extension of this methodology to multi-domain and formulation in terms of dimensional characteristic variables in order to clearly highlight the physical significance of the governing equations. Based on the assessment by Yang [13] on various TVD schemes to predict the thermal wave propagation, it can be been shown that TVD schemes were able to provide oscillation-free and accurate numerical results. Third-order TVD schemes are considered and explored in this present study.

2. Mathematical formulation

In order to account for the microscopic effect such as the phonon–electron interaction, the DPL model for heat transfer introduces two phase lags or lumped time parameters, also known as the relaxation times, to both heat flux and temperature gradient. The corresponding macro-scale lagging behaviour can be described as:

$$\boldsymbol{q}(\boldsymbol{R}, t+t_q) = -k\nabla T(\boldsymbol{R}, t+t_T). \tag{1}$$

The above equation constitutes that the temperature gradient being established at a position $\boldsymbol{R}$ at time $t+t_T$ causes the heat to propagate at a different instant of time $t+t_q$.

From a mathematical viewpoint, the heat flux precedes the temperature gradient when $t_q<t_T$, whereas the temperature gradient precedes the heat flux for $t_q>t_T$. From a physical viewpoint, the case of $t_q<t_T$ presents the premise of unacceptable conclusions as it has been argued by Zhou et al. [14] that the DPL model may violate the second law of thermodynamics implying that heat can spontaneously flow from a low-temperature to a high-temperature. However, the specific case of $t_q<t_T$ especially for ultrafast pulse-laser heating can be considered since such phenomenon can be corroborated by the non-equilibrium entropy production theory [15]. Taking a first order Taylor series expansion on both sides of Eq. (1) with reference to time t yields

$$\boldsymbol{q}(\boldsymbol{R}, t)+t_q\frac{\partial \boldsymbol{q}}{\partial t}(\boldsymbol{R}, t) = -k\left[\nabla T(\boldsymbol{R}, t)+t_T\frac{\partial}{\partial t}(\nabla T(\boldsymbol{R}, t))\right]. \tag{2}$$

The energy conservation with constant properties can be written as

$$\rho C_p\frac{\partial T}{\partial t}(\boldsymbol{R}, t) = -\nabla\cdot\boldsymbol{q}(\boldsymbol{R}, t)+Q(\boldsymbol{R}, t) \tag{3}$$

Taking the grad of Eq. (3) yields

$$\rho C_p\frac{\partial}{\partial t}(\nabla T(\boldsymbol{R}, t)) = -\nabla[\nabla\cdot\boldsymbol{q}(\boldsymbol{R}, \boldsymbol{t})]+\nabla Q(\boldsymbol{R}, t). \tag{4}$$

Comparing with the classical diffusion ($t_q=t_T=0$), the phase lag of the heat flux is responsible for the wave nature of the non-Fourier heat transfer. On the other hand, the phase lag of the temperature gradient t_T brings an additional diffusion-like feature into the thermal wave equation ($t_q\neq 0$ and $t_T=0$).

For one-dimensional problems, Eqs. (2)–(4) take the form in the Cartesian coordinate system as

$$\rho C_p\frac{\partial T}{\partial t}(x, t) = -\frac{\partial q}{\partial x}(x, t)+Q(x, t) \tag{5}$$

$$q(x, t)+t_q\frac{\partial \boldsymbol{q}}{\partial t}(x, t) = -k\left[\frac{\partial T}{\partial x}(x, t)+t_T\frac{\partial(\nabla T(x, t))}{\partial t}\right] \tag{6}$$

$$\rho C_p\frac{\partial}{\partial t}(\nabla T(x, t)) = -\frac{\partial^2 q}{\partial x^2}(x, t)+\frac{\partial Q}{\partial x}(x, t) \tag{7}$$

and in the Spherical coordinate system as

$$\rho C_p\frac{\partial T}{\partial t}(r, t) = -\frac{1}{r^2}\frac{\partial(r^2\boldsymbol{q})}{\partial r}(r, t)+Q(r, t) \tag{8}$$

