

## Nonlinear dissipation and nonequilibrium gas flows

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Rayleigh and Onsager showed that in the regime where the flows are small and the thermodynamic forces vary slowly, the entropy generation rate is linearly related to the flows, and the flows are related to the gradient of the forces. Hence, the Rayleigh-Onsager dissipation is only applicable to linear irreversible thermodynamics. We introduce the extension of Rayleigh-Onsager dissipation to highly nonlinear dissipation to treat nonlinear irreversible thermodynamics. This extension fulfills the positive entropy generation criterion. To demonstrate this nonlinear dissipation, we apply it to obtain the generalized hydrodynamics from the kinetic theory according to Eu theory. Specifically, it provides an alternative evolution for a stress tensor and heat flux. The challenging problems of nonlinear irreversible thermodynamics, as represented by nonequilibrium flows, are investigated. The result implies that this study provides a promising alternative to obtain a unified framework for modeling both equilibrium and nonequilibrium gas flows.

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### I. INTRODUCTION

In 1872, Boltzmann described the statistical behavior of kinetic systems governing particle motion at molecular scales [1]. His description considered a probability distribution function  $f$  for the position and momentum of a typical particle at the position  $\mathbf{r}$ , the velocity of which is nearly equal to a given velocity vector  $\mathbf{v}$  at time  $t$ . In the last century, Curtiss [2] added the moment of inertia  $I$  and angular momentum  $\mathbf{j}$  to consider diatomic molecules in particular, leading to the Boltzmann-Curtiss equation at the molecular level (in the absence of external forces for a gas):

$$\left[ \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi} \right] f(\mathbf{v}, \mathbf{r}, t) = R[f]. \quad (1)$$

In this equation,  $\psi$ ,  $j$ , and  $R[f]$  represent the azimuthal angle associated with the orientation of the molecular level, the magnitude of the angular momentum vector, and the collision integral of the interparticle interactions, respectively,

$$R[f] = \frac{1}{2\pi m_{ab}^2} \int (f_a^* f_b^* - f_a f_b) \left( \frac{j_b j_r}{|\mathbf{v}_b - \mathbf{v}_a|} \right) d\Gamma_a, \quad (2)$$

where  $m_{ab}$  denotes the reduced mass of the collision pair  $a$  and  $b$ ; the superscript asterisk  $*$  stands for the postcollision value. The collision volume element is defined by  $d\Gamma_a = \sin \beta_b d\psi_a d\alpha_b d\beta_b d\psi_b dj_b d\gamma_r dj_r$ , where  $\psi_a$  and  $\psi_b$  are the values of phase angles  $\gamma_a$  and  $\gamma_b$ , respectively, at the point of closest approach of the collision pair. The Euler angles  $\alpha$  and  $\beta$  are determined by the condition of the molecular rotation in the rotated frame.  $\mathbf{j}$  is aligned with the  $z$  axis. For details, we refer the reader to Curtiss' paper [2], which contains the derivation of the collision integral for a rigid

rotator gas. The important point to note about (1) is that  $R[f]$  extends the collision integrals in the original Boltzmann equation for monatomic gases to rigid rotator fluids, but it still remains irreversible and satisfies the Boltzmann  $H$ -theorem. Additionally, since it breaks time-reversal invariance symmetry and hence is irreversible, it makes it possible to formulate a thermodynamically consistent hydrodynamics theory. This is the principal reason why we choose the Boltzmann-Curtiss kinetic equation (1) to derive the unified framework of transport processes in the rigid rotator fluid.

The nonconserved variables  $\Phi^{(k)}$  such as the viscous stress tensor  $\mathbf{\Pi}$ , excess normal stress  $\Delta$ , and heat flux vector  $\mathbf{Q}$  can be defined by molecular expressions as given by  $\mathbf{\Pi} = \langle h^{(1)} f \rangle$ ,  $h^{(1)} = m[\mathbf{c}\mathbf{c}]^{(2)}$ ;  $\Delta = \langle h^{(2)} f \rangle$ ,  $h^{(2)} = \frac{1}{3} m\mathbf{c}^2 - \frac{p}{n}$ ;  $\mathbf{Q} = \langle h^{(3)} f \rangle$ ,  $h^{(3)} = (\frac{1}{2} m\mathbf{c}^2 + H_{\text{rot}} - m\hat{h})\mathbf{c}$ . Here,  $\langle \rangle$  denotes the integration over the velocity space,  $\mathbf{c}$  is the particular velocity of the gas particle defined by  $\mathbf{c} = \mathbf{v} - \mathbf{u}$ ,  $H_{\text{rot}}$  denotes the rotational Hamiltonian of the molecule,  $m$  is the molecular mass,  $p$  is the pressure, and  $n$  is the number density.  $\hat{h}$  represents the enthalpy density per unit mass, and the symbol  $[\mathbf{A}]^{(2)}$  denotes the traceless symmetric part of second-rank tensor  $\mathbf{A}$ .

