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On defects of Taylor series approximation in heat conduction models

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ABSTRACT

Taylor series approximation like $q(t+\tau) \approx q + \tau \frac{\partial q}{\partial t}$ are often used to derive, extend or interpret typical heat conduction models. Researchers may take it for granted that the single-phase-lagging (SPL) model can be considered as an extension of the Cattaneo–Vernotte (CV) model because there is such approximation relationship between them. We point out in this paper that this Taylor series approximation itself has some defects based on analyses in mathematics, physics and some examples first. Then, we show essential differences in both mathematics and physics between the CV and SPL models. It is found that their mathematical characteristics and accordance with the laws of thermodynamics are significantly different, which indicates that using this approximation to connect the two models may be defective in some cases. What's more, higher order approximation can't solve these problems and defects.

1. Introduction

Fourier's law of heat conduction is often used to describe normal heat conduction problems in engineering. In recent years, the limitations of Fourier's law have been revealed [1–6] that Fourier's law predicts an unphysically infinite speed of heat perturbation propagation and it fails to characterize supertransient and high heat flux processes well. Several modified heat conduction models were proposed to get over these limitations. The Cattaneo–Vernotte (CV) model [7,8] is the most typical one which leads to hyperbolic heat conduction equation and wave-like transport in heat conduction processes, called thermal wave. Jeffrey model [2] can be considered as an extension of the CV model since it takes into account the influence of temperature relaxation. Tzou [9] proposed the single-phase-lagging (SPL) model which can reduce to the CV model by taking first-order Taylor series approximation. Anisinov et al. [10] proposed a model for metals by regarding the interactions of electron and phonon. Guyer et al. [11] developed a representative model for pure phonon heat conduction. There are also further modifications and improvements of these classical models. Tzou [12] proposed a dual-phase-lagging model to add the influence of temperature lag on the basis of the single-phase-lagging model. Coleman et al. [13] improved the changing rate of the heat energy. Most of these models are linear and predict limited heat conduction speed, getting over the infinite speed problem in Fourier's law. There are also some non-linear models which predict limited heat conduction speed. Thermomass theory [14–17] for heat conduction under extreme conditions is just one of them based on relativity and mass-energy equation. Alternative approaches to the analysis of the diffusion equation [18–20] is another non-linear model whose equation can be changed to Burger's equation and therefore, some existing conclusions in math can be used to analyze heat conduction problems.

We have seen from the above brief review that Taylor series approximation is adopted in several heat conduction models. Here the CV and SPL models are taken as typical examples. The CV model is expressed as

$$q + \tau \frac{\partial q}{\partial t} + \lambda \nabla T = 0, \tag{1}$$

where τ is the thermal relaxation time, q is the heat flux density, λ is the thermal conductivity and T is the temperature. The CV model is used to describe the supertransient heat conduction and also agrees well with some of experiments and simulations. Consider the single-phase-lagging model [9]

$$q(x, y, z, t+\tau) + \lambda \nabla T = 0. \tag{2}$$

Comparing Eq. (2) with the CV model Eq. (1), we find that for $q(x, y, z, t+\tau)$, if we use first-order Taylor series approximation

$$q(t+\tau) \approx q + \tau \frac{\partial q}{\partial t}. \tag{3}$$

Eq. (2) will reduce to Eq. (1). Because of this approximation relationship between them, the SPL model is considered as an extension or explanation of the CV model and similar approximation methods, such as temperature Taylor series approximation, are

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also used in deriving other typical heat conduction models [21–25]. This approximation method is assumed to cause negligibly small influence because the relaxation time is very small.

In this paper, however, we note that the Taylor series approximation can lead to very large difference no matter how small the relaxation time is. Even if the relaxation time is very small, the deviation between the two sides of Eq. (3) can be very large, and there are also some essential differences in mathematics and physics between the CV and SPL models. Their mathematical characteristics and accordance of the laws of thermodynamics are very different, which shows that using this approximation to connect the two models is defective. In addition, higher order approximation can't solve the mathematical and physical problems caused by first-order approximation.

2. Influence of Taylor series approximation

2.1. Deviation of heat flux field

In the approximation of heat flux Eq. (3), $q(t+\tau)$ doesn't equal to $q+\tau\frac{\partial q}{\partial t}$ strictly. Therefore, this approach is considered as a special Taylor series approximation when the relaxation time τ is very small. But in fact, the deviation between the two sides of Eq. (3) is uncertain in mathematics. First, not all functions have Taylor series, even infinitely differentiable functions. For these functions which don't have Taylor series, Taylor series approximation is infeasible because the remainders don't tend to zero. Therefore the deviation between the Taylor series and function is not sure. In addition, Taylor series approximation is feasible only in their convergence regions. That is to say, even if a function has Taylor series, the approximation only exists in some certain regions. Second, even if we can make sure that Taylor series approximation exists and the relaxation time τ is very small, the deviation between the two sides of Eq. (3) is not necessarily very small. This is because the relaxation time τ is a physical property. It must be a real number, not an "infinitesimal" in mathematics. As long as τ is not an infinitesimal, the deviation between $q(t+\tau)$ and $q+\tau\frac{\partial q}{\partial t}$ can still be very large because the higher order derivative terms $\tau^n\frac{\partial^n q}{\partial t^n}$ are unknown. Although τ^n are very small, $\frac{\partial^n q}{\partial t^n}$ can also be very large and, their products are uncertain. Because of these uncertain higher order derivative terms, the deviation between $q(t+\tau)$ and $q+\tau\frac{\partial q}{\partial t}$ is uncertain either. In summary, even if the relaxation time τ is very small, the deviation between the two sides of Eq. (3) can still be very large. As examples, we will discuss this problem below in some common functions which often appear in heat conduction problems. Consider the heat conduction equations of Fourier's law Eq. (4) and the CV model Eq. (5)

$$\frac{\partial T}{\partial t}=\frac{\lambda}{\rho c_V}\nabla^2 T, \tag{4}$$

$$\frac{\partial T}{\partial t}+\tau\frac{\partial^2 T}{\partial t^2}=\frac{\lambda}{\rho c_V}\nabla^2 T. \tag{5}$$

For Eq. (4), a general method is to make a separation of variables $T=f(t)g(x)$. Substituting it into Eq. (4) gives

$$\frac{f'}{f}=\frac{g''}{g}=-\lambda_n, \tag{6}$$

$$f'(t)+\lambda_n f(t)=0. \tag{7}$$

Solving this ordinary differential equation, we obtain $f(t)=Ce^{-\lambda_n t}$. The part determined by time of temperature field has a form of exponential function. For Eq. (5), we can also make a separation of variables $T=f(t)g(x)$. Substituting it into Eq. (5) gives

$$\frac{\frac{1}{\tau}f'+f''}{f}=\frac{\lambda}{\rho c_V\tau}\frac{g''}{g}=-\lambda_n, \tag{8}$$

$$\frac{1}{\tau}f'+f''+\lambda_n f=0. \tag{9}$$

There will be different cases. When $\frac{1}{\tau^2}-4\lambda_n>0$, the solution is $f(t)=A_1e^{x_1t}+B_1e^{x_2t}$ which also has a form of exponential function. $x_1,\ x_2$ are the real roots of $x^2+\frac{1}{\tau}x+\lambda_n=0$. When $\frac{1}{\tau^2}-4\lambda_n<0$, the solution is $f(t)=e^{x_3t}(A_2\sin x_4t+B_2\cos x_4t)$. $x_3+x_4i,\ x_3-x_4i$ are the complex roots of $x^2+\frac{1}{\tau}x+\lambda_n=0$. We can find that not only exponential function but also trigonometric function appears. From the above analyses we can find that the part of temperature field determined by time can be expressed by exponential and trigonometric functions in the method of separation of variables. So, we can make sure the deviation between the two sides of Eq. (3) in these functions to show this deviation in heat conduction problems.

