Modeling shock waves in an ideal gas: Combining the Burnett approximation and Holian's conjecture

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We model a shock wave in an ideal gas by combining the Burnett approximation and Holian's conjecture. We use the temperature in the direction of shock propagation rather than the average temperature in the Burnett transport coefficients. The shock wave profiles and shock thickness are compared with other theories. The results are found to agree better with the nonequilibrium molecular dynamics (NEMD) and direct simulation Monte Carlo (DSMC) data than the Burnett equations and the modified Navier-Stokes theory.

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The strong gradients within a shock wave lead to a number of associated effects of scientific and technological relevance, which have attracted the attention of theoreticians and experimentalists for a long time. Though the main features of shock waves are well understood, much remains to be done to complete the prediction of their quantitative aspects. The Navier-Stokes (NS) model can be used to provide a description for several shock wave propagation phenomena. But this model is valid only for Mach numbers (M) up to 1.8 because it is based on the essential idea that the viscous tensor and the heat flux generated in the fluid due to a perturbation are expressed by the linear laws: Newton's law of friction and Fourier's law of heat conduction. Holian [1] introduced a slight modification to the Navier-Stokes model to account for the fact that the component of temperature $T=(T_{xx}+T_{yy}+T_{zz})/3$ in the direction of shock propagation always exceeds the total average temperature T. This modification, designated as Holian's conjecture, consists of replacing T by T_{xx} in the Navier-Stokes transport coefficients and leads to a substantial improvement of the agreement with the molecular dynamics results over the standard Navier-Stokes equations [2]. A kinetic foundation for Holian's conjecture has been explored by Uribe *et al.* [3]. There are also some other theories for shock waves, such as the Burnett theory [4–6], the bimodal distribution of Mott-Smith [7], and the Bhatnagar-Gross-Krook (BGK) model [8,9]. Especially the Burnett constitutive equations, obtained by Chapman and Cowling, in which the second-order terms of fluxes are considered, can significantly improve over the Navier-Stokes model. Since the Burnett model is the next-order corrections of the Navier-Stokes model, a natural question is whether the modification of the Burnett theory with Holian's conjecture, as the modification of Navier-Stokes theory made by Holian, can improve the description of the shock wave profiles.

The accuracy of the Burnett equations for $M>2$ in a dilute gas has been validated by Salomons and Mareschal [10] in 1992 using both the nonequilibrium molecular dynamics (NEMD) and Bird's direct simulation Monte Carlo (DSMC) method [11,12] to compute shock wave profiles. Chapman has also pointed out that the Burnett corrections to the NS theory are important by comparing the Burnett and DSMC results [5,6]. In 1998, Uribe *et al.* [13] have gone one step further and obtained velocity and temperature profiles using the Burnett equations; the theoretical results are very close to the NEMD results except for the small deviations near the unshocked region. Since shear viscosity is the most important of the transport coefficients in the accurate description of a fluid shock wave profile [1], using T_{xx} rather than T in the transport coefficients (Holian's conjecture) would increase the viscosity and broaden the profile, and this solution would more closely approximate the NEMD and DSMC results.

For plane shock waves it is convenient to choose a reference frame moving with the front, so that the shock is stationary in this frame. Under this condition, and taking the x axis as the shock wave direction, the hydrodynamic balance equations yield

$$\rho(x)u(x)=\rho_0 u_0, \tag{1}$$

$$P_{xx}=P_0+\rho_0 u_0[u_0-u(x)], \tag{2}$$

$$E(x)+\frac{q_x}{\rho_0 u_0}=E_0+\frac{1}{2}[u_0-u(x)]^2+\frac{P_0}{\rho_0 u_0}[u_0-u(x)], \tag{3}$$

where ρ is the mass density, u is the x component of the flow velocity, P_{xx} is the relevant element of the pressure tensor, E is the internal energy per mass unit, and q_x is the x component of the heat flux. The initial unshocked equilibrium state (cold region) is labeled by subscript 0, while the final shocked state far behind the shock front (hot region) will be labeled by subscript 1.

