

Nanoscale Heat Transfer using Phonon Boltzmann Transport Equation

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Abstract: COMSOL Multiphysics was used to solve a phonon Boltzmann transport equation (BTE) for nanoscale heat transport problems. One-dimensional steady-state and transient BTE problems were successfully solved based on finite element and discrete ordinate methods for spatial and angular discretizations, respectively, by utilizing the built-in feature of the COMSOL, *Coefficient Form of PDE*. A sensitivity study was conducted with various discretization refinements for different values of the Knudsen number, which is a measure of the nanoscale regime. It was found that sufficient refinement for angular discretization is critical in obtaining accurate solutions of the BTE.

Keywords: Nanoscale heat transport, phonon Boltzmann transport equation, finite element method, discrete ordinates method.

1. Introduction

For the last two centuries, many heat conduction problems have been modeled successfully by a Fourier diffusive equation (FDE). The equation can be derived using a conservation law of energy and Fourier's linear approximation of heat flux using a temperature gradient. The FDE is a parabolic equation reflecting a diffusive nature of heat transport. An underlying assumption is that the heat is effectively transferred between localized regions through sufficient scattering events of phonons within a medium. Therefore, the FDE does not hold when the number of scatterings is negligible, which could happen when a mean free path of phonon is similar or a larger order of magnitude than a domain size of interest, significant boundary scattering occurs at material interfaces causing thermal resistance, etc. Another problem of the FDE is that it admits an infinite speed of the heat transport, which is contradictory to the theory of relativity. Therefore, the FDE is inappropriate for the heat transfer problems at small time and spatial scales.

To resolve the issue of the infinite speed of heat carrier, hyperbolic equations, such as a Cattaneo equation (Telegraph equation) [1] or a relativistic heat equation [2], are often used to reflect a wave nature of the heat transport for cases of small speed of heat propagation (e.g., low temperature, low conductive medium, thermal insulator, phase transition, etc.) and/or high speed of heat flux (e.g., pico- or femto-second pulsed-laser heating.) Despite some issues [1], these hyperbolic equations can be used to consider the finite speed of phonons for a short time scale. However, they still cannot be used for small spatial scale.

For the nanoscale heat transfer analysis, one needs equations and methods for small-scale simulation in terms of both time and space. A molecular dynamics (MD) simulation can be a useful and accurate method in this regard. However, the MD simulation is usually computationally expensive, so it is suitable for systems having a few atomic layers or several thousand atoms, but not suitable for device-level thermal analysis. Alternatively, a phonon Boltzmann transport equation (BTE), a first-order partial differential equation for a phonon distribution function, has been used for this purpose [3-5]. The distribution function is a scalar quantity in the six-dimensional phase space (three space coordinates and three wave-vector coordinates). The phonon BTE is also called an equation of phonon radiative transfer (EPRT) when the phonon distribution function is replaced with a phonon intensity function [3]. The BTE is known to be difficult to solve, and thus often simplified with a relaxation time approximation. The BTE can predict a ballistic nature of heat transfer under an assumption that particle-like behaviors of phonon are much more significant than its wave-like behaviors, which make the BTE valid for structures larger than the wavelength of phonons. The BTE can be solved analytically for simple geometries [4, 6, 7], or numerically for complex geometries by using either deterministic methods (e.g., discrete ordinates method, spherical harmonics method,

finite volume method [8], etc.) or statistical methods (e.g., Monte Carlo simulation [9, 10]). In general, solving the BTE is much more efficient than the MD, and the predictions agree well with experimental data [10, 11].

In the present study, we will solve the BTE with the relaxation time approximation for one-dimensional heat transport problems using the COMSOL Multiphysics. We will combine the finite element (FE) capability of the COMSOL with the DOM to solve both steady-state and transient heat transfer problems. The numerical results will be compared with analytical ones for the steady-state problem. A sensitivity study will be conducted for various scale measures to show the difference between the BTE solutions with the conventional FDE ones. Furthermore, we will determine a suitable discretization scheme for spatial and angular spaces in order to obtain reliable transient solutions in using the COMSOL.

