Derivation of stable Burnett equations for rarefied gas flows

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A set of constitutive relations for the stress tensor and heat flux vector for the hydrodynamic description of rarefied gas flows is derived in this work. A phase density function consistent with Onsager's reciprocity principle and H theorem is utilized to capture nonequilibrium thermodynamics effects. The phase density function satisfies the linearized Boltzmann equation and the collision invariance property. Our formulation provides the correct value of the Prandtl number as it involves two different relaxation times for momentum and energy transport by diffusion. Generalized three-dimensional constitutive equations for different kinds of molecules are derived using the phase density function. The derived constitutive equations involve cross single derivatives of field variables such as temperature and velocity, with no higher-order derivative in higher-order terms. This is remarkable feature of the equations as the number of boundary conditions required is the same as needed for conventional Navier-Stokes equations. Linear stability analysis of the equations is performed, which shows that the derived equations are unconditionally stable. A comparison of the derived equations with existing Burnett-type equations is presented and salient features of our equations are outlined. The classic internal flow problem, force-driven compressible plane Poiseuille flow, is chosen to verify the stable Burnett equations and the results for equilibrium variables are presented.

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I. INTRODUCTION

Accurate description of rarefied gas flows is required for various microelectromechanical systems and vacuum applications [1–5]. These flows are characterized by high Knudsen number Kn (the ratio of the mean free path to the characteristic length scale). The governing equation describing flow in the transition regime ($\mathrm{Kn} \geqslant 0.1$) is however not available. The Navier-Stokes equations do not describe the physics of gas flows in the transition regime due to the failure of the continuum hypothesis, fundamental to the derivation of these equations. A second-order slip model at the walls can push the limit of the Navier-Stokes equations to the initial transition regime but not beyond [6–8]. Therefore, alternate transport models, namely, Burnett and Grad 13-moment equations have been derived, with kinetic theory playing the central role. The search for accurate transport models is however far from over, as the proposed models are plagued by several severe shortcomings, which explains the reason for the existence of their numerous variants. Derivation of accurate continuum transport models is invaluable as they provide a theoretical description of the problem (thereby opening the exciting possibility of obtaining an analytical solution) and serve as an alternative to performing expensive simulations [the most popular being the direct simulation Monte Carlo (DSMC) technique].

The Boltzmann equation describes the dynamics of gas flow over the entire Knudsen number range [1–3,9]; however, solving this equation is rather involved. Linearization of the equation reduces the complexity to some extent; however, this simplification is only possible for weak departures from equilibrium, while significant deviations from equilibrium requires the solution of the full Boltzmann equation. Computational techniques to solve the Boltzmann equation are not as well developed as, for example, the Navier-Stokes equations in computational fluid dynamics. The Chapman-Enskog expansion of the distribution function (with Knudsen number as the small parameter) is used to construct an approximate solution of the full Boltzmann equation. Nonlinear constitutive relations for the stress tensor and heat flux vector are obtained by retaining second-order-accurate terms in the Chapman-Enskog series [1,2]. These constitutive relations provide a computationally inexpensive alternative for describing gas flow in the rarefied regime ($\mathrm{Kn} \gg 0.001$) and capture many rarefied gas flow phenomena [4,5,10–14]. The truncation of the Chapman-Enskog expansion to second-order results in Burnett equations, which yield linearly unstable rest states [15,16], is a major drawback of the Chapman-Enskog expansion approach.

Zhong [17] derived augmented Burnett equations by adding linearly stabilizing terms from super-Burnett equations. The augmented equations provide more accurate solutions in the shock layer than the Navier-Stokes equations [15,18]. However, these equations involve derivatives of fourth order, thereby requiring several additional boundary conditions for their solution. Moreover, the H theorem (or entropy consistency) is not proven for these set of equations. Interestingly, generalized Burnett equations that do not contain third-order derivatives of velocity and temperature have been found to be better than the classical Burnett equations [19]. Welder *et al.* [20] discussed the instability of Burnett equations in view of the nonlinear terms present. This instability has been addressed by Jin and Slemrod [21] with a viscoelastic relaxation approximation. The proposed system satisfies entropy inequality, ensuring irreversibility of the relaxation process. Jin and Slemrod [21] obtained a system of weakly parabolic equations, with a hyperbolic convection part, by relaxing the pressure tensor and heat flux vector through rate equations. The resulting equations were found to be linearly stable and yield Burnett equations when expanded via the Chapman-Enskog expansion. Agarwal *et al.* [15] employed the Bhatnagar-Gross-Krook (BGK) model to represent the

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nonlinear collision integral in deriving entropy consistent equations. The BGK model assumes the same time for thermal and momentum diffusion leading to a Prandtl number of unity.

The Chapman-Enskog expansion assumes small Knudsen number in its derivation, which makes its validity questionable in transition and free molecular regimes, where Kn exceeds unity. Burnett equations contain third-order derivatives of velocity requiring additional boundaries that are not available. Burnett equations suffer from many other issues [17,22–24]. For example, Struchtrup and Torrilhon [25] showed that small oscillations at a point results in large oscillations at other points. Burnett equations do not yield a solution to the Boltzmann equation in the Knudsen layer [26,27]. We have recently provided an analytical solution of Burnett equations for Couette flow [28], planar flow [29], and cylindrical Poiseuille flow [6]. Apart from these nonlinear constitutive relationships, for a description of rarefied gas flows, equations for higher-order moments such as Grad's moment [30], regularized 13-moment equations [25,31], or regularized 26-moment equations [32,33] have also been derived. These equations have been shown to have success in predicting many rarefied gas flow phenomena. Those derivations have ignored some of the key nonequilibrium thermodynamics ideas such as Onsager-Casimir relations [34–36]. We have recently proposed 13-moment equations [37], where we close equations for higher-order moments using Onsager's principle consistent distribution function.

Sharipov [38] expanded the Boltzmann equation in terms of power series of thermodynamic forces and utilized Onsager's reciprocal relations in its construction. The phase density function relaxing to a Maxwellian distribution in the absence of any thermodynamic force at any Knudsen number makes the approach interesting. Other classes of transport equations that comply with nonequilibrium thermodynamics deal with maximization of entropy production. For instance, Dadzie [39] introduced an additional moment for a variable that accounts for the local number of molecules and their spatial distribution. He did not employ the Chapman-Enskog approach nor did he solve the Boltzmann equation. Öttinger [40] proposed 13 parameter solutions of Boltzmann's kinetic equation and provided a closure.

These earlier attempts that have not been entirely successful motivated us to construct continuum models whose core lies in satisfying the principles of nonequilibrium thermodynamics [24,35,40]. In order to capture strong deviations from equilibrium, the transport equations should (a) represent the approximate solution of the full Boltzmann equation and (b) have closure based on principles of nonequilibrium thermodynamics (such as maximum entropy production and symmetry in thermodynamic fluxes). The core idea of our approach is to satisfy these requirements, thus making the definition of the entropy production and thermodynamic fluxes consistent with Gibbs' relation. The evaluation procedure of the phase density function ensures that the function is in agreement with the solution of the Boltzmann equation and satisfies the H theorem. We recently derived the distribution function [37] that we utilize further in the present work. This phase density function, derived without invoking the Chapman-Enskog series, is then utilized to obtain generalized three-dimensional constitutive equations. Interestingly, no additional boundary conditions are needed to solve the proposed Burnett-type equations. The phase density function provides the correct value of Prandtl number. The derivation does not put any cap on the Knudsen number, making it possible to apply the proposed equations to the transition regime, Kn > 0.1.

II. CONSTITUTIVE RELATIONSHIPS: DERIVATION PROCEDURE

The single-particle distribution function f, which expresses the probability of finding the molecules in phase space element $d\mathbf{x}d\mathbf{c}$, can be obtained from the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{c}\cdot\nabla_{\mathbf{x}} f + \mathbf{G}\cdot\nabla_{\mathbf{c}} f = J_m(f,f), \tag{1}$$

where $\mathbf{x}$ is the space vector, $\mathbf{c}$ is the molecular velocity, $\mathbf{G}$ is the external force, which is considered to be independent of the molecular velocity $\mathbf{c}$, and $J_m(f,f)$ is the binary particle collision integral. The Maxwellian distribution that corresponds to the equilibrium distribution is

$$f_0 = \frac{\rho}{m}\left(\frac{\beta}{\pi}\right)^{3/2} \exp[-\beta(\mathbf{c}-\mathbf{u})^2], \tag{2}$$

where $\beta = 1/2RT$, R is the specific gas constant, T is the absolute temperature, $\mathbf{u}$ is the bulk velocity, ρ is the density, and m is the molecular mass.

