Abstract

We model a shock wave in an ideal gas by solving a modified version of the compressible Navier-Stokes equations of hydrodynamics, where, following an earlier conjecture by Holian [Phys. Rev. **A 37**, 2562 (1988)], we use the temperature in the direction of shock propagation T_{xx}, rather than the average temperature $T=(T_{xx}+T_{yy}+T_{zz})/3$, in the evaluation of the linear transport coefficients. The results are found to agree much better with the molecular-dynamics simulations of Salomons and Mareschal [Phys. Rev. Lett. **69**, 269 (1992)] than standard Navier-Stokes theory.

RAPID COMMUNICATIONS

PHYSICAL REVIEW E VOLUME 47, NUMBER 1 JANUARY 1993

Modeling shock waves in an ideal gas: Going beyond the Navier-Stokes level

B. L. Holian and C. W. Patterson
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

M. Mareschal and E. Salomons
Centre Européen de Calcul Atomique et Moléculaire, Université Paris-Sud, 91405 Orsay CEDEX, France
(Received 28 September 1992)

We model a shock wave in an ideal gas by solving a modified version of the compressible Navier-Stokes equations of hydrodynamics, where, following an earlier conjecture by Holian [Phys. Rev. A **37**, 2562 (1988)], we use the temperature in the direction of shock propagation T_{xx}, rather than the average temperature $T=(T_{xx}+T_{yy}+T_{zz})/3$, in the evaluation of the linear transport coefficients. The results are found to agree much better with the molecular-dynamics simulations of Salomons and Mareschal [Phys. Rev. Lett. **69**, 269 (1992)] than standard Navier-Stokes theory.

PACS number(s): 51.10.+y, 47.40.Nm, 47.45.−n

I. INTRODUCTION

Shock waves in dense fluids are remarkably well approximated by solving the compressible Navier-Stokes (NS) equations of hydrodynamics [1,2]. Nonequilibrium molecular-dynamics (MD) calculations by Holian *et al.* [2] and by Klimenko and Dremin [3] for shock waves in the Lennard-Jones (LJ) fluid were compared to the NS solution, which requires as input the LJ equation of state (EOS) (the equilibrium pressure P as a function of internal energy E and density ρ) and the linear transport coefficients (shear viscosity η_S, bulk viscosity η_V, and thermal conductivity κ as functions of ρ and temperature T). The EOS was determined from earlier equilibrium MD and Monte Carlo calculations [4], while the transport coefficients were obtained either from previous equilibrium MD simulations, evaluating Green-Kubo fluctuation formulas [5], or from more reliable nonequilibrium MD simulations of fluxes in response to imposed external fields [6]. In subsequent work, Holian [7] noted that any discrepancy between NS and nonequilibrium MD shock-wave simulation profiles, such as particle velocity $u(x)$, could be at least qualitatively explained by the thermal dependence of the shear viscosity at the steepest part of the shock front (located approximately at the point where u is halfway between initial and final values), since shear viscosity is the most important of the transport coefficients in the accurate description of a fluid shock-wave profile. In all cases thus far simulated (either fluid or solid), the component of temperature in the direction of shock propagation T_{xx} always exceeds the average temperature $T=(T_{xx}+T_{yy}+T_{zz})/3$, even exhibiting a peak $T_{xx}\approx 1.3T$ near the middle of the shock front. T_{xx} is defined by the x component of the peculiar kinetic energy

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

where the local fluid velocity has been subtracted from the momenta of N particles in the thin slab of material (volume V) in this equation, so that the p_{ix} are peculiar momenta, i.e., thermal fluctuations only (m is the atomic mass, k is Boltzmann's constant). At the lower shock strengths [3], the density and temperature states remain in the dense-fluid regime, where the shear viscosity decreases with increasing temperature; consequently, using T_{xx} rather than T would lower the viscosity and steepen the profile. On the other hand, for the strongest shock wave [2], where the final temperature is sufficiently high that the LJ system begins to approach ideal-gas behavior, using T_{xx} rather than T would increase the viscosity and broaden the profile. In both cases, the modified NS solution would more closely approximate reality, i.e., the nonequilibrium MD results.

