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A general framework for the inverse design of mesoscopic models based on the Boltzmann equation

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Abstract

In this paper, we present a general framework for the inverse-design of mesoscopic models based on the Boltzmann equation. Starting from the single-relaxation-time Boltzmann equation with an additional source term, two model Boltzmann equations for two reduced distribution functions are obtained, each then also having an additional undetermined source term. Under this general framework and using Navier-Stokes-Fourier (NSF) equations as constraints, the structures of the distribution functions are obtained by the leading-order Chapman-Enskog analysis. Next, five basic constraints for the design of the two source terms are obtained in order to recover the Navier-Stokes-Fourier system in the continuum limit. These constraints allow for adjustable bulk-to-shear viscosity ratio, Prandtl number as well as a thermal energy source. The specific forms of the two source terms can be determined through proper physical considerations and numerical implementation requirements. By employing the truncated Hermite expansion, one design for the two source terms is proposed. Moreover, three well-known mesoscopic models in the literature are shown to be compatible with these five constraints. In addition, the consistent implementation of boundary conditions is also explored by using the Chapman-Enskog expansion at the NSF order. Finally, based on the higher-order Chapman-Enskog expansion of the distribution functions, we derive the complete analytical expressions for the viscous stress tensor and the heat flux. Some underlying physics can be further explored under this framework.

Keywords: Mesoscopic CFD methods; Boltzmann equation; inverse design; the Navier-Stokes-Fourier system; Chapman-Enskog analysis; structure of distribution function; thermal forcing; boundary condition; bulk viscosity; Prandtl number

1 Introduction

The Boltzmann equation is of vital importance in the kinetic theory of dilute gases [1]. The original collision operator in the Boltzmann equation is a complex integral term, which makes direct numerical simulation of the system very costly. The simplest choice is to replace the original collision operator with the Bhatnager-Gross-Krook (BGK) model [2]. It should be noted that the original collision operator is directly based on the physical description of molecule interactions while the BGK model describes the fact that the distribution of the molecules relaxes to the local equilibrium state through particle collisions without considering the detailed molecule interactions. It has long been recognized that such an approximation works well beyond its theoretical limit as long as the relaxation time can be made to capture the relevant physics [3, 4].

By applying the Chapman-Enskog expansion to the Boltzmann equation with the BGK collision operator, the NSF system can be recovered, but with a unit Prandtl number which does not obey the physical reality. Hence, some improved models have been developed to overcome this limitation from different physical considerations, such as the Shakhov (SH) model [5], the ellipsoidal statistical (ES) model [6], the internal energy double-distribution-function (IEDDF) model [7], the total energy double-distribution-function (TEDDF) model [8], and the Rykov (R) model [9, 10, 11]. Further, we notice that, for example, the ratio between the bulk to shear viscosity in SH model is always less than $2/D$, where D is the dimension of the hydrodynamic velocity space. Therefore, for a fixed specific heat ratio, the SH model cannot be used to investigate the physical effect of the bulk-to-shear viscosity ratio.

Some merits and drawbacks of these models are briefly discussed below. The SH model may encounter a negative value of the particle distribution function because of the modified equilibrium distribution to accommodate arbitrary Prandtl number, while the ES model and the TEDDF model can avoid such unphysical deficiency. However, Chen *et al.* [12] showed that the SH model may yield more accurate solutions than that from the ES model in the transition regime and they proposed a generalized model which combines the advantages of the SH model and ES model. For both IEDDF and TEDDF models, two distribution functions are introduced with different relaxation times for the non-equilibrium part of the particle distribution function because the momentum and energy have different relaxation time scales during the collision process as suggested by Wood [13]. In the TEDDF model, spatial and time derivatives of the hydrodynamic velocity are not involved in the source terms while they are involved in the source terms of the IEDDF model which may introduce some numerical errors and lead to some unphysical phenomena in fluid systems containing large spatial gradients. In the R model, by considering the elastic and non-elastic particle collision processes, the hydrodynamic flow variables corresponding to the translational and rotational processes can be evaluated separately. Both the total internal energy and the total heat flux are the sum of the contributions from the two processes. The bulk-to-shear viscosity ratio can be modified in the R model through the ratio of the total number of translational and rotational collisions to that of rotational collisions.

During the past few decades, the BGK model has been widely used to simulate different flows such as homogeneous isotropic turbulence [14], turbulent channel flows [15] and multiphase flows [16], by different numerical approaches such as the lattice Boltzmann method (LBM) [17], the gas kinetic scheme (GKS) [18], the unified gas kinetic scheme (UGKS) [19], and the discrete unified gas kinetic scheme (DUGKS) [20, 21]. Recently, Liu *et al.* [22] claimed that the predictions based on the BGK model for highly nonequilibrium flows are only qualitatively correct in the transitional regime since the BGK model filters out the information of the detailed molecular-interaction processes. They compare the Boltzmann equation and its model equations through some test cases where the distribution functions are far from equilibrium. From these tests, they found that information contained in the nonequilibrium moments and the different relaxation rates of high- and low-speed molecules is essential in adjusting the behaviors of model collision terms. However, many existing works have shown that the BGK model is adequate in simulating many flows accurately for both the continuum and rarefied regimes [14, 15, 23, 16, 24, 25].

In this paper, we focus on the inverse design of the source term in the model Boltzmann equation. Following the work done by Guo *et al.* [21], an adjustable parameter representing the internal degree of freedom of molecules is introduced to the Maxwellian equilibrium distribution function. We will demonstrate that the two source terms in the two reduced model Boltzmann equations can be redesigned to attain the following objectives. First, the NSF system can be recovered in the continuum limit by applying the Chapman-Enskog analysis. Second, the model Boltzmann system can have flexible Prandtl number as well as adjustable bulk-to-shear viscosity ratio. Third, an arbitrary thermal source/sink term can be added to the internal energy equation.