2.1.1. Deviation in trigonometric function

Consider a heat conduction problem with heat source $\phi=-\frac{2n\pi q_0\rho c_V x}{\lambda\tau}\cos\frac{2n\pi t}{\tau}$. In this case, the energy conservation equation is expressed as

$$\frac{\partial q}{\partial x}=-\rho c_V\frac{\partial T}{\partial t}+\phi. \tag{10}$$

Substituting it into Eq. (2) leads to

$$\frac{\rho c_V}{\lambda}\frac{\partial q(t+\tau)}{\partial t}+\frac{\partial\phi}{\partial x}=\nabla^2 q. \tag{11}$$

The initial condition is taken $q|_{t=0}=0$ and the boundary conditions are taken $q|_{x=0,l}=q_0\sin\frac{2n\pi t}{\tau}$. For this problem, we can get its classical solution

$$q(x,t)=q_0\sin\frac{2n\pi t}{\tau}. \tag{12}$$

It is worth mentioning that for this problem, Eq. (12) is also equivalent to Fourier's Law because $q(x,t)=q(x,t+\tau)$. Then we can use Eq. (12) to show the deviation in Eq. (3). For the heat flux expressed by Eq. (12), we can get its Taylor series approximation

$$q+\tau\frac{\partial q}{\partial t}=q_0\left(\sin\frac{2n\pi t}{\tau}+2n\pi\cos\frac{2n\pi t}{\tau}\right). \tag{13}$$

The relative deviation between $q(t+\tau)$ and $q+\tau\frac{\partial q}{\partial t}$ is

$$\eta=\frac{q+\tau\frac{\partial q}{\partial t}-q(t+\tau)}{q(t+\tau)}=2n\pi\cot\frac{2n\pi t}{\tau}. \tag{14}$$

We find that Eq. (14) is a periodic function and its value can reach infinity. No matter how small the relaxation time τ is (larger than zero), the relative deviation can still be very large. The large deviation will always appear because Eq. (14) is a periodic function. Fig. 1 shows the heat flux fields with the form of trigonometric function which belongs to original heat flux $q(t+\tau)$ and heat flux with Taylor approximation $q+\tau\frac{\partial q}{\partial t}$ (q is expressed by Eq. (12) and $n=1$). In Fig. 1, the heat flux with Taylor approximation has far larger amplitude than the original heat flux. Therefore, the deviation caused by Taylor approximation can be very large and we find that the difference between the two heat flux fields is in periodical vibration. In fact, Fig. 1 is for the case of $n=1$, and the difference between them will be larger and larger with the increase of n.

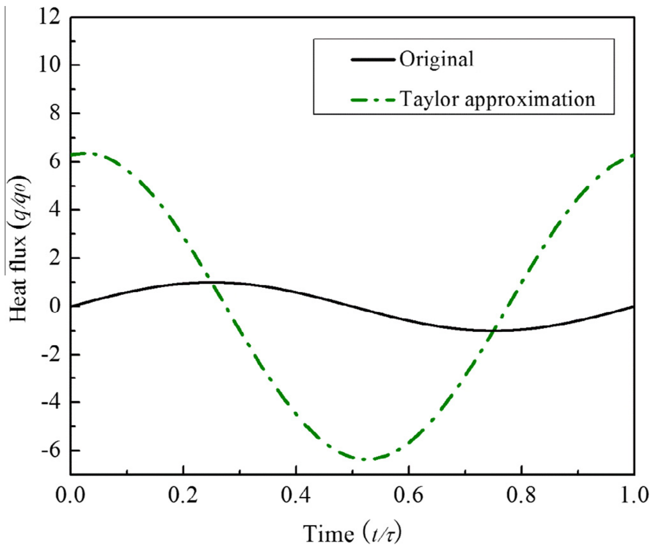

Fig. 1. Heat flux fields with the form of trigonometric function.

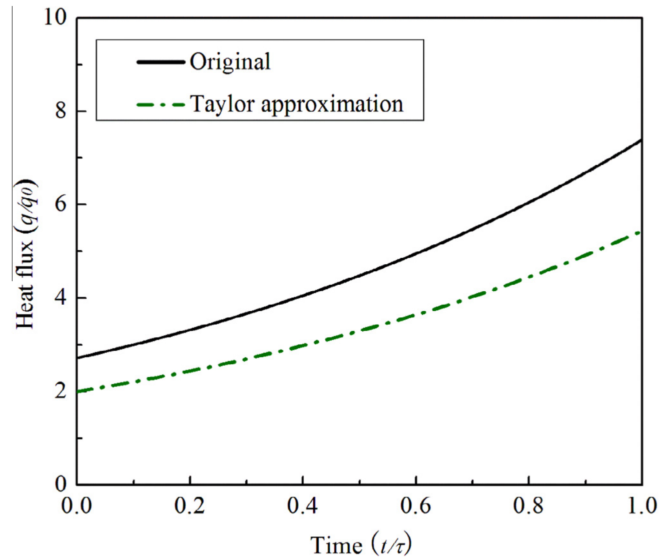

Fig. 2. Heat flux fields with the form of exponential function.

2.1.2. Deviation in exponential function

Consider a heat conduction problem with heat source $\phi = -\frac{a^{\frac{t}{\tau}} \ln a q_0 \rho c_V x}{\lambda \tau}$. The heat conduction equation is still Eq. (11). The initial condition is taken $q|_{t=0} = q_0$ and the boundary conditions are taken $q|_{x=0,l} = q_0 a^{\frac{t}{\tau}}$. For this problem, we can get its classical solution

$$q(x,t) = q_0 a^{\frac{t}{\tau}}. \tag{15}$$

Then we can use Eq. (15) to show the deviation in Eq. (3). For heat flux expressed by Eq. (15), we can get its Taylor series approximation

$$q + \tau \frac{\partial q}{\partial t} = q_0 a^{\frac{t}{\tau}} (1 + \ln a). \tag{16}$$

The relative deviation between $q(t+\tau)$ and $q + \tau \frac{\partial q}{\partial t}$ is

$$\eta = \frac{q + \tau \frac{\partial q}{\partial t} - q(t+\tau)}{q(t+\tau)} = \frac{1 + \ln a - a}{a}. \tag{17}$$

This relative deviation is a constant which has nothing to do with the relaxation time τ. From the above analyses we can find that for some common functions in heat conduction problems, the relative deviation between $q(t+\tau)$ and $q + \tau \frac{\partial q}{\partial t}$ can be very large no matter how small the relaxation time τ is. Fig. 2 shows the heat flux fields with the form of exponential function which belong to original heat flux $q(t+\tau)$ and heat flux with Taylor approximation $q + \tau \frac{\partial q}{\partial t}$ (q is expressed by Eq. (15) and $a = e$). In Fig. 2, the original heat flux is larger than the heat flux with Taylor approximation. In addition, the difference between them will be larger and larger as time goes on but the relative deviation is a constant, i.e. Eq. (17).