The moments of the single-particle distribution function with Ψ $(= m\{1, c_i, \frac{1}{2}|\mathbf{C}|^2\})$ upon its inner product $\langle\Psi, f\rangle \equiv \int \Psi f d\mathbf{c}$ yield variables that are assumed to describe the state of the gas completely ($\mathbf{C}$ is the peculiar velocity, $\mathbf{C} = \mathbf{c} - \mathbf{u}$). The inner product results in density $\rho = m\int f d\mathbf{c}$, momentum $\rho u_i = m\int c_i f d\mathbf{c}$, and energy $\rho\epsilon = \frac{3}{2}\rho kT/m = m\int |\mathbf{C}|^2 f d\mathbf{c}$, where k is the Boltzmann constant. These moments of the Boltzmann equation result in conservation laws for the macroscopic quantities [30,41]. For instance, if $f = f_0$, the approach yields the Euler equations. The resulting generalized conservation equations are

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0, \tag{3}$$

$$\rho\frac{\partial u_i}{\partial t} + \rho u_k\frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = \rho G_i, \tag{4}$$

$$\rho\frac{\partial \epsilon}{\partial t} + \rho u_k\frac{\partial \epsilon}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + p\frac{\partial u_k}{\partial x_k} + \sigma_{ij}\frac{\partial u_i}{\partial x_j} = 0, \tag{5}$$

where G_i is the external body force, p is the pressure, and p_{ij} and q_i are

$$p_{ij} = p\delta_{ij} + \sigma_{ij} = m\int C_i C_j f d\mathbf{c}, \quad q_i = m\int |\mathbf{C}|^2 C_i f d\mathbf{c}, \tag{6}$$

which still need to be evaluated.

III. ONSAGER'S PRINCIPLE CONSISTENT PHASE DENSITY FUNCTION

A. Onsager's reciprocity principle and earlier approaches

In this section we construct the phase density function that is consistent with Onsager's principle of reciprocity. We do not construct higher-order corrections to the equilibrium distribution function using the Chapman-Enskog expansion or Grad's approach of using a Hermite polynomial.

The entropy produced in any process can be expressed in terms of the thermodynamic forces X_i and fluxes J_i. Onsager [42,43] proposed the phenomenological linear law to relate these fluxes and forces: $J_i = \sum_{k=1}^{n} L_{ik} X_k$, where $L_{ik} = L_{ki}$ also holds. De Groot and Mazur [35] have shown that only a first approximation of the phase density function in the Chapman-Enskog series that yields Navier-Stokes constitutive relationships satisfies Onsager's symmetry principle. Furthermore, the second approximation of the Chapman-Enskog expansion, which leads to Burnett-type higher-order continuum equations, leads to entropy production and fluxes different from Gibbs' relation and do not satisfy the symmetry principle [34–36,44]. These thermodynamic inconsistencies of the distribution function may cause generation of unstable modes observed in Burnett-type hydrodynamic equations [16,45,46]. Therefore, we derive a distribution function preserving Onsager's symmetry by expressing it in terms of appropriate thermodynamic forces and fluxes.

B. Derivation of the distribution function

The first-order distribution function obtained from the Chapman-Enskog expansion can be cast in terms of thermodynamic forces X_i and fluxes Υ_j around the local equilibrium distribution in the following way [35,47]:

$$f^{(1)} = f_0 - (\Upsilon_\tau : X_\tau + \Upsilon_q \cdot X_q), \tag{7}$$

$$\Upsilon_j = -f_0 t_{r(j)} \bar{\Upsilon}_j, \tag{8}$$

$$\bar{\Upsilon}_\tau = -\{\mathbf{C} \otimes \mathbf{C} - \tfrac{1}{2}[|\mathbf{C}|^2(\gamma - 1)]\mathbf{I}\},$$

$$\bar{\Upsilon}_q = -\left(\frac{5}{2\beta} - |\mathbf{C}|^2\right)\mathbf{C}, \tag{9}$$

$$X_\tau = \beta[\nabla \otimes \mathbf{u} + (\nabla \otimes \mathbf{u})^T], \quad X_q = \nabla\beta, \tag{10}$$

where $\otimes$ is the outer product, $t_{r(\tau)}$ is the relaxation time for momentum transport ($= \mu/p$), $t_{r(q)}$ is the relaxation time for energy transport [$= \kappa(\gamma - 1)/R\gamma p$], subscripts τ and q have been used with both flux and force associated with stress and heat flux, respectively, μ is the viscosity, κ is the thermal conductivity, and γ is the ratio of specific heat. Macroscopic thermodynamic flux can be obtained as $J_i = \langle \bar{\Upsilon}_i, f\rangle$. This form of distribution function is standard and has been shown to yield constitutive relationships that satisfy Onsager's symmetry principle [35]. Note that the thermodynamic forces and fluxes for the precise form of distribution function in Eqs. (7)–(10) can also be obtained from the following Chapman-Enksog-like expansion [47,48]:

$$\Upsilon_j \odot X_j = t_{r(j)}\left(\frac{\partial f_0}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{c} f_0)\right)_{X_j = 0 \forall j \neq i}, \tag{11}$$

where $\odot$ denotes full tensor contraction of Υ_i and X_i of the same tensorial order. This formulation assumes the standard BGK collision model with two different time scales corresponding to momentum and thermal diffusion. Thermodynamic forces (X_τ and X_q) relax the nonequilibrium state to the equilibrium state in these two characteristic time scales. The variation of the momentum diffusion and thermal diffusion time scales is taken into account using $\mu = \mu_0(T/T_0)^\varphi$ and $\kappa = \kappa_0(T/T_0)^\varphi$, where μ_0 and κ_0 are the viscosity and thermal conductivity at reference temperature and φ depends on the interaction type between molecules (for example, $\varphi \approx 0.75$ for air). Any assumption about the type of molecule is not required in this formulation. Note that two different relaxation times (for momentum transport and energy transport) are involved above, which resolves the issue of the Prandtl number being nonunity for most gases.

Since the first-order correction satisfies the symmetry principle owing to the form in which the distribution function is constructed, we keep the functional form of the distribution function in terms of forces and fluxes and then derive a second-order correction to the Maxwellian distribution. The distribution function with a second-order correction therefore can be expanded in terms of $\Upsilon_i \odot X_i$ as follows (also in [47]):

$$f = f_0 - \sum_j \Upsilon_j \odot X_j + \sum_{k,j} (\Upsilon_{kj} \odot X_k) \odot X_j + \cdots. \tag{12}$$

The second-order correction to the distribution function in Eq. (12) is evaluated in a manner similar to Eq. (11), with the Maxwellian distribution replaced by the first-order correction function [48]

$$\Upsilon_{kj} \odot X_k = t_{r(j)}\left(\frac{\partial \Upsilon_j}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{c}\Upsilon_j)\right)_{X_j = 0 \forall j \neq i}. \tag{13}$$

The second-order corrections can be obtained from Eq. (13) in a form consistent with the first-order correction as

$$\Upsilon_{jj} = f_0 t_{r(j)}^2 \bar{\Upsilon}_{jj}, \tag{14}$$

where

$$\begin{aligned}
\bar{\Upsilon}_{\tau\tau} \odot X_\tau
&= -\overbrace{C_i\left[\mathbf{C} \otimes \frac{\partial \mathbf{u}}{\partial x_i} + \left(\mathbf{C} \otimes \frac{\partial \mathbf{u}}{\partial x_i}\right)^T\right]}^{\omega_1} + \overbrace{\frac{1}{2\beta}[\mathbf{C} \otimes \nabla g + (\mathbf{C} \otimes \nabla g)^T]}^{\omega_2} - \left[\overbrace{\frac{1}{2\beta}(\gamma - 1)\mathbf{C} \cdot \nabla g}^{\omega_3} - \overbrace{\frac{1}{2\beta}(\gamma - 1)(\mathbf{C} \otimes \mathbf{C}) : X_\tau}^{\omega_4}\right]\mathbf{I} \\
&\quad - \overbrace{\bar{\Upsilon}_\tau\left(\frac{1}{t_{r(\tau)}}\sum_j \Upsilon_j \odot X_j\right)}^{\omega_5} + \overbrace{\bar{\Upsilon}_\tau\left\{[\varphi(\gamma - 1) - \gamma]\nabla \cdot \mathbf{u} + \frac{\varphi}{\beta}\mathbf{C} \cdot \nabla\beta + \mathbf{C} \cdot \nabla g\right\}}^{\omega_6},
\end{aligned} \tag{15}$$

