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IMPLEMENTATION OF DUAL-PHASE LAG MODEL AT DIFFERENT KNUDSEN NUMBERS WITHIN SLAB HEAT TRANSFER

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ABSTRACT

One dimensional problem of heat conduction for the Knudsen numbers more than 0.1 corresponding to nano-structures is implemented utilizing the Dual-Phase-Lag (DPL) model and its special case, Cattaneo and Vernotte (CV) model as well as the Fourier law. The results are compared with the results obtained from the Ballistic-Diffusive Equations (BDE) model, which considered being an accurate approximation of the Boltzmann equation. It is observed that in Knudsen numbers of order one, the DPL model, with considering the real value of the ratio of temperature to heat flux time lag, leads to better results than the CV model in which this ratio is considered to be equal to zero whereas in the greater values of Knudsen number there is no advantage between two approaches. In the smaller values of Knudsen number the curves obtained from the DPL and CV models match to each other, and lay very close to the curves obtained from the Fourier law

Keywords: Dual-phase Lag model, Ballistic-Diffusive equations, Cattaneo and Vernotte model, Nano-scale slap modeling and Simulation

INTRODUCTION

The problem of self-heating in microelectronic 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. Solving the Boltzmann equation is the most correct 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 the finite speed of heat propagation and effects of boundaries into account.

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 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 effect of finite relaxation time by using 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 hyperbolic equation in which the temperature phase lag is omitted is utilized.

So far the advantages of the DPL model over the CV [7, 8] model have been proven in the field of heat transfer in processed meat [9].

The present study develops heat transfer regime maps by using different values for Knudsen number which makes a comparison between results of the DPL and the BDE model, for a thin slab. The results are developed for relaxation time ratios between 0.0, the case of CV, to 0.05, and for Knudsen numbers from 0.1 to 10 to find how accurate the prediction of DPL model response in the heat conduction of nano-structure. Clearly explain the nature of the problem, previous work, purpose, and contribution of the paper.

MATHEMATICAL MODELING

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 $t+t_q$ corresponds to the temperature gradient at the same point at time $t+t_t$, or:

$$q(X,t+t_q) = -k\nabla T(X,t+t_t) \tag{1}$$

where t_q and t_t stand for the heat flux and temperature gradient phase lags respectively, both are positive and intrinsic properties of the material are shown in Table 1.

Using a Taylor series expansion of Eq. (1) respect to t yields:

$$q(X,t)+t_q\frac{\partial q}{\partial t}(X,t) \cong -k\left[\nabla T(X,t)+t_t\frac{\partial}{\partial t}[\nabla T(X,t)]\right] \tag{2}$$

Table 1: Thermal properties of some materials at room temperature [4]

	$k\ (W/mK)$	$t_t\ (ps)$	$t_q\ (ps)$
Cu	386	70.833	0.4348
Ag	419	89.286	0.7438
Au	315	89.286	0.7438
Pb	35	12.097	0.1670

Eq. (3) is combined with energy equation:

$$-\nabla q(X,t) = \rho c_p \frac{\partial T}{\partial t}(x,t) \qquad (3)$$

Eliminating of the heat flux between Eqs. (2) and (3) lead to the heat conduction equation under the DPL effect:

$$\nabla^2 T + \tau_t \frac{\partial}{\partial t}(\nabla^2 T) = \frac{1}{\alpha}\frac{\partial T}{\partial t} + \frac{\tau_q}{\alpha}\frac{\partial^2 T}{\partial t^2}$$
(4)

It is obvious that the Eq. (4) is reduced to CV equation in the case of $t_t = 0$.