2.2. Influence on entropy production rate

From Eq. (2) we can obtain

$$\nabla T = -\frac{q(t+\tau)}{\lambda}. \tag{18}$$

Substituting it into the expression of the entropy production rate $\dot{S} = -\frac{q \nabla T}{T^2}$ leads to

$$\dot{S} = \frac{q q(t+\tau)}{\lambda T^2}. \tag{19}$$

According to the second law of thermodynamics, the entropy production rate must be positive or zero. (We will discuss if Eq. (19) is positive or zero in Section 3.3) If we use the Taylor series approximation in Eq. (3), the expression of the entropy production rate turns to

$$\dot{S}' = \frac{q(q + \tau \frac{\partial q}{\partial t})}{\lambda T^2}. \tag{20}$$

From the above analyses we know that the deviation between $q(t+\tau)$ and $q + \tau \frac{\partial q}{\partial t}$ can be very large, even infinite. So it is possible that one is positive and the other is negative. Therefore, the Taylor series approximation in Eq. (3) may lead the original positive entropy production rate to be negative. Next, we will provide a simple example about this problem. Consider a heat conduction problem without heat source, i.e. $\phi = 0$. The heat conduction equation is still Eq. (11). The initial condition is taken $q|_{t=0} = q_0 \sin \frac{\pi x}{l}$, the boundary conditions are taken $q|_{x=0,l} = 0$, and physical properties satisfy $\frac{\lambda \pi^2}{\rho c_V l^2} = \frac{2}{e^2 \tau}$. For this problem, we can get its classical solution

$$q(x,t) = q_0 e^{-\frac{2t}{\tau}} \sin \frac{\pi x}{l}. \tag{21}$$

Substituting Eq. (21) into Eq. (19), we can get the original entropy production rate

$$\dot{S}_{\mathrm{I}} = \frac{q q(t+\tau)}{\lambda T^2} = \frac{e^{-2} q^2(x,t)}{\lambda T^2}. \tag{22}$$

Obviously, this original entropy production rate expressed by Eq. (22) is greater than or equal to zero at any time and place. Eq. (22) equals to zero only when the heat flux is zero and therefore, the original heat flux field satisfies the second law of thermodynamics. Substitute Eq. (21) into Eq. (20), and then, we get the entropy production rate which belongs to the heat flux with Taylor series approximation

$$\dot{S}_{\mathrm{II}} = -\frac{q^2(x,t)}{\lambda T^2} \leqslant 0. \tag{23}$$

This entropy production rate which belongs to the heat flux field with Taylor series approximation is less than or equal to zero at any time and place. This result has nothing to do with the relaxation time τ. Obviously, it violates the second law of thermodynamics but the original entropy production rate doesn't. So this violation of the second law of thermodynamics is caused by the Taylor series approximation in Eq. (3). That is another big problem of this approximation.

In addition, this problem is adiabatic and it's an isolated system. According to the second law of thermodynamics, this system's entropy must increase. But the negative entropy production rate in Eq. (23) means that the entropy decreases, which is contradictory. From Eq. (21) we find that the heat flux attenuates and therefore, the system tends to equilibrium. The negative entropy production rate in Eq. (23) means that equilibrium state has the least entropy which is also non-physical. So the approximation in Eq. (3) is defective not only in mathematics but also in physics. Fig. 3 shows the entropy production rates which belong to original heat flux $q(t+\tau)$ and heat flux with Taylor approximation $q+\tau\frac{\partial q}{\partial t}$. Here $x=\frac{l}{2}$, $\alpha=\frac{q_0^2}{\lambda T^2}$ and $S'=\dot{S}_{\mathrm{I}}(\frac{l}{2},t)$ or $\dot{S}_{\mathrm{II}}(\frac{l}{2},t)$. From Fig. 3, it is not difficult to find that the original entropy production is always positive but the entropy production rates belonging to Taylor approximation is always negative. In summary, for the entropy production rate problem, the single-phase-lagging model is better than the CV model. It is necessary to point out that the entropy production rates in this paper are evaluated based on classical irreversible thermodynamics (CIT). However, there are further discussion about this in extended irreversible thermodynamics [30] which beyond our ability.

3. Difference between SPL and CV models

Although a certain "approximation" relationship exists between the single-phase-lagging model and the CV model, some essential differences also exist between them. Considering the single-phase-lagging model as an extension or explanation of the CV model and using the single-phase-lagging model to derive or cover the CV model will be defective because of these essential differences. On balance, this Taylor series approximation is only for determined functions but we need suitable boundary and initial conditions to determine the heat flux fields. Without these suitable boundary and initial conditions, the heat flux fields are not determined functions. Therefore, this approximation is defective because we do not even know if the time differential $\frac{\partial q}{\partial t}$ exists. What's more, even if we have these boundary and initial conditions, the heat flux fields may not be existent, unique or differentiable either. So, this Taylor series approximation method is greatly influenced by the boundary and initial conditions and a very small relaxation time is not enough to predict the influence of this approximation. That is the reason why there are essential differences between the two models.

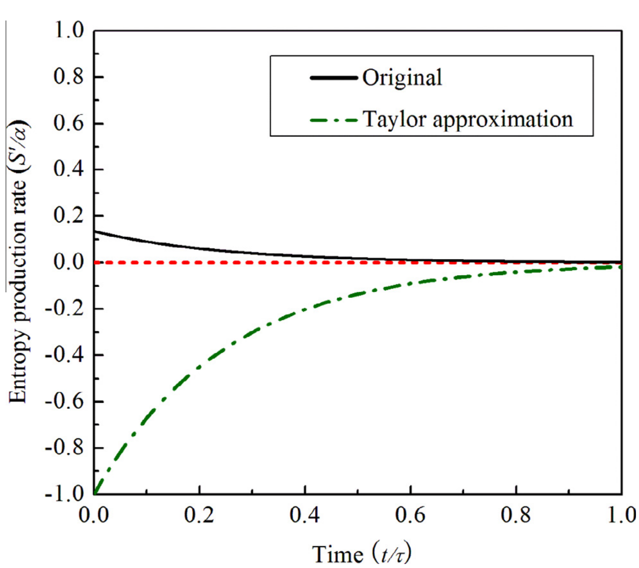

Fig. 3. Entropy production rates belonging to original and Taylor approximation heat fluxes.

