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Effect of boundary phonon scattering on Dual-Phase-Lag model to simulate micro- and nano-scale heat conduction

J. Ghazanfarian, A. Abbassi *

Amirkabir University of Technology, Mechanical Engineering Department, P.O. Box 15916-34311 Tehran, Iran

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ABSTRACT

In this paper, one-dimensional heat conduction within a thin slab for Knudsen numbers more than 0.1 is implemented using the Dual-Phase-Lag (DPL) model including phonon scattering boundary condition. The Dual-Phase-Lag equation is solved with a stable and convergent finite difference scheme. Also the Laplace transformation technique is employed to solve DPL equation analytically. The results show that in the smaller values of Knudsen number, the results of the DPL model lay very close to the solution of the Boltzmann equation. Also, it is shown that moving towards the steady state, the DPL model reduces to the Cattaneo and Vernotte (CV) model and has results more accurate than the Ballistic-Diffusive Equations (BDE). It is also shown that the temperature distribution is closer to the results of Boltzmann equation relative to the heat flux distribution. Due to the simplicity of derivation of the DPL model formulation and its possibility for developing to higher dimensions, using the DPL model with new boundary condition is recommended to simulate nano- and micro-scale heat conduction. To investigate the accuracy of the DPL model, its results are compared with the results obtained from BDE model, and Boltzmann equation.

1. Introduction

The problem of self-heating in micro-electronic devices or for situations involving very low temperature near absolute zero, heat source, such as laser, heat is found to propagate at a finite speed. The solution of the Boltzmann equation is the most accurate option to model heat transfer in such problems. However, the Boltzmann equation is too difficult to solve in general, so many other models have been proposed so far to take into account the finite speed of heat propagation and the effects of boundaries.

One of the best approximations of Boltzmann equation is Ballistic-Diffusive Equations (BDE) derived by Chen [1] in which the heat transfer is divided at any point into two parts, one represents the ballistic nature of heat conduction originating from the boundary scattering of heat carriers, and the other characterizes the diffusive behavior with heat flux time-lag phenomenon taken into account only. The BDE approximation shows a good agreement with Boltzmann equation in both one and two-dimensional problems as shown by Chen et al. [2,3].

Another well-known approximation of non-Fourier heat conduction is the Dual-Phase-Lag (DPL) model first proposed by Tzou [4,5]. This model considers only the effect of finite relaxation time by using the heat flux and temperature phase lags where the former is caused by micro structural interactions such as phonon scattering and the latter is interpreted as the relaxation time due to fast-transient effects of thermal inertia [6]. However, in many problems the Cattaneo and Vernotte (CV) model is applied in which the temperature phase lag is omitted.

In recent years, utilization of Dual-Phase-Lag model to simulate heat transfer in micro- or nano-structures has been considered by researchers. One-dimensional problem of heat conduction for the Knudsen numbers more than 0.1 corresponding to nano-structures was implemented by Basirat et al. [7] using the Dual-Phase-Lag (DPL) model and its special case, CV model as well as the Fourier law. In this paper their results were compared with the results obtained from the BDE model, which considered being an accurate approximation of the Boltzmann equation. It is observed that in Knudsen numbers of order of one, the DPL model, including the real value of the ratio of the temperature to the heat flux time lag, leads to better results than the CV model. This ratio is considered to be equal to zero while in the greater values of Knudsen number, there is no advantage between two approaches. In the smaller values of Knudsen number the results obtained from the DPL and CV models match to each other, and lay very close to the results obtained from the Fourier law.

The transient thermal behavior of a stagnant gas confined in a horizontal micro-channel was studied analytically under the effect of the Dual-Phase-Lag heat conduction model by Al-Nimr and

* Corresponding author. Tel.: +98 (21)64543425.
E-mail addresses: j.ghazanfarian@aut.ac.ir (J. Ghazanfarian), abbassi@aut.ac.ir (A. Abbassi).

