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Size effects in non-linear heat conduction with flux-limited behaviors

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ABSTRACT

Size effects are discussed for several non-linear heat conduction models with flux-limited behaviors, including the phonon hydrodynamic, Lagrange multiplier, hierarchy moment, nonlinear phonon hydrodynamic, tempered diffusion, thermon gas and generalized nonlinear models. For the phonon hydrodynamic, Lagrange multiplier and tempered diffusion models, heat flux will not exist in problems with sufficiently small scale. The existence of heat flux needs the sizes of heat conduction larger than their corresponding critical sizes, which are determined by the physical properties and boundary temperatures. The critical sizes can be regarded as the theoretical limits of the applicable ranges for these non-linear heat conduction models with flux-limited behaviors. For sufficiently small scale heat conduction, the phonon hydrodynamic and Lagrange multiplier models can also predict the theoretical possibility of violating the second law and multiplicity. Comparisons are also made between these non-Fourier models and non-linear Fourier heat conduction in the type of fast diffusion, which can also predict flux-limited behaviors.

1. Introduction

As a phenomenological model, Fourier's law of heat conduction has been proved by numerous experiments and widely used in engineering. It describes a constitutive relation between the temperature gradient and heat flux

$$\boldsymbol{q} = -\lambda \nabla T, \quad (1)$$

where $\boldsymbol{q}$ is the heat flux, λ is the thermal conductivity and T is the temperature. In statistical mechanics, Fourier's law has been derived approximately through several given theoretical assumptions, which also implies its possible restrictions, i.e., near-equilibrium region. Especially in nanoscale heat transport [1–6], the effects of far-from-equilibrium can play an important role because the characteristic size can be comparable to the mean free path of heat carriers. The non-Fourier effects in nanoscale can be classified into three types [7]: relaxation, nonlocality and nonlinearity. Relaxation in heat conduction is first introduced by the Cattaneo–Vernotte (CV) model [8,9], whose hyperbolic governing equation predicts a finite wave velocity of heat propagation. It should be noted that in non-linear Fourier heat conduction [12,13], there also exist hyperbolic or wave-like characteristics. For instance, fast (superfast) diffusion [14], where $\lambda = \lambda(T) \propto T^{-\alpha}$ $(0 < \alpha < 2$ is a constant), also has the travelling wave solution $T(x,t) = T_1(x - Ut) + T_2(x + Ut)$ with a finite wave velocity U. Thus, hyperbolic or wave-like characteristics are not enough to distinguish non-Fourier relaxation models and Fourier's law. In the spirit of relaxation, the CV model has been generalized to different non-Fourier models, i.e., the Jeffrey model [10,11], a linear superposition of the CV and Fourier heat conductions. The constitutive relations of these relaxation models can usually be summarized as memory behaviors [10,11], where the heat flux is depended on the integrated history of the temperature gradient. Different constitutive models can be given through different choices of the integral kernels. Most of the memory kernels are exponential type or Dirac delta function (or their linear superposition) [10,11]. Power-law kernels can also be applied, which will lead to fractional differential operators [15,16]. The hyperbolic heat conduction models, i.e., the CV model, might predict non-positive values of the absolute temperature which seems unphysical. Recently, hyperbolic heat conductions paired with this behavior have been further discussed by introducing a new class of stochastic processes [17,18], generalized Poisson–Kac processes. The nonlocal and nonlinear effects are mainly found in the models related to phonon hydrodynamics [19,20]. Most of these models are on the basis of phonon Boltzmann transport equation and relaxation approximations, while the thermon gas model [21–24] takes a different method, which considers Einstein's mass–energy relation in phonon hydrodynamics. The second spatial derivatives of the heat flux including $\nabla^2\boldsymbol{q}$ and $\nabla(\nabla \bullet \boldsymbol{q})$ [19,20] are the most common nonlocal terms. For steady-state cases, the relaxation

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terms will disappear as $\frac{\partial}{\partial t}=0$ but nonlocality might still exist due to $\nabla^2\boldsymbol{q}\neq\boldsymbol{0}$, which means that the nonlocal models would not reduce to Fourier's law.

In contrast with relaxation and nonlocality, nonlinearity, which might be unignorable in nanoscale heat transport, is not much studied [25–29]. The nonlinear effects predict significant and interesting phenomenon, i.e., flux-limited behavior [29], where the heat flux tends to a finite upper bound with the temperature gradient increasing. The flux-limited behaviors in heat conduction caused by nonlinearity have been well discussed and reviewed by Guo et al. [25]. They have summarized the nonlinear models with flux-limited behaviors into three categories according to their theoretical foundations: phonon hydrodynamics, nonequilibrium thermodynamics, and phenomenological methods. These models expressed by the local temperature and heat flux distributions aim at providing constitutive relations for nanoscale heat transport. However, from the viewpoint of physics, it is obvious that they cannot be applied to the heat conduction problem with arbitrarily small size because the definitions of the local temperature and heat flux will be debatable or even undefinable for sufficiently small size. Therefore, besides the value of the heat flux varying along with the increasing temperature gradient, the applicable size of a heat conduction model should also be limited, which remains an open question.

In this work, it is found that this limitation of size can also be predicted by the nonlinear regime in the models with flux-limited behaviors, mainly including the phonon hydrodynamic [30,31] and Lagrange multiplier [32] models. For 1D steady-state heat conduction, where flux-limited behaviors are usually discussed, there will exist a critical size determined by the boundary temperatures, and the heat flux will exist only when the size is larger than the critical size. The critical sizes of these non-linear models can be regarded as the theoretical limits of their applicable ranges. The size and boundary effects for the existence of heat flux show different features from Fourier heat conduction, which can always guarantee the existence of heat flux for arbitrary boundary temperatures and size. It means that even in the limit of small heat flux (or small temperature gradient), these non-Fourier models with flux-limited behaviors will not reduce to Fourier's law and the nonlinear effects could not be negligible.