The Burnett corrections to the pressure tensor and the heat flux were taken from the book by Chapman and Cowling [4] and its form is adopted as Uribe's [14]. The coefficients that appear in the expressions for the pressure tensor and the heat flux are also the same as Uribe's [14]. We also adopt the same dimensionless variables as Holian [2], so the dimensionless expressions for $P_{xx}\equiv P_{xx}^{(0)}+P_{xx}^{(1)}+P_{xx}^{(2)}$ and $q_x\equiv q_x^{(0)}+q_x^{(1)}+q_x^{(2)}$ are the same as Uribe's [14].

Now we modify the Burnett equations according to Holian's conjecture; we replace T in the transport coefficients by T_{xx}. T_{xx} is defined by the x component of the peculiar energy

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$$NkT_{xx}=\sum_{i=1}^{N} p_{ix}^2/m, \tag{4}$$

where the local fluid velocity has been subtracted from the momenta of N particles in the thin slab of material in the equation, so that the p_{ix} are peculiar momenta, i.e., thermal fluctuations only. m is the atomic mass and k is the Boltzmann's constant. For the ideal gas there is no potential contribution, so that $P_{xx}=\rho kT_{xx}$. Hence, we get T_{xx} as follows:

$$T_{xx}=\frac{P_0+\rho_0 u_0[u_0-u(x)]}{\rho k}. \tag{5}$$

The modified dimensionless expressions for P_{xx} and q_x turn out to be given by

$$P_{xx}^*\equiv\frac{P_{xx}}{\rho_0 u_0^2}=\frac{\tau}{u^*}-[u^*(\tau_0+1-u^*)]^{1/2}\frac{du^*}{ds}+\Bigg\{[2\omega_1/3 - 14\omega_2/9+2\omega_6/9]\left(\frac{du^*}{ds}\right)^2-\frac{2}{3}\omega_2\frac{d}{ds}\left[u*\frac{d}{ds}(\tau/u^*)\right] + \frac{2}{3}\omega_3\frac{d^2\tau}{ds^2}+\frac{2}{3}\omega_4\frac{u^*}{\tau}\frac{d}{ds}\left(\frac{\tau}{u^*}\right)\frac{d\tau}{ds}+\frac{2}{3}\frac{\omega_5}{\tau}\left(\frac{d\tau}{ds}\right)^2\Bigg\}\frac{9u^*}{16}, \tag{6}$$

$$q_x^*\equiv\frac{q_x}{\rho_0 u_0^3} = -\frac{45}{16}[u^*(\tau_0+1-u^*)]^{1/2}\frac{d\tau}{ds}+\Bigg\{[\theta_1-8\theta_2/3+2\theta_5]\frac{du^*}{ds}\frac{d\tau}{ds} + \frac{2}{3}[\theta_4-\theta_2]\tau\frac{d_2u^*}{ds^2}+\frac{2\theta_3 u^*}{3}\frac{du^*}{ds}\frac{d}{ds}\left(\frac{\tau}{u^*}\right)\Bigg\}\frac{9u^*}{16}. \tag{7}$$

Here $u^*\equiv u/u_0$ is the reduced velocity, $\tau\equiv kT/mu_0^2$ is the reduced temperature, and s is equal to x/l, with $l=5m/(12\rho_0\sigma^2\sqrt{\pi})$, which will turn out to be close to the mean free path of the initial state of the ideal gas. We would like to point out that only the first-order terms of the pressure and heat in Eqs. (6) and (7) are corrected using Holian's conjecture for simplicity, as only a few of the second-order terms of the pressure and heat are actually dependent on the temperature and they are small compared with the first terms.