$$\bar{\Upsilon}_{qq}\odot X_q = -\overbrace{\bar{\Upsilon}_q\left(\frac{1}{t_{r(q)}}\sum_j \Upsilon_j\odot X_j\right)}^{\xi_1} - \left\{\overbrace{\frac{1}{\beta}[\mathbf{C}\cdot\nabla g]}^{\xi_2} - \overbrace{\frac{1}{\beta}(\mathbf{C}\otimes\mathbf{C}):X_\tau}^{\xi_3} + \overbrace{\left(\frac{5}{2\beta}\right)(\gamma-1)\nabla\cdot\mathbf{u}}^{\xi_4} + \overbrace{\left(\frac{5}{2\beta^2}\right)(\mathbf{C}\cdot\nabla\beta)}^{\xi_5}\right\}\mathbf{C}$$
$$-\overbrace{\left[\frac{5}{2\beta}-|\mathbf{C}|^2\right]\left[\frac{1}{2\beta}\nabla g\right]}^{\xi_6} - \overbrace{\left[\frac{5}{2\beta}-|\mathbf{C}|^2\right][\mathbf{C}\otimes\nabla\mathbf{u}]}^{\xi_7} + \overbrace{\bar{\Upsilon}_q\left\{[\varphi(\gamma-1)-\gamma]\nabla\cdot\mathbf{u} + \frac{\varphi}{\beta}\mathbf{C}\cdot\nabla\beta + \mathbf{C}\cdot\nabla g\right\}}^{\xi_8}, \quad (16)$$

and $g = \log(\rho/\beta)$. Note that the terms ω_6 and ξ_8 are obtained from the variation of time scales. The distribution function with known contractions of forces and fluxes can therefore be expressed as

$$f = f_0 - (\Upsilon_\tau : X_\tau + \Upsilon_q\cdot X_q + (\Upsilon_{\tau\tau}\odot X_\tau):X_\tau + (\Upsilon_{qq}\odot X_q)\cdot X_q). \quad (17)$$

The terms capturing deviations from equilibrium should also satisfy the additional constraint of the additive invariants property of kinetic theory:

$$\langle\Psi,(f-f_0)\rangle = 0. \quad (18)$$

The obtained second-order correction to the distribution function however does not satisfy Eq. (18) in the present form. The function is therefore modified in such a way that it satisfies the additive invariance property without breaking Onsager's symmetry. Details of the modification procedure for satisfying the additive invariance property are available in our recent work [37]. For brevity, we present here only the final form of the distribution function:

$$f' = f_0 - [\Upsilon_\tau : X_\tau + \Upsilon_q\cdot X_q + (\Upsilon'_{\tau\tau}\odot X_\tau):X_\tau + (\Upsilon'_{qq}\odot X_q)\cdot X_q], \quad (19)$$

where

$$\bar{\Upsilon}'_{\tau\tau}\odot X_\tau = \bar{\Upsilon}_{\tau\tau}\odot X_\tau + \overbrace{\frac{\Delta}{t_{r(\tau)}}(\Upsilon_q\cdot X_q)\bar{\Upsilon}_\tau}^{\omega_7} + \left(\frac{5}{2\beta}-|\mathbf{C}|^2\right)\left(\overbrace{\Lambda(\omega_6+\omega_1)}^{\omega_8}\right),$$

$$\bar{\Upsilon}'_{qq}\odot X_q = \bar{\Upsilon}_{qq}\odot X_q + \overbrace{\frac{\Delta}{t_{r(q)}}(\Upsilon_\tau : X_\tau)\bar{\Upsilon}_q}^{\xi_9} + \left(\frac{5}{2\beta}-|\mathbf{C}|^2\right)\left(\overbrace{\Omega\mathbf{C}\cdot\nabla\beta\mathbf{C}}^{\xi_{10}}\right),$$

$$\Omega = \varphi+2, \quad \Lambda = -\frac{2}{5}, \quad \Delta = -\varphi\frac{t_{r(\tau)}}{t_{r(q)}} - \frac{t_{r(q)}}{t_{r(\tau)}} + 2, \quad \Upsilon'_{jj} = f_0 t^2_{r(j)}\bar{\Upsilon}'_{jj}.$$

The collision invariance property (18) of the distribution function (19) has been explicitly shown to be satisfied [37]. With this final Onsager principle consistent distribution (19), we close conservation equations (3)–(6) in the next section.

IV. ONSAGER PRINCIPLE CONSISTENT BURNETT REGIME CONSTITUTIVE EQUATIONS

The phase density function (19) is substituted in Eq. (6) to evaluate the Burnett order constitutive relationships. The employed distribution function being consistent with the principles of nonequilibrium thermodynamics has the promise of yielding more accurate higher-order continuum transport equations. Note that the second-order correction to the distribution function involves a huge number of terms as apparent from Eqs. (15) and (16). Some simplification is however possible by realizing that odd moments of peculiar velocity with equilibrium distribution function are zero:

$$\Theta = m\int C_i^{\lambda_1} C_j^{\lambda_2}\, C_k^{\lambda_3}|\mathbf{C}|^{\lambda_4} f\, d\mathbf{c}, \quad (20)$$

i.e., all the exponents λ_1, λ_2, λ_3, and λ_4 need to be even simultaneously.

We now present a detailed derivation for the new expression of σ^B_{11} (where the superscript B indicates Burnett order). It can be readily seen from Eq. (20) that the ω_2, ω_3, ξ_3, ξ_4, and ξ_7 terms do not contribute to the integral in Eq. (6). The contributions of the remaining ω_i and ξ_i terms to the integrals are as follows:

$$m\int C_1^2\omega_1 : X_\tau f_0 t^2_{r(\tau)} d\mathbf{c} = -4\frac{\mu^2\beta}{\rho}\left[3u_x^2 + v_y^2 + w_z^2 + 2\left(u_y v_x + u_z w_x + \frac{1}{2}v_z w_y\right) + \frac{1}{2}\left(u_y^2+u_z^2+v_z^2+w_y^2+3w_x^2+3v_x^2\right)\right], \quad (21)$$

$$m\int C_1^2\omega_4 : X_\tau f_0 t^2_{r(\tau)} d\mathbf{c} = 4\frac{\mu^2\beta}{\rho}\frac{(\gamma-1)}{2}\left[3u_x^2+v_y^2+w_z^2+2(2u_x v_y + 2u_x w_z + v_y w_z)\right], \quad (22)$$

$$m\int C_1^2\omega_5 : X_\tau f_0 d\mathbf{c}$$
$$= 4\frac{\mu^2\beta}{\rho}\bigg[\frac{3}{2}u_y^2+\frac{3}{2}u_z^2+\frac{3}{2}v_x^2+\left(\frac{35\gamma^2-154\gamma+179}{8}\right)u_x^2+\frac{1}{2}v_z^2+\left(\frac{35\gamma^2-98\gamma+75}{8}\right)\left(v_y^2+w_z^2\right)$$
$$+\frac{3}{2}w_x^2+v_z+\frac{1}{2}w_y^2+3u_yv_x+3u_zw_x+\left(\frac{35\gamma^2-126\gamma+103}{4}\right)(u_xv_y+u_xw_z)+\left(\frac{35\gamma^2-98\gamma+67}{4}\right)v_yw_z\bigg], \quad (23)$$

$$m\int C_1^2\omega_6 : X_\tau f_0 t_{r(\tau)}^2 d\mathbf{c} = -4\frac{\mu^2\beta}{\rho}\left(\frac{\varphi(\gamma-1)-\gamma}{4}\right)[(5\gamma-11)u_x^2+(5\gamma-7)u_xv_y+(5\gamma-7)u_xw_z+(5\gamma-11)u_yu_x$$
$$+(5\gamma-7)u_yv_y+(5\gamma-7)u_yw_z+(5\gamma-11)u_zu_x+(5\gamma-7)u_zv_y+(5\gamma-7)u_zw_z], \quad (24)$$

$$m\int C_1^2\Lambda\omega_8 : X_\tau f_0 t_{r(\tau)}^2 d\mathbf{c} = \Lambda 4\frac{\mu^2\beta}{\rho}\frac{1}{5}\big[(-9+3\gamma)u_x^2+4(-1+\gamma)u_xv_y+4(-1+\gamma)u_xw_z+(-3+\gamma)\left(v_y^2+w_z^2\right)$$
$$+2(-1+\gamma)v_yw_z-4u_yv_x-4u_zw_x-u_y^2-u_z^2-v_y^2-w_z^2-2v_yw_z\big], \quad (25)$$