The rest of the paper is organized as follows. In Section 2, the model Boltzmann equation with an additional source term is introduced. By introducing two reduced distribution functions, two reduced model Boltzmann equations are obtained. Some notations and conventions are given in Section 3. In Section 4, the structures of the Boltzmann equations are obtained by applying the first-order Chapman-Enskog expansion. Next, five requirements for the two reduced source terms are given in Section 5. In Section 6, we present one design for the two source terms by applying the Hermite expansion to the two source terms. In Section 7, we show that the SH model, the TEDDF model as well as the R model are compatible with the five derived constraints. Then we discuss the derivation of the proper implementation of the hydrodynamic boundary conditions in Section 8. Next, we derive the complete analytical expression for the viscous stress and the heat flux based on the second-order Chapman-Enskog expansion in the following three sections. Major conclusions are drawn in Section XII. In Appendix A, we include the details on the Hermite polynomials and Hermite expansion. Appendix B provides the widely used models for the thermal cooling function and the shear viscosity in the literature. Appendix C provides some details on the Chapman-Enskog expansion of the particle distribution functions. Appendix D contains the derivations of the requirements for the two reduced source terms. Appendix E documents some details on the Rykov model.

2 The reduced model Boltzmann system with source terms

The Boltzmann equation with an additional source term can be expressed as

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} f + \boldsymbol{a} \cdot \boldsymbol{\nabla}_{\boldsymbol{\xi}} f = \Omega_f + S_f, \tag{1}$$

where $f(\boldsymbol{x}, \boldsymbol{\xi}, \boldsymbol{\eta}, \boldsymbol{\zeta}, t)$ is the particle distribution function, $\boldsymbol{x} = (x_1, ..., x_D)$ is the spatial location, t is the time, $\boldsymbol{\xi} = (\xi_1, ..., \xi_D)$ is the particle velocity in $D-$dimensional space, $\boldsymbol{\eta} = (\eta_{D+1}, ..., \eta_3)$ is the particle velocity in the remaining $(3 - D)$ dimensional space, $\boldsymbol{\zeta} = (\zeta_1, ..., \zeta_K)$ represents $K-$dimensional internal degree of freedom. $\boldsymbol{a}$ represents the body force per unit mass, which can vary with the spatial location $\boldsymbol{x}$ and the time t. The single-relaxation-time Bhatnager-Gross-Krook (BGK) model [2] is used for the collision operator, *i.e.* $\Omega_f = (f^{eq} - f)/\tau$. $\tau = \mu/p$ is the molecular relaxation time, μ is the shear viscosity and p is the pressure. S_f is a source term to be designed, which will allow for modification of both the fluid Prandtl number Pr as well as the bulk viscosity μ_V.

By assuming that the particle motion in $(\boldsymbol{\eta}, \boldsymbol{\zeta})$ subspace is at local equilibrium, the local Maxwellian equilibrium distribution function can be written as [21]

$$f^{eq} = \frac{\rho}{(2\pi RT)^{(K+3)/2}} \exp\left(-\frac{c^2 + \eta^2 + \zeta^2}{2RT}\right), \tag{2}$$

where ρ is the density of the fluid, R is the specific gas constant, T is the temperature, $\boldsymbol{c} = \boldsymbol{\xi} - \boldsymbol{u}$ is the peculiar velocity with $\boldsymbol{u}$ being the hydrodynamic velocity. The pressure p is related to the density ρ and the temperature T through an ideal-gas equation of state (EOS), namely, $p = \rho RT$.

The conservative variables are defined as the moments of the particle distribution function

$$\begin{aligned} &\rho = \int f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta},\ \rho \boldsymbol{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta}, \\ &\rho E = \frac{1}{2}\rho u^2 + \rho\epsilon = \int \frac{\xi^2 + \eta^2 + \zeta^2}{2} f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta}, \end{aligned} \tag{3}$$

where $\epsilon = C_v T$ is the internal energy per unit mass, C_v is the specific heat capacity at constant volume, ρE is the total energy per unit volume which is the sum of the internal energy and the kinetic energy. All relations in Eq. (3) remain valid if f is replaced by f^{eq}. C_v and the specific heat at constant pressure C_p are determined by the number of the internal degrees of freedom, K, and the gas constant, R. By integrating the energy moment of the equilibrium distribution, we can obtain

$$C_v = \frac{(K+3)R}{2},\ C_p = \frac{(K+5)R}{2}, \tag{4}$$

which implies that the specific heat ratio and thus the Prandtl number are

$$\gamma = \frac{C_p}{C_v} = \frac{K+5}{K+3}, \ Pr = \frac{\mu C_p}{\kappa}, \tag{5}$$

where κ is the thermal conductivity.

In addition, by comparing the first-order moment of the model Boltzmann equation with the Navier-Stokes equation, it can be shown that the viscous stress tensor $\boldsymbol{\sigma}$ is determined by the non-equilibrium part of the particle distribution function as

$$\boldsymbol{\sigma} = -\int \boldsymbol{c}\boldsymbol{c}(f - f^{eq}) d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta}, \tag{6}$$

and, by comparing the energy moment of the Boltzmann equation with the macroscopic energy equation, the heat flux $\boldsymbol{q}$ can be determined as

$$\boldsymbol{q} = \frac{1}{2} \int \boldsymbol{c}(c^2 + \eta^2 + \zeta^2) f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta}. \tag{7}$$

The physical conservative requirements can be expressed through the moments of the collision operator Ω_f, which reads

$$\begin{aligned} &\int \Omega_f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta} = 0, \ \int \boldsymbol{\xi} \Omega_f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta} = \mathbf{0}, \\ &\int \frac{1}{2} \left(\xi^2 + \eta^2 + \zeta^2\right) \Omega_f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta} = 0. \end{aligned} \tag{8}$$

Therefore, provided that the mass conservation and the momentum conservation laws are observed, we have the following basic requirements for the source term

$$\begin{aligned} &\int S_f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta} = 0, \ \int \boldsymbol{\xi} S_f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta} = \mathbf{0}, \\ &\int \frac{1}{2} (c^2 + \eta^2 + \zeta^2) S_f d\boldsymbol{\xi} d\boldsymbol{\eta} d\boldsymbol{\zeta} = -\rho \Lambda, \end{aligned} \tag{9}$$

where Λ represents a source term applied to the macroscopic energy equation, an example of which is the thermal cooling or heating function, see Appendix B for details.