2. Use of COMSOL Multiphysics

The BTE equation under a relaxation time approximation is written as

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \left(\frac{\partial f}{\partial t} \right)_{\text{scat}} \approx \frac{f_o - f}{\tau_o}, \quad (1)$$

where f is the carrier distribution function, f_o the equilibrium distribution, \mathbf{v} the carrier group velocity vector, and τ_o the relaxation time. The EPRT in terms of the phonon intensity is written as

$$\frac{\partial I_\omega}{\partial t} + \mathbf{v} \cdot \nabla I_\omega = \frac{I_{\omega o} - I_\omega}{\tau_o}, \quad (2)$$

where the phonon intensity is expressed as $I_\omega(t, \mathbf{v}, \mathbf{r}) = |\mathbf{v}| \hbar \omega f(t, \mathbf{v}, \mathbf{r}) D(\omega) / 4\pi$, where \hbar is the reduced Planck constant, ω the phonon angular frequency, and $D(\omega)$ the density of state per unit volume. An equilibrium phonon intensity in Eq. (2) is written as

$$I_{\omega o} = \frac{1}{4\pi} \int_{\Omega=4\pi} I_\omega d\Omega. \quad (3)$$

For one-dimensional problems, Eq. (2) becomes

$$\frac{\partial I_\omega}{\partial t} + v \cos \theta \frac{\partial I_\omega}{\partial x} = \frac{I_{\omega o} - I_\omega}{\tau_o}, \quad (4)$$

where θ is a polar angle between a phonon propagation direction and the global heat transfer direction (x).

A solution process of the 1-D BTE in Eq. (4) along with Eq. (3) can be summarized as follows: With an initial value of $I_{\omega o}$, Eq. (4) is solved for the phonon intensity field, $I_\omega(t, x)$, for a particular phonon propagation angle, θ . After obtaining the solutions for all possible solid angles, 4π , $I_{\omega o}$ can be calculated using Eq. (3). With this updated value of $I_{\omega o}$, the solution process repeats until the convergence of I_ω and $I_{\omega o}$. Therefore, the BTE and thus the EPRT are highly nonlinear equations to solve. Once the phonon intensity is solved, heat flux and an equivalent temperature can be obtained by integrating the phonon intensity over the solid angles, 4π , such that

$$q = \int_{\Omega=4\pi} I_\omega \cos \theta d\Omega \quad \text{and} \quad (5)$$

$$T \approx \frac{u}{c} = \int_{\Omega=4\pi} \frac{I_\omega}{c|\mathbf{v}|} d\Omega = \frac{4\pi I_{\omega o}}{c|\mathbf{v}|}, \quad (6)$$

where c is the volumetric specific heat.

One of the most widely used methods for solving the BTE numerically is the discrete ordinates method (DOM). The DOM is a tool to transform the equation of radiative transfer into a set of simultaneous partial differential equations. This is based on a discrete representation of directional variation of intensity. A solution to the transport problem can be found by solving the equation of radiative transfer for a set of discrete directions spanning the entire solid angle. The integrals over the solid angle can be approximated by numerical integration using Gauss-Legendre quadratures.

The BTEs in Eqs. (3)-(4) were solved by the DOM using a built-in feature of *Coefficient Form PDEs* in COMSOL Multiphysics. The spatial domain (x) was discretized into n elements as a normal FE mesh refinement, while the angular domain (Ω), referred to as ordinates, was discretized in the directional coordinates by dividing the angular space into a finite number, m . The angular domain was discretized at Gaussian quadrature points within $-1 \leq \mu = \cos \theta \leq 1$. For each polar angle (θ_m), we solved the system of nonlinear equations for the phonon intensity, $I_\omega(t, x, \mu_m)$, and then updated the equilibrium phonon intensity, $I_{\omega o}(t, x)$, using

I_ω for all angles. Eqs. (3) and (5) can be written in discrete forms as

$$I_{\omega o}(t, x) = \frac{1}{2} \sum_m I_\omega(t, x, \mu_m) w_m \quad \text{and} \quad (7)$$

$$q(t, x) = 2\pi \sum_m I_\omega(t, x, \mu_m) \mu_m w_m, \quad (8)$$

respectively. The weight satisfies $\sum_m w_m = 2$.

The solver used for the steady-state and transient analyses was a built-in direct solver, UMFPAK. Default values were used for the solver parameters except that strict time steps were taken by the solver and a maximum BDF order was set to 1. When the relative error of the calculated value of the equivalent equilibrium intensity between two iteration steps was less than a present tolerance, we considered the problem was converged and then calculated the equivalent temperature and heat flux using Eqs. (6) and (8), respectively.

5. Results and Discussion

We have solved the BTE equations with the COMSOL under both steady-state and transient states. Spatial and angular domains were discretized into n elements and m quadrature points, respectively. A quadratic Lagrange element was used for the spatial FE mesh. The total degree of freedom for the 1-D problem becomes $2m(n+1/2)$. For the steady-state problems, it was observed that the well-converged solutions were obtained with a relatively coarse mesh (15 elements) while using 16 quadrature points. The sensitivity of mesh and quadrature points for the transient analysis will be stated later in this section.