$$m\int C_1^2\xi_1\cdot X_q f_0 t_{r(q)}^2 d\mathbf{c} = \left(\frac{2\kappa\beta(\gamma-1)}{R\rho\gamma}\right)^2\left[\frac{9}{8\beta^3}\left(3\beta_x^2+\beta_y^2+\beta_z^2\right)\right], \quad (26)$$

$$m\int C_1^2\xi_2\cdot X_q f_0 t_{r(q)}^2 d\mathbf{c} = -\left(\frac{2\kappa\beta(\gamma-1)}{R\rho\gamma}\right)^2\left[\frac{1}{4\beta^2}(3\beta_xg_x+\beta_yg_y+\beta_zg_z)\right], \quad (27)$$

$$m\int C_1^2\xi_5\cdot X_q f_0 t_{r(q)}^2 d\mathbf{c} = -\left(\frac{2\kappa\beta(\gamma-1)}{R\rho\gamma}\right)^2\left[\frac{5}{8\beta^3}\left(3\beta_x^2+\beta_y^2+\beta_z^2\right)\right], \quad (28)$$

$$m\int C_1^2\xi_6\cdot X_q f_0 t_{r(q)}^2 d\mathbf{c} = 0, \quad (29)$$

$$m\int C_1^2\xi_8\cdot X_q f_0 t_{r(q)}^2 d\mathbf{c} = \left(\frac{2\kappa\beta(\gamma-1)}{R\rho\gamma}\right)^2\left[\frac{\varphi}{4\beta^3}\left(3\beta_x^2+\beta_y^2+\beta_z^2\right)+\frac{1}{4\beta^2}(3\beta_xg_x+\beta_yg_y+\beta_zg_z)\right], \quad (30)$$

$$m\int C_1^2\Omega\xi_{10}\cdot X_q f_0 t_{r(q)}^2 d\mathbf{c} = -\Omega\left(\frac{2\kappa\beta(\gamma-1)}{R\rho\gamma}\right)^2\left[\frac{1}{4\beta^3}\left(3\beta_x^2+\beta_y^2+\beta_z^2\right)\right], \quad (31)$$

$$m\int C_1^2\Delta(\omega_7 : X_\tau+\xi_9\cdot X_q) f_0 t_{r(q)}^2 d\mathbf{c} = 0. \quad (32)$$

In these equations, u, v, and w are the velocity components along the x, y, and z directions, respectively.

The addition of Eqs. (21)–(32) yields the expression for σ_{11}^B. In a similar manner, expressions for other elements of the stress tensor and heat flux vector can be derived. For the sake of brevity, we present only the final expressions for other stress and heat flux components. The proposed constitutive relationships therefore are

$$\sigma_{11}^B = 4\frac{\mu^2\beta}{\rho}\bigg[\left(\frac{125\gamma^2-576\gamma+\varphi(110-160\gamma+50\gamma^2)+643}{40}\right)u_x^2+\frac{4}{5}\left(u_y^2+u_z^2\right)+\frac{1}{5}(u_yv_x+u_zw_x)-\frac{3}{5}\left(w_x^2+v_x^2\right)$$
$$+\left(\frac{125\gamma^2-392\gamma+\varphi(70-120\gamma+50\gamma^2)+291}{40}\right)\left(v_y^2+w_z^2\right)+\left(\frac{125\gamma^2-392\gamma+\varphi(70-120\gamma+50\gamma^2)+307}{40}\right)v_yw_z$$
$$+\left(\frac{100\gamma^2-484\gamma+\varphi(90-140\gamma+50\gamma^2)+459}{20}\right)(u_xv_y+u_xw_z)-\frac{2}{5}(v_zw_y)-\frac{1}{5}\left(w_y^2+v_z^2\right)\bigg], \quad (33)$$

$$\sigma_{12}^B = 4\frac{\mu^2\beta}{\rho}\left(\frac{-1}{10}\right)[(23\gamma+5\gamma\varphi-5\varphi-37)(u_xu_y+v_xv_y)-10u_zv_z+(23\gamma+5\gamma\varphi-5\varphi-51)(u_xv_x+u_yv_y+4w_xw_y)$$
$$-3(v_zw_x+u_zw_y)+(23\gamma+5\gamma\varphi-5\dot{\omega}-37)(u_yw_z+v_xw_z)], \quad (34)$$

$$q_1^B = 4\frac{\mu^2\beta}{\rho}\bigg[\left(\frac{-47+25\gamma}{8}\right)\frac{g_x u_x}{\beta} + \varphi\left(\frac{49-35\gamma}{8\beta^2}\right)(\beta_x v_y + \beta_x w_z) - \frac{1}{2\beta}(g_y u_y + g_y v_x + g_z w_x) + \varphi\left(\frac{77-35\gamma}{8}\right)\frac{\beta_x u_x}{\beta^2} + \frac{7\varphi}{4\beta^2}(\beta_y u_y + \beta_z u_z + \beta_y v_x + \beta_z w_x) + \left(\frac{-39+25\gamma}{8\beta}\right)(g_x v_y + g_x w_z)\bigg] + \left(\frac{2\kappa(\gamma-1)}{R\gamma}\right)^2 \frac{1}{\rho\beta}\bigg[-\beta_y v_x - \beta_z w_x\left(\frac{-77+35\gamma+10\varphi(-1+\gamma)}{8}\right)\beta_x u_x - \frac{7}{4}(\beta_y u_y + \beta_z u_z) + \left(\frac{-59+35\gamma+10\varphi(-1+\gamma)}{8}\right)(\beta_x v_y + \beta_x w_z)\bigg]. \tag{35}$$

The full stress tensor and heat flux vector can be obtained by a suitable change of variables in the equations for σ_{11}^B, σ_{12}^B, and q_1^B. For completeness, we note that the expression for σ_{22}^B can be evaluated from the expression for σ_{11}^B in Eq. (33) by performing an appropriate change of variables $u \to v, x \to y, v \to u$, and $y \to x$. The expression for σ_{33}^B can be evaluated from the expression for σ_{11}^B in Eq. (33) as $u \to w, x \to z, w \to u$, and $z \to x$. The expression for σ_{23}^B can be evaluated from the expression for σ_{12}^B in Eq. (34) by replacing $u \to v, x \to y, v \to w, y \to z, w \to u$, and $z \to x$ and the expression for σ_{31}^B by $u \to w, x \to z, v \to u, y \to x, w \to v$, and $z \to y$. Similarly, to obtain the heat flux vectors q_2^B and q_3^B we replace $u \to v, x \to y, v \to u$, and $y \to x$ and $u \to w, x \to z, w \to u$, and $z \to x$ in Eq. (35), respectively.

V. PROPOSED BURNETT ORDER EQUATIONS

In this section we present the final set of conservation equations for mass, momentum, and energy, closed with consistent Onsager symmetry principle thermodynamic fluxes, stress tensor, and heat flux vector

$$\frac{\partial\rho}{\partial t} + \frac{\partial\rho u_k}{\partial x_k} = 0, \tag{36}$$

$$\rho\frac{\partial u_i}{\partial t} + \rho u_k\frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \frac{\partial\sigma_{ik}}{\partial x_k} = \rho G_i, \tag{37}$$

$$\rho\frac{\partial\epsilon}{\partial t} + \rho u_k\frac{\partial\epsilon}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + p\frac{\partial u_k}{\partial x_k} + \sigma_{ij}\frac{\partial u_i}{\partial x_j} = 0, \tag{38}$$

with expressions for σ_{11}, σ_{12}, and q_1 are given below, obtained by adding the corresponding Navier-Stokes and Burnett terms

$$\sigma_{11} = \sigma_{11}^{NS} + \sigma_{11}^B = \mu\delta_1 u_x + \mu\delta_2 v_y + \mu\delta_2 w_z + 4\frac{\mu^2\beta}{\rho}\big[\alpha_1 u_x^2 + \alpha_2 u_y^2 + \alpha_3 u_z^2 + \alpha_4 u_y v_x + \alpha_5 u_z w_x + \alpha_6 w_x^2 + \alpha_7 v_x^2 + \alpha_8 u_x v_y + \alpha_9 v_y^2 + \alpha_{10} w_z^2 + \alpha_{11} v_y w_z + \alpha_{12} u_x w_z + \alpha_{13} v_z w_y + \alpha_{14} w_y^2 + \alpha_{15} v_z^2\big], \tag{39}$$