BDE model
Chen [2] developed one dimensional Ballistic-Diffusive equation for phonons so that:

$$t\frac{\partial^2 u_m}{\partial t^2} + \frac{\partial u_m}{\partial t} = \frac{k}{rc_p}\frac{\partial u_m}{\partial x^2} - \frac{\partial q_b}{\partial x}$$
(5)

$$T = \frac{1}{rc_p}(u_m + u_b)$$
(6)

$$q_b = \begin{cases} \dfrac{rc_p v\Delta T}{2}\displaystyle\int_{m_t}^{1} m e^{-(x/\Lambda m)} dm + q_{b0}(x,0), 0 \le m_t \le 1 \\ q_{b0}(x,0) \qquad other m \end{cases} \qquad (7)$$

$$m_t = x/(vt)$$

To obtain the normalized equations, the following non-dimensional parameters are suggested:

$$q = \frac{T - T_0}{\Delta T} \quad q^* = \frac{q - q_0}{rc_p v\Delta T} \quad t^* = t/t_q$$
$$B = t_t/t_q h = x/L \quad Kn = \Lambda/L \qquad (8)$$

Now, Eqs. (4) and (2) can be rewritten as:

$$\frac{\partial q}{\partial t^*} + \frac{\partial^2 q}{\partial t^{*2}} = \frac{Kn^2}{3}\frac{\partial^2 q}{\partial h^2} + B\left(\frac{Kn^2}{3}\right)\frac{\partial^3 q}{\partial t^* \partial h^2} \qquad (9)$$

$$q^* + \frac{\partial q^*}{\partial t^*} = -\frac{Kn}{3}\frac{\partial q}{\partial h} - B\frac{Kn}{3}\frac{\partial^2 q}{\partial h \partial t^*} \qquad (10)$$

with the following boundary and initial conditions:

$$h = 0 \quad ,q(0,t^*) = 1, \frac{\partial q}{\partial t}(0,t^*) = 0$$
$$h = 1 \quad ,q(1,t^*) = 0, \frac{\partial q}{\partial t}(1,t^*) = 0 \qquad (11)$$
$$t^* = 0 \quad ,q(h,0) = 0, \frac{\partial q}{\partial t}(h,0) = 0$$

The normalized BDE equations are presented in [2] as:

$$\frac{\partial^2 q_m}{\partial t^{*2}} + \frac{\partial q_m}{\partial t^*} = \frac{Kn^2}{3}\frac{dq_m}{dh^2} - Kn\frac{dq_b^*}{dh}$$
(12)

and:

$$q_b^* = \begin{cases} \dfrac{1}{2}\displaystyle\int_{m_t}^{1} m e^{-(h/Knm)} dm \qquad 0 \le m_t \le 1 \\ 0 \qquad other m \end{cases} \qquad (13)$$

$$q_b = \begin{cases} \dfrac{1}{2}\displaystyle\int_{m_t}^{1} e^{-(x/\Lambda m)} dm + q_{b0}(x,0) \qquad 0 \le m_t \le 1 \\ q_{b0}(x,0) \qquad other m \end{cases} \qquad (14)$$

where

$$q = \frac{T - T_0}{\Delta T}, \quad q_b^* = \frac{q - q_0}{rc_p v\Delta T}, \quad t^* = t/t_q$$
$$m_t = x/(vt), \quad h = x/L, \quad Kn = \Lambda/L \qquad (15)$$

Numerical scheme
Eq.(9) is one of parabolic type. To solve it a second order fully implicit finite difference scheme was used in which discretization of all derivatives was central. The other equations to be solved were that of the BDE model. In this model we are to solve two coupled set of equations. First, Eqs. (13), (14) should be numerically solved. For this, four point Gauss-quadrature integration method was utilized. The results of Eq.(13) was considered as source term in Eq.(12), which is a hyperbolic type equation obtained by adding source terms of ballistic heat conduction to the CV equation. It is observed that the convergence of numerical method is improved by decreasing Knudsen number, so that in high Kn numbers the solution strongly depends on the marching step size.