The general evolution equations of nonconserved variables can be obtained by multiplication of the Boltzmann-Curtiss equation (1) with subsequent integration over the velocity space, yielding  $\langle h^{(k)} \frac{\partial f}{\partial t} \rangle + \langle h^{(k)} \mathbf{v} \cdot \nabla f \rangle + \langle h^{(k)} \frac{j}{I} \frac{\partial f}{\partial \psi} \rangle = \langle h^{(k)} R[f] \rangle$ . Using  $\mathbf{v} = \mathbf{c} + \mathbf{u}$ ,  $\nabla \cdot \mathbf{v} = \mathbf{0}$ , the mass conservation equation and substantial time derivative  $D/Dt$ , this general evolution equation can be expressed as  $\rho \frac{D}{Dt} \left( \frac{h^{(k)} f}{\rho} \right) + \nabla \cdot \langle \mathbf{c} h^{(k)} f \rangle - Z^{(k)} = \Lambda^{(k)}$ . Here,  $\rho$  is the density.  $\langle \mathbf{c} h^{(k)} f \rangle$ , the flux of  $\langle h^{(k)} f \rangle$ , denotes the high-order moments and can be neglected.  $\Lambda^{(k)} = \langle h^{(k)} R[f] \rangle$  is the dissipation term

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that accounts for the energy dissipation accompanying the irreversible process.  $Z^{(k)} = \langle f(\frac{D}{Dt} + \mathbf{c} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi})h^{(k)} \rangle$  represents the kinematic term arising from the hydrodynamic streaming effect, which can be expressed as the shear stress, as given by

$$\begin{aligned} Z^{(\Pi)} &= \left\langle f \frac{D}{Dt} h^{(1)} \right\rangle + \langle f \mathbf{c} \cdot \nabla h^{(1)} \rangle + \left\langle f \frac{j}{I} \frac{\partial}{\partial \psi} h^{(1)} \right\rangle \\ &= -2(p + \Delta)[\nabla \mathbf{u}]^{(2)} - 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} \\ Z^{(\Delta)} &= -2\gamma'(\Pi + \Delta \mathbf{I}) : \nabla \mathbf{u} - \frac{2}{3}\gamma' \nabla \cdot \mathbf{u} \\ Z^{(\mathbf{Q})} &= -\mathbf{Q} \cdot \nabla \mathbf{u} + \Pi \cdot C_p \nabla T - (p + \Delta)C_p \nabla T, \end{aligned}$$

where  $\gamma' = (5 - 3\gamma)/2$ , where  $\gamma$  is the specific-heat ratio,  $C_p$  is the specific heat at constant pressure, and  $T$  is the temperature.

Finally, the constitutive equations, all of which are derived from the Boltzmann-Curtiss equation, can be expressed in compact form as

$$\rho \frac{D\Phi^{(k)}/\rho}{Dt} - Z^{(k)} = \Lambda^{(k)} (k \geq 1). \quad (3)$$

## II. NONLINEAR DISSIPATION, RAYLEIGH-ONSAGER DISSIPATION, AND ENTROPY GENERATION

The local equilibrium Maxwell distribution function is defined as

$$f^{(e)} = n \left( \frac{m}{2\pi k_B T} \right)^{3/2} \exp(Z_0) = \frac{\exp(Z_0)}{n^{-1} \langle \exp(Z_0) \rangle}, \quad (4)$$

where  $k_B$  is the Boltzmann constant and  $Z_0 = -\frac{1}{k_B T} [\frac{1}{2} m \mathbf{c}^2 + H_{\text{rot}}]$ . We note that  $\langle f^{(e)} \rangle = n$ , and we then have  $(\frac{m}{2\pi k_B T})^{3/2} = \frac{1}{\langle \exp(Z_0) \rangle}$ . In view of the H-theorem, it is convenient to search for the form of the nonequilibrium distribution function, namely the thermodynamic branch, in an exponential form. Additionally, the exponential form can be proved based on the maximum entropy principle [3]. The nonequilibrium effect is the source of the dissipation term and thus gives rise to the viscous stress, excess normal stress, and heat flux. Then, we use the exponential forms of the viscous stress, excess normal stress, and heat flux  $Z_1 = -\frac{1}{k_B T} [\sum X^{(k)} \odot h^{(k)}]$  to represent the nonequilibrium part [4,5],

$$f = \frac{\exp(Z_0) \exp(Z_1)}{n^{-1} \langle \exp(Z_0) \exp(Z_1) \rangle}. \quad (5)$$