Physically, the evolution of the particle distribution function only depends on the $D-$dimensional particle velocity space. In order to remove the dependence of the passive variables and also reduce the computational cost in the practical implementation, two independent, reduced distribution functions g and h, residing in lower dimensional phase space, are introduced [21]

$$g = \int f d\boldsymbol{\eta} d\boldsymbol{\zeta}, \; h = \int (\eta^2 + \zeta^2) f d\boldsymbol{\eta} d\boldsymbol{\zeta}. \tag{10}$$

Therefore, the two model Boltzmann equations residing in lower dimensional space can be obtained

$$\frac{\partial g}{\partial t} + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} g + \boldsymbol{a} \cdot \boldsymbol{\nabla}_{\boldsymbol{\xi}} g = \Omega_g + S_g, \tag{11a}$$

$$\frac{\partial h}{\partial t} + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} h + \boldsymbol{a} \cdot \boldsymbol{\nabla}_{\boldsymbol{\xi}} h = \Omega_h + S_h. \tag{11b}$$

In Eqs. (11a) and (11b), the collision operators are

$$\Omega_g = \frac{g^{eq} - g}{\tau}, \; \Omega_h = \frac{h^{eq} - h}{\tau}, \tag{12}$$

and the two source terms are given by

$$S_g = \int S_f d\boldsymbol{\eta} d\boldsymbol{\zeta}, \; S_h = \int (\eta^2 + \zeta^2) S_f d\boldsymbol{\eta} d\boldsymbol{\zeta}, \tag{13}$$

where the equilibrium distribution functions g^{eq} and h^{eq} are

$$g^{eq} = \int f^{eq} d\boldsymbol{\eta} d\boldsymbol{\zeta} = \frac{\rho}{(2\pi RT)^{D/2}} \exp\left[-\frac{c^2}{2RT}\right], \tag{14a}$$

$$h^{eq} = \int \left(\eta^2 + \zeta^2\right) f^{eq} d\boldsymbol{\eta} d\boldsymbol{\zeta} = (3 - D + K) RT g^{eq}. \tag{14b}$$

Based on Eq. (8), the conservation laws can be recasted in terms of the collision operators Ω_g and Ω_h, as follows,

$$\int \Omega_g d\boldsymbol{\xi} = 0, \ \int \boldsymbol{\xi}\Omega_g d\boldsymbol{\xi} = \mathbf{0}, \ \int \left(\xi^2\Omega_g + \Omega_h\right) d\boldsymbol{\xi} = 0. \tag{15}$$

From Eq. (9), the two reduced source terms must satisfy the following requirements

$$\int S_g d\boldsymbol{\xi} = 0, \ \int \boldsymbol{\xi} S_g d\boldsymbol{\xi} = \mathbf{0}, \ \int \frac{1}{2}(c^2 S_g + S_h) d\boldsymbol{\xi} = -\rho\Lambda. \tag{16}$$

In addition, from Eq. (3), we find that the conservative variables can be evaluated as

$$\rho = \int g d\boldsymbol{\xi}, \ \rho\boldsymbol{u} = \int \boldsymbol{\xi} g d\boldsymbol{\xi}, \ \rho E = \frac{1}{2}\int (\xi^2 g + h) d\boldsymbol{\xi}. \tag{17}$$

Moreover, from Eqs. (6) and (7), the viscous stress $\boldsymbol{\sigma}$ and the heat flux $\boldsymbol{q}$ become

$$\boldsymbol{\sigma} = -\int \boldsymbol{cc}(g - g^{eq}) d\boldsymbol{\xi}, \ \boldsymbol{q} = \frac{1}{2}\int \boldsymbol{c}(c^2 g + h) d\boldsymbol{\xi}. \tag{18}$$

Several well-known models for the shear viscosity μ and thermal cooling function Λ are briefly introduced in Appendix B.

3 Notations and conventions

For convenience, two time derivatives are introduced

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \boldsymbol{\xi}\cdot\boldsymbol{\nabla} + \boldsymbol{a}\cdot\boldsymbol{\nabla}_{\boldsymbol{\xi}}, \quad \frac{d}{dt} \equiv \frac{\partial}{\partial t} + \boldsymbol{u}\cdot\boldsymbol{\nabla}, \tag{19}$$

where D/Dt is the time derivative along the phase-space trajectory of a particle subjected to a body force $\boldsymbol{a}$ per unit mass and d/dt is the rate of change of a physical quantity along the path of a fluid element in the physical space. Three variables including the time t, the spacial location $\boldsymbol{x}$, and the particle velocity $\boldsymbol{\xi}$ are assumed to be independent when these time derivatives act on the distribution functions $g(\boldsymbol{x}, \boldsymbol{\xi}, t)$ and $h(\boldsymbol{x}, \boldsymbol{\xi}, t)$.

In addition, a symmetrical tensor $\boldsymbol{S}$ and an antisymmetric tensor $\boldsymbol{\Omega}$ can be defined based on the velocity gradient

$$\boldsymbol{S} = \frac{1}{2}\left(\nabla \boldsymbol{u}^T + \nabla \boldsymbol{u}\right), \ \boldsymbol{\Omega} = \frac{1}{2}\left(\nabla \boldsymbol{u}^T - \nabla \boldsymbol{u}\right), \tag{20}$$

where $\boldsymbol{S}$ is called the strain rate tensor which describes the deformation of a fluid element and $\boldsymbol{\Omega}$ is called the rotation tensor representing the directionally-averaged rate of local rotation.

The Newtonian constitutive relation for the viscous stress $\boldsymbol{\sigma}^{(NS)}$ and the Fourier's law for the heat flux $\boldsymbol{q}^{(NS)}$ are, respectively,

$$\boldsymbol{\sigma}^{(NS)} = 2\mu\left(\boldsymbol{S} - \frac{1}{D}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right) + \mu_V(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}, \ \boldsymbol{q}^{(NS)} = -\kappa\boldsymbol{\nabla}T. \tag{21}$$

where $\boldsymbol{I}$ represents the unit tensor of which the components are δ_{ij} in the Cartesian coordinate system.

In addition, the ratio of bulk to shear viscosity is defined as $\chi = \mu_V/\mu$.

4 The structure of the particle distribution functions

In the continuum flow limit, the relaxation time τ, when normalized by the acoustic time scale l_0/c_0, is proportional to the Knudsen number, where l_0 is a system length scale and c_0 is the speed of the sound at a reference temperature T_0. Therefore, τ may be taken as a small parameter in the Boltzmann equation. At the level of NSF equations, terms higher than $O(\tau)$ in the distribution functions can be neglected.