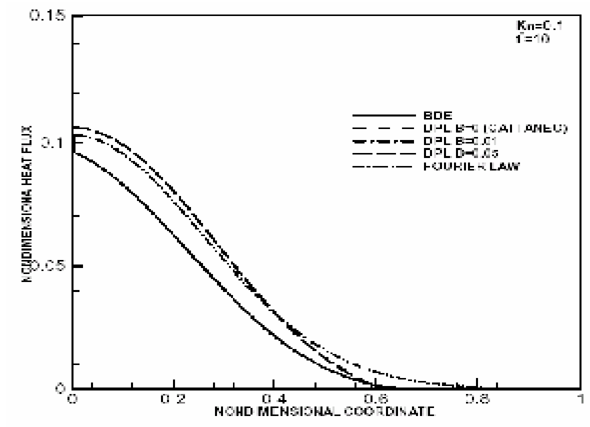
ANALYSIS AND DISCUSSION
The numerical simulations of the above equations are presented in Figs. 1 to 3. Each figure shows the non-dimensional temperature and heat flux distribution from the three models including the Fourier law, the ballistic-diffusive equations, and the Dual Phase Lag model. In all figures the DPL model is presented in three cases each of which represents a certain ratio of temperature phase lag to heat flux phase lag, or *B*. It should be kept in mind that the value of *B* is an intrinsic property of the material, so it is evident that for a certain medium of

heat conduction there is a unique solution of DPL equation.

Here, the DPL model with *B=0,* i.e. the case of less complicated CV model, is compared with the model with non-zero values of *B* to find out the trend of the real ratio of phase lags could affect the results of calculation. It is worth saying that based on the work of Chen [2] 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, so verification is based on the results obtained from other models with the BDE.

Fig. 1 shows the non-dimensional temperature and heat flux from various models for the Knudsen number of 0.1. It is obvious that for this value of Knudsen number the results based on the DPL model with non-zero values of *B* doesn't deviates considerably from that of the CV model. In this case the results of DPL model are very close to that of Fourier law especially the temperature distribution. The DPL model has shown better agreement, in all points, with the BDE model than the Fourier law for the prediction of temperature; however in the prediction of heat flux the DPL model is shown to be closer at the points far from the left boundary.

Figs. 2 and 3 the non-dimensional temperature and heat flux by using various models for Knudsen number of 1 at t*=1 and 2 could be observed. Figs. 2,3(a) show that an abrupt drop in temperature and heat flux is arisen based on the prediction of the DPL model, and this drop makes the attained results closer to the results of the BDE model at the points near the right boundary when compared with the curves of the Fourier law. In this case one could recognize that taking advantage of DPL model with non-zero values of *B* results in a more prediction of both temperature and heat flux distribution. In Figs. 2,3 (b) it could be seen that when moving toward the steady state

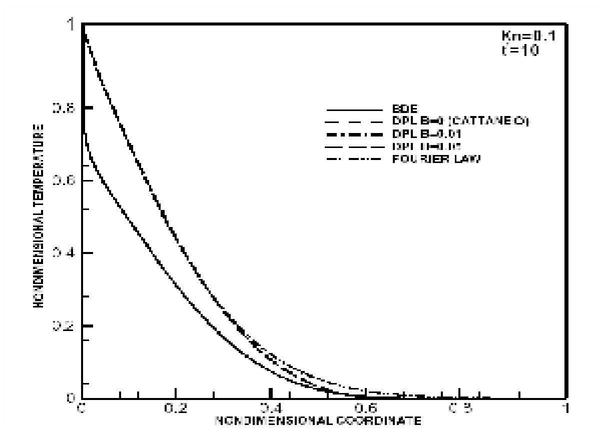


(b)

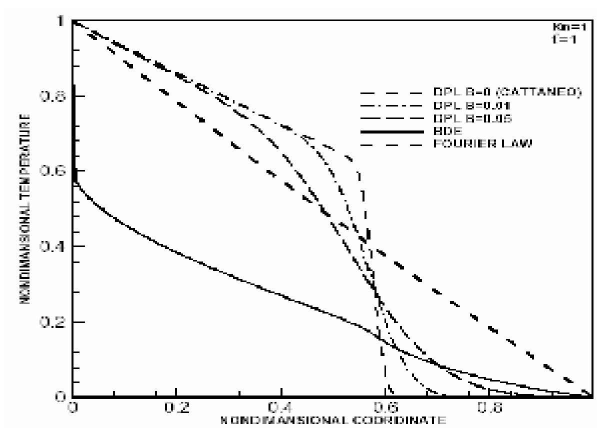
Fig. 1 Comparison of temperature (a) and heat flux (b) distribution obtained from various models for *Kn*=0.1

the DPL model keeps it's advantages over the CV model; however in the prediction of temperature distribution these models are by no means more accurate than the Fourier law.