We note that  $\exp(Z_0)$  is the equilibrium term and  $\exp(Z_1)$  is the nonequilibrium term. The unknown conjugate variables  $X^{(k)}$  can be obtained by generalizing the equilibrium Gibbs ensemble theory that provides the relationship between the thermodynamic variables and the partition functions to nonequilibrium processes. Such a nonequilibrium generalization was previously developed [4]. Then,  $X^{(k)}$  can be calculated in terms of the macroscopic flux  $\langle h^{(n)} f \rangle$ . The leading-order approximate solutions are known to be  $X^{(1)} = -\frac{\Pi}{2p}$ ,  $X^{(2)} = -\frac{3}{2} \frac{\Delta}{p}$ ,  $X^{(3)} = -\frac{\mathbf{Q}}{pC_p T}$ . This form of the nonequilibrium distribution function can be proven to fulfill the conservation laws and the positive entropy generation

criterion. The entropy generation  $\sigma_{\text{ent}}$  can be obtained as

$$\sigma_{\text{ent}} = -k_B \langle \ln f R[f] \rangle = \frac{1}{T} \sum X^{(k)} \Lambda^{(k)}. \quad (6)$$

Additionally,  $\sigma_{\text{ent}}$  can be derived by rewriting the nonequilibrium distribution function  $f$  as

$$f = f^{(e)} \exp(-x). \quad (7)$$

Here,  $\exp(-x) = \frac{\exp(Z_1) \langle \exp(Z_0) \rangle}{\langle \exp(Z_0) \exp(Z_1) \rangle}$ . If we use subscripts 1 and 2 to denote the collision pair of the molecule, we obtain

$$\begin{aligned} \sigma_{\text{ent}} &= -k_B \langle \ln f R[f] \rangle \\ &= \frac{1}{4} k_B \int f^{(e_1)} f^{(e_2)} (x_{12} - x_{12}^*) [\exp(x_{12}^*) - \exp(x_{12})] \\ &= Z_2 / 4T \langle \langle (x_{12} - x_{12}^*) [\exp(x_{12}^*) - \exp(x_{12})] \rangle \rangle \\ &= Z_2 / T \kappa^2 q(\kappa, \kappa_1, \kappa_2, \dots) \\ &= Z_2 / T \kappa^2 q(\kappa). \end{aligned} \quad (8)$$

Here,  $Z_2 = \frac{\sqrt{2} p^2 d^2}{\sqrt{m k_B T}}$ .  $d$  and  $m$  denote the diameter of the molecule and the molecular mass, respectively.  $\kappa = \frac{1}{2} \langle \langle (x_{12} - x_{12}^*) \rangle \rangle^{1/2}$ .  $\kappa_i (i \geq 1)$  are high-order terms and they can be neglected. If  $x_{12} \rightarrow x_{12}^*$ , then we obtain

$$\lim_{\kappa \rightarrow 0} \kappa^2 q(\kappa) = \kappa^2. \quad (9)$$

Thus,  $\kappa^2$  should be a Rayleigh-Onsager-type function [6],

$$\kappa = \frac{1}{\sqrt{Z_2}} \left[ \frac{\Pi : \Pi}{2\eta} + \gamma' \frac{\Delta^2}{\eta_b} + \frac{\mathbf{Q} \cdot \mathbf{Q}}{\lambda T} \right]^{1/2}. \quad (10)$$

Combining Eqs. (6), (8), and (10), we obtain

$$\sum X^{(k)} \Lambda^{(k)} = \left[ \frac{\Pi : \Pi}{2\eta} + \gamma' \frac{\Delta^2}{\eta_b} + \frac{\mathbf{Q} \cdot \mathbf{Q}}{\lambda T} \right] q(\kappa) \quad (11)$$

and we then have

$$\begin{bmatrix} \Lambda^{(\Pi)} \\ \Lambda^{(\Delta)} \\ \Lambda^{(\mathbf{Q})} \end{bmatrix} = \begin{bmatrix} -\frac{p}{\eta} \Pi q(\kappa) \\ -\frac{2}{3} \gamma' \frac{p}{\eta_b} \Delta q(\kappa) \\ -\frac{p C_p}{\lambda} \mathbf{Q} q(\kappa) \end{bmatrix} \quad (12)$$

and

$$\sigma_{\text{ent}} = \frac{1}{T} \left[ \frac{\Pi : \Pi}{2\eta} + \gamma' \frac{\Delta^2}{\eta_b} + \frac{\mathbf{Q} \cdot \mathbf{Q}}{\lambda T} \right] q(\kappa) \geq 0. \quad (13)$$