Specializing to the case of the ideal gas, the equation of state (EOS) is

$$P(\rho,T)=\rho\frac{kT}{m}, \quad E(\rho,T)=\frac{3}{2}\frac{kT}{m}. \tag{8}$$

By substituting Eqs. (6) and (7) into the conservation equations (2) and (3), one derives a closed system of two second-order differential equations for u^* and τ. These equations are transformed to first-order equations in Uribe's way [14]. In terms of $y_1(s)=u^*(s)$, $y_2(s)=\tau(s)$, $y_3(s)=u^*(s)'$, and $y_4(s)=\tau(s)'$, the first-order system can be written as

$$y'=\boldsymbol{F}(y(s),\tau_0), \tag{9}$$

where the prime denotes the derivative with respect to s and the vector field $\boldsymbol{F}(y)$ is given by $\boldsymbol{F}_1(y,\tau_0)=y_3$, $\boldsymbol{F}_2(y,\tau_0)=y_4$,

$$\boldsymbol{F}_3(y,\tau_0)=\frac{3}{2y_1^2y_2(\theta_4-\theta_2)}\Bigg[\frac{40}{9}\tau_0y_1-\frac{16}{9}\tau_0y_1^2+\frac{8}{9}y_1-\frac{16}{9}y_1^2 + \frac{8}{9}y_1^3-\frac{8}{3}y_1y_2+5y_1y_4\sqrt{y_1(\tau_0+1-y_1)} - y_3y_4y_1^2\left(\theta_1-\frac{8}{3}\theta_2+\frac{2}{3}\theta_3+2\theta_5\right)+\frac{2}{3}y_1\theta_3y_3^2y_2\Bigg], \tag{10}$$

$$\boldsymbol{F}_4(y,\tau_0)=\frac{1}{y_1^2y_2(c_2+c_3)}\Bigg[\frac{16}{9}\tau_0y_1y_2+\frac{16}{9}y_1y_2-\frac{16}{9}y_1^2y_2 - \frac{16}{9}y_2^2+y_1y_2^2c_2F_3(y,\tau_0) + \frac{16}{9}y_1y_2y_3\sqrt{y_1(\tau_0+1-y_1)}-y_3^2(y_1^2y_2c_1+y_2^2c_2) - y_4^2y_1^2(c_4+c_5)+y_3y_4y_1y_2(c_2+c_4)\Bigg], \tag{11}$$

and $c_1=\frac{2}{3}\omega_1-\frac{14}{9}\omega_2+\frac{2}{9}\omega_6$, $c_2=-\frac{2}{3}\omega_2$, $c_3=\frac{2}{3}\omega_3$, $c_4=\frac{2}{3}\omega_4$, $c_5=\frac{2}{3}\omega_5$. The coefficients ω's and θ's are given by

$$\omega_1=1.014\times 4, \quad \omega_2=1.014\times 2,$$
$$\omega_3=0.806\times 3, \quad \omega_4=0.681,$$
$$\omega_5=0.806\times 3/2-0.99, \quad \omega_6=0.928\times 8,$$
$$\theta_1=1.035\times 45/4, \quad \theta_2=1.035\times 45/8,$$
$$\theta_3=-1.03\times 3, \quad \theta_4=0.806\times 3,$$
$$\theta_5=8.3855. \tag{12}$$

We have to use numerical methods to solve Eq. (9) because in nonlinear phenomena it is rather often the only way to go. Because the mathematical stability of the system of equations is directional [15], the numerical integration has to start at the shocked state. Notice the boundary conditions can be obtained from the Rankine-Hugoniot jump conditions

$$u_1^*=\frac{5}{4}\tau_0+\frac{1}{4}, \quad \tau_1=\frac{7}{8}\tau_0+\frac{3}{16}-\frac{5}{16}\tau_0^2, \quad u_0^*=1. \tag{13}$$

We also use the Mach number $M=\sqrt{0.6/\tau_0}$ to characterize the hydrodynamic profiles. For the purpose of comparing with the NEMD work of Salomons and Mareschal [10] ($M=134$), we make the reasonable and simplifying assumption that the initial temperature is zero($M=\infty$, $\tau_0=0$). We would like point out that shock wave profiles for all Mach numbers can be generated. We have used the Runge-Kutta method to solve Eq. (9) setting $u^*(s_0)=u_1^*+6\times 10^{-6}$, $\tau(s_0)=\tau_1$. The initial values for derivatives were taken to be zero.