The derivatives of the equilibrium distribution function g^{eq} will be multiplied by τ to form the $O(\tau)$ terms in the distribution functions. Therefore, we only need to evaluate them to $O(1)$. Direct evaluation yields the derivatives of the equilibrium distribution function g^{eq} as

$$\frac{\partial g^{eq}}{\partial t} = \left[\frac{1}{\rho}\frac{\partial \rho}{\partial t} + \left(\frac{c^2}{2RT} - \frac{D}{2}\right)\frac{1}{T}\frac{\partial T}{\partial t} + \frac{\partial \boldsymbol{u}}{\partial t}\cdot\frac{\boldsymbol{c}}{RT}\right] g^{eq}, \tag{22a}$$

$$\boldsymbol{\nabla} g^{eq} = \left[\frac{1}{\rho}\boldsymbol{\nabla}\rho + \left(\frac{c^2}{2RT} - \frac{D}{2}\right)\frac{1}{T}\boldsymbol{\nabla}T + \boldsymbol{\nabla}\boldsymbol{u}\cdot\frac{\boldsymbol{c}}{RT}\right] g^{eq}, \tag{22b}$$

$$\nabla_{\boldsymbol{\xi}} g^{eq} = -\frac{\boldsymbol{c}}{RT} g^{eq}. \tag{22c}$$

The three coefficients in three derivatives are found to be polynomials of the peculiar velocity $\boldsymbol{c}$ and are related to the time t and spatial location $\boldsymbol{x}$ through the relation $\boldsymbol{c} = \boldsymbol{\xi} - \boldsymbol{u}$.

By employing the Euler equations in Appendix D to replace the time derivatives with spatial derivatives of the hydrodynamic variables in Eq. (22a), we obtain the expression for Dg^{eq}/Dt to the leading order, as

$$\frac{Dg^{eq}}{Dt} = G g^{eq} + O(\tau), \tag{23}$$

where the operator G contains three parts, *i.e.* $G = G_1 + G_2 + G_3$. They are given explicitly as

$$G_1 = \left(\frac{c^2}{2RT} - \frac{D+2}{2} \right) \boldsymbol{c} \cdot \left(\frac{1}{T} \nabla T \right), \tag{24a}$$

$$G_2 = \frac{\boldsymbol{c} \cdot \boldsymbol{S} \cdot \boldsymbol{c}}{RT} - \frac{1}{K+3} \left(\frac{c^2}{RT} + 3 - D + K \right) \nabla \cdot \boldsymbol{u}, \tag{24b}$$

$$G_3 = -\left(\frac{c^2}{2RT} - \frac{D}{2} \right) \frac{\Lambda}{C_v T}. \tag{24c}$$

Similarly, for Dh^{eq}/Dt, we have

$$\frac{Dh^{eq}}{Dt} = (G + \Phi_1) h^{eq} + O(\tau), \tag{25}$$

where the new operator Φ_1 is given as

$$\Phi_1 = \boldsymbol{c} \cdot \left(\frac{1}{T} \nabla T \right) - \frac{2}{K+3} \nabla \cdot \boldsymbol{u} - \frac{\Lambda}{C_v T}. \tag{26}$$

Therefore, up to the order $O(\tau)$ in the Chapman-Enskog expansion [1], the structure of the distribution functions g and h can be obtained and they are

$$g = (1 - \tau G)g^{eq} + \tau S_g + O(\tau^2), \tag{27a}$$

$$h = (1 - \tau G - \tau \Phi_1)h^{eq} + \tau S_h + O(\tau^2). \tag{27b}$$

5 Five basic requirements for the two source terms

Based on the structure of the distribution function, we shall now propose five basic requirements for the two source terms, S_g and S_h. The requirements are given as follows and the details for their derivations are included in Appendix D. If these five requirements are satisfied up to the order of $O(\tau)$, then the NSF system can be recovered by applying the Chapman-Enskog expansion to the two model Boltzmann equations.

The first requirement comes from the continuity equation

$$\int S_g d\boldsymbol{\xi} = 0. \tag{28a}$$

The second requirement emerges from the continuity equation and the momentum equation

$$\int \boldsymbol{c} S_g d\boldsymbol{\xi} = \int \boldsymbol{\xi} S_g d\boldsymbol{\xi} = \mathbf{0}. \tag{28b}$$

The third requirement is used to modify the bulk viscosity in the viscous stress term, and it is

$$\int \boldsymbol{\xi\xi} S_g d\boldsymbol{\xi} = \int \boldsymbol{cc} S_g d\boldsymbol{\xi} = -\left(\chi - \frac{2(3 - D + K)}{D(K+3)}\right) p(\boldsymbol{\nabla} \cdot \boldsymbol{u})\boldsymbol{I} - \frac{p\Lambda}{C_v T}\boldsymbol{I}. \tag{28c}$$

The fourth requirement follows from the energy equation and it is

$$\int S_h d\boldsymbol{\xi} = -\int \xi^2 S_g d\boldsymbol{\xi} - 2\rho\Lambda. \tag{28d}$$

The fifth requirement is expressed as

$$\int \boldsymbol{c} S_h d\boldsymbol{\xi} = \frac{2\left(1 - Pr\right)\boldsymbol{q}^{(NS)}}{\tau} - \int \boldsymbol{c}c^2 S_g d\boldsymbol{\xi}, \tag{28e}$$

which is needed to modify the heat flux and thus the resulting Prandtl number.

As a result the design constraints, Eqs. (28a) – (28e), the model Boltzmann equation will yield the following NSF system

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0, \tag{29a}$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}^{(NS)} + \rho \boldsymbol{a} + \boldsymbol{O}(\tau^2), \tag{29b}$$

$$\begin{aligned} &\frac{\partial \left(\rho E\right)}{\partial t} + \nabla \cdot (\rho E \boldsymbol{u}) = \\ &-\boldsymbol{\nabla} \cdot \boldsymbol{q}^{(NS)} - \boldsymbol{\nabla} \cdot (p\boldsymbol{u}) + \boldsymbol{\nabla} \cdot (\boldsymbol{\sigma}^{(NS)} \cdot \boldsymbol{u}) + \rho \boldsymbol{a} \cdot \boldsymbol{u} - \rho \Lambda + O(\tau^2). \end{aligned} \tag{29c}$$

The equation for the internal energy can be obtained from Eqs. (29b) and (29c), which reads

$$\rho C_v \frac{dT}{dt} = -p \boldsymbol{\nabla} \cdot \boldsymbol{u} - \boldsymbol{\nabla} \cdot \boldsymbol{q}^{(NS)} + \boldsymbol{\sigma}^{(NS)} : \boldsymbol{S} - \rho \Lambda + O(\tau^2). \tag{30}$$

6 A possible design of the two reduced source terms

There are many possible ways to design the specific form of the two source terms. By applying the Hermite expansion to the two source terms, a new mesoscopic model with both adjustable Prandtl number and bulk viscosity is proposed next. Any reasonable design of the two source terms should satisfy the five basic requirements presented in Eqs. (28a) to (28e).