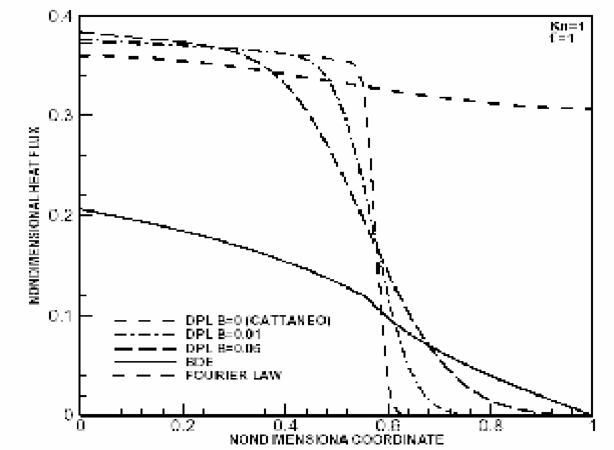
Fig. 4 compares the temperature and heat flux obtained from the models for Knudsen number of 10. In this figure one could simply find out that using both DPL and Fourier equations leads to a large error in the prediction of the temperature and heat flux. This may be interpreted as a result of disregarding the effects of boundaries in DPL model and its special case, the CV model. Like the Figs. 2,3 (b), in this Figs. the DPL results are more accurate compared with the Fourier one only in the prediction of heat flux, and there is no significant advantage for either of models regarding to the temperature. Clearly indicate advantages, limitations, and possible applications.



(a)

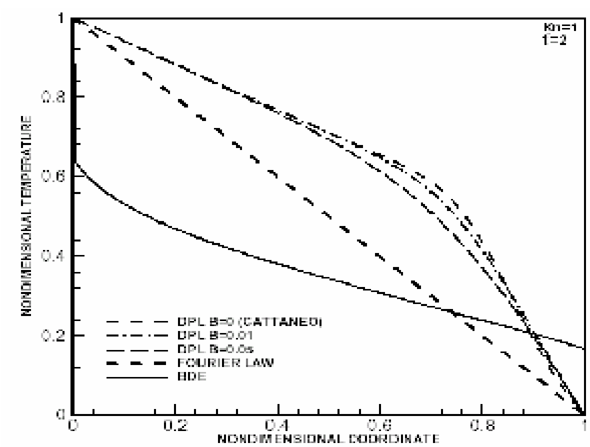


(a)

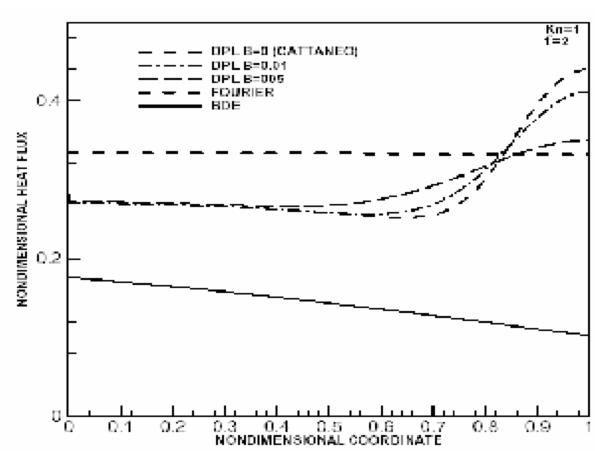


(b)