The  $\eta$ ,  $\eta_b$ , and  $\lambda$  are the Chapman-Enskog shear viscosity, bulk viscosity, and thermal conductivity, respectively. We note that the molecular-based derivation of the nonlinear entropy generation Eqs. (13) has been well-developed by Peters [7,8]. The nonlinear nature of the entropy generation follows phenomenological arguments as shown in the textbook by Bird, Stewart, and Lightfoot [9].

Following Peters's approach [7,8] to the nonequilibrium entropy conservation, we introduce the Chapman-Enskog perturbation expansion  $f_i = f^{(e)}(1 + \phi_i)$ , where  $\phi_i$  are the perturbation functions. The derivation of the perturbation functions requires the conservation of mass, momentum, and energy for the  $f^{(e)}$  distribution. The first-order perturbation function,

$\phi_1$ , can be expressed in terms of velocity and temperature gradients as

$$\phi_1 = -\mathbf{A} : \nabla \mathbf{u} - \frac{1}{T} \mathbf{B} \cdot \nabla T, \quad (14)$$

where  $\mathbf{A}$  and  $\mathbf{B}$  are obtained by an expansion in series of Sonine polynomials. According to Peters's nonequilibrium entropy conservation [8], we obtain the entropy generation term in dilute gases,

$$\begin{aligned} \sigma_{\text{ent}} = & \int (\mathbf{A} : \nabla \mathbf{u}) f^{(e)} ([mcc]^{(2)} : \nabla \mathbf{u}) \frac{1}{T} d\mathbf{v} \\ & - \int (\mathbf{B} \cdot \nabla T) f^{(e)} \left( \frac{5}{2} - \frac{(m\mathbf{c})^2}{2k_B T} \right) (m\mathbf{c} \cdot \nabla T) \frac{1}{T^2} d\mathbf{v}. \end{aligned} \quad (15)$$

As derived in Eq. 40 in [8], it can be shown that this Boltzmann entropy generation yields the phenomenological result

$$\sigma_{\text{ent}} = \frac{1}{T} (\mathbf{\Pi} : \nabla \mathbf{u}) - \frac{1}{T^2} (\mathbf{Q} \cdot \nabla T). \quad (16)$$

Also, it can be expressed as

$$\sigma_{\text{ent}} = \frac{1}{T} \left( \frac{\mathbf{\Pi} : \mathbf{\Pi}}{2\eta} + \frac{\mathbf{Q} \cdot \mathbf{Q}}{\lambda T} \right). \quad (17)$$

It implies that Chapman-Enskog expansion represents the low  $\kappa$  limit of Eq. (13). This derivation has been well developed by Peters, and we refer the reader to Peters's papers [7,8].

If we use the BGK operator [10] and the approximation of molecular relaxation time  $\tau_0 = \frac{\eta}{p}$ , the dissipation term  $\mathbf{\Lambda}^{(k)}$  can be expressed as

$$\begin{bmatrix} \mathbf{\Lambda}^{(\Pi)} \\ \mathbf{\Lambda}^{(\Delta)} \\ \mathbf{\Lambda}^{(\mathbf{Q})} \end{bmatrix} = \begin{bmatrix} \langle h^{(1)} \frac{f^{(e)} - f}{\tau_0} \rangle \\ \langle h^{(2)} \frac{f^{(e)} - f}{\tau_0} \rangle \\ \langle h^{(3)} \frac{f^{(e)} - f}{\tau_0} \rangle \end{bmatrix} = \begin{bmatrix} -\frac{\rho}{\eta} \mathbf{\Pi} \\ -\frac{2}{3} \gamma' \frac{\rho}{p} \Delta \\ -\frac{pC_p}{\lambda} \mathbf{Q} \end{bmatrix}. \quad (18)$$

This also implies that the linear BGK operator represents the low  $\kappa$  limit of the dissipation term  $\mathbf{\Lambda}^{(k)}$ .