$$\sigma_{12} = \sigma_{12}^{NS} + \sigma_{12}^B = \mu\delta_3 u_y + \mu\delta_3 v_x + 4\frac{\mu^2\beta}{\rho}\big[\beta_1 u_x u_y + \beta_2 v_x v_y + \beta_3 u_z v_z + \beta_4 u_x v_x + \beta_5 u_y v_y + \beta_6 w_x w_y + \beta_7 v_z w_x + \beta_8 u_z w_y + \beta_9 u_y w_z + \beta_{10} v_x w_z\big], \tag{40}$$

$$q_1 = q_1^{NS} + q_1^B = \delta_4\kappa\frac{\beta_x}{2R\beta^2} + 4\frac{\mu^2\beta}{\rho}\bigg[\gamma_1\frac{g_x u_x}{\beta} + \gamma_2\frac{\beta_x v_y}{\beta^2} + \gamma_3\frac{\beta_x w_z}{\beta^2} + \gamma_4\frac{1}{\beta}g_y u_y + \gamma_5\frac{1}{\beta}g_y v_x + \gamma_6\frac{1}{\beta}g_z w_x + \gamma_7\frac{\beta_x u_x}{\beta^2} + \gamma_8\frac{1}{\beta^2}\beta_y u_y + \gamma_9\frac{1}{\beta^2}\beta_z u_z + \gamma_{10}\frac{1}{\beta^2}\beta_y v_x + \gamma_{11}\frac{1}{\beta^2}\beta_z w_x + \gamma_{12}\frac{g_x v_y}{\beta} + \gamma_{13}\frac{g_x w_z}{\beta}\bigg] + \left(\frac{2\kappa(\gamma-1)}{R\gamma}\right)^2\frac{1}{\rho\beta}[\gamma_{14}\beta_y v_x + \gamma_{15}\beta_z w_x + \gamma_{16}\beta_x u_x + \gamma_{17}\beta_y u_y + \gamma_{18}\beta_z u_z + \gamma_{19}\beta_x v_y + \gamma_{20}\beta_x w_z]. \tag{41}$$

The constants appearing in front of the derivatives of flow field variables are as follows:

$$\delta_1 = -\frac{4}{3},\quad \delta_2 = \frac{2}{3},\quad \alpha_1 = \left(\frac{125\gamma^2 - 576\gamma + \varphi(110 - 160\gamma + 50\gamma^2) + 643}{40}\right),\quad \alpha_2 = \frac{4}{5},\quad \alpha_3 = \frac{4}{5},\quad \alpha_4 = \frac{1}{5},$$

$$\alpha_5 = \frac{1}{5},\quad \alpha_6 = -\frac{3}{5},\quad \alpha_7 = -\frac{3}{5},\quad \alpha_8 = \left(\frac{100\gamma^2 - 484\gamma + \varphi(90 - 140\gamma + 50\gamma^2) + 459}{20}\right),$$

$$\alpha_9 = \left(\frac{125\gamma^2 - 392\gamma + \varphi(70 - 120\gamma + 50\gamma^2) + 291}{40}\right), \quad \alpha_{10} = \alpha_9,$$

$$\alpha_{11} = \alpha_9 + \frac{18}{40}, \quad \alpha_{12} = \alpha_{11}, \quad \alpha_{13} = -\frac{2}{5}, \quad \alpha_{14} = -\frac{1}{5}, \quad \alpha_{15} = \alpha_{14},$$

$$\delta_3 = -1, \quad \beta_1 = \frac{23\gamma + 5\gamma\varphi - 5\varphi - 37}{10}, \quad \beta_2 = \beta_1, \quad \beta_3 = -1, \quad \beta_4 = \beta_1 - \frac{14}{10},$$

$$\beta_5 = \beta_4, \quad \beta_6 = 4\beta_4, \quad \beta_7 = -\frac{3}{10}, \quad \beta_8 = \beta_7, \quad \beta_9 = \beta_1,$$

$$\delta_4 = 1, \quad \gamma_1 = \left(\frac{-47 + 25\gamma}{8}\right), \quad \gamma_2 = \varphi\left(\frac{49 - 35\gamma}{8}\right), \quad \gamma_3 = \gamma_2, \quad \gamma_4 = -\frac{1}{2}, \quad \gamma_5 = \gamma_4, \quad \gamma_6 = \gamma_4, \quad \gamma_7 = +\varphi\left(\frac{77 - 35\gamma}{8}\right),$$

$$\gamma_8 = \frac{7\varphi}{4}, \quad \gamma_9 = \gamma_8, \quad \gamma_{10} = \gamma_9, \quad \gamma_{11} = \gamma_8, \quad \gamma_{12} = \left(\frac{-39 + 25\gamma}{8}\right), \quad \gamma_{13} = \gamma_{12}, \quad \gamma_{14} = -1, \quad \gamma_{15} = \gamma_{14},$$

$$\gamma_{16} = \left(\frac{-77 + 35\gamma + 10\varphi(-1 + \gamma)}{8}\right), \quad \gamma_{17} = -\frac{7}{4}, \quad \gamma_{18} = \gamma_{17}, \quad \gamma_{19} = \frac{-59 + 35\gamma + 10\varphi(-1 + \gamma)}{8}, \quad \gamma_{20} = \gamma_{19}.$$

These coefficients are a function of the type of gas, such as monatomic and diatomic, and the interaction potential variable φ between molecules. Substitution of these stress and heat flux terms in Eqs. (36)–(38) completes the derivation of our proposed Burnett-type equations.

VI. LINEAR STABILITY ANALYSIS

A linear stability analysis of the equations derived in the preceding section is now performed. The analysis is performed for a one-dimensional wave about the following equilibrium state: $u = 0$, $\rho = \rho_0$, and $T = T_0$. Assume small perturbations around equilibrium

$$\begin{aligned} u &= u'(x,t), \\ \rho &= \rho_0 + \rho'(x,t), \\ T &= T_0 + T'(x,t) \end{aligned} \tag{42}$$

(where X' denotes small quantities away from equilibrium) and substitute Eq. (42) in the governing equations (36)–(38). This yields the following set of equations upon linearization:

$$\frac{\partial \rho'}{\partial t} + \rho_0 \frac{\partial u'}{\partial x} = 0, \tag{43}$$

$$\rho_0 \frac{\partial u'}{\partial t} + \rho_0 R \frac{\partial T'}{\partial x} + R T_0 \frac{\partial \rho'}{\partial x} + \frac{4}{3}\mu \frac{\partial^2 u'}{\partial x^2} = 0, \tag{44}$$

$$\frac{3}{2}\rho_0 R \frac{\partial T'}{\partial t} - \kappa \frac{\partial^2 T'}{\partial x^2} + p_0 \frac{\partial u'}{\partial x} = 0. \tag{45}$$

It is remarkable to note that there are no Burnett order terms in the above equations. This ensures that the stability of the derived equations is the same as that for the Navier-Stokes equations.

The above stems from the fact that Eqs. (33)–(35) involve only the cross product of the derivative of velocity, temperature, and pressure. Therefore, the σ_{11}^B, σ_{12}^B, and q_1^B terms all become identically zero for small perturbation. In contrast, the presence of second derivatives of velocity and temperature in the stress tensor and heat flux vector in Burnett equations leads to the problem of stability.

VII. FORCE-DRIVEN PLANE POISEUILLE FLOW

Force-driven plane Poiseuille flow, an example of classic internal flow, is chosen as the standard case to verify the stable Burnett equations. Several nonintuitive and nonequilibrium thermodynamic phenomena such as a nonconstant pressure profile in the transverse direction, a characteristic temperature dip at the center, and tangential heat flux are observed in force-driven plane Poiseuille flow. The inability of Navier-Stokes-Fourier equations to capture these effects has been widely reported in the literature [15,24,49].

Uribe and Garcia [50] performed a comprehensive study analyzing the flow characteristics of force-driven compressible plane Poiseuille flow by Burnett equations for Knudsen numbers equal to 0.025, 0.05, and 0.1. To validate these results, they also conducted numerical simulations using the DSMC technique. In order to establish the validity of the presently derived stable Burnett equations, the problem is defined in exactly the same way as by Uribe and Garcia [50] so as to compare the results from the stable Burnett equations with DSMC data and the conventional Burnett equations.