3.1. Difference in physical meaning

Eq. (2) shows that there is a time lag between the temperature gradient and the heat flux response, which means that the speed of the heat flux response to temperature gradient is not infinite. However, for the CV model, the heat conduction equation is a wave equation which means that the speed of temperature perturbation itself is not infinite. The two heat conduction models both mean that some certain speeds are not infinite but the underlying meanings of the speed are different. From observing Eq. (1), we find that for the CV model, the temperature gradient at a certain moment must influence the heat flux at the same moment. However, in Eq. (2), the temperature gradient at a certain moment influences the heat flux at the moment τ later. In other words, the heat flux only depends on the instantaneous temperature gradient τ ago in Eq. (2). However, for the CV model, the heat flux depends on not only the instantaneous temperature gradient but also the preceding heat conduction process which is reflected in $\tau\frac{\partial q}{\partial t}$. Next, we will provide a simple example. Consider a case which satisfies $q|_{t=0}=q_0$ and $\nabla T=0,\ t\geqslant 0$. For Eq. (2), because of $\nabla T|_{t=0}=0$, we can obtain $q|_{t=\tau}=0$ which has nothing to do with the initial heat flux $q|_{t=0}$. However, for the CV model, we obtain $q=q_0e^{-\frac{t}{\tau}}$ and $q|_{t=\tau}=\frac{q_0}{e}$. Obviously, for the CV model, $q|_{t=\tau}$ depends on $q|_{t=0}$. In fact, the CV model means that there is a phase difference θ between the temperature gradient and the heat flux response in fact. However, there is a time lag not phase difference in Eq. (2). At a fixed location, this phase difference θ can be expressed as Eqs. (24) and (25) in mathematics

$$\nabla T=C\sin\xi(t), \tag{24}$$

$$q=-\lambda C\sin[\xi(t)+\theta]. \tag{25}$$

3.2. Difference in mathematics

For the single-phase-lagging model, the heat conduction equation without heat source is

$$\frac{\rho c_V}{\lambda}\frac{\partial T}{\partial t}=\nabla^2 T(t-\tau). \tag{26}$$

In Eq. (26), there is only a first-order time derivative term. So for a single-phase-lagging problem, we only need to give one initial condition to determine the solution in general. However, a second-order time derivative term appears in Eq. (5). Therefore, we need two initial conditions to determine the solution for the CV model. The number of initial conditions needed to determine the solution is different. That is one of the most obvious difference between the two models. In addition, Eq. (26) doesn't have the uniqueness of solution but Eq. (5) does. For the problem of uniqueness, Eq. (5) is a telegrapher's equation and if we provide enough boundary conditions $T|_{\Gamma}=f_{\Gamma}$ and initial conditions $T|_{t=0}=f_0$ and $\frac{\partial T}{\partial t}|_{t=0}=f_{t0}$, the solution will be unique. However, the problem of uniqueness is more complex for Eq. (26). In some special circumstances, even if we give enough boundary and initial conditions, the solutions are still not unique. Next, we will provide a simple example. Consider a one-dimensional problem where the physical properties satisfy $\frac{2\tau n^2\pi}{\rho c_V l^2}=1$ (n is an integer). The boundary conditions are taken $T|_{x=0,l}=f_{\Gamma}$, and the initial condition is taken

$T|_{t=0} = f_0$. Consider a solution $A\sin\frac{n\pi x}{l}\sin\frac{\pi t}{2\tau}$, where A is a constant. This solution satisfies Eq. (26), boundary conditions $T|_{\Gamma} = T|_{x=0,l} = 0$ and initial condition $T|_{t=0} = 0$. This means that if a solution $T_{\Lambda}(x,t)$ satisfies Eq. (26), boundary conditions $T|_{x=0,l} = T|_{\Gamma} = f_{\Gamma}$ and initial condition $T|_{t=0} = f_0$, other solutions expressed by $T'_{\Lambda}(x,t) = T_{\Lambda}(x,t) + A\sin\frac{n\pi x}{l}\sin\frac{\pi t}{2\tau}$ will also satisfy Eq. (26) and all conditions. Therefore, the solution of this problem is not unique. This example shows that Eq. (26) doesn't have the uniqueness in some cases, which is another great difference between the two models.

It's a very complex and frontier problem about well-posedness problem of the differential delay equation like Eq. (26) in mathematics and it is beyond our ability to make more mathematical analyses on it. Here, we will provide a physical method to guarantee the uniqueness of the solution for Eq. (26). We can consider a heat conduction process beginning at $t = 0$, and there is no heat conduction when $t < 0$. That is to say, the systems are in thermal equilibrium and the whole temperature field is uniform when $t < 0$. The mathematical representations are $T(x,t) = C_0, t < 0$. Let $\varphi = T - C_0$ and φ also satisfies $\frac{\rho c_V}{\lambda}\frac{\partial\varphi}{\partial t} = \nabla^2\varphi(t-\tau)$. The boundary and initial conditions of φ are $\varphi|_{\Gamma} = T|_{\Gamma} - C_0$ and $\varphi|_{t=0} = T|_{t=0} - C_0$. Consider the Laplace transform $F = \int_0^{+\infty}\varphi e^{-pt}dt$. Substituting it into $\frac{\rho c_V}{\lambda}\frac{\partial\varphi}{\partial t} = \nabla^2\varphi(t-\tau)$, and according to the Time-Shift Theorem, we can get

$$e^{-p\tau}\nabla^2 F = \frac{\rho c_V}{\lambda}(pF - \varphi|_{t=0}). \tag{27}$$

Eq. (27) is an elliptic differential equation and its solution is unique when the boundary conditions are determined and continuous. $F = \int_0^{+\infty}\varphi e^{-pt}dt$ is unique, and φ must be continuous in time because there is a time differential $\frac{\partial\varphi}{\partial t}$ in the heat conduction equation. Based on the continuity of φ, we can determine that φ is unique from Lerch's Theorem. Finally, we can get a unique temperature field for the heat conduction problem. In summary, we can't guarantee that the solutions of Eq. (26) are unique in general but we can guarantee the uniqueness by considering no heat conduction exists when $t < 0$.

For Fourier's law, the heat conduction equation Eq. (4) is a parabolic equation and its maximum principle guarantees that the maximum values of temperature fields must appear in boundary or initial conditions. However, for the CV model, the heat conduction equation Eq. (5) is a wave equation which doesn't have such maximum principle in mathematics. It's easy to understand this result in physics. Consider a vibration of a fixed–fixed string without initial displacement. As long as the initial velocity is not zero, the displacement will be not always zero. Because the displacement is zero in boundary and initial conditions, the maximum values don't appear in boundary or initial conditions. For Eq. (26), we have mentioned that if the physical properties satisfy $\frac{2\tau n^2\pi}{\rho c_V l^2} = 1$, the solution with the form of $A\sin\frac{n\pi x}{l}\sin\frac{\pi t}{2\tau}$ satisfies Eq. (26), boundary conditions $T|_{\Gamma} = T|_{x=0,l} = 0$ and initial condition $T|_{t=0} = 0$. Obviously, the maximum values of this solution are $\pm|A|$ which don't appear in the boundary or initial conditions. Therefore, Eq. (26) doesn't have maximum principle either. The physical problems related to maximum principle in mathematics will be discussed in Section 3.4.