Recently, Salomons and Mareschal [8] performed the first MD simulations of a shock wave in an ideal gas of hard spheres. The ideal gas regime is very difficult for MD, since the mean free path l_0 can become large compared to the molecular size σ. Hence, the simulation requires a large system, whose minimum linear dimension is many mean free paths. They also undertook to check the direct-simulation Monte Carlo (DSMC) method of solving the Boltzmann equation [9]; the results literally could not be distinguished from MD, confirming the validity of DSMC. Then, they compared their results (MD and/or DSMC) to the standard Navier-Stokes shock-wave solution, and found rather good agreement, though, as in the strong dense-fluid case, the NS profiles were too steep when compared to the exact solution (MD). They estimated the Burnett correction to the heat flux, using the observed MD gradients in velocity, temperature, and pressure, and found that it helped explain the observed deviations from Fourier's Law.

The ideal gas is, in fact, an ideal candidate for testing Holian's conjecture (that T_{xx} should be used in a modification to Navier-Stokes theory, rather than T), since a self-consistent solution is possible; that is, there is no ambiguity about extracting T_{xx} from the normal component of the pressure tensor P_{xx}, the general expression for which is

$$P_{xx}V=\sum_{i=1}^{N}(p_{ix}^2/m+F_{ix}x_i)=NkT_{xx}+\sum_{i=1}^{N}F_{ix}x_i\,. \tag{2}$$

For the ideal gas there is no potential contribution, only kinetic ($F_{ix} \equiv 0$), so that $P_{xx} = \rho k T_{xx}/m$ (the mass density is $\rho = Nm/V$). In the next section, we review the NS equations as they apply to a planar shock wave, exhibit the EOS and transport coefficients for an ideal gas, and outline the solution method for the modified NS equations, where T_{xx} replaces T in the thermal dependence of the transport coefficients. Finally, we compare the modified Navier-Stokes solution to molecular dynamics and conclude with some comments.

II. BEYOND THE NAVIER-STOKES LEVEL

The Navier-Stokes equations of hydrodynamics [10] are given by the conservation (continuity equations) of mass, momentum, and energy in a volume element (the mass density is ρ, $\mathbf{u}$ is the fluid velocity, $\vec{\mathbf{P}}$ is the pressure tensor, E is the internal energy per unit mass, i.e., excluding the kinetic energy associated with the fluid motion, and $\mathbf{q}$ is the heat flux vector),

$$\begin{aligned} &\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 , \\ &\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla \cdot \vec{\mathbf{P}} , \\ &\frac{\partial}{\partial t}[\rho(E + \tfrac{1}{2}u^2)] + \nabla \cdot [\rho(E + \tfrac{1}{2}u^2)\mathbf{u}] = -\nabla \cdot (\mathbf{u} \cdot \vec{\mathbf{P}} + \mathbf{q}) , \end{aligned} \tag{3}$$

where the Navier-Stokes constitutive equations specify a linear relation between momentum flux (pressure tensor $\vec{\mathbf{P}}$) and components of the rate-of-strain tensor $\nabla \mathbf{u}$, as well as a linear relation between the heat flux vector $\mathbf{q}$ and the temperature gradient ∇T (Fourier's law of heat conduction). Note that in the solution of Eqs. (3) for any practical hydrodynamics problem, the local equilibrium temperature T has to be obtained by inverting the equation of state. That is, the hydrostatic pressure P is obtained from ρ and E in Eqs. (3), whereas in the usual representations of the EOS, P and E are expressed in terms of the independent variables ρ and T. (Similarly, the linear NS transport coefficients are usually expressed as functions of ρ and T.)