In the present study, we consider a steady-state one-dimensional flow confined between two infinite and stationary plane parallel walls, as shown in Fig. 1. The walls are located at $y = \pm L/2$ and maintained at a constant temperature T_R. An external body force a in the x direction drives the flow. The velocity normal to the stationary walls (v) and the third component of velocity (w) are both zero. All the flow variables are assumed to be functions of the y direction only [50]. With these assumptions, we have the following conditions:

$$u_i = \{u(y),0,0\}, \quad \frac{\partial u_k}{\partial x_k} = 0, \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + u_k \frac{\partial}{\partial x_k} = 0. \tag{46}$$

In the two-dimensional framework of the problem, i.e., the flow quantities independent of the third direction, the stress

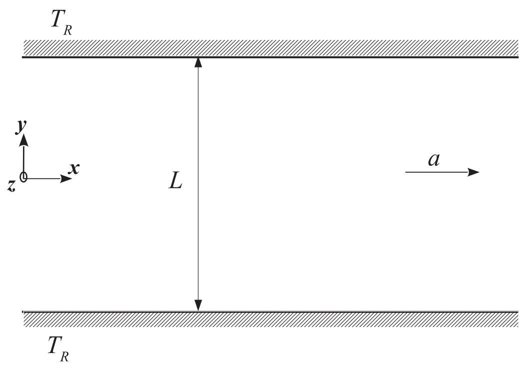

FIG. 1. Schematic of plane Poiseuille flow driven by an external force a.

tensor and heat flux vector reduce to

$$\sigma_{ij} = \begin{bmatrix} \sigma_{11}(y) & \sigma_{12}(y) & 0 \\ \sigma_{12}(y) & \sigma_{22}(y) & 0 \\ 0 & 0 & -\sigma_{11}(y) - \sigma_{22}(y) \end{bmatrix},$$

$$q_i = [q_1(y), \quad q_2(y), \quad 0]. \tag{47}$$

Conservation equations for momentum and energy [Eqs. (37) and (38)] with the above simplifications and using the constitutive relations for the stress tensor and heat flux vector [Eqs. (39)–(41)] with suitable change of variables reduce to

$$-\frac{d}{dy}\left(\mu\frac{du}{dy}\right) = \rho a, \tag{48}$$

$$\frac{dp}{dy} + \frac{d}{dy}\left[2\mu^2\alpha_7\frac{1}{p}\left(\frac{du}{dy}\right)^2\right] = 0, \tag{49}$$

$$\frac{d}{dy}\left(\kappa\frac{dT}{dy}\right) + \mu\left(\frac{du}{dy}\right)^2 = 0. \tag{50}$$

The expressions for dynamic viscosity and thermal conductivity for a dilute gas of rigid spheres are given as [1]

$$\mu = \frac{5c_\mu}{16\sigma^2}\left(\frac{mkT(y)}{\pi}\right)^{1/2}, \quad \kappa = \frac{75c_\lambda}{64\sigma^2}\left(\frac{k^3T(y)}{\pi m}\right)^{1/2}, \tag{51}$$

where σ is the particle diameter and accurate values of $c_\mu = 1.016\,034$ and $c_\lambda = 1.025\,13$ are known [1]. The variables are nondimensionalized as [50]

$$s = \frac{y}{L}, \quad p^*(s) = \frac{p(y)}{p(0)}, \quad T^*(s) = \frac{T(y)}{T_R},$$

$$u^*(s) = \frac{u(y)}{(2kT_R/m)^{1/2}}, \tag{52}$$

where T_R is the temperature of the walls. Using the ideal gas equation $p = \rho RT$ in the x-momentum equation to eliminate density, the nondimensionalized form of the equations is given as

$$\frac{d^2u^*}{ds^2} = -\frac{1}{2T^*}\frac{dT^*}{ds}\frac{du^*}{ds} + \frac{b_0 p^*}{T^{*3/2}}, \tag{53}$$

$$\frac{d^2T^*}{ds^2} = -\frac{8c_\mu}{15c_\lambda}\left(\frac{du^*}{ds}\right)^2 - \frac{1}{2T^*}\left(\frac{dT^*}{ds}\right)^2, \tag{54}$$

$$\frac{dp^*}{ds} = \frac{-\frac{2T^*}{p^*}\frac{du^*}{ds}\left[-\frac{1}{2T^*}\frac{dT^*}{ds}\frac{du^*}{ds} + \frac{b_0 p^*}{T^{*3/2}}\right] + \left(\frac{du^*}{ds}\right)^2\frac{1}{p^*}\frac{dT^*}{ds}}{b_2 - \frac{T^*}{p^{*2}}\left(\frac{du^*}{ds}\right)^2}. \tag{55}$$

The coefficients are

$$b_0 = -\frac{8}{5}\frac{L^2 a\sqrt{2\pi}\,p(0)m\sigma^2}{c_\mu k^2 T_R^2},$$

$$b_2 = \frac{64}{25}\left(\frac{p(0)L}{kT_R}\frac{\sigma^2}{c_\mu}\right)^2\frac{\pi}{\alpha_7}. \tag{56}$$

The above system of three ordinary coupled differential equations can be expressed as five coupled first-order differential equations. The inherent symmetry in the problem provides us with two initial conditions $\frac{du^*}{ds}|_{s=0} = 0$ and $\frac{dT^*}{ds}|_{s=0} = 0$. The centerline values taken from DSMC simulations [50] are specified as

$$u^*(0) = u_0, \quad T^*(0) = T_0, \quad p^*(0) = 1, \tag{57}$$

Table I shows the values of the different parameters [$p(0)$, a, and L] as defined in the problem statement and the initial conditions [$u^*(0)$, $T^*(0)$, and $p^*(0)$] for three different Knudsen numbers as taken from Uribe and Garcia [50]. In order to simplify the comparison with the DSMC results, the authors [50] specified $m = \sigma = T_R = 1$ and $k = \frac{1}{2}$ for all the simulations.

The results of the conserved variables (u^*, p^*, and T^*) for the stable Burnett equations are compared with those of the Burnett equations and the DSMC results obtained by Uribe and Garcia [50] at Kn = 0.025, 0.05, and 0.1. The variation of pressure in the cross stream direction at Kn = 0.025 is shown in Fig. 2(a). The genesis of the nonconstant pressure profile can be explained when we closely examine the y-momentum equation. On integrating the y-momentum equation, we have $p + \sigma_{22} = p(0)$. The contribution to the normal stress comes only from the Burnett order terms and hence the classical Navier-Stokes-Fourier theory is unable to capture the nonconstant pressure profile. Another striking feature of the pressure profile is evident in Fig. 2(a), which shows very unusual bimodal behavior near the wall in the case

TABLE I. Values of different parameters as defined in the problem statement and initial conditions [50].

	Parameters			Initial conditions		
Kn	$p(0)$	a	L	$u^*(0)$	$T^*(0)$	$p^*(0)$
0.025	$(6.555\times10^{-4})2kT_R/\sigma^3$	$(1.0\times10^{-5})2kT_R/m\sigma$	7440σ	0.689452	1.09814	1.0
0.05	$(6.727\times10^{-4})2kT_R/\sigma^3$	$(4.0\times10^{-5})2kT_R/m\sigma$	3720σ	0.7575	1.1293	1.0
0.1	$(7.13394\times10^{-4})2kT_R/\sigma^3$	$(1.6\times10^{-4})2kT_R/m\sigma$	1860σ	0.90287	1.2052	1.0