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Nomenclature

B	phase-lag ratio	Γ	mean free path of careers, m
k	heat conduction coefficient, W/m °C	ρ	density, kg/m^3
L	length, m	η	non-dimensional coordinate
T	temperature, K	τ	relaxation time, s
x	direction, m		
C_P	specific heat, J/kg °C	*Superscript*	
Kn	Knudsen number	$*$	non-dimensional condition
q	heat flux, W/m^2		
t	time, s	*Subscript*	
		b	ballistic
Greek		q	heat flux
α	BC coefficient and thermal diffusion coefficient, m^2/s	m	diffusive
θ	non-dimensional temperature	t	gradient temperature

Khadrawi [9]. The effects of the Knudsen number Kn, the thermal relaxation time τ_q, and the thermal retardation time τ_t on the micro-channel thermal behavior were investigated using three heat conduction models. It was found that the deviations between the predictions of the parabolic and the hyperbolic models are insignificant. On the other hand, the deviations between the parabolic and Dual-Phase-Lag models are significant under the same operating conditions. In the other study, Khadrawi and Al-Nimr considered the unsteady hydrodynamics and thermal behavior of fluid flow in an open-ended vertical parallel-plate micro-channel semi-analytically under the effect of the Dual-Phase-Lag heat conduction model [8]. However, attempts to simulate one-dimensional heat conduction in micro- and nano-scale geometries have been led to unsatisfying results.

In order to achieve a general model for micro- and nano-scale heat conduction, in this paper, a new boundary condition is developed to use along with DPL model to improve the obtained results of micro- and nano-scale heat conduction. So, heat transfer regimes for a thin slab has been analyzed by using different values for Knudsen number which enables a comparison between the results of DPL model with new boundary condition and the BDE model. The results are developed for relaxation time ratios between 0.0, the case of CV, to 0.1, and for Knudsen numbers from 0.1 to 10 to find how accurate the prediction of DPL model responses in the heat conduction of micro- and nano-structures.

2. Mathematical modeling

Cattaneo [10] and Vernotte [11] suggested independently a modified heat flux model in the form (CV model),

$$\vec{q}(t+\bar{\tau}_q,\vec{r}) = -k\vec{\nabla}T(t,\vec{r}), \tag{1}$$

where $\vec{q}$ is the heat flux vector, k is the thermal conductivity, and $\bar{\tau}_q$ is the phase-lag in the heat flux vector. The constitutive law of Eq. (1) assumes that the heat flux vector (the effect) and the temperature gradient (the cause) across a material volume occur at different instants of time, and the time delay between the heat flux and the temperature gradient is the relaxation time $\bar{\tau}_q$.

In 1995 Tzou [4] proposed a non-Fourier approximation for heat conduction in which the heat flux vector at a point in material at time $t+\tau_q$ corresponds to the temperature gradient at the same point at time $t+\tau_t$, or:

$$\vec{q}(t+\bar{\tau}_q,\vec{r}) = -k\vec{\nabla}T(t+\bar{\tau}_T,\vec{r}), \tag{2}$$

where $\bar{\tau}_q$ and $\bar{\tau}_t$ stand for the heat flux and temperature gradient phase lags, respectively, both are positive and intrinsic properties of the material. Values of the two phase lags like the thermal conductivity and the thermal diffusivity must be determined experimentally and were tabulated for engineering materials under various conditions, including the elevated temperature and the same medium with different microstructures. Tzou [5] has presented some analytical correlations and Basirat et al. [7] have reported values for phase lags corresponding to some metal films.

Using Taylor series expansion of Eq. (2) with respect to time yields:

$$q+\tau_q\frac{\partial q}{\partial t} = -k\frac{\partial T}{\partial x} - \tau_t\frac{\partial^2 T}{\partial t\partial x}. \tag{3}$$

Eq. (3) is combined with the energy equation:

$$-\frac{\partial q}{\partial x} = c\frac{\partial T}{\partial t}, \tag{4}$$

where c is specific heat of the material. Eliminating of the heat flux between above equations, lead to the heat conduction equation under the DPL effect:

$$\frac{\partial T}{\partial t}+\tau_q\frac{\partial^2 T}{\partial^2 t} = \frac{k}{c}\left(\frac{\partial^2 T}{\partial^2 x}+\tau_t\frac{\partial^3 T}{\partial t\partial^2 x}\right). \tag{5}$$

The Dual-Phase-Lag model allows either the temperature gradient (cause) to precede the heat flux vector (effect) or the heat flux vector (cause) to precede the temperature gradient (effect) in the transient process. There are actually three characteristic times involved in the DPL model. The instant of time $(t+\tau_t)$ at which the temperature gradient is established across a metal volume, $(t+\tau_q)$ for the onset of the heat flow, and the time for the occurrence of the heat transfer. It is Obvious that Eq. (5) is reduced to the CV equation in the case of $\tau_t = 0$. It should be noted that the DPL model is capable of taking about solids, liquids and gases.