We assume that the source terms, S_g and S_h, are functions of the spatial location $\boldsymbol{x}$, the particle velocity $\boldsymbol{\xi}$ and the time t, *i.e.*, $S_g = S_g\left(\boldsymbol{x}, \boldsymbol{\xi}, t\right)$, $S_h = S_h\left(\boldsymbol{x}, \boldsymbol{\xi}, t\right)$. Due to the desire to keep the order of Gauss-Hermite quadrature as low as feasible in the numerical implementation, we further require

$$\int \boldsymbol{\xi\xi\xi} S_g d\boldsymbol{\xi} = \mathbf{0}. \tag{31}$$

By using Eqs. (28b) and (31), we have

$$\int S_g \mathscr{H}^{(3)}(\boldsymbol{\xi}, T_0)\, d\boldsymbol{\xi} = \mathbf{0}. \tag{32}$$

The Eqs. (28a)–(28c) can also be written as

$$\int S_g \mathscr{H}^{(0)}(\boldsymbol{\xi}, T_0)\, d\boldsymbol{\xi} = 0, \quad \int S_g \mathscr{H}^{(1)}(\boldsymbol{\xi}, T_0)\, d\boldsymbol{\xi} = \mathbf{0},$$
$$\int S_g \mathscr{H}^{(2)}(\boldsymbol{\xi}, T_0)\, d\boldsymbol{\xi} = -\left(\chi - \frac{2(3-D+K)}{D(K+3)}\right)\frac{p\boldsymbol{\nabla}\cdot\boldsymbol{u}}{RT_0}\boldsymbol{I} - \frac{p}{RT_0}\frac{\Lambda}{C_vT}\boldsymbol{I}, \tag{33}$$

where T_0 is a reference temperature and the velocity are scaled with $\sqrt{RT_0}$.

Therefore, by using Eqs. (32) and (33) and keeping the Hermite expansion (see Appendix A) of the source term S_g up to the third-order, we obtain

$$S_g(\boldsymbol{x}, \boldsymbol{\xi}, t) = \frac{1}{2!}\omega(\boldsymbol{\xi}, T_0)\, \boldsymbol{a}^{(2)}(\boldsymbol{x}, t) : \mathscr{H}^{(2)}(\boldsymbol{\xi}, T_0)$$
$$= -\omega(\boldsymbol{\xi}, T_0)\left[\left(\chi - \frac{2(3-D+K)}{D(K+3)}\right)\frac{p\boldsymbol{\nabla}\cdot\boldsymbol{u}}{2RT_0} + \frac{p}{2RT_0}\frac{\Lambda}{C_vT}\right]\left(\frac{\xi^2}{RT_0} - D\right). \tag{34}$$

From Eqs. (28a)–(28c) and Eq. (31), we can obtain

$$\int \boldsymbol{c}c^2 S_g d\boldsymbol{\xi} = (D+2)\left(\chi - \frac{2(3-D+K)}{D(K+3)}\right)p\boldsymbol{u}\boldsymbol{\nabla}\cdot\boldsymbol{u} + (D+2)\frac{p\Lambda}{C_vT}\boldsymbol{u}. \tag{35}$$

Combination of Eqs. (28d), (28e) and (35) yields

$$\int \boldsymbol{\xi} S_h d\boldsymbol{\xi} = \frac{2(1-Pr)\boldsymbol{q}^{(NS)}}{\tau} + \boldsymbol{u}\int S_h d\boldsymbol{\xi} - \int \boldsymbol{c}c^2 S_g d\boldsymbol{\xi}$$
$$= \frac{2(1-Pr)\boldsymbol{q}^{(NS)}}{\tau} - 2\left(\chi - \frac{2(3-D+K)}{D(K+3)}\right)p\boldsymbol{u}\boldsymbol{\nabla}\cdot\boldsymbol{u} - 2\cdot\frac{K+5}{K+3}\rho\Lambda\boldsymbol{u}. \tag{36}$$

Therefore, we obtain

$$\int S_h \mathscr{H}^{(1)}\left(\boldsymbol{\xi}, T_0\right) d\boldsymbol{\xi} = \frac{2(1-Pr)\boldsymbol{q}^{(NS)}}{\tau\sqrt{RT_0}}$$
$$-2\left(\chi - \frac{2(3-D+K)}{D(K+3)}\right)\frac{\boldsymbol{u}}{\sqrt{RT_0}} p\boldsymbol{\nabla}\cdot\boldsymbol{u} - 2\cdot\frac{K+5}{K+3}\frac{\boldsymbol{u}}{\sqrt{RT_0}}\rho\Lambda. \tag{37}$$

Eqs. (28c) and (28d) together imply that

$$\int S_h \mathscr{H}^{(0)}\left(\boldsymbol{\xi}, T_0\right) d\boldsymbol{\xi} = D\left(\chi - \frac{2(3-D+K)}{D(K+3)}\right) p\boldsymbol{\nabla}\cdot\boldsymbol{u} + D\frac{p\Lambda}{C_v T} - 2\rho\Lambda. \tag{38}$$

Combination of Eqs. (37) and (38) yields one design for the source term S_h

$$S_h = \omega\left(\boldsymbol{\xi}, T_0\right)\left[\begin{array}{l}\dfrac{2(1-Pr)\boldsymbol{q}^{(NS)}\cdot\boldsymbol{\xi}}{\tau RT_0} + \left(D - 2\dfrac{\boldsymbol{u}\cdot\boldsymbol{\xi}}{RT_0}\right)\left(\chi - \dfrac{2(3-D+K)}{D(K+3)}\right)p\boldsymbol{\nabla}\cdot\boldsymbol{u} \\ -2\left(\dfrac{3-D+K}{K+3} + \dfrac{K+5}{K+3}\dfrac{\boldsymbol{u}\cdot\boldsymbol{\xi}}{RT_0}\right)\rho\Lambda\end{array}\right]. \tag{39}$$

Eqs. (34) and (39) provide one possible choice for the two source terms.