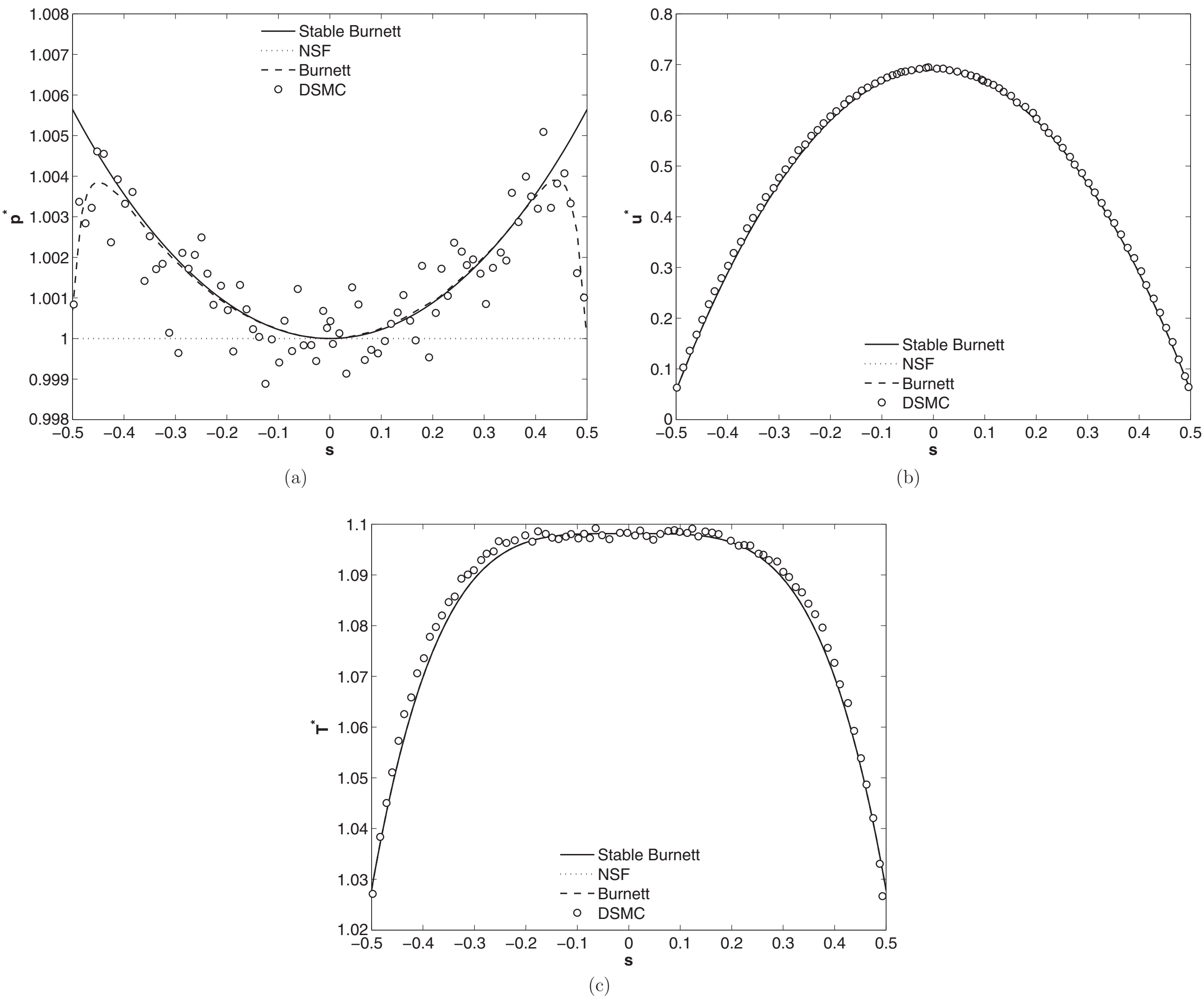

FIG. 2. (a) Pressure, (b) velocity, and (c) temperature distribution in the cross stream direction in force-driven compressible plane Poiseuille flow at Kn = 0.025. In the case of velocity and temperature variation, the results of NSF equations, Burnett equations, and stable Burnett equations overlap.

of DSMC and Burnett equations. As compared to this bimodal behavior, the stable Burnett equations predict a monotonic pressure profile with a minimum at the center. However, it should be noted that the pressure profile according to Burnett equations is constructed such that it closely follows the DSMC profile by tweaking one of the coefficients in the differential equation of pressure. Nonetheless, excellent agreement is observed in the bulk region, whereas approximately 0.5% deviation is observed near the wall when compared with the DSMC results. It is worth mentioning here that the recent molecular dynamics simulations performed by Rana *et al.* [51] at $\mathrm{Kn} = 0.1$ also predicted a similar monotonic behavior, thereby lending support to the monotonic pressure profile as predicted by the stable Burnett equations.

Figure 2(b) shows the variation of velocity in the cross stream direction at $\mathrm{Kn} = 0.025$ with Navier-Stokes-Fourier (NSF) equations, Burnett equations, stable Burnett equations, and DSMC simulations, all predicting the same trend, i.e., quadratic variation with a maximum at the center. The x-momentum equation for Burnett equations and stable Burnett equations reduces to the classical NSF equations and hence the velocity profiles obtained from NSF theory, Burnett equations, and stable Burnett equations are virtually indistinguishable. It is quite evident from Fig. 2(b) that the velocity profile predicted by the stable Burnett equations is in excellent agreement with the DSMC results.

The variation of temperature in the cross stream direction at $\mathrm{Kn} = 0.025$ is shown in Fig. 2(c). The energy equation in the case of Burnett and stable Burnett equations reduces to the classical NSF equations and the resulting temperature profile is quartic with a maximum appearing at the center. The temperature profile predicted by the stable Burnett equations is found to be in excellent agreement with the DSMC results, as shown in Fig. 2(c).

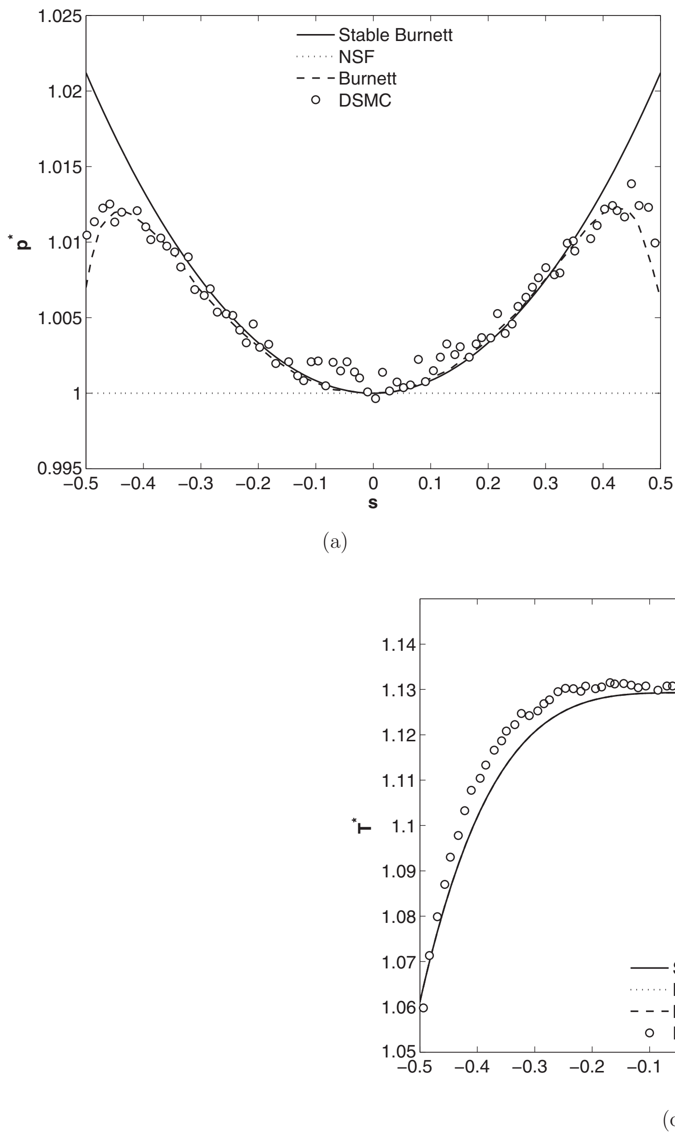

FIG. 3. (a) Pressure, (b) velocity, and (c) temperature distribution in the cross stream direction in force-driven compressible plane Poiseuille flow at $\mathrm{Kn} = 0.05$. In the case of velocity and temperature variation, the results of NSF equations, Burnett equations, and stable Burnett equations overlap.

Similar trends are observed for all the conserved variables at Knudsen number equal to 0.05. The results of stable Burnett equations are found to be in excellent agreement with DSMC results in the case of velocity and temperature, as shown in Fig. 3. However, in the case of a pressure profile as shown in Fig. 3(a), a deviation of about 1% is observed near the wall, while in the bulk region the results are in good agreement with the DSMC results.

At $\mathrm{Kn} = 0.1$, i.e., in the transition regime, there is a maximum deviation of 4% near the walls in the case of a pressure profile when compared with the DSMC results as shown in Fig. 4(a). Again, the bimodal pressure profile as predicted by DSMC and Burnett equations is not captured by the stable Burnett equations. However, when we compare with the molecular dynamics results of Rana *et al.* [51], the monotonic pressure profile as predicted by the stable Burnett equations compares well with the molecular dynamics simulation results. Rana *et al.* [51] suggested that the stochastic mesoscopic DSMC simulations are inadequate to capture the gas-wall interactions precisely and hence the pressure profile is contaminated near the walls. With these recent findings exposing some of the flaws associated with the DSMC simulations, the monotonic pressure profile as predicted by the stable Burnett equations is well justified by the MD simulations as against the bimodal behavior predicted by the DSMC simulations and the Burnett equations.