To obtain the normalized equations, the following non-dimensional parameters were considered:

$$\theta = \frac{T-T_0}{T_w-T_0}, \quad t^* = \frac{t}{\tau_q}, \quad B = \frac{\tau_t}{\tau_q}, \quad \eta = \frac{x}{L} \quad Kn = \frac{\lambda}{L}, \tag{6}$$

where λ and L are the mean molecular mean free path and characteristic length, respectively.

Now, Eq. (5) can be rewritten as:

$$\frac{\partial\theta}{\partial t^*}+\frac{\partial^2\theta}{\partial^2 t^*} = \frac{Kn^2}{3}\frac{\partial^2\theta}{\partial^2\eta}+B\frac{Kn^2}{3}\frac{\partial^3\theta}{\partial t^*\partial^2\eta}. \tag{7}$$

As explained before, Chen [1] developed one-dimensional Ballistic-Diffusive Equations for phonons which for simplicity was not included here. In the next section, the results of this model will be used to verify the accuracy of results of our new model.

2.1. New boundary condition

All phase-lag models mentioned in the previous sections, were supposed to be solved with no temperature jumps on the boundaries. Since, the DPL model neglects the effects of boundary phonon scattering, obtained results with imposing no-jump boundary condition lead to unsatisfying results especially near the boundaries. In this section it is to propose a new boundary condition in which the boundaries are allowed to include temperature jump. The new boundary condition to use along with the DPL model is as follows;

$$\theta_s - \theta_w = -\alpha Kn\left(\frac{\partial\theta}{\partial n^*}\right)_w \tag{8}$$

where θ_s is the wall's jumped temperature, θ_w is the boundary temperature, and α is a coefficient which should be tuned. Values of two unknown parameters α and B, should be determined in a way that results of the DPL model coincides with the solution of the Boltzmann equation. It was interesting that values of these parameters were turned out to be independent of the Knudsen number and merely vary with time and can be computed from Eqs. (9) and (10).

$$B = \begin{cases} 0 & t^* > 1 \\ 0.1t^* & t^* \leqslant 1 \end{cases} \tag{9}$$

$$\alpha = \begin{cases} 0.5 & t^* > 0.1 \\ 0.7t^* & t^* \leqslant 0.1 \end{cases} \tag{10}$$

It is worth noting that these equations stem from numerical results and are appropriate for engineering applications, so they have no specific mathematical derivations. Since $\tau_q > \tau_t$, the temperature gradient precedes heat flux vector in the process of heat transport. However, using these constants along with the Dual-Phase-Lag model helps us to model heat transfer phenomenon in small structures with many time scales only with two time scales.

From Eqs. (9) and (10), it was obvious that for the initial time periods and by moving towards the steady state, the CV model as a special case of DPL model has been achieved with $\alpha = 0$ and $\alpha = \frac{1}{2}$, respectively. It means that the DPL model and the CV model are used to simulate transient and steady state behavior of the micro- and nano-scale heat conduction, respectively. In addition, in the limiting case for $\alpha = 0$ the new boundary conditions changes to no-slip boundary condition. So, by marching in time the value of α increases. It means that in initial times, mixed boundary condition alters to no-slip condition, but by the increase in time, definition of the new boundary condition is more vital.

Important limitations of this model are constant physical properties such as thermal conductivity, thermal diffusivity, and phase lags, one dimensionality, no heat source, and iso-temperature boundary condition.

3. Numerical solution

To solve Eq. (5) a second order fully implicit finite difference scheme was used in which discretization of all derivatives was central. In this way, a stable and convergent three-level finite difference scheme has been used which was introduced by Dai et al. [12]. It should be pointed out that in this method; a weighted average was used for stability and convergence. It was observed that the convergence of the numerical method was improved by decreasing Knudsen number, so that at high Kn numbers the solution strongly depends on the marching step size. In addition, a mesh independency test has been carried out in order to investigate numerical convergence of the results in all above cases which are not included in the paper.