Figure 1 shows steady-state temperature distributions via nondimensional emissive power (e_o^*) along the 1-D domain for various Knudsen numbers (Kn). For comparison purpose, an analytical solution was also obtained by using an analogy to the radiation heat transfer [5] by solving an integral equation,

$$2e_o^*(\eta) = E_2(\eta) + \int_0^\xi e_o^*(\eta') E_1(|\eta - \eta'|) d\eta', \quad (9)$$

where $\eta = x/L$ is the nondimensional coordinate, where L is the length of the domain, $E_n(x) = \int_0^1 \mu^{n-2} \exp(-x/\mu) d\mu$ the exponential integral, ξ the optical thickness, which is an

inverse of the Knudsen number, $Kn = \Lambda/L$, where Λ is the average mean free path of phonons, and $e_o^*(\eta) = [e_o(\eta) - J_{q2}^-] / [J_{q1}^+ - J_{q2}^-]$ is the emissive power nondimensionalized by a difference of boundary heat fluxes (J_{q2}^- and J_{q1}^+) at both ends of the 1-D domain. In Figure 1, the analytic and numerical solutions for various Kn ($= 0.1, 1, 10, 100$) were drawn with markers and lines, respectively, which shows an excellent agreement of the solutions with each other. While the conventional Fourier solution would yield the temperature gradient varying from 1 at $\eta = 0$ to 0 at $\eta = 1$, the solution from the BTE yields a reduced temperature gradient. The larger the Knudsen number, the smaller the temperature gradient, which is attributed from more ballistic phonon transport as compared to the diffusive one.

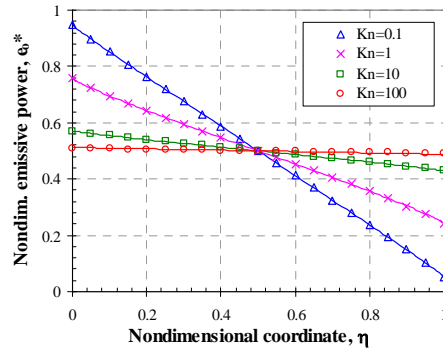


Figure 1. Steady-state nondimensionalized emissive power distribution for various Knudsen numbers.

We studied the effects of refinements in terms of spatial FE meshes and angular quadrature points on the time-dependent transient BTE solutions. The transient time (t) was nondimensionalized by the relaxation time of phonons (τ_o), so that $t^* = t/\tau_o$. Figure 2 shows nondimensionalized temperature distributions at $t^* = 0.1$ along the 1-D domain for $Kn = 10$. We used three different FE meshes (15, 60 and 120 elements) and a fixed angular division with 16 Gaussian points ($n_{gp} = 16$). The three FE meshes yield nearly identical temperature solutions with a decreasing trend from the hot side ($\eta = 0$) to the cold side ($\eta = 1$).

Smooth solutions were obtained except at a region near the hot boundary. An inset rectangular area in Figure 2 within $0 \leq \eta \leq 0.3$ was zoomed in and replotted in Figure 3, which clearly shows significant wiggles near the hot boundary. Therefore, the FE mesh refinement does not help smoothing out the wiggles at all. The wiggling of the solution, called a ray effect, is known to be attributed to insufficient refinement in the angular domain, and thus cannot be smoothed out with the FE mesh refinement in the spatial domain.

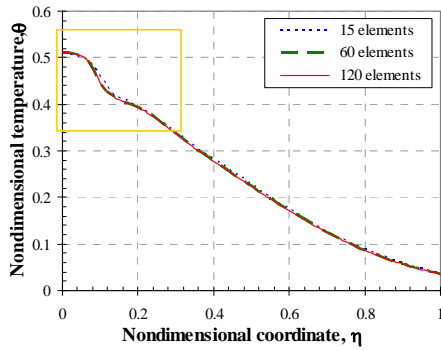


Figure 2. Transient nondimensional temperature distribution predicted with 15, 60 and 120 finite elements and 16 Gaussian points.

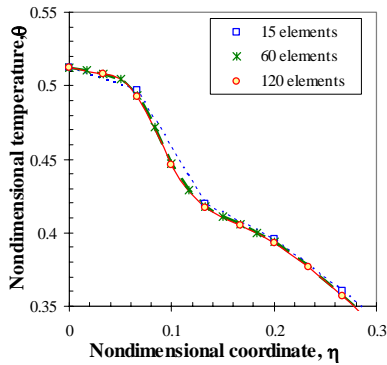


Figure 3. A magnified view of Figure 2 within $0 \leq \eta \leq 0.3$.