The present model [Eqs. (11) and (12)] extends the dissipation terms  $\mathbf{\Lambda}^{(n)}$  from the linear Rayleigh-Onsager dissipation to the high nonlinear form by a factor of  $q(\kappa)$ . This form renders a clear, physical interpretation of entropy production: entropy production is a direct measure of the stress and heat dissipation arising from molecular collisions in the system. The factor  $q(\kappa)$  in the dissipative terms is defined by the Rayleigh-Onsager dissipation function

$$q(\kappa) \equiv \frac{\sinh \kappa}{\kappa} = \left( 1 + \frac{1}{3!} \kappa^2 + \frac{1}{5!} \kappa^4 + \dots \right), \quad (19)$$

$\kappa$  plays an important role in connecting the equilibrium and nonequilibrium and then in connecting molecular-level and continuum-level fluids. We note that the physical meaning of  $q(\kappa)$  is obvious because it denotes the linear "1" and nonlinear " $\frac{1}{3!} \kappa^2 + \frac{1}{5!} \kappa^4 + \dots$ " parts of the dissipation term.

To show the relevance of the present model to the nonequilibrium gas flows in the simplest manner, we assume that the shear stress evolution is not coupled to the evolutions of  $\Delta$

and  $\mathbf{Q}$ ,

$$\rho \frac{D\mathbf{\Pi}/\rho}{Dt} = -2p[\nabla \mathbf{u}]^{(2)} - 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} - \frac{p}{\eta} \mathbf{\Pi} q(\kappa),$$

and we appropriately reduce the variables of the evolution equation for  $\mathbf{\Pi}$ , which consequently takes the following form:

$$\frac{D\mathbf{\Pi}}{Dt} = N_\delta \left( \mathbf{\Pi}_{\text{NSF}} + \left[ \frac{\mathbf{\Pi}}{p} \cdot \mathbf{\Pi}_{\text{NSF}} \right]^{(2)} \right) - N_\delta \mathbf{\Pi} q(\kappa)$$

or the dimensionless steady-state form,

$$\mathbf{\Pi} = \mathbf{\Pi}_{\text{NSF}} + N_\delta \left( \mathbf{\Pi}_{\text{NSF}} + \left[ \frac{\mathbf{\Pi}}{p} \cdot \mathbf{\Pi}_{\text{NSF}} \right]^{(2)} \right) - N_\delta \mathbf{\Pi} [q(\kappa) - 1],$$

where  $\mathbf{\Pi}_{\text{NSF}} = -2\eta[\nabla \mathbf{u}]^{(2)}$  is the Newton viscous stress, as it appears in the NSF framework.  $N_\delta = \sqrt{\frac{2\gamma}{\pi}} \text{MaKn}$ , where Ma is the Mach number and Kn is the Knudsen number. All variables in the equation are dimensionless reduced variables, including Rayleigh dissipation function  $\kappa$ . Therefore, as  $q(\kappa) = 1 + \sum_{i=1}^n \frac{1}{(2i+1)!} \kappa^{2i}$  [see Eq. (19)], the evolution equation for  $\mathbf{\Pi}$  tends to the steady-state form

$$\mathbf{\Pi} = \mathbf{\Pi}_{\text{NSF}} + N_\delta [f_1(\mathbf{\Pi}) - \kappa^2 f_2(\mathbf{\Pi})], \quad (20)$$

where  $f_1(\mathbf{\Pi}) = \mathbf{\Pi}_{\text{NSF}} + [\frac{\mathbf{\Pi}}{p} \cdot \mathbf{\Pi}_{\text{NSF}}]^{(2)}$  and  $f_2(\mathbf{\Pi}) = \mathbf{\Pi} [q(\kappa) - 1]$ . Note that as  $\text{Kn} \rightarrow \infty$ ,  $N_\delta \rightarrow \infty$ , then  $\mathbf{\Pi} \rightarrow \mathbf{0}$ . Meanwhile, as  $\text{Kn} \rightarrow \text{Kn}_0$ ,  $f_1(\mathbf{\Pi}) \rightarrow \kappa^2 f_2(\mathbf{\Pi})$ , then  $\mathbf{\Pi} \rightarrow \mathbf{\Pi}_{\text{NSF}}$ . In fact, when Kn decreases, the viscous stress tends to the Newton viscous stress, which shows that the flow becomes continuum (laminar). This feature is also shown in Fig. 1.