4. Analytical solution

In this section, Eq. (7) with boundary condition (8) are solved by using the Laplace transformation technique. Now, with the notation that $L\{\theta(t^*,\eta)\} = F_T(s,\eta)$, the Laplace transformation of Eqs. (7) and (8) yields:

$$s^2F_T + sF_T = \frac{Kn^2}{3}\frac{d^2F_T}{d\eta^2} + Bs\frac{Kn^2}{3}\frac{d^2F_T}{d\eta^2}, \tag{11}$$

$$\eta = 0; \quad F_T - \frac{1}{s} = Kn\alpha\frac{dF_T}{d\eta},$$

$$\eta = 1; \quad F_T = -Kn\alpha\frac{dF_T}{d\eta}. \tag{12}$$

According to the boundary conditions, Eq. (11) is solved to give;

$$F_T = C_1\sinh(A\eta) + C_2\cosh(A\eta), \tag{13}$$

where

$$A = \sqrt{\frac{s(1+s)}{\frac{Kn^2}{3}(1+Bs)}},$$

$$C_1 = -\frac{1}{s}\frac{\cosh(A) + Kn\alpha A\sinh(A)}{\sinh(A)(1+Kn^2\alpha^2A^2) + 2Kn\alpha A\cosh(A)},$$

$$C_2 = \frac{1}{s}\frac{\sinh(A) + Kn\alpha A\cosh(A)}{\sinh(A)(1+Kn^2\alpha^2A^2) + 2Kn\alpha A\cosh(A)}. \tag{14}$$

Eq. (13) is inverted in terms of the Riemann-sum approximation as

$$\theta(t^*,\eta) = \frac{e^{\epsilon t^*}}{t^*}\left\{\frac{1}{2}F_T(\epsilon,\eta) + Re\left[\sum_{n=1}^{N}F_T\left(\epsilon + \frac{in\pi}{t^*},\eta\right)(-1)^n\right]\right\}, \tag{15}$$

where Re refers to the "real part of" and $i^2 = -1$ is the imaginary number, N is the number of terms used in the Riemann-sum approximation, and ϵ is the real part of the Bromwich contour that is used in inverting Laplace transforms. The Riemann-sum approximation for the Laplace inversion involves a single summation for the numerical process. For faster convergence, however, numerous numerical experiments have shown that a value which satisfies the relation $\epsilon t^* = 1.3$, gives the most satisfactory results [9].

5. Results and discussions

The numerical simulation of the above equations are presented in Figs. 1–3. The non-dimensional temperature and heat flux distribution from the two models including the BDE and the DPL model, and the Boltzmann equation has been shown in the right and the left columns, respectively. In all cases, the DPL model is presented with certain ratio of temperature phase lag to heat flux phase lag, or B and α which could be computed from Eqs. (9) and (10). It is worth noting that based on the work of Chen [1], the BDE model is considered as an accurate approximation of Boltzmann equation in the range of time and Knudsen numbers in which the problem is solved. Verification of the results is based on the results obtained from the solution of Boltzmann equation.

Fig. 1 shows the non-dimensional temperature and heat flux from mentioned models for the Knudsen number of 0.1. Since, the propagation of energy into the solid material is so slow and also in order to produce observable temperature distribution, in this case results are presented for long periods of time. It is evident that for $Kn = 0.1$ the DPL model has shown better agreement, in all points, with the BDE model especially near the boundaries which are so important in present analysis. By comparison of the results of Boltzmann equation [1] with predictions of DPL model, it is also seen that at the non-dimensional time of $t^* = 100$, the prediction of DPL model with new boundary condition is more accurate than BDE results. So that, the undesirable curvature noticed in BDE