2. Critical size for heat flux in non-Fourier heat conduction

The flux-limited behaviors are mainly discussed for 1D steady-state boundary value problems in $[0,l]$ [25–29], where $T|_{x=0}=T_1$ and $T|_{x=l}=T_2$ (without loss of generality, $T_1<T_2$). In 1D steady-state problems, the heat flux the heat flux reduces to a constant scalar $q=-C$ and in consideration of $T_1<T_2$, only positive C can satisfy the second law (the positive direction of the coordinate is from $x=0$ to $x=l$).

2.1. Phonon hydrodynamic model

We start from the phonon hydrodynamic model [30,31], which is derived from Callaway's relaxation approximation and maximum entropy principle

$$\boldsymbol{q}+\tau_R\frac{\partial\boldsymbol{q}}{\partial t}+\lambda\nabla T=-\tau_R\nabla\bullet\left(\frac{3v_g\langle\boldsymbol{qq}\rangle}{2v_gc_VT+\sqrt{4v_g^2c_V^2T^2-3\boldsymbol{q}^2}}\right),\tag{2}$$

where $\langle\boldsymbol{qq}\rangle$ is the deviatoric part of tensor $\boldsymbol{qq}$, τ_R is the relaxation time of phonon resistive scattering, v_g is the average phonon group speed and c_V is the heat capacity per unit volume. In 1D steady-state heat conduction, the governing equation of the phonon hydrodynamic model can be simplified to

$$C=\lambda\left[5-\frac{4}{\sqrt{1-\left(\frac{\sqrt{3}C}{2v_gc_VT}\right)^2}}\right]\frac{dT}{dx}.\tag{3}$$

In 1D steady-state problems, Eq. (3) is derived from Eq. (2), which can be found in Ref. [25] (see Eqs. (9)–(11) of Ref. [25]). From Eq. (3), it is obvious that the upper bound of the heat flux should be limited $|C|<\frac{2v_gc_VT}{\sqrt{3}}$ in mathematics. What's more, the second law of thermodynamics requires a non-negative effective thermal conductivity $\lambda[5-\frac{4}{\sqrt{1-\left(\frac{\sqrt{3}C}{2v_gc_VT}\right)^2}}]\geq 0$, which will give a smaller upper bound $|C|\leq\frac{2\sqrt{3}}{5}v_gc_VT$. Similar upper bounds determined by v_gc_VT can also be found in other models. The corresponding physical meaning is that the heat flux cannot be higher than the product of the energy density c_VT and the maximum phonon speed $\sup(v_g)$. The relation between the boundary temperatures and heat flux can be given by the integration of Eq. (3)

$$5(T_2-T_1)-4\left[\sqrt{T_2^2-\left(\frac{\sqrt{3}C}{2v_gc_V}\right)^2}-\sqrt{T_1^2-\left(\frac{\sqrt{3}C}{2v_gc_V}\right)^2}\right]=\frac{Cl}{\lambda}.\tag{4}$$

In the cases of $C>0$, set $\frac{\sqrt{3}|C|}{2v_gc_V}=u_1$ $(0\leq u_1\leq T_1)$ and Eq. (4) is then rewritten as

$$5(T_2-T_1)-4\left(\sqrt{T_2^2-u_1^2}-\sqrt{T_1^2-u_1^2}\right)=\frac{2v_gc_Vl}{\sqrt{3}\lambda}u_1.\tag{5}$$

To determine the existence of u_1 in $[0,T_1]$, an auxiliary function is introduced as follows

$$f_1(u_1)=5(T_2-T_1)-4\left(\sqrt{T_2^2-u_1^2}-\sqrt{T_1^2-u_1^2}\right)-\frac{2v_gc_Vl}{\sqrt{3}\lambda}u_1,\tag{6}$$

whose first-order derivative is

$$\frac{df_1(u_1)}{du_1}=4u_1\left(\frac{1}{\sqrt{T_2^2-u_1^2}}-\frac{1}{\sqrt{T_1^2-u_1^2}}\right)-\frac{2v_gc_Vl}{\sqrt{3}\lambda}.\tag{7}$$

For $T_2>T_1$, we have $\frac{df_1(u_1)}{du_1}<0$ and hence, there is at most one solution. Due to $f_1(0)=(T_2-T_1)>0$, the existence of u_1 in $[0,T_1]$ needs

$$f_1(T_1)=5(T_2-T_1)-4\sqrt{T_2^2-T_1^2}-\frac{2v_gc_Vl}{\sqrt{3}\lambda}T_1\leq 0,\tag{8}$$

but inequality (8) is not necessarily satisfied, i.e., $\lim_{T_1\to 0}f_1(T_1)\to T_2>0$. In order to guarantee the existence of heat flux, the size should satisfy the following inequality

$$l\geq l_{c1}=\frac{\sqrt{3}\lambda}{2v_gc_V}\left[5\left(\frac{T_2}{T_1}-1\right)-4\sqrt{\frac{T_2^2}{T_1^2}-1}\right].\tag{9}$$

When $1<\frac{T_2}{T_1}\leq\frac{41}{9}$, we find $l_{c1}\leq 0$ and therefore, inequality (9) always holds, which means that the heat flux of this case must exist. For $\frac{41}{9}<\frac{T_2}{T_1}$, l_{c1} is positive and only when the size is larger than l_{c1}, the heat flux will exist. Accordingly, a size effect about the existence of heat flux is found for $\frac{41}{9}<\frac{T_2}{T_1}$. l_{c1}, which is determined by the ratio of boundary temperatures, can be regarded as a critical

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