The velocity profile for $M=\infty$ is shown in Fig. 1 for NEMD computer experiments, the Holian's modified NS

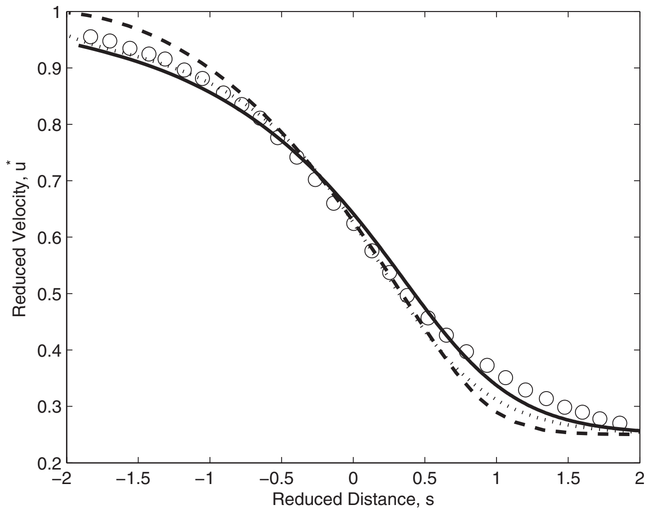

FIG. 1. Reduced velocity profile $u^*(s)$ for shock wave in an ideal gas for $M=\infty$. Circles: NEMD ($M=134$); dashed line: Burnett; long-dashed line: modified NS; solid line: modified Burrnett; the reduced shock thickness is, respectively, 2.35, 1.97, 2.07 and 2.38.

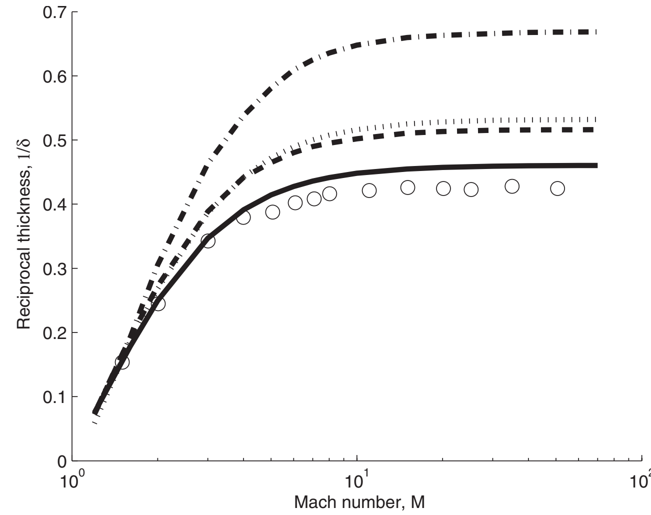

FIG. 3. Reciprocal thickness as a function of Mach number. Circles: DSMC; long-dashed line: modified NS; dashed line: Burnett; solid line: modified Burrnett; dot-dashed line: standard NS.

theory, the Burnett theory, and our results (we will refer to it as the modified Burnett theory following). It is found that the modified Burnett equations improve the agreement with the NEMD data as compared to other theories for lager M. The Burnett equations are superior in the cold region with a small discrimination. However, the performance on the hot region of the shock front is better if one uses the modified Burnett equations. The velocity profile for $M=2$ is also shown in Fig. 2. It is found both that the Burnett theory and the modified Burnett theory agree with the DSMC data well for small Mach number. To make a further comparison, we have calculated the shock wave reciprocal thickness as it has been taken as a criterion to assess different theories in the literature. Shock thickness is defined as $\delta=(u_0^*-u_1^*)/\max(|du^*/ds|)$. In Fig. 3 we display shock reciprocal thickness for different theories. It can be seen that the modified Burnett results are in much closer agreement to DSMC results than the other three theories for all Mach numbers. Especially, for $M=\infty$ the calculation results for DSMC, modified Burnett, Burnett, and modified NS are 2.35, 2.38, 1.97, and 2.07, respectively. So the modified Burnett equations give a very good description especially for strong shock waves.