For a planar shock wave, such as that generated by a piston pushed in the x direction at a steady velocity into a material initially at rest, the overall motion is one dimensional. When the shock wave achieves a steady profile, due to the dissipative effects of viscosity (in fluids) and thermal conductivity, the partial time derivatives vanish, and the conservation equations simplify

$$\begin{aligned} &\rho(x)u(x) = \text{const} , \\ &P_{xx}(x) + \rho(x)u^2(x) = \text{const} , \\ &\rho(x)[E(x) + \tfrac{1}{2}u^2(x)]u(x) + u(x)P_{xx}(x) + q(x) = \text{const} . \end{aligned} \tag{4}$$

The initial unshocked equilibrium state will be labeled by subscript 0, while the final shocked state far behind the shock front is at a hotter, denser equilibrium state, which will be labeled by subscript 1. Both equilibrium states are characterized by zero gradients, so that the normal component of the pressure tensor (in the direction of shock propagation) is equal to the hydrostatic pressure, and the heat flux vector is zero. Thus, Eq. (4) becomes

$$\begin{aligned} &\rho(x)u(x) = \rho_0 u_0 = \rho_1 u_1 , \\ &P_{xx}(x) + \rho_0 u_0 u(x) = P_0 + \rho_0 u_0^2 = P_1 + \rho_1 u_1^2 , \\ &E(x) + \tfrac{1}{2}u^2(x) + \frac{P_{xx}(x)}{\rho(x)} + \frac{q(x)}{\rho_0 u_0} \\ &\qquad = E_0 + \tfrac{1}{2}u_0^2 + \frac{P_0}{\rho_0} = E_1 + \tfrac{1}{2}u_1^2 + \frac{P_1}{\rho_1} , \end{aligned} \tag{5}$$

where the latter relations between initial and final equilibrium states are the Rankine-Hugoniot jump conditions. We interpret the initial and final velocities for this steady shock wave as follows: A piston, pushed from the right at a steady velocity $-u_p$ into material initially at rest, generates a shock wave moving to the left, out in front of the piston, at a steady velocity $-u_s$. We can ride along with the shock front by adding u_s to all velocities; in this coordinate system, the location of the front is fixed at $x = 0$, with cold material rushing from the left ($x \ll 0$) toward the piston at fluid velocity $u_0 = u_s$, while the hot material stagnates against the piston, receding to the right ($x \gg 0$) at velocity $u_1 = u_s - u_p$.

The Navier-Stokes constitutive equation relating the pressure tensor to the strain rate, i.e., gradient of the velocity u', is (P is the hydrostatic pressure, or $\frac{1}{3}$ the trace of the pressure tensor)

$$\begin{aligned} &P_{xx}(x) = P(x) - \eta_L(x)u'(x) , \\ &\eta_L = \eta_V + \tfrac{4}{3}\eta_S , \end{aligned} \tag{6}$$

where the longitudinal viscosity η_L is a combination of bulk η_V and shear η_S viscosities. Fourier's law relates the heat flux to the temperature gradient T' by

$$q(x) = -\kappa(x)T'(x) . \tag{7}$$

Thus, the one-dimensional NS equations for momentum and energy in a steady shock wave become

$$\begin{aligned} &P(x) - \eta_L(x)u'(x) = P_0 + \rho_0 u_0[u_0 - u(x)] , \\ &E(x) - \frac{\kappa(x)T'(x)}{\rho_0 u_0} = E_0 + \tfrac{1}{2}[u_0 - u(x)]^2 \\ &\qquad + \frac{P_0}{\rho_0 u_0}[u_0 - u(x)] . \end{aligned} \tag{8}$$

Specializing to the case of the ideal gas, the EOS is

$$P(\rho,T) = \rho\frac{kT}{m}, \quad E(\rho,T) = \frac{3}{2}\frac{kT}{m} , \tag{9}$$

and the Navier-Stokes transport coefficients for hard spheres of diameter σ are given by

$$\begin{aligned} &\eta_V(\rho,T) = 0 , \\ &\eta_S(\rho,T) = \frac{5m}{16\sigma^2}\left(\frac{kT}{\pi m}\right)^{1/2} \Rightarrow \eta_L = \frac{5m}{12\sigma^2}\left(\frac{kT}{\pi m}\right)^{1/2} , \\ &\kappa(\rho,T) = \frac{75k}{64\sigma^2}\left(\frac{kT}{\pi m}\right)^{1/2} = \frac{45}{16}\frac{k}{m}\eta_L . \end{aligned} \tag{10}$$

Note that the ideal-gas bulk viscosity is zero, and that both the shear viscosity and thermal conductivity increase with the square root of the temperature.