$$q(r, t)+t_q\frac{\partial \boldsymbol{q}}{\partial t}(r, t) = -k\left[\frac{\partial T}{\partial r}(r, t)+t_T\frac{\partial(\nabla T(r, t))}{\partial t}\right] \tag{9}$$

$$\rho C_p\frac{\partial}{\partial t}(\nabla T(r, t)) = -\frac{\partial}{\partial r}\left[\frac{1}{\boldsymbol{r}^2}\frac{\partial(\boldsymbol{r}^2\boldsymbol{q})}{\partial \boldsymbol{r}}(\boldsymbol{r}, \boldsymbol{t})\right]+\frac{\partial Q}{\partial r}(r, t) \tag{10}$$

or

$$\rho C_p\frac{\partial T}{\partial t}(r, t) = -\frac{\partial \boldsymbol{q}}{\partial r}(r, t)-\frac{2\boldsymbol{q}}{r}(r, t)+Q(r, t) \tag{11}$$

$$q(r, t)+t_q\frac{\partial \boldsymbol{q}}{\partial t}(r, t) = -k\left[\frac{\partial T}{\partial r}(r, t)+t_T\frac{\partial(\nabla T(r, t))}{\partial t}\right] \tag{12}$$

$$\rho C_p\frac{\partial}{\partial t}(\nabla T(r, t)) = -\frac{\partial^2 q}{\partial r^2}(r, t)-\frac{2}{r}\frac{\partial \boldsymbol{q}}{\partial r}(r, t)+\frac{2\boldsymbol{q}}{r^2}(r, t)+\frac{\partial Q}{\partial r}(r, t). \tag{13}$$

For the sake of brevity, the above equations can be written in vector form as

$$\frac{\partial \boldsymbol{E}}{\partial t}+A\frac{\partial \boldsymbol{E}}{\partial \xi} = \boldsymbol{S}. \tag{14}$$

In the Cartesian coordinate system, where $\xi=x$,

$$E = \begin{bmatrix}\sqrt{\rho C_p}\;T\\ \sqrt{\frac{t_q}{\boldsymbol{k}}}\;q\end{bmatrix},\quad A = \begin{bmatrix}0 & \sqrt{\frac{k}{\rho C_p t_q}}\\ \sqrt{\frac{k}{\rho C_p t_q}} & 0\end{bmatrix},$$
$$S = \begin{bmatrix}\frac{Q}{\sqrt{\rho C_p}}\\ -\frac{\boldsymbol{q}}{\sqrt{kt_q}}-\sqrt{\frac{\boldsymbol{k}}{t_q}}t_T\frac{\partial(\nabla T(r, t))}{\partial t}\end{bmatrix}. \tag{15}$$

In the Spherical coordinate system, where $\xi=r$,

$$E = \begin{bmatrix}\sqrt{\rho C_p}\;T\\ \sqrt{\frac{t_q}{\boldsymbol{k}}}\;q\end{bmatrix},\quad A = \begin{bmatrix}0 & \sqrt{\frac{k}{\rho C_p t_q}}\\ \sqrt{\frac{k}{\rho C_p t_q}} & 0\end{bmatrix},$$
$$S = \begin{bmatrix}-\frac{1}{\sqrt{\rho C_p}}\frac{2\boldsymbol{q}}{r}+\frac{Q}{\sqrt{\rho C_p}}\\ -\frac{\boldsymbol{q}}{\sqrt{kt_q}}-\sqrt{\frac{\boldsymbol{k}}{t_q}}t_T\frac{\partial(\nabla T(r, t))}{\partial t}\end{bmatrix} \tag{16}$$

In Eq. (15), it should be noted that $\frac{\partial(\nabla T(x,t))}{\partial t}$ is determined from the right hand side of Eq. (7). Analogously, $\frac{\partial(\nabla T(r,t))}{\partial t}$ in Eq. (16) is determined