3.3. On negative entropy production rate

For Fourier's Law $q + \lambda\nabla T = 0$, we have $\dot{S} = -\frac{q\nabla T}{T^2} = \frac{q^2}{\lambda T^2} \geqslant 0$. Therefore, the entropy production rate of heat conduction is always positive or zero, which is required by the second law of thermodynamics. Next, we will discuss if the entropy production rate is positive or zero in the SPL and CV models.

For the single-phase-lagging model, the entropy production rate is Eq. (19). In general, we can't guarantee that $q(x,y,z,t+\tau)$ and $q(x,y,z,t)$ are all positive or negative at the same time. Therefore, we can't guarantee the entropy production rate is positive or zero either. However, q must be continuous in time because there is a time differential $\frac{\partial q}{\partial t}$ in the heat conduction equation. Based on the continuity of q, we can obtain that there is a $\tau_0 > 0$, and when $\tau < \tau_0$, $q(x,y,z,t)q(x,y,z,t+\tau) \geqslant 0$. Therefore, for the single-phase-lagging model, the entropy production rate will be positive or zero as long as the relaxation time is enough small. It should be pointed out that this condition is just a prerequisite or hypothesis for avoiding negative entropy production rate in the SPL model. It is possible that although the relaxation time is very small, the condition $\tau < \tau_0$ is still not satisfied which will still cause negative entropy production rate problem. For the CV model, there is a phase difference θ between the temperature gradient and the heat flux response expressed by Eqs. (24) and (25). Substituting Eqs. (24) and (25) into the expression of the entropy production rate $\dot{S} = -\frac{q\nabla T}{T^2}$ leads to

$$\dot{S} = -\frac{q\nabla T}{T^2} = \frac{\lambda C^2\sin[\xi(t)+\theta]\sin\xi(t)}{T^2}. \tag{28}$$

Obviously, we can't guarantee that $\sin\xi(t)$ and $\sin[\xi(t)+\theta]$ are all positive or negative at the same time either. We can see that the entropy production rate is not necessarily positive or zero for the CV model. Unlike the single-phase-lagging model, the entropy production rate is still not positive or zero for the CV model no matter how small the relaxation time is (larger than zero). That is because as long as the relaxation time is larger than zero, the phase difference θ will exist and this phase difference depends on not only the relaxation time but also other physical properties, the initial and boundary conditions. So the phase difference is not necessarily very small no matter how small the relaxation time is. In addition, if $\sin\xi(t)$ and $\sin[\xi(t)+\theta]$ are all positive or negative at the same time depends on not only the phase difference but also $\xi(t)$. For example, when $\xi(t) = 2N\pi - \frac{\theta}{2}$, where N is an integer, the entropy production rate turns to $\dot{S} = -\frac{q\nabla T}{T^2} = -\frac{\lambda C^2\sin^2\left(\frac{\theta}{2}\right)}{T^2} \leqslant 0$. In summary, compared with the single-phase-lagging model, the CV model is more likely to lead to the negative entropy production rate. Next, we will provide an example. Consider a heat conduction problem without heat source. The initial condition is taken $T|_{t=0} = T_0(1+\sin\frac{\pi x}{l})$, the boundary conditions are taken $T|_{x=0,l} = T_0$ and the physical properties satisfy $\frac{\lambda\tau\pi^2}{\rho c_V l^2} = \frac{1}{2\sqrt{e}}$. For this problem, if we use the single-phase-lagging model, we can get the classical solution

$$T_1(x,t) = T_0\left(1 + e^{-\frac{t}{2\tau}}\sin\frac{\pi x}{l}\right). \tag{29}$$

Then we can obtain the entropy production rate $\dot{S}_1$

$$\dot{S}_1 = -\frac{q\nabla T}{T^2} = \frac{\sqrt{e}\lambda(\nabla T)^2}{T^2} \geqslant 0. \tag{30}$$

From Eq. (30) we find that the entropy production rate of the single-phase-lagging model is positive or zero. Therefore, for this problem, the single-phase-lagging model satisfies the second law of thermodynamics. From Eq. (29) we find $T_1(x,t) > 0$ and therefore, the single-phase-lagging model also satisfies the third law of thermodynamics. The heat conduction equation satisfies first law of thermodynamics naturally. So for this problem, the single-phase-lagging model satisfies all the three laws of thermodynamics. For the CV model, we have mentioned that two initial conditions are needed to determine the solution. So if we use the CV model, we need an extra initial condition. To make the two models' initial states have a certain "consistency", we can let they have the same initial heat flux. So this extra initial condition for the CV model is $q_2|_{t=0} = q_1|_{t=0} = -\frac{\lambda T_0 \pi \sqrt{e}}{l}$, where $q_1|_{t=0}$ is the initial heat flux of the single-phase-lagging model determined by the classical solution Eq. (29), $q_2|_{t=0}$ is the initial heat flux of the CV model and $q_2|_{t=0} = -\frac{\lambda T_0 \pi \sqrt{e}}{l}$ is the extra initial condition. In addition, this extra initial condition is not unique, and we can also give other initial conditions. With this extra initial condition, we can obtain the classical solution of the CV model

$$T_2(x,t) = T_0\left[1 + e^{-\frac{t}{2\tau}} \sin\frac{\pi x}{l} \cos\left(\frac{\sqrt{\frac{2}{\sqrt{e}} - 1}}{2\tau} t\right)\right]. \tag{31}$$

Obviously, $T_2(x,t) > 0$ and so, for this problem, the CV model satisfies the third law of thermodynamics. Then we can obtain the entropy production rate $\dot{S}_2$ of the CV model

$$\dot{S}_2 = \frac{\rho c_V T_0^2 e^{-\frac{t}{\tau}}}{4\tau T^2} \cos^2\frac{\pi x}{l}\left[-\cos\left(\frac{\sqrt{\frac{2}{\sqrt{e}} - 1}}{\tau} t\right) + \left(\sqrt{\frac{2}{\sqrt{e}}} - 1\right) \sin\left(\frac{\sqrt{\frac{2}{\sqrt{e}} - 1}}{\tau} t\right) + 1\right]. \tag{32}$$