If we define the origin such that $u(x=0)=(u_0+u_1)/2$, then scale x by a convenient factor l (which will turn out to be close to the mean free path l_0 of the initial state of the ideal gas), scale density by its initial value ρ_0, and scale the fluid velocity by the shock velocity $u_0=u_s$:

$$\mathcal{R}(s)=\frac{\rho(x)}{\rho_0},\quad s=\frac{x}{l},$$
$$\mathcal{U}(s)=\frac{u(x)}{u_0}\Rightarrow u'(x)=\frac{du}{dx}=u_0\frac{d\mathcal{U}}{ds}\frac{ds}{dx}$$
$$=\frac{u_0}{l}\mathcal{U}'(s), \tag{11}$$
$$\mathcal{T}(s)=\frac{kT(x)}{mu_0^2},\quad \mathcal{T}_{xx}(s)=\frac{kT_{xx}(x)}{mu_0^2},$$

then the standard NS equations [Eqs. (8)] for a steady shock wave in the ideal gas become

$$\mathcal{R}(s)=\frac{1}{\mathcal{U}(s)},$$
$$\frac{\mathcal{T}(s)}{\mathcal{U}(s)}-\mathcal{T}^{1/2}(s)\mathcal{U}'(s)=\mathcal{T}_0+1-\mathcal{U}(s)\quad\left[\equiv\frac{\mathcal{T}_{xx}(s)}{\mathcal{U}(s)}\right],$$
$$\tfrac{3}{2}\mathcal{T}(s)-\tfrac{45}{16}\mathcal{T}^{1/2}(s)\mathcal{T}'(s)=\tfrac{3}{2}\mathcal{T}_0+\tfrac{1}{2}[1-\mathcal{U}(s)]^2$$
$$+\mathcal{T}_0[1-\mathcal{U}(s)]. \tag{12}$$

The definition of l in these rescaled NS equations is chosen to be

$$l=\frac{5m}{12\rho_0\sigma^2\sqrt{\pi}}=\frac{5}{12}\sqrt{2\pi}l_0\approx 1.04l_0, \tag{13}$$

where l_0 is the mean free path in the initial state of the ideal gas of hard spheres.

Finally, to go beyond the Navier-Stokes level according to Holian's conjecture, we replace T in the transport coefficients by T_{xx}, i.e., wherever $\mathcal{T}^{1/2}$ appears in Eq. (12), we replace it with $\mathcal{T}_{xx}^{1/2}=[\mathcal{U}(\mathcal{T}_0+1-\mathcal{U})]^{1/2}$:

$$\frac{\mathcal{T}}{\mathcal{U}}-[\mathcal{U}(\mathcal{T}_0+1-\mathcal{U})]^{1/2}\mathcal{U}'=\mathcal{T}_0+1-\mathcal{U},$$
$$\tfrac{3}{2}\mathcal{T}-\tfrac{45}{16}[\mathcal{U}(\mathcal{T}_0+1-\mathcal{U})]^{1/2}\mathcal{T}'=\tfrac{3}{2}\mathcal{T}_0+\tfrac{1}{2}(1-\mathcal{U})^2 \tag{14}$$
$$+\mathcal{T}_0(1-\mathcal{U}).$$

In order to solve Eqs. (12) or (14) numerically, we start integrating at the hot piston end (remembering that heat flows naturally from hot to cold and that the mathematical stability is similarly directional [2]). For the purpose of comparing with the MD work of Salomons and Mareschal [8], we make the reasonable and simplifying assumption that the initial temperature is zero, i.e., $T_0=0\Rightarrow E_0=0$ and $P_0=0$; hence, from the Hugoniot relations, $\mathcal{U}_1=\frac{1}{4}$ ($\Rightarrow\mathcal{R}_1=4$) and $\mathcal{T}_1=\frac{3}{16}$. A simple first-order difference scheme is adequate, with starting values $\mathcal{U}=\mathcal{U}_1+6\times10^{-6}$ and $\mathcal{T}=\mathcal{T}_1$, and an integration step of $\Delta s=10^{-4}$.