The balance equations for mass  $\rho$ , momentum  $\rho \mathbf{u}$ , and energy  $\rho e$  can be derived by differentiating the statistical formulas for these three quantities with time and then substituting the Boltzmann-Curtiss equation. These processes and equations are very similar to those in the NSF framework. They do not have contributions from the Boltzmann collision integral because the three quantities are conserved variables for which the molecular expressions are the collisional invariants of the Boltzmann collision integral. The generalized hydrodynamics [4] can be obtained by the balance equations (21), (22), and (23) of the conserved variable and constitutive Eqs. (6),

$$\rho \frac{D(1/\rho)}{Dt} = \nabla \cdot \mathbf{u}, \quad (21)$$

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla \cdot (\mathbf{\Pi} + \Delta), \quad (22)$$

$$\rho \frac{De}{Dt} = -\nabla \cdot \mathbf{Q} - (\mathbf{\Pi} + \Delta) : \nabla \mathbf{u}. \quad (23)$$

### III. RESULTS

Direct simulation Monte Carlo (DSMC) models of fluid flows using simulation molecules that represent a large number of real molecules in a probabilistic simulation are used to solve the Boltzmann kinetic equation. DSMC is widely used to study highly nonequilibrium conditions, such as rarefied gas dynamics [12,13]. In a typical application, the particle

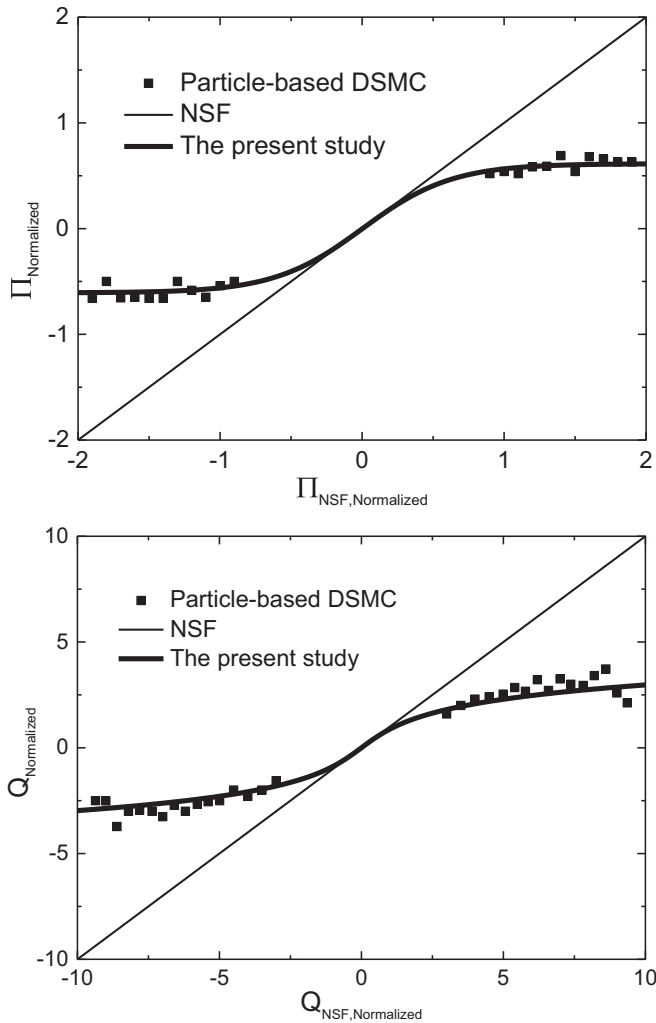


FIG. 1. Comparisons of the shear viscous stress (top) and heat flux (bottom) in the present model; NSF and DSMC results via the Bird code [11].

simulators may have internal degrees of freedom. Two rotational degrees of freedom are applied for diatomic gas in this study. As the first case study, we provide comparisons of one-dimensional dimensionless viscous stress (one-dimensional shock for nitrogen gas) in the present study at a steady state, the classical Navier-Stokes-Fourier (NSF) framework, and the particle-based DSMC results via the Bird code [11]. The following observations are made:

(i) The present model shows nonlinear relations of viscous stress that are quite different from the NSF equation. However, the present model has the same linear relations as those of Newton's laws near the equilibrium state. In other words, the NSF equation can be regarded as a low-order approximation of the present model.

(ii) The present model has different nonlinear trends for viscous stress. This finding was validated by a DSMC model, as shown in Fig. 1. This feature indicates that the present model can be used to describe the gas flow in the far-from-equilibrium state.

(iii) The present model also shows nonlinear relations for the heat flux, which are similar to those of Fourier's laws near