The entropy production rate in Eq. (32) is not always positive or zero. For example, when $\tan\left[(t\sqrt{2/\sqrt{e} - 1})/\tau\right] = -(\sqrt{2/\sqrt{e}} - 1)$ and $x = 0$, we can obtain $\dot{S}_2 = \frac{\rho c_V T_0^2 e^{-\frac{t}{\tau}}}{4\tau T^2}\left(1 - \sqrt{2/\sqrt{e}}\right) < 0$. We also find that no matter how small the relaxation time is, the negative entropy production rate still appears. In summary, the entropy production rate must be positive or zero in Fourier's Law, and for the single-phase-lagging model, the entropy production rate will be positive or zero if the relaxation time is enough small. However, for the CV model, no matter how small the relaxation time is, the negative entropy production rate still appears. Fig. 4 shows the entropy production rates which belong to the CV and SPL models. Here $\gamma = \frac{\rho c_V T_0^2 e^{-\frac{t}{\tau}}}{4\tau T^2} \cos^2 \frac{\pi x}{l}$ and $S' = \dot{S}_1$ or $\dot{S}_2$. Obviously, $\gamma > 0$ and thus, we can judge if the entropy production rate is positive everywhere from S'/γ. It is not difficult to find that the entropy production rate of the single-phase-lagging model is positive everywhere. However, we find negative values appear in the entropy production rate of the CV model. Negative values in S'/γ mean that the

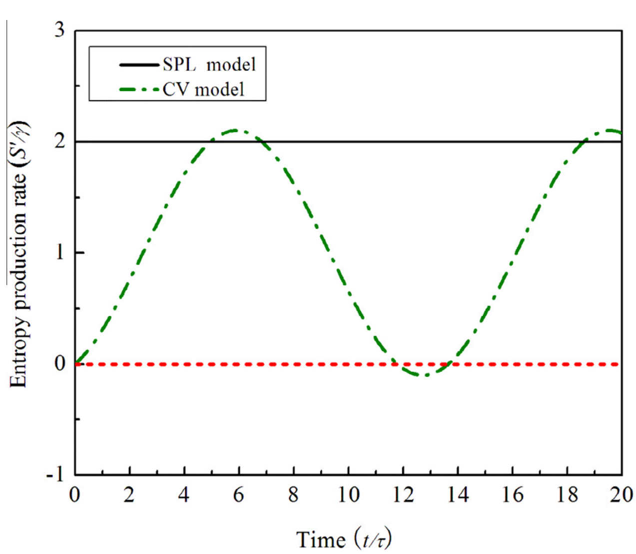

Fig. 4. Entropy production rates for the CV and SPL models.

entropy production rate is negative everywhere because for everywhere, $\gamma > 0$. In summary, for the entropy production rate problem, the single-phase-lagging model seems better than the CV model. In addition, the violation of the second law of thermodynamics by the CV model has been discussed by researchers [31–34]. It is also worth noting that the negative entropy production rate problem caused by the CV model can be avoided in the framework of extended irreversible thermodynamics [30].

Besides positive entropy production rate, the second law of thermodynamics requires that systems must tend to equilibrium spontaneously. For the CV model, the definition of energy integral [26] for Eq. (5) showing the vibration amplitude of the temperature field is

$$E(t) = \int\int\int\left[\left(\frac{\partial T}{\partial r}\right)^2 + \frac{\lambda}{\rho c_V \tau}(\nabla T)^2\right] dV. \tag{33}$$

The changing rate of energy integral can be written as

$$\frac{dE(t)}{dt} = -\frac{2}{\tau}\int\int\int\left(\frac{\partial T}{\partial t}\right)^2 dV, \tag{34}$$

which is negative or zero and shows that the vibration amplitude of systems is always dissipative. In addition, if there is no initial temperature perturbation and difference, a system must keep equilibrium because the initial energy integrals are zero, and are not able to decrease. However, for the single-phase-lagging heat conduction model, the solutions in Section 3.1 have the form of boundary conditions $T|_\Gamma = T|_{x=0,l} = 0$ and initial condition $T|_{t=0} = 0$. These solutions mean that a system in equilibrium will destroy the equilibrium without any perturbation spontaneously, which violates the second law of thermodynamics. Therefore, although the CV model as well as the single-phase-lagging model doesn't follow the second law of thermodynamics in the problem of entropy production rate, it does better in physical meaning. However, the two models both violate the second law of thermodynamics in classical irreversible thermodynamics.

3.4. On negative temperature

In Section 3.2, we have mentioned that for Fourier's Law, the heat conduction equation has maximum principle which guarantees that the maximum values of temperature field must appear in boundary and initial conditions. Therefore, Fourier's Law won't lead to absolute negative or zero temperature. In general, the temperature field is continuous and therefore, absolute negative temperature will lead to absolute zero temperature. Obviously, this violates the third law of thermodynamics. So, we need to discuss this problem in the two models. In addition, the negative absolute temperature problem of the CV model were studied by numerical calculations [27–29] and we will discuss this problem by analytical solutions.

In mathematics, the heat conduction equation of the CV model doesn't have maximum principle and so, the maximum values of temperature may not appear in boundary or initial conditions, which means that positive temperature in boundary and initial conditions cannot guarantee positive temperature in the whole temperature field. In physics, if the initial temperature change rate $\frac{\partial T}{\partial t}|_{t=0}$ is enough large, the amplitude of temperature will be very large, which means that the temperature field can reach much lower or higher than the initial temperature. Therefore, the CV model can't guarantee that temperature fields are always positive. We have mentioned that the heat conduction equation of the single-phase-lagging model doesn't have maximum principle either. Therefore, the single-phase-lagging model can't guarantee that the temperature fields are positive either. The solution

$A\sin\frac{n\pi x}{l}\sin\frac{\pi t}{2\tau}$ in Section 3.2 is an example which can lead to negative temperature because A is arbitrary. In Section 3.2 we guarantee the uniqueness of Eq. (26) by considering that there is no heat conduction when $t<0$ and the Laplace transform. We can also use the Laplace transform to get more conclusions about the problem of negative temperature. For Eq. (26), we have got Eq. (27) and for Eq. (5), the Laplace transform is

$$\frac{\lambda}{\rho c_V}\nabla^2 F-(p+p^2\tau)F+(p\tau+1)T|_{t=0}+\tau\left.\frac{\partial T}{\partial t}\right|_{t=0}=0. \tag{35}$$

Eq. (27) contains only the initial temperature $T|_{t=0}$, but Eq. (35) contains not only the initial temperature $\varphi|_{t=0}$ but also the initial temperature change rate $\frac{\partial T}{\partial t}|_{t=0}$. This means that for the single-phase-lagging model, the temperature field is only determined by the initial and boundary temperature but for the CV model, the initial temperature change rate will also take effect. So, the CV model needs the initial temperature change rate to guarantee positive temperature but the single-phase-lagging model doesn't need. However, for general problems, we only require $T|_{t=0}>0$ and there is no special requirement for initial temperature change rate $\frac{\partial T}{\partial t}|_{t=0}$ (for some temperature jump problems, $\frac{\partial T}{\partial t}|_{t=0}$ could even be infinite). Therefore, the CV model is more likely to lead to negative or zero temperature than the single-phase-lagging model because of the influence of the initial temperature change rate. Next, we will provide an example. Consider a heat conduction problem with heat source

$$\phi=T_0\sin\frac{\pi x}{l}\left(\frac{2\pi\rho c_V}{\tau}\cos\frac{2\pi t}{\tau}+\frac{\lambda\pi^2}{l^2}\sin\frac{2\pi t}{\tau}\right). \tag{36}$$