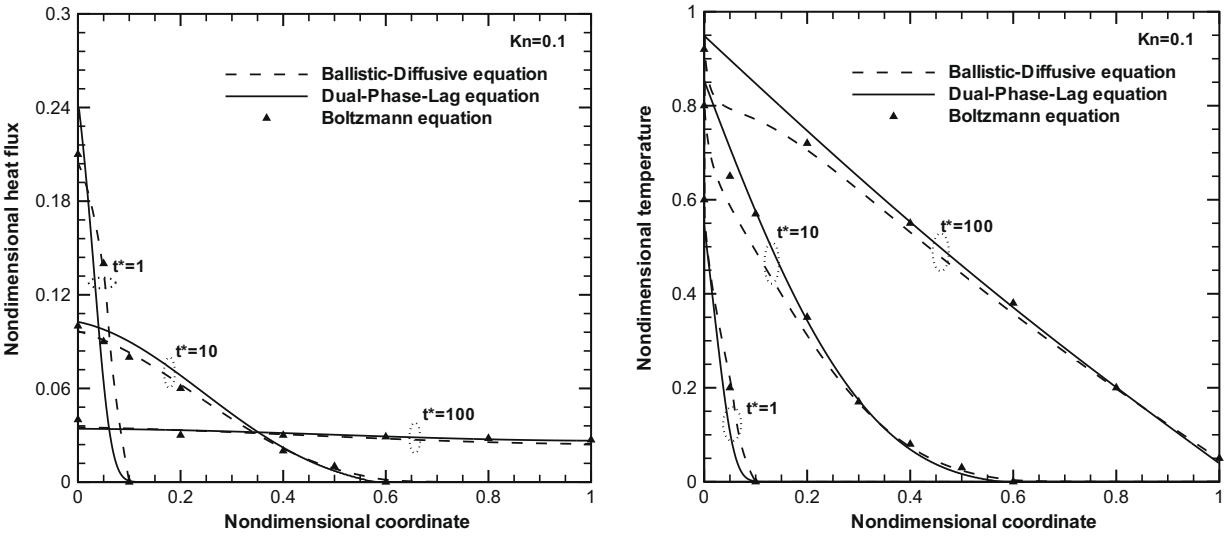

Fig. 1. Comparison of temperature (right column) and heat flux (left column) distribution obtained from BDE model and DPL with new boundary condition for different instantaneous times and $Kn = 0.1$.

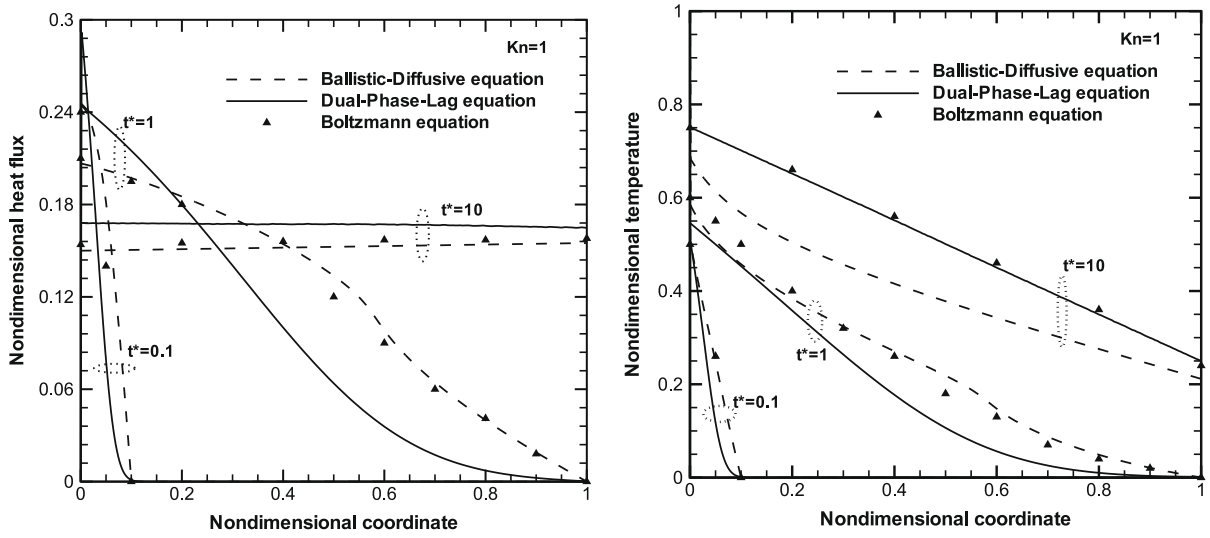

Fig. 2. Comparison of temperature (right column) and heat flux (left column) distribution obtained from BDE model and DPL with new boundary condition for different instantaneous times and $Kn = 1$.