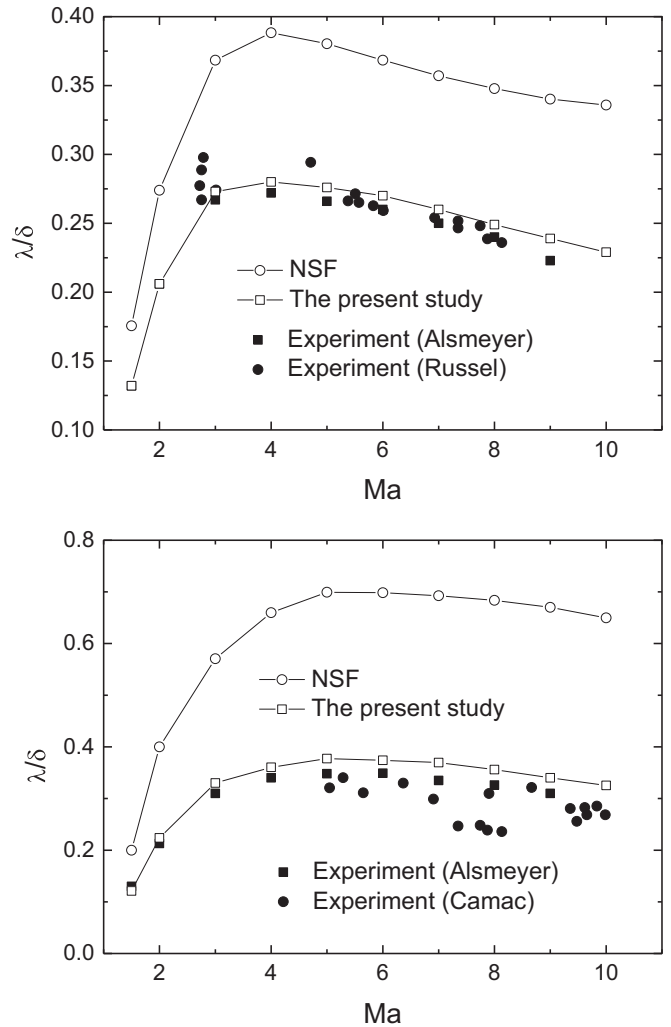


FIG. 2. 1D shock structure problem: computed inverse shock density thickness profile of argon (top) and nitrogen (bottom) gas, and the experimental data [14–16].

the equilibrium state. By contrast, this result indicates that the low trends are similar to those of NSF, indicating that NSF overestimates the heat flux in far-from-equilibrium states.

In physics, a shock is a type of propagating disturbance that moves faster than the local speed of sound in a medium. Unlike solitons, the energy and speed of a shock alone dissipate relatively quickly with distance. When a shock passes through matter, energy is preserved but entropy increases. Thus, a shock is a strongly irreversible process and a typical nonequilibrium flow. The shock density thickness is known to be an important parameter regarding the accuracy of models; therefore, the solutions of the present model for argon and nitrogen gas are compared experimentally [14–16] in Fig. 2. It is shown that the present model can capture the shock density thickness. Excess studies on the shock density thickness and shock vortex interaction can also be found in our previous work [17,18].

The Knudsen number ( $Kn$ ) is a dimensionless number defined as the ratio of the molecular mean free path length to a representative physical length scale. The Knudsen number helps determine whether the fluid is in a continuum or

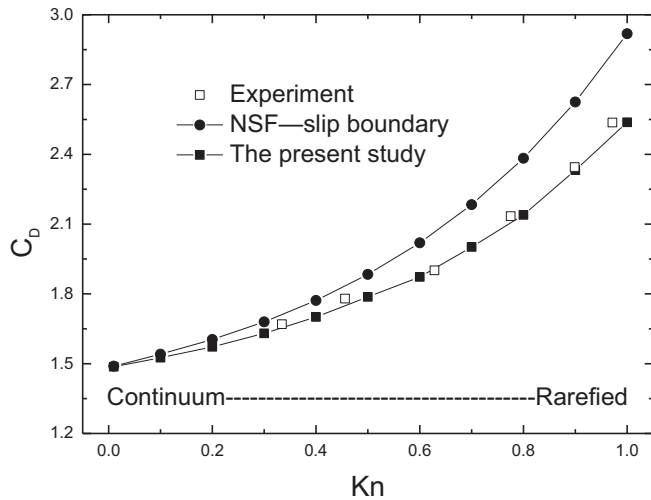


FIG. 3. The drag coefficients of cylinder vs Knudsen numbers at  $Ma = 2.0$ .

rarefied (nonequilibrium) region. We applied the Langmuir slip boundary conditions [19] in the present approach and the NSF framework. Figure 3 shows the drag coefficients as a function of the Knudsen number. In addition, the experiments of Maslach [20] are also plotted for comparison. The results of NSF agree well with the experiments at a Knudsen number less than 0.1. However, it overpredicts the drag coefficients for the high Knudsen number cases. When the Knudsen number becomes appreciable and greater than 0.1, the NSF fails to describe the nonequilibrium gas flows. The agreement from the present study is expected to be observed with experiments over the whole studied region.