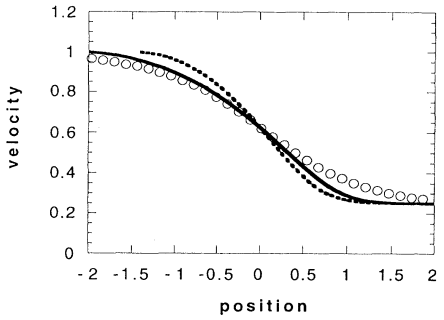

FIG. 1. Velocity profile $u(x)$ (in units of $u_0=u_s$) vs position x [in units of l, see Eq. (13)] for a shock wave in an ideal gas: standard NS (dashed line), modified NS (solid line), and MD (circles); the shock thickness λ/l is, respectively, 1.53, 2.08, and 2.35 [$\lambda=-u_p/u'(0)$].

III. COMPARISON OF MOLECULAR DYNAMICS, NAVIER-STOKES THEORY, AND BEYOND

As can be seen from Eqs. (12) and (14), the velocity and temperature profiles are the independent ones, since the normal component of the pressure tensor and the density can be easily obtained from the velocity. The velocity profile is shown in Fig. 1 for MD (DSMC) nonequilibrium computer experiments, standard NS theory, and the modified NS theory. For fluids, the velocity profile exhibits a great deal of symmetry, and the maximum slope occurs at the shock front ($x=0$). Consequently, the shock-wave thickness can be defined by $\lambda=-u_p/u'(0)$, which is much more closely approximated by the modified NS theory (namely, $2.08l$, compared to the exact MD value of $2.35l$; in comparison, the standard NS value is $1.53l$). In Fig. 2, the density profile (inverse of the velocity) is displayed. In Fig. 3, the normal P_{xx} and shear $\tau=(P_{xx}-P_{yy})/2$ pressure-tensor components are shown. The ratio of the total rise in pressure to the maximum shear pressure $P_1/\tau_{\max}$ is roughly 6 in all cases, compared to about 10 in the dense fluid and solid [7]. In these first three figures, the principal remaining discrepancy between MD and modified NS is in the hot end, rather than the cold end.

The average temperature T and the normal component

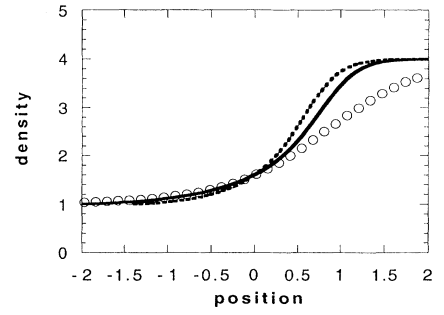

FIG. 2. Density profile $\rho(x)$ (in units of ρ_0) vs position x (in units of l) for a shock wave in an ideal gas: standard NS (dashed lines), modified NS (solid line), and MD (circles).

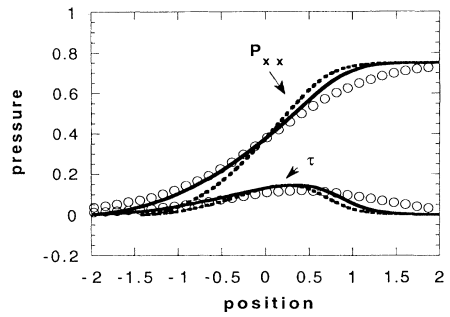

FIG. 3. Normal component of pressure tensor $P_{xx}(x)$ (in units of $\rho_0 u_0^2$) vs position x (in units of l) for a shock wave in an ideal gas: standard NS (dashed line), modified NS (solid line), and MD (circles); also, shear component $\tau = (P_{xx} - P_{yy})/2$. The ratio of the final pressure rise P_1 to the maximum shear pressure τ_{max} is, respectively, 5.4, 5.4, and 6.0.