The initial conditions are taken $T|_{t=0}=T_0, T|_{t=0^+}=T_0(1+\beta)$, the boundary conditions are taken $T|_{x=0,l}=T_0(1+\beta),\ \beta>0$ and the physical properties satisfy $\frac{\lambda\tau}{\rho c_V l^2}=4$. For this problem, if we use the single-phase-lagging model, we can get its classical solution

$$T_3(x,t)=T_0\left(1+\beta\,\mathrm{sgn}t+\sin\frac{2\pi t}{\tau}\sin\frac{\pi x}{l}\right). \tag{37}$$

It is worth mentioning that if we use Fourier's Law, the solution is still Eq. (37). Obviously, $T_3(x,t)>0$ and for this problem, the single-phase-lagging model satisfies the third law of thermodynamics. We have mentioned that the CV model needs two initial conditions to determine the solution. So if we use the CV model, we need an extra initial condition and this extra initial condition should make the two models' initial state have a certain "consistency". This time, we let them have the same initial temperature change rate

$$\left.\frac{\partial T_3}{\partial t}\right|_{t=0}=\left.\frac{\partial T_4}{\partial t}\right|_{t=0}=\frac{2\pi T_0}{\tau}\cos\frac{2\pi t}{\tau}\sin\frac{\pi x}{l}=\frac{2\pi T_0}{\tau}\sin\frac{\pi x}{l}. \tag{38}$$

$\frac{\partial T_3}{\partial t}|_{t=0}$ is the initial temperature change rate of the single-phase-lagging model determined by classical solution Eq. (37), and $\frac{\partial T_4}{\partial t}|_{t=0}$ is the initial temperature change rate of the CV model. Then we can get $\frac{\partial T_4}{\partial t}|_{t=0}=\frac{2\pi T_0}{\tau}\cos\frac{2\pi t}{\tau}\sin\frac{\pi x}{l}=\frac{2\pi T_0}{\tau}\sin\frac{\pi x}{l}$. This extra initial condition is not unique and for telegrapher's equations, the most common initial conditions are initial temperature change rate and initial temperature. That's why we give this extra initial condition. With this extra initial condition, we can get the classical solution of the CV model

$$T_4(x,t)=T_0\begin{bmatrix}1+\beta\,\mathrm{sgn}t+(4\pi^2+1)\sin\frac{2\pi t}{\tau}\sin\frac{\pi x}{l}\\ +\frac{4\pi}{\sqrt{16\pi^2-1}}e^{-\frac{t}{2\tau}}\sin\frac{\sqrt{16\pi^2-1}}{2\tau}t\sin\frac{\pi x}{l}\end{bmatrix}. \tag{39}$$

$T_4(x,t)$ in Eq. (39) is not always positive. For example, for $t=\frac{3}{4}\tau+n\tau$, if n tends to infinity, t will also tend to infinity and the term $\frac{4\pi}{\sqrt{16\pi^2-1}}e^{-\frac{t}{2\tau}}\sin\frac{\sqrt{16\pi^2-1}}{2\tau}t\sin\frac{\pi x}{l}$ will tend to zero. Then we get

$$T_4(x,t)\to T_0\left[1+\beta\,\mathrm{sgn}t+(4\pi^2+1)\sin\frac{2\pi t}{\tau}\sin\frac{\pi x}{l}\right]. \tag{40}$$

Let β be very small and $x=\frac{l}{2}$, and then we get $T_4(x,t)\to T_0(1-4\pi^2)<0$ which has nothing to do with the relaxation time. We find that for this problem, the CV model leads to negative temperature no matter how small the relaxation time is but the single-phase-lagging model doesn't.

In addition, although this is an unsteady heat conduction problem whose temperature and heat flux fields are both unsteady, the single-phase-lagging model and Fourier's Law lead to exactly same temperature and heat flux fields. Obviously, it is impossible for the CV model. That is because if the temperature and heat flux fields satisfy both Fourier's Law and the CV model, $\frac{\partial q}{\partial t}$ must be zero. For this problem, the relative deviation between the CV and SPL models (or Fourier's law) is

$$\eta=\frac{T_2(x,t)-T_1(x,t)}{T_1(x,t)}=\frac{4\pi^2\sin\frac{2\pi t}{\tau}\sin\frac{\pi x}{l}+\frac{4\pi}{\sqrt{16\pi^2-1}}e^{-\frac{t}{2\tau}}\sin\frac{\sqrt{16\pi^2-1}}{2\tau}t\sin\frac{\pi x}{l}}{\left(1+\beta\,\mathrm{sgn}t+\sin\frac{2\pi t}{\tau}\sin\frac{\pi x}{l}\right)}. \tag{41}$$

When time tends to infinity, Eq. (40) tends to $(4\pi^2\sin\frac{2\pi t}{\tau}\sin\frac{\pi x}{l})/(1+\beta\,\mathrm{sgn}t+\sin\frac{2\pi t}{\tau}\sin\frac{\pi x}{l})$. It is still not small. For example, when $t=\frac{3}{4}\tau+n\tau,\ x=\frac{l}{2}$ and n tends to infinity, this relative deviation tends to $-\frac{4\pi^2}{\beta}$. If β is very small, the relative deviation will still be very large and this result has nothing to do with the relaxation time either. Therefore, the deviation between the CV model and the single-phase-lagging model (or Fourier's law) can also be very large no matter how small the relaxation time is and won't decay over time. Fig. 5 shows the temperature at $x=l/2$ ($\beta=0.5$) which belongs to the CV model $[T_4(l/2,t)]$ and the single-phase-lagging model $[T_3(l/2,t)]$. Obviously, negative temperature appears in the solution of the CV model which has far larger amplitude than the solution of the single-phase-lagging model. However, Eq. (37) and Fig. 5 show that the solution of the single-phase-lagging model must be positive. From Fig. 5, we find that the CV model leads to a far stronger temperature vibration than the single-phase-lagging model, and this phenomenon causes negative temperature problem in the CV model rather than the single-phase-lagging model.

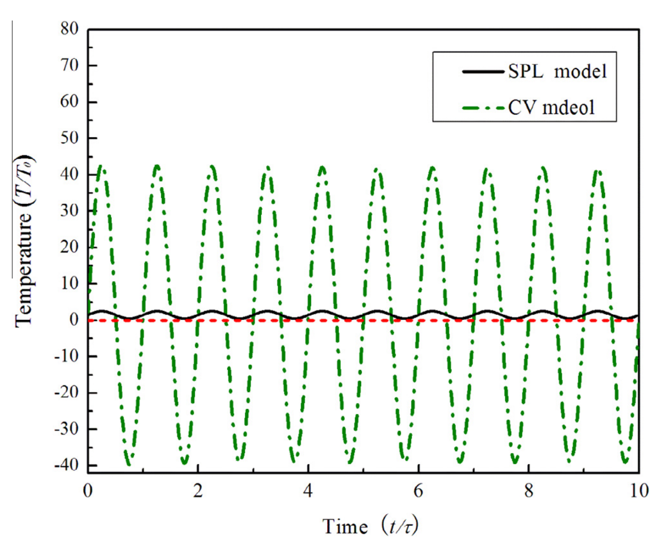

Fig. 5. Temperature of the CV and SPL models at $x=l/2$.