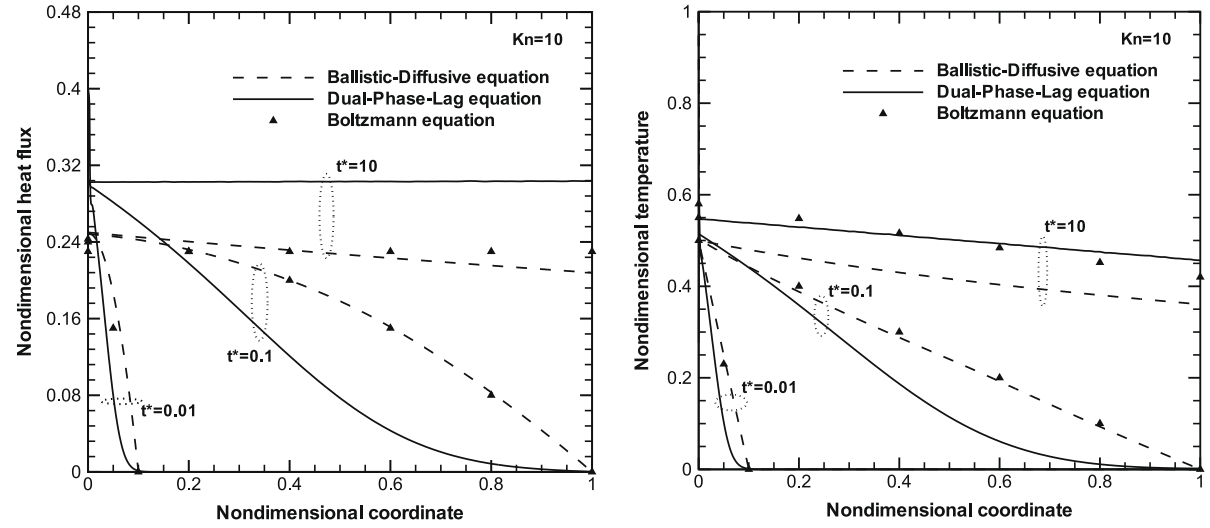

Fig. 3. Comparison of temperature (right column) and heat flux (left column) distribution obtained from BDE model and DPL with new boundary condition for different instantaneous times and $Kn = 10$.

results in the vicinity of the left boundary is omitted by the aim of DPL model. As mentioned before, moving towards the steady state, proposed DPL model has been reduced to CV model. The DPL model has also shown good agreement in all points with the BDE model in order to predict the heat flux value.

Fig. 2 compares the temperature and heat flux distribution obtained from the models for the Knudsen number of 1 corresponding to micro-scale heat conduction. Similar to the Knudsen number of 0.1 by marching in time, the accuracy of DPL model prediction increases relative to the BDE model. Also, it is noticed that the accuracy of prediction of heat flux has been decreased by increase in the Knudsen number. It should be mentioned that by changing coefficients α and B, better agreement can be obtained. But, in order to have unique coefficients for various cases an optimum coefficient tuning has been performed. So, this model needs an extra modification for heat flux to agree well with exact results.

In order to investigate nano-scale heat conduction, in Fig. 3 the Knudsen number has been increased to 10. It is seen that the disagreement between the BDE and the DPL models is more considerable especially for heat flux computation. In spite of this fact, due to the simplicity of derivation of the DPL model formulation and its possibility of developing to the higher dimensions, using the DPL model with the new boundary condition is recommended by the authors to simulate the nano- and micro-scale heat conduction. As is obvious from Figs. 1–3, the steady state temperature and heat flux distribution turned out to be linear. So, in all above cases for different Kn numbers, it is easy to present a compact formula for steady state temperature and heat flux distribution for the design purposes of micro-electro-mechanical systems (MEMS).

Comparing analytical and numerical results, non-dimensional temperature distribution for three different Knudsen numbers has been plotted in Fig. 4. From this figure, it is obvious that the analytical solution coincides with numerical results perfectly which verifies the numerical results. The discrepancy of numerical and analytical results is expectable and stems from the numerical error of computing the inverse Laplace transformation and spatial and temporal truncation errors in finite difference scheme.

6. Conclusion

This paper established a new boundary condition for transient DPL equations of heat conduction, which was divided in two cases of the CV equation and the general DPL equation with non-zero ra-