7 An examination of three existing mesoscopic models in our design framework

7.1 The Shakhov model

In this section, we will prove that the well-known Shakhov model [21, 5] can be considered as a special example in our general framework. Through the Chapman-Enskog analysis, it can be verified that the ratio of bulk viscosity to shear viscosity in the Shakhov model is $\mu_V/\mu = 2(1/D - 1/(K+3))$. In addition, no cooling function is considered, *i.e.*, $\Lambda = 0$. Therefore, the five general requirements (Eqs. (28a) to (28e)) for the two source terms can be reduced as

$$\int S_g d\boldsymbol{\xi} = 0, \ \int \boldsymbol{c} S_g d\boldsymbol{\xi} = \boldsymbol{0}, \ \int \boldsymbol{c}\boldsymbol{c} S_g d\boldsymbol{\xi} = \boldsymbol{0}, \ \int S_h d\boldsymbol{\xi} = 0, \tag{40a}$$

$$\int \boldsymbol{c} c^2 S_g d\boldsymbol{\xi} + \int \boldsymbol{c} S_h d\boldsymbol{\xi} = \frac{2(1-Pr)\boldsymbol{q}^{(NS)}}{\tau}. \tag{40b}$$

By using Eq. (40), the source term S_g can be assumed as

$$S_g = \frac{1}{3!}\omega(\boldsymbol{c},T)\boldsymbol{a}^{(3)}(\boldsymbol{x},t) : \mathscr{H}^{(3)}(\boldsymbol{c},T), \tag{41}$$

where $\omega(\boldsymbol{c},T)$ is the peculiar-velocity-based weighting function, $\boldsymbol{a}^{(3)}(\boldsymbol{x},t)$ is the coefficient and $\mathscr{H}^{(3)}(\boldsymbol{c},T)$ is the third order Hermite polynomial.

Note that $\boldsymbol{a}^{(3)}(\boldsymbol{x},t) \equiv \int S_g \mathscr{H}^{(3)}(\boldsymbol{c},T)d\boldsymbol{\xi}$ is also symmetrical with respect to the components of $\boldsymbol{c}$ because $\mathscr{H}^{(3)}(\boldsymbol{c},T)$ remains unchanged under the permutation operation, the simplest way is to assume that the coefficient $\boldsymbol{a}^{(3)}$ takes the following form,

$$a^{(3)}_{ijk} = A_i\delta_{jk} + A_j\delta_{ki} + A_k\delta_{ij}, \tag{42}$$

where $\boldsymbol{A}(\boldsymbol{x},t) = (A_1, A_2, A_3)$ is a vector coefficient to be determined.

Substitution of Eq. (42) into Eq. (41) gives

$$S_g = \frac{1}{2}\omega(\boldsymbol{c},T)A_i\mathscr{H}^{(3)}_{ijj}(\boldsymbol{c},T) = \frac{1}{2}\omega(\boldsymbol{c},T)\boldsymbol{A}\cdot\frac{\boldsymbol{c}}{\sqrt{RT}}\left(\frac{c^2}{RT} - D - 2\right), \tag{43}$$

Moreover, it can be shown that

$$\int \boldsymbol{c}c^2 S_g d\boldsymbol{c} = (D+2)\boldsymbol{A}(RT)^{3/2}. \tag{44}$$

Similarly, the source term S_h can be designed as

$$S_h = \omega(\boldsymbol{c},T)\boldsymbol{B}\cdot\mathscr{H}^{(1)}(\boldsymbol{c},T) + \frac{1}{2}\omega(\boldsymbol{c},T)\boldsymbol{C}\cdot\frac{\boldsymbol{c}}{\sqrt{RT}}\left(\frac{c^2}{RT} - D - 2\right). \tag{45}$$

Therefore, the coefficient $\boldsymbol{A}$ and $\boldsymbol{B}$ should satisfy the following relation,

$$(D+2)(RT)^{3/2}\boldsymbol{A} + \sqrt{RT}\boldsymbol{B} = \frac{2(1-Pr)\boldsymbol{q}^{(NS)}}{\tau}, \tag{46}$$

and $\boldsymbol{C}$ is a vector coefficient to be determined.

If the coefficients $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ are chosen specifically as

$$\boldsymbol{A} = \frac{2}{5}\frac{(1-Pr)\boldsymbol{q}^{(NS)}}{\tau(RT)^{3/2}},\ \boldsymbol{B} = \frac{2(3-D)}{5}\frac{(1-Pr)\boldsymbol{q}^{(NS)}}{\tau(RT)^{1/2}},$$
$$\boldsymbol{C} = \frac{2(3-D+K)}{5}\frac{(1-Pr)\boldsymbol{q}^{(NS)}}{\tau(RT)^{1/2}}, \tag{47}$$

then Eq. (46) is satisfied and the two source terms S_g and S_h are given as

$$S_g = \frac{1-Pr}{\tau}\frac{\boldsymbol{c}\cdot\boldsymbol{q}^{(NS)}}{5pRT}\left(\frac{c^2}{RT} - D - 2\right)g^{eq}, \tag{48a}$$

$$S_h = \frac{1-Pr}{\tau}\frac{\boldsymbol{c}\cdot\boldsymbol{q}^{(NS)}}{5p}\left((3-D+K)\left(\frac{c^2}{RT} - D\right) - 2K\right)g^{eq}. \tag{48b}$$

In the Shakhov model, the source term S_f corresponding to the original distribution function f is given by

$$S_f = \frac{f^{Pr}}{\tau} = \frac{1-Pr}{\tau}\frac{\boldsymbol{c}\cdot\boldsymbol{q}^{(NS)}}{5pRT}\left(\frac{c^2+\eta^2}{RT} - 5\right)f^{eq}. \tag{49}$$

Substitution of Eq. (49) into Eq. (13) yields the same results given in Eqs. (48a) and (48b). Therefore, the Shakhov model is indeed just a special design of the source terms in our general framework.