To eliminate the ray effect, we made further refinement in the angular domain by using more quadrature points. Figure 4 shows nondimensionalized temperature distributions at

$t^* = 0.1$ along the 1-D domain for $Kn = 10$ predicted with six different Gaussian quadrature points ($n_{gp} = 4, 8, 16, 32, 64, 128$). We utilized a Matlab-scripting feature of COMSOL to implement the large n_{gp} in building the system of equations. A fixed spatial division with 240 FE elements was used in these calculations. An inset rectangular area within $0 \leq \eta \leq 0.3$ was magnified and replotted in Figure 5. Although a highly refined FE mesh (240 elements) was used, the coarse angular divisions alleviate the wiggling of the solution (e.g., $n_{gp} = 4$). The wiggles near the hot end gradually decrease with the increase of n_{gp} , and thus the ray effect. Therefore, we found that the spatial and angular refinements are independent of each other, and thus do not recommend to use the highly refined spatial mesh with the coarse angular mesh.

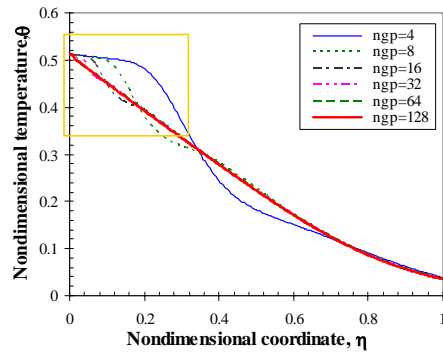


Figure 4. Transient nondimensional temperature distribution predicted with 240 finite elements and six Gaussian quadrature points (n_{gp}) for angular discretization.

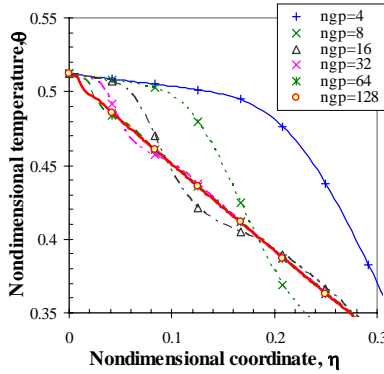


Figure 5. A magnified view of Figure 5 within $0 \leq \eta \leq 0.3$.

Figure 6 and Figure 7 show the temperature and heat flux distributions, respectively, at various time scales with three different Knudsen numbers. The result successfully reproduced the one reported earlier by Chen [4], but this time using the FE method using the COMSOL. The figures show the heat transfer from the hot side to the cold side with the finite speed of phonon as the short term (small t^*) solutions indicate, which cannot be predicted by the FDE. While constant temperatures were applied as boundary conditions at both sides, we can observe the temperature jump at these boundaries. The higher the Kn , the larger the jump. The reason for the temperature jump at these emissive boundaries was well explained in earlier work [7]. For a small Knudsen number at $Kn = 0.1$, the temperature solution approaches that of the steady-state FDE as the time increases, while for

a large Knudsen number at $Kn = 10$, the temperature solution approaches a nearly horizontal line, which indicates the ballistic heat transfer rather than the diffusive one, and results in a small temperature gradient and thus a large thermal conductivity.

6. Conclusions

We have solved the phonon Boltzmann transport equation for the nanoscale heat transfer problems with the COMSOL Multiphysics. One-dimensional steady-state and transient problems were successfully solved using FEM and DOM for spatial and angular discretizations, respectively, by utilizing the built-in feature of the COMSOL, *Coefficient Form of PDE*.

A sensitivity study was conducted with various discretization refinements for different values of the Knudsen number, which is a measure of the nanoscale regime. Significant ray effects were found with coarse angular discretizations. However, false scattering due to coarse spatial discretization was not severe with the COMSOL solution. It was found that the spatial and angular refinements were independent of each other, and it was not recommended to use the highly refined spatial mesh with the coarse angular mesh in solving the BTE with the COMSOL. The present success with the 1-D simulation encourages us to apply it for multidimensional cases.