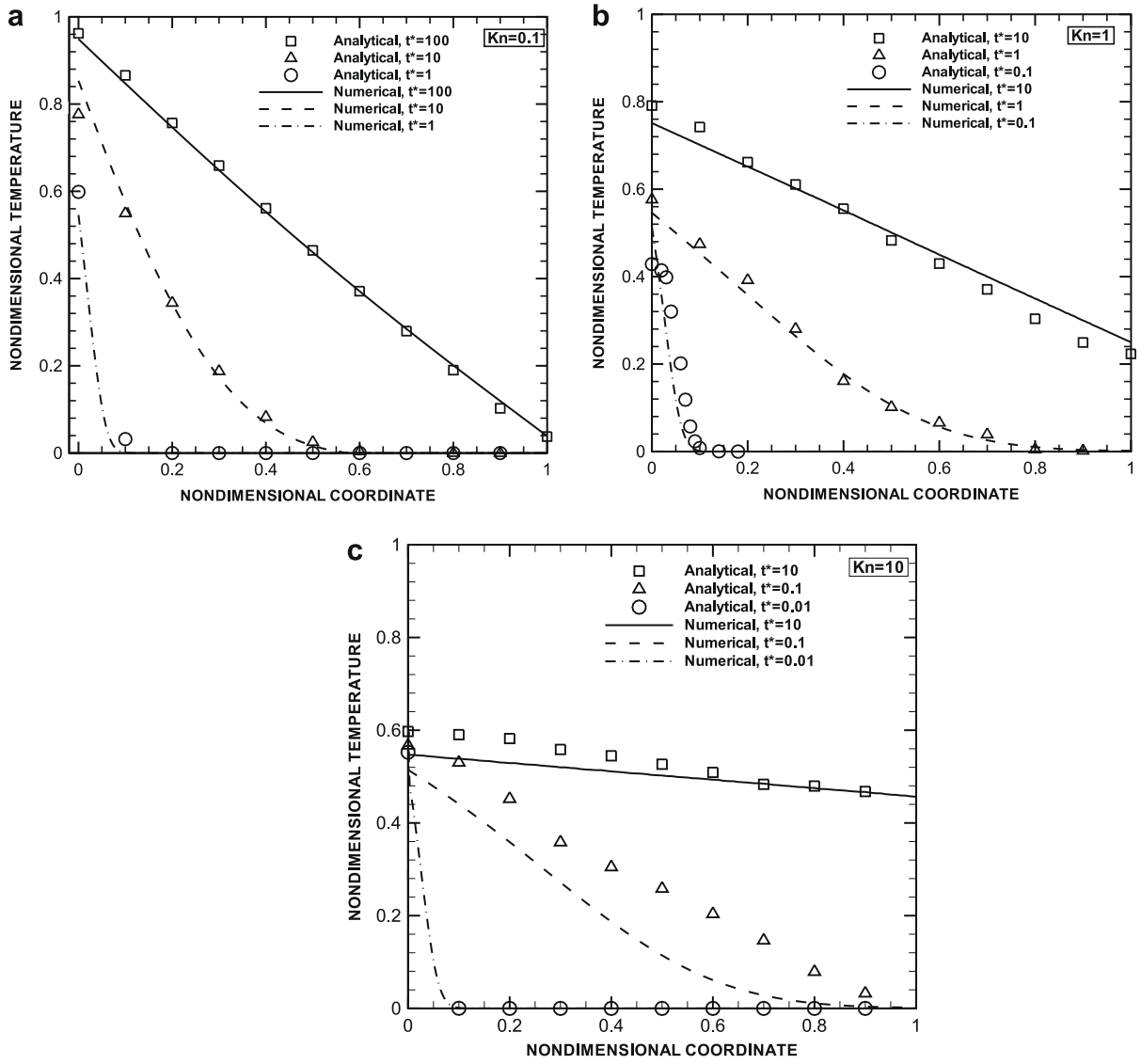

Fig. 4. Comparison of temperature distribution obtained from the numerical and analytical methods for different times and (a) $Kn = 0.1$, (b) $Kn = 1$, (c) $Kn = 10$.

tio of time lags, for the Knudsen numbers more than 0.1 corresponding to micro- and nano-scale geometries.

Computational results of this model applied to a thin slab were compared with the results obtained from Ballistic-Diffusive Equations and Boltzmann equation. Since, the new boundary condition considers the effects of the boundary phonon scattering, good agreement between the BDE and the DPL models was observed in the vicinity of the boundaries as well as the part of the domain that is far from the boundaries. This agreement was not seen by employing no-jump boundary condition. It was shown that moving towards the steady state, the CV model as an especial case of the DPL model with temperature jump ($\alpha = \frac{1}{2}$), could be used and has the results much more accurate than the BDE model. But, for initial time steps, employing the DPL model with non-zero temperature gradient phase lag is essential. It was also noticed that by solving DPL model the predictions of the temperature distribution with respect to the BDE results was improved much more than the heat flux distribution.

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