7.2 The total energy double-distribution-function model

The total energy double-distribution-function model (TEDDF) is originally proposed by Guo et al. [8] and then generalized by Liu et al. [26] to simulate thermal compressible flows. The TEDDF model is briefly introduced as follows. From the original particle distribution function f, two new distribution functions g and b are introduced.

$$g = \int f d\boldsymbol{\eta} d\boldsymbol{\zeta},\ b = \frac{1}{2}\int(\xi^2+\eta^2+\zeta^2) f d\boldsymbol{\eta} d\boldsymbol{\zeta}. \tag{50}$$

Therefore, this kinetic system can be expressed as

$$\frac{\partial g}{\partial t} + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} g + \boldsymbol{a} \cdot \boldsymbol{\nabla}_{\boldsymbol{\xi}} g = \frac{g^{eq} - g}{\tau_g}, \tag{51}$$

$$\frac{\partial b}{\partial t} + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} b + \boldsymbol{a} \cdot \boldsymbol{\nabla}_{\boldsymbol{\xi}} b = \frac{b^{eq} - b}{\tau_b} + \left(\boldsymbol{\xi} \cdot \boldsymbol{u} - \frac{1}{2}u^2\right) \frac{g - g^{eq}}{\tau_{bg}} + g\boldsymbol{\xi} \cdot \boldsymbol{a}, \tag{52}$$

where the relaxation times are computed as

$$\tau = \tau_g = \mu/p, \ \tau_b = \tau_g/Pr, \ \tau_{bg} = \tau_b\tau_g/(\tau_g - \tau_b). \tag{53}$$

Through the Chapman-Enskog expansion, the bulk viscosity of this model is

$$\mu_V = \left(\frac{2}{D} - \frac{2}{K+3}\right)\mu, \tag{54}$$

The equilibrium g^{eq} is the same as that in Eq. (14a). With h^{eq} defined in Eq. (14b), the equilibrium b^{eq} can be written as

$$b^{eq} = \frac{1}{2}\left(\xi^2 g^{eq} + h^{eq}\right). \tag{55}$$

From Eq. (51), we find that the definition of g is the same as that in Eq. (10) and the relation $2b = \xi^2 g + h$ holds. The expressions for the hydrodynamic variables are the same as those given in Eqs. (17) and (18). By using the reduced distribution functions introduced in Eq. (10), the kinetic system Eqs. (51) and (52) can be rewritten as

$$\frac{\partial g}{\partial t} + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} g + \boldsymbol{a} \cdot \boldsymbol{\nabla}_{\boldsymbol{\xi}} g = \Omega_g, \tag{56a}$$

$$\frac{\partial h}{\partial t} + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} h + \boldsymbol{a} \cdot \boldsymbol{\nabla}_{\boldsymbol{\xi}} h = \Omega_h - (1 - Pr)\left(c^2\Omega_g + \Omega_h\right). \tag{56b}$$

Therefore, the two source terms are

$$S_g = 0,\ \ S_h = -(1 - Pr)(c^2\Omega_g + \Omega_h). \tag{57}$$

Eq. (57) indicates that the source terms in the TEDDF model is designed based on the collision operators.

By noticing that the conservation law for the internal energy,

$$\int (c^2\Omega_g + \Omega_h) d\boldsymbol{\xi} = 0, \tag{58}$$

and the heat flux can be expressed as the moments of the collision operators,

$$\boldsymbol{q} = -\frac{1}{2}\tau \int \boldsymbol{c}(c^2\Omega_g + \Omega_h) d\boldsymbol{\xi}, \tag{59}$$

we find that the five general conditions given by Eqs. (28a) – (28e) are satisfied.

Therefore, we conclude that the TEDDF model is also a special design of the two source terms. Although two relaxation times are used to modify the Prandtl number, the TEDDF model is equivalent to a mesoscopic model with a single relaxation time.

7.3 The Rykov model

The well-known Rykov model for diatomic gases with rotational degrees of freedom is originally obtained by Rykov [9, 10]. Recently, Wu *et al.* [11] has generalized this model to polyatomic gases. The elastic and non-elastic collision processes are considered respectively in this model. By integrating the particle distribution function f with respect to the rotational energy e, the following two-equation kinetic system can be established.

$$\frac{\partial f_0}{\partial t} + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} f_0 = \frac{1}{\tau Z}\left(f_0^r - f_0\right) + \frac{1}{\tau}\left(1 - \frac{1}{Z}\right)\left(f_0^t - f_0\right), \tag{60a}$$

$$\frac{\partial f_1}{\partial t} + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} f_1 = \frac{1}{\tau Z}\left(f_1^r - f_1\right) + \frac{1}{\tau}\left(1 - \frac{1}{Z}\right)\left(f_1^t - f_1\right), \tag{60b}$$

where the equilibrium distribution functions corresponding to the elastic and nonelastic processes are

$$f_0^r = f_M(T)\left[1-\omega_0 \boldsymbol{q}^t\cdot\boldsymbol{a}(T)\right],\ f_0^t = f_M(T_t)\left[1-\boldsymbol{q}^t\cdot\boldsymbol{a}(T_t)\right], \tag{61a}$$

$$\begin{aligned} f_1^r &= RTf_M(T)\left[1-\omega_0 \boldsymbol{q}^t\cdot\boldsymbol{a}(T)+(1-\delta)\omega_1\frac{\boldsymbol{q}^r\cdot\boldsymbol{c}}{pRT}\right] \\ &= RTf_0^r+\omega_1 RTf_M(T)(1-\delta)\frac{\boldsymbol{q}^r\cdot\boldsymbol{c}}{pRT}, \end{aligned} \tag{61b}$$

$$\begin{aligned} f_1^t &= RT_rf_M(T_t)\left[1-\boldsymbol{q}^t\cdot\boldsymbol{a}(T_t)+(1-\delta)\frac{\boldsymbol{q}^r\cdot\boldsymbol{c}}{p_tRT_r}\right] \\ &= RT_rf_0^t+RT_rf_M(T_t)(1-\delta)\frac{\boldsymbol{q}^r\cdot\boldsymbol{c}}{p_tRT_r}, \end{aligned} \tag{61c}$$

with

$$f_M(T)=\frac{\rho}{(2\pi RT)^{3/2}}\exp\left(-\frac{c^2}{2RT}\right),\ \boldsymbol{a}(T)=\frac{2}{15}\frac{\boldsymbol{c}}{pRT}\left(\frac{5}{2}-\frac{c^2}{2RT}\right). \tag{61d}$$

Here f_0 is the velocity distribution function and f_1 is the distribution for rotational energy. f_0^t and f_0^r denote the equilibrium distributions of the elastic and nonelastic collision processes for f_0, respectively. Similarly, f_1^t and f_1^r denote the equilibrium distributions of the elastic and nonelastic collision processes for f_1, respectively. f_M is the Maxwellian equilibrium distribution function. T_t is the translational temperature corresponding to the translational degrees of freedom of particles, T_r is the rotational temperature corresponding to the rotational degrees of freedom, T is the total temperature in the local equilibrium state. $\boldsymbol{q}^t$ is the translational heat flux and $\boldsymbol{q}^r$ is the rotational heat flux. The total heat flux is decomposed as $\boldsymbol{q}=\boldsymbol{q}^t+\boldsymbol{q}^r$.