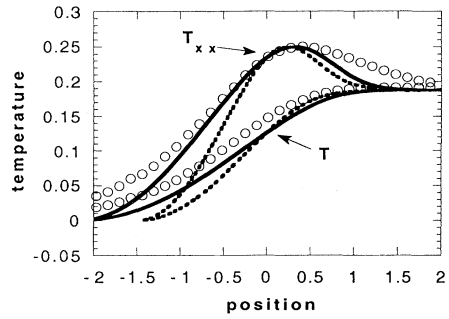

FIG. 4. Average temperature $T = (T_{xx} + T_{yy} + T_{zz})/3$ (in units of mu_0^2/k vs position x (in units of l) for a shock wave in an ideal gas: standard NS (dashed line), modified NS (solid line), and MD (circles); also, normal component of temperature T_{xx}. Note that in both standard and modified NS, T_{xx} exhibits a peak of $\frac{1}{4}$, which is $\frac{4}{3}$ the final temperature.

T_{xx} are displayed in Fig. 4. Perhaps the clearest sign of superiority of the modified NS theory is seen here, namely, in the agreement of the gradient T' and in the width of T_{xx}, when compared with the nonequilibrium MD. Nevertheless, the MD simulations exhibit a longer relaxation time in the approach to the final temperature T_1 than is seen in either standard NS or the modified version. It is clear, however, that the modified NS captures this relaxation phenomenon more faithfully than the standard NS theory.

IV. CONCLUSIONS

We have modeled shock waves in the ideal gas, using both Navier-Stokes theory and a modification based on a conjecture by Holian, namely, that the temperature in the direction of shock-wave propagation is superior to the spatially averaged value when evaluating the linear transport coefficients, and compared them with exact molecular dynamics and direct simulation Monte Carlo (Boltzmann equation solution). It appears that on the hot side of the shock front, there is yet an additional relaxation mechanism beyond that predicted by the modified version of the Navier-Stokes theory.

ACKNOWLEDGMENTS

This work was performed by B.L.H. and C.W.P. at Los Alamos National Laboratory, which is operated by the University of California for the Department of Energy under Contract No. W-7405-36. E.S. and M.M. gratefully acknowledge the support of CECAM. M.M. acknowledges the financial support of the Fonds National de la Recherche Scientifique (Belgium). We thank Bill Hoover for helpful discussions and encouragement in our quest beyond Navier-Stokes theory.

[1] W. G. Hoover, Phys. Rev. Lett. **42**, 1531 (1979).

[2] B. L. Holian, W. G. Hoover, B. Moran, and G. K. Straub, Phys. Rev. A **22**, 2798 (1980).

[3] V. Y. Klimenko and A. N. Dremin, in *Detonatsiya, Chernogolovka*, edited by O. N. Breusov *et al.* (Akademik Nauk, Moscow, 1978), p. 79.

[4] F. H. Ree, J. Chem. Phys. **73**, 5401 (1980), and references therein.

[5] D. Levesque, L. Verlet, and J. Kurkijarvi, Phys. Rev. A **7**, 1690 (1973).

[6] W. T. Ashurst, Ph.D. thesis, University of California, Davis, 1975 (unpublished); W. G. Hoover and W. T. Ashurst, in *Theoretical Chemistry*, edited by R. N. Dixon and C. Thomson (Academic, New York, 1975), Vol. I, p. 1; W. G. Hoover, A. J. C. Ladd, R. B. Hickman, and B. L. Holian, Phys. Rev. A **21**, 1756 (1980); W. G. Hoover, D. J. Evans, R. B. Hickman, A. J. C. Ladd, W. T. Ashurst, and B. Moran, *ibid.* **22**, 1714 (1980).

[7] B. L. Holian, Phys. Rev. A **37**, 2562 (1988); B. L. Holian, in *Microscopic Simulations of Complex Hydrodynamic Phenomena*, edited by M. Mareschal and B. L. Holian (Plenum, New York, 1992), p. 75.

[8] E. Salomons and M. Mareschal, Phys. Rev. Lett. **69**, 269 (1992).

[9] G. A. Bird, *Molecular Gas Dynamics* (Clarendon, Oxford, 1976), pp. 118–142; G. A. Bird, Progr. Astronaut. Aeronaut. **118**, 211 (1989).

[10] See, for example, discussion by M. Mareschal and B. L. Holian, in *Microscopic Simulations of Complex Hydrodynamic Phenomena* (Ref. [7]), p. 1.