#### IV. DISCUSSION

Rayleigh [21] and Onsager [6] showed that the entropy generation rate is linearly related to the flows, and the flows are related to the gradient of the forces when the irreversible

process are linear and thus the system is near equilibrium, which leads to the Rayleigh Onsager dissipation. The second law of thermodynamics requires that the matrix in the relation of the flows and the force gradient be positive-definite. Statistical mechanics involving microscopic reversibility of dynamics implies that this matrix is symmetric. This fact is the so-called Onsager reciprocal relations. All known results of linear irreversible thermodynamics follow the approach based on Rayleigh-Onsager dissipation; however, the theory is open for nonlinear generalization [22]. This study extends the Rayleigh-Onsager dissipation to a highly nonlinear dissipation. This extension fulfills the positive entropy generation criterion. To demonstrate this extension, we applied it to obtain the generalized hydrodynamics from the kinetic theory, and we investigated the typical nonlinear irreversible thermodynamics as represented by nonequilibrium flows. The predictions are found to agree well with the experimental results.

A nonequilibrium gas flow [23–25] is commonly observed in nature and engineering. A nonequilibrium gas flow is considered to be one of the challenging problems in physics. For more than 150 years, flow dynamics has usually been formulated in terms of the Navier-Stokes-Fourier (NSF) framework. Unfortunately, NSF has serious limitations in capturing the correct flow physics under high nonequilibrium conditions. This study reports an alternative option for nonequilibrium analysis, namely generalized hydrodynamics. This theory is derived from kinetic theory according to the Eu method [4,5] in such a manner that it is thermodynamically consistent. The result implies that it provides a promising alternative to obtain a unified framework for modeling both equilibrium and nonequilibrium gas flows.

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- [1] L. Boltzmann, *Kinetische Theorie II* (Springer, Berlin, 1970), pp. 115–225.
- [2] C. Curtiss, *J. Chem. Phys.* **75**, 376 (1981).
- [3] M. Chen, *J. Math. Phys.* **41**, 7445 (2000).
- [4] B. C. Eu, *Kinetic Theory and Irreversible Thermodynamics* (Wiley-Interscience, New York, 1992).
- [5] B. C. Eu, *Kinetic Theory of Nonequilibrium Ensembles, Irreversible Thermodynamics, and Generalized Hydrodynamics: Volume 1. Nonrelativistic Theories* (Springer, Heidelberg, 2016).
- [6] L. Onsager, *Phys. Rev.* **37**, 405 (1931).
- [7] M. Peters, *Entropy* **21**, 330 (2019).
- [8] M. Peters, *Ind. Eng. Chem. Res.* **48**, 166 (2009).
- [9] R. Byron Bird, W. E. Stewart, and E. Lightfoot, *Transport Phenomena* (Wiley International, New York, 1960).
- [10] P. L. Bhatnagar, E. P. Gross, and M. Krook, *Phys. Rev.* **94**, 511 (1954).
- [11] G. Bird, *The DSMC Method* (CreateSpace Independent Publishing Platform, Charlestone, 2013).
- [12] K. H. Lee, *Comput. Fluids* **173**, 88 (2018).
- [13] M. Usami and K. Teshima, *Trans. Jpn. Soc. Mech. Eng.* **42**, 369 (1999).
- [14] H. Alsmeyer, *J. Fluid Mech.* **74**, 497 (1976).
- [15] W. C. Feldman, R. L. Tokar, J. Birn, W. E. Hones, and S. J. Bame, *J. Geophys. Res. Space Phys.* **92**, 83 (1987).
- [16] M. Camac, in *Aerospace Sciences Meeting, New York* (AIAA, New York, 1964).
- [17] H. Xiao and R. Myong, *Comput. Fluids* **105**, 179 (2014).
- [18] N. Le, H. Xiao, and R. Myong, *J. Comput. Phys.* **273**, 160 (2014).

- [19] D. K. Bhattacharya and B. C. Eu, *Phys. Rev. A* **35**, 821 (1987).
- [20] G. J. Maslach and S. A. Schaaf, *Phys. Fluids* **6**, 32 (1963).
- [21] J. Rayleigh, *Proc. London Math. Soc.* **S1-1**, 357 (1871).
- [22] V. N. Pokrovskii, *ISRN Thermodynamics* **2013**, 1 (2013).
- [23] D. A. Lockerby, M. A. Gallis, and J. M. Reese, *AIAA J.* **43**, 1391 (2005).
- [24] S. Succi, *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond* (Clarendon Press, Oxford, 2001).
- [25] S. Takata, *J. Stat. Phys.* **136**, 751 (2009).