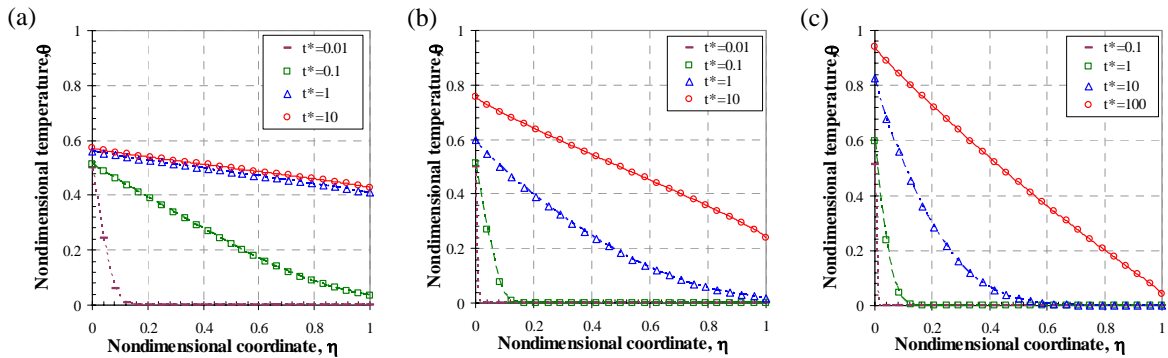


Figure 6. Temperature distributions at different time scales. (a) $Kn = 10$, (b) $Kn = 1$ and (c) $Kn = 0.1$.

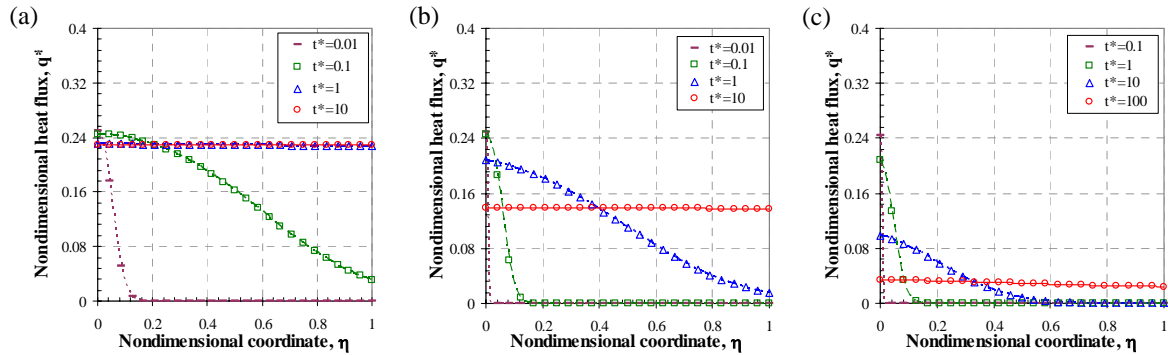


Figure 7. Heat flux distributions at different time scales. (a) $Kn = 10$, (b) $Kn = 1$ and (c) $Kn = 0.1$.

8. References

1. C. Bai, et al., On Hyperbolic Heat Conduction and the Second Law of Thermodynamics, *Journal of Heat Transfer*, **117**(2), 256-263 (1995).
2. Y. M. Ali, et al., Relativistic Heat Conduction, *International Journal of Heat and Mass Transfer*, **48**(12), 2397-2406 (2005).
3. A. Majumdar, Microscale Heat Conduction in Dielectric Thin Films, *Journal of Heat Transfer*, **115**(1), 7-16 (1993).
4. G. Chen, Ballistic-Diffusive Equations for Transient Heat Conduction from Nano to Macroscales, *Journal of Heat Transfer*, **124**(2), 320-328 (2002).
5. G. Chen, *Nanoscale Energy Transport and Conversion: A Parallel Treatment of Electrons, Molecules, Phonons and Photons*, Oxford University Press (2005).
6. G. Chen, Nonlocal and Nonequilibrium Heat Conduction in the Vicinity of Nanoparticles, *Journal of Heat Transfer*, **118**(3), 539-545 (1996).
7. R. Yang, et al., Simulation of Nanoscale Multidimensional Transient Heat Conduction Problems Using Ballistic-Diffusive Equations and Phonon Boltzmann Equation, *Journal of Heat Transfer*, **127**(3), 298-306 (2005).
8. J. Y. Murthy, et al., Computation of Sub-Micron Thermal Transport Using an Unstructured Finite Volume Method, *Journal of Heat Transfer*, **124**(6), 1176-1181 (2002).
9. M.-S. Jeng, et al., Modeling the Thermal Conductivity and Phonon Transport in

Nanoparticle Composites Using Monte Carlo Simulation, *Journal of Heat Transfer*, **130**(4), 042410-042411 (2008).

10. S. Mazumder, et al., Monte Carlo Study of Phonon Transport in Solid Thin Films Including Dispersion and Polarization, *Journal of Heat Transfer*, **123**(4), 749-759 (2001).

11. G. Chen, Size and Interface Effects on Thermal Conductivity of Superlattices and Periodic Thin-Film Structures, *Journal of Heat Transfer*, **119**(2), 220-229 (1997).

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