4. About higher order terms

In this section, we will discuss whether using higher order approximation or measuring the quantity $\frac{\partial^n q}{\partial t^n}$ can reduce the defection caused by first-order approximation and increase the approximation degree. It is necessary to point out that Taylor series approximation of $q(x, y, z, t + \tau)$ needs the existence of differential term(s) when $\tau \to 0$. Unfortunately, this condition is usually invalid. For example, in Sections 2.1.1 and 2.1.2, it is not difficult to find that although boundary and initial conditions are infinitely differentiable for any $\tau > 0$, $\lim_{\tau\to 0}\frac{\partial q}{\partial t}$ doesn't exist. Because differential term(s) $\frac{\partial^n q}{\partial t^n}$ may not exist when $\tau \to 0$, Taylor series approximation may be meaningless either. This problem is caused by the boundary conditions $T(t)|_\Gamma$. Because the heat flux fields are not determined functions without boundary and initial conditions, it is better to express $q(x, y, z, t)$ as

$$q(x,y,z,t) = q(T(t)|_\Gamma, T(x,y,z)|_{t=0}), \tag{42}$$

and express $q(x, y, z, t + \tau)$ as

$$q(x,y,z,t+\tau) = q(T(t+\tau)|_\Gamma, T(x,y,z)|_{t=0}). \tag{43}$$

Formally speaking, first-order approximation of $q(x, y, z, t + \tau)$ can be written as

$$\begin{aligned} q(x,y,z,t+\tau) &= q(T(t+\tau)|_\Gamma, T(x,y,z)|_{t=0}) \\ &= q + \tau \frac{\partial q}{\partial (T|_\Gamma)} \frac{\partial (T|_\Gamma)}{\partial t} + R(\tau), \end{aligned} \tag{44}$$

where $R(\tau)$ is the remainder. This approximation needs the existence of $\frac{\partial q}{\partial (T|_\Gamma)}$ and $\frac{\partial (T|_\Gamma)}{\partial t}$ when $\tau \to 0$. However, as counterexamples, Sections 2.1.1 and 2.1.2 show that $\lim_{\tau\to 0}\frac{\partial (T|_\Gamma)}{\partial t}$ may not exist even if $T|_\Gamma$ are infinitely differentiable for any $\tau > 0$. What's more, whether the remainder $R(\tau)$ satisfies $\lim_{\tau\to 0}\frac{R(\tau)}{\tau} \equiv 0$ also depends on boundary conditions.

On the other hand, higher order approximation leads to higher order time derivative terms in the heat conduction equation. For the SPL model, there is only a first-order time derivative term $\frac{\partial T}{\partial t}$ in the heat conduction equation. However, nth-order approximation will lead to higher order derivative terms from second-order to $(n+1)$th-order $\frac{\partial^2 T}{\partial t^2}, \frac{\partial^3 T}{\partial t^3} \ldots \frac{\partial^{n+1} T}{\partial t^{n+1}}$. Therefore, higher order approximation will lead to more initial conditions needed to determine the solution, and stronger influence on solutions will be caused by initial conditions. It seems that the higher the order of the approximation is, the larger the difference between the approximate equation and original equation Eq. (26) is. In Section 3.4, we have mentioned that the CV model is more likely to cause unphysical problems than the SPL model because of the influence by the initial temperature change rate $\frac{\partial T}{\partial t}\big|_{t=0}$. However, for higher order approximation, higher order temperature change rates $\left(\frac{\partial^2 T}{\partial t^2}\Big|_{t=0}, \frac{\partial^3 T}{\partial t^3}\Big|_{t=0} \ldots\right)$ will also have an impact. From the physical point of view, the ordinary physical meaning without approximation is time lagging. However, the physical meaning of first-order approximation can be considered as impedance or damping. Higher order approximation will lead to higher order damping or impedance terms. Therefore, from physical point of view, higher order approximation can't reduce or even increase the physical difference.

Therefore, using higher order approximation or measuring the quantity $\frac{\partial^n q}{\partial t^n}$ can neither reduce the deviation caused by first-order approximation nor avoid unphysical problems. The application of higher order terms is not enough to discuss the approximation degree problem and might be impossible because the boundary conditions will also have an influence on the remainder $R(\tau)$ and the existence of $\lim_{\tau\to 0}\frac{\partial^n q}{\partial t^n}$ also depends on the boundary conditions."

5. Conclusions

In this paper we demonstrate that Taylor series approximation itself has some defects when used in heat conduction models. First, the relative deviation between $q(t + \tau)$ and $q + \tau\frac{\partial q}{\partial t}$ can be very large no matter how small the relaxation time τ is. Second, this approximation can lead the originally positive entropy production rate to be negative, which violates the second law of thermodynamics. Using Taylor series approximation to derive or extend heat conduction models may be defective because it will cause large deviation and essential difference in mathematics and physics. Although there is a certain "approximation" relationship between the single-phase-lagging model and the CV model, there are essential differences between them as follows:

1. Their physical meanings are different. The single-phase-lagging model means that there is a time lag between the temperature gradient and the heat flux response, and the speed of the heat flux response to the temperature gradient is not infinite. The CV model means that there is a phase difference between the temperature gradient and the heat flux, and the speed of temperature perturbation itself is not infinite.
2. Great difference in mathematics exists between them. For the CV model, more initial conditions are needed than the single-phase-lagging model for getting their solutions. In addition, the solution of the heat conduction equation of the CV model has the uniqueness but for the single-phase-lagging model, this uniqueness does not exist in some cases. However, for the single-phase-lagging model, we can guarantee the uniqueness by considering that there is no heat conduction process when $t < 0$, and using the method of the Laplace transform.
3. The single-phase-lagging model can guarantee the entropy production rate to be positive as long as the relaxation time is enough small. However, for the CV model, no matter how small the relaxation time is, the negative entropy production rate may appear. The CV and SPL models may both lead to negative or zero temperature, and the CV model is more likely to lead to negative or zero temperature than the single-phase-lagging model.
4. For an unsteady problem whose temperature and heat flux fields are both unsteady, the single-phase-lagging model and Fourier's law can lead to exactly same temperature and heat flux fields, but quite different for the CV model. The deviation between the CV model and the single-phase-lagging model (or Fourier's law) can also be very large no matter how small the relaxation time is, and it won't decay over time.
5. In mathematics, higher order approximation will lead to larger difference between the approximate equation and original equation than first-order approximation. It also complicates the existence problem of differential term(s) and influence by the initial conditions. In physics, higher order approximation will lead to higher order damping or impedance terms which can't reduce or even increase the physical meaning difference. Therefore, higher order approximation can't solve the mathematical and physical problems caused by first-order approximation.

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