Fig. 2 Comparison of temperature (a) and heat flux (b) distribution obtained from various models for *Kn*=1 at t^{*}=1



(a)



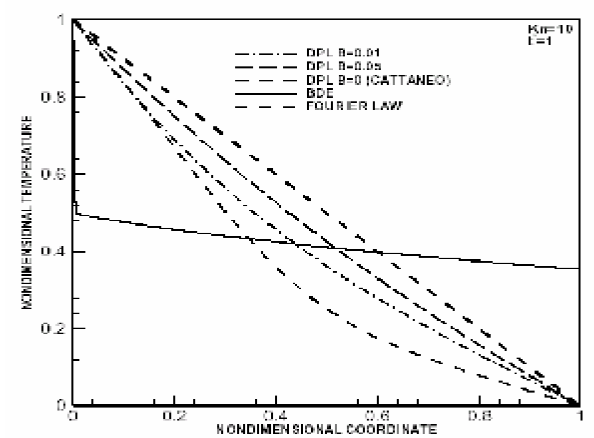
(b)

Fig. 3 Comparison of temperature (a) and heat flux (b) distribution obtained from various models for *Kn*=1 at t^{*}=2

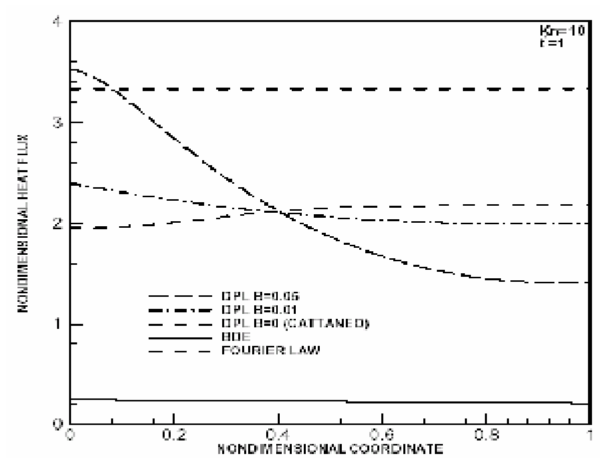
CONCLUSIONS

The present paper established the discussion of the transient the DPL equations of heat conduction, which divided into two cases of the CV equation and the general DPL equation with non-zero ratio of time lags, for Knudsen numbers more than 0.1 corresponding to nanoscale geometries.

Computational results of this model applied to a thin slab were compared with the results obtained from ballistic-diffusive equations, and from the Fourier law was also presented for a more comprehensive investigation. Since the DPL model neglects the effects of boundary phonon scattering, good agreement between BDE and DPL models was observed in the part of the domain that is far from the left boundary. This agreement wasn't seen in the Fourier law and the CV equations. It was shown that in the Knudsen numbers of order one the general DPL model have better agreement with BDE model, when compared with the CV equation; however in the larger values of Knudsen number no significant advantage could be observed for any of the two models. It was also found that in Knudsen numbers of order one and more



(a)



(b)

Fig. 4 Comparison of temperature (a) and heat flux (b) distribution obtained from various models for *Kn*=10 the DPL model is able to give predictions more accurate than the Fourier law only for heat flux distribution.

NOMENCLATURE

B	phase lag ratio
C_p	specific heat, J/kg°C
K	heat conduction coefficient, W/m°C
Kn	Knudsen No.
L	length, m
q	heat flux, W/m^2
T	temperature, ^oC
t	time, s
U	internal energy, J/Kg
V	group velocity of heat careers, m/s
X	direction, m

Greek Letters

α	thermal diffusion coefficient, m^2/s
ρ	density, kg/m^3
q	non-dimensional temperature
h	non-dimensional coordinate
Λ	mean free path of careers, m
μ	directional cosine
t	relaxation time, s
n	kinematic viscosity, m^2/s
Δ	difference
∇	gradient

Subscripts

b	ballistic
m	diffusive
q	heat flux
t	gradient temperature
o	equilibrium state

Superscripts

*	non-dimensional condition

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