At Knudsen number equal to 0.1, a deviation of about 20% is observed in the slip velocity as shown in Fig. 4(b). However, in the bulk region, the velocity profile according to the stable Burnett equations is in good agreement with the DSMC results. The bimodal behavior of temperature with a characteristic dip at the center is quite noticeable at $\mathrm{Kn} = 0.1$ [see Fig. 4(c)] according to DSMC results, however this dip is not captured by the stable Burnett equations. It has been pointed out that this characteristic dip in temperature is probably a super-Burnett effect [50,52], and since the Burnett equations as well as

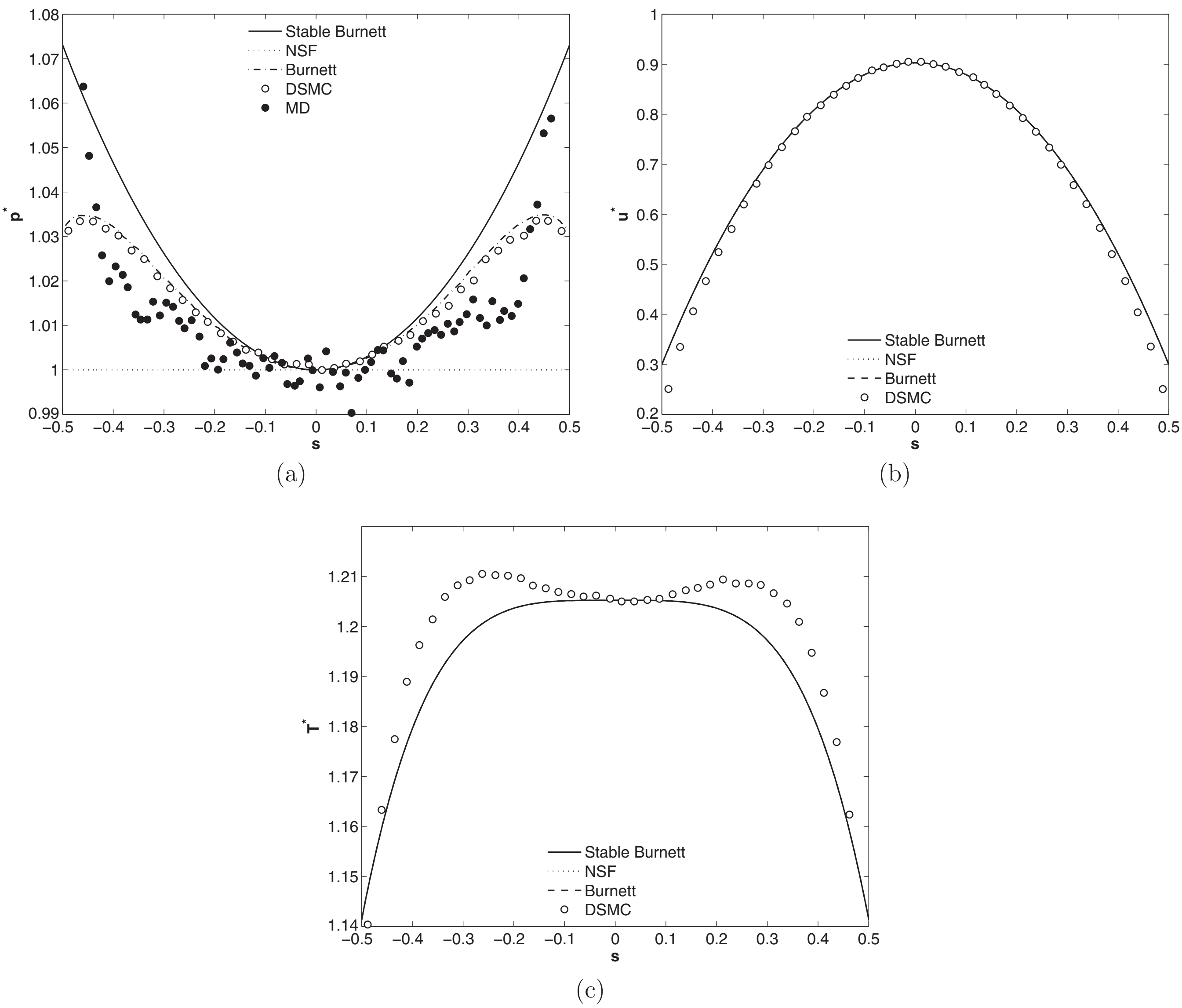

FIG. 4. (a) Pressure, (b) velocity, and (c) temperature distribution in the cross stream direction in force-driven compressible plane Poiseuille flow at $\mathrm{Kn} = 0.1$. In the case of velocity and temperature variation, the results of NSF equations, Burnett equations, and stable Burnett equations overlap.

stable Burnett equations are only second-order accurate, their inability to capture this temperature dip at the center is not surprising. Nonetheless, the maximum discrepancy between the DSMC results and the stable Burnett results is found to be about 1%.

In summary, we can safely say that the stable Burnett equations are indeed able to capture nonequilibrium phenomena that are observed in force-driven plane Poiseuille flow with the exception of a peculiar temperature dip at the center where the difference in value is less than 1%. This dip is due to the super-Burnett effect and therefore is not expected to be captured by the present equations.

VIII. COMPARISON WITH EXISTING BURNETT-TYPE EQUATIONS

There are differences in the structure of the proposed and all available equations in the literature [1,15,17,21,22,53]. First, the proposed constitutive equations do not contain second-order derivatives of velocity that are there in existing Burnett-type equations. Along with resolving the issue of stability discussed above, this circumvents the need to find additional boundary condition for the proposed equations. That is, the proposed equations require the same number of boundary conditions as the Navier-Stokes equations for their solution. This remarkable feature will broaden the range of applications to which the equations can be applied by altering the constitutive relationships. Bobylev *et al.* [19] showed improved performance in capturing shock profiles with generalized Burnett equations, which do not contain third-order derivatives of velocity and temperature.

The second feature of the proposed equations is the absence of temperature gradient terms in the stress tensor. In contrast, temperature gradients are present in the stress tensor of all Burnett-type equations. This reduced coupling between velocity and temperature allows for complete solution of the mass and momentum equations in certain cases (such as incompressible forced convection problems) before solving the energy equation.

Third, note the appearance of two different relaxation times [coefficient $(\frac{2\kappa(\gamma-1)}{R\gamma})^2\frac{1}{\rho\beta}$, which can also be expressed as $1/\mathrm{Pr}^2(\mu/p)^2$, where Pr is Prandtl number] in the expression of heat flux. Although the problem of deducing the correct Prandtl number has been addressed [53] by assuming two different relaxation times for momentum transport and energy transport, those approaches are at the macroscopic level and appear arbitrary. Here it is straightforward and natural to assume two different relaxation times for momentum transport and energy transport in Eq. (17) and then evaluate expressions for the stress tensor and heat flux vector accordingly.

IX. CONCLUSION

In this work, a set of stable Burnett-type higher-order continuum transport equation has been derived. An approach involving Onsager's reciprocity principle consistent phase density function is utilized towards this end. The employed phase density function satisfies the collision invariance properties and also satisfies the linearized form of the Boltzmann equation. The phase density function therefore satisfies the features of nonequilibrium thermodynamics.

The phase density function is then utilized to evaluate the Burnett order constitutive relations. It is interesting to note that the phase density function naturally involves two different relaxation times for momentum and energy transport, thereby ensuring the correct value of Prandtl number for any gas. The derived equations are found to be second order, therefore these equations do not require more boundary conditions beyond the Navier-Stokes equations for their complete solution. In addition, the absence of temperature gradient terms in the stress tensor is noted. The presence of terms with two relaxation time scales in the heat flux vector is a different feature of our equations.

Because our derivation process does not involve the Chapman-Enskog expansion, the validity of these equations is not restricted to small Knudsen number. The problem of stability that plagues the existing Burnett equations is not there with the derived equations; the equations are shown to be unconditionally stable. These are a generalized set of Burnett-type equations applicable to any kind of molecule.

The derivation of these three-dimensional higher-order continuum equations is an important achievement as it captures departures from equilibrium in transport phenomena and establishes the importance of ideas from nonequilibrium thermodynamics. The validity of these equations is established by analyzing the results of equilibrium variables in the case of force-driven compressible plane Poiseuille flow. However, these equations need to be tested rigorously to fully establish their potential in capturing rarefied gas flow physics.

ACKNOWLEDGMENT

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