The average temperature τ and the normal component τ_{xx} for $M=\infty$ are displayed in Fig. 4. In all theories, τ_{xx} exhibits a peak of 0.25, which is 4/3 the final temperature. τ and τ_{xx} both provide good agreements with the NEMD results in the hot region. Since transport coefficients are proportional to $\sqrt{T}$, the discriminations in the cold region may have small effect on the shock wave profile and shock wave thickness because of the small absolute value of temperature.

In summary, in this paper we have modeled shock waves in the ideal gas, combining the Burnett equations and the

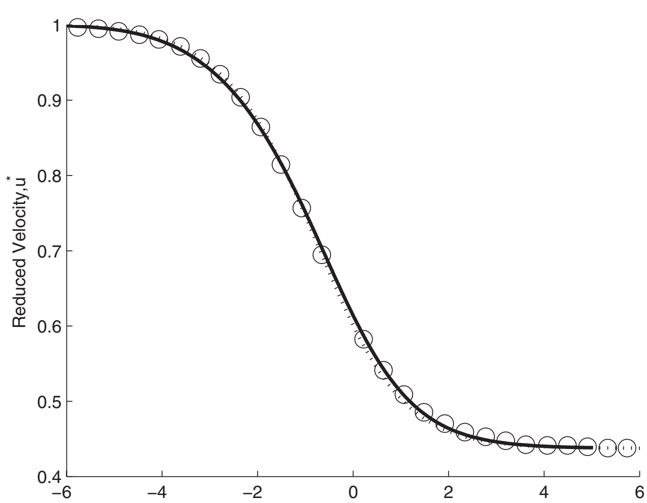

FIG. 2. Reduced velocity profile $u^*(s)$ for shock wave in an ideal gas for $M=2$. Circles: DSMC; dashed line: Burnett; solid line: modified Burrnett.

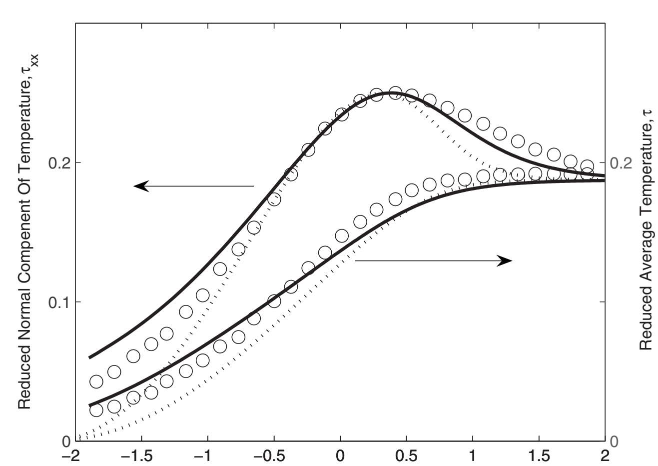

FIG. 4. Reduced average temperature τ and reduced normal component of temperature τ_{xx} vs reduced distance s for a shock wave in an ideal gas. Circles: NEMD; dashed line: modified NS; solid line: modified Burnett.

conjecture by Holian. Namely, since the temperature in the direction of shock propagation always exceeds the total average temperature T, we have used T_{xx} to replace T in the Burnett transport coefficients. We also have compared the shock wave profiles and shock thickness of different theories and found that the modified Burnett equations could provide a good description of the shock wave profile, especially for strong shock waves.

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