The relaxation time τ is related to the shear viscosity μ and pressure p through the relation $\tau=\mu/p$ with $p=\rho RT$. Physically, the relaxation time τ is related to the translational temperature T_t instead of the rotational temperature T_r. Therefore, in analogy to the case of a monatomic gas, the following assumption is used,

$$\tau=\mu_t/p_t,\ \mu_t=\mu(T_t),\ p_t=\rho RT_t,\ p_r=\rho RT_r. \tag{62}$$

Z indicates the ratio of the total number of translational and rotational collisions to that of rotational collisions. We will realize that Z is proportional to the ratio of bulk to shear viscosity χ and thus provides a reasonable physical interpretation for the origin of bulk viscosity μ_V. $\delta = (\mu_t/\rho)\, D$, where D is the gas self-diffusion coefficient. ω_0 and ω_1 are two parameters which can be selected to achieve proper relaxation of the heat fluxes.

The hydrodynamic variables are defined by the following relationships.

$$
\begin{aligned}
&\rho = \int f_0 d\boldsymbol{\xi},\ \rho\boldsymbol{u} = \int \boldsymbol{\xi} f_0 d\boldsymbol{\xi},\\
&\frac{3}{2}\rho RT_t = \frac{1}{2}\int c^2 f_0 d\boldsymbol{\xi},\ \rho RT_r = \int f_1 d\boldsymbol{\xi},\\
&\frac{5}{2}\rho RT = \frac{3}{2}\rho RT_t + \rho RT_r = \frac{1}{2}\int (c^2 f_0 + 2f_1) d\boldsymbol{\xi},\\
&\boldsymbol{q}^t = \int \frac{1}{2}\boldsymbol{c}c^2 f_0 d\boldsymbol{\xi},\ \boldsymbol{q}^r = \int \boldsymbol{c} f_1 d\boldsymbol{\xi},\\
&\boldsymbol{q} = \boldsymbol{q}^t + \boldsymbol{q}^r = \frac{1}{2}\int \boldsymbol{c}\left(c^2 f_0 + 2f_1\right) d\boldsymbol{\xi}.
\end{aligned}
\tag{63}
$$

In order to use our general results, we first notice $D = 3,\ K = 2,\ \Lambda = 0$ in this case. Then we introduce two new distribution functions, $g = f_0$ and $h = 2f_1$.

Two new collision operators are defined as

$$
\Omega_g = \frac{1}{\tau}\left[f_M(T) - g\right],\ \Omega_h = \frac{1}{\tau}\left[2RTf_M(T) - h\right]. \tag{64}
$$

Two new source terms are given by

$$
\begin{aligned}
S_g &= \frac{1}{\tau}\left[\frac{1}{Z}f_0^r + \left(1 - \frac{1}{Z}\right) f_0^t - f_M(T)\right],\\
S_h &= \frac{1}{\tau}\left[\frac{2}{Z}f_1^r + 2\left(1 - \frac{1}{Z}\right) f_1^t - 2RTf_M(T)\right].
\end{aligned}
\tag{65}
$$

The expressions for the hydrodynamic variables in Eq. (63) can be rewritten in terms of g and h, which are found to be the same as Eqs. (17) and (18). From Eqs. (63) and (64), we confirm that the newly defined collision operators, Ω_g and Ω_h, still satisfy the conservative requirements in Eq. (15). Furthermore, it can be shown that S_g and S_h indeed satisfy five basic requirements in Eqs. (28a) – (28e). The details of proof are provided in Appendix E in which we can confirm that the ratio of bulk to shear viscosity χ is determined by the collision ratio Z through $\chi = 4Z/15$.

In addition, the Prandtl number can be identified as

$$Pr = \frac{7R\mu}{2(\kappa^t + \kappa^r)} = \frac{\mu C_p}{\kappa}, \tag{66}$$

where the tranlational and rotational thermal conductivity coefficients κ^t and κ^r as well as the total thermal conductivity coefficient are shown to be

$$\begin{aligned} \kappa^t &= \frac{15R\mu_t}{4A},\ A = 1 + 0.5\frac{1-\omega_0}{Z}, \\ \kappa^r &= \frac{R\mu_t}{B},\ B = \delta + \frac{1}{Z}(1-\delta)(1-\omega_1), \\ \kappa &= \kappa^t + \kappa^r. \end{aligned} \tag{67}$$

Therefore, we conclude that, from an inverse-design viewpoint, the Rykov model is also compatible with our general design framework. One of the advantages of the Rykov model is that the hydrodynamic variables being relevant to the translational and rotational processes can be investigated separately by considering the elastic and non-elastic collision processes. In comparison, the total hydrodynamic flow variables can still be evaluated correctly in our inverse-design new mesoscopic model through the adjustable parameters.

8 Implementation of macroscopic hydrodynamic and thermodynamic boundary conditions

When numerically implementing mesoscopic methods based on a model Boltzmann equation, a challenge is to properly determine the unknown distribution functions near a solid boundary, such that the resulting scheme is fully consistent with the NSF system near the boundary. Since the NSF system is derived from the Chapman-Enskog expansion up to $O(\tau)$, it follows that the proper implementation of the boundary condition should be based on a consistent application of the Chapman-Enskog expansion up to $O(\tau)$. In the literature, this requirement is often not checked and thus not met rigorously, leading to degradation of the accuracy of a mesoscopic method. Furthermore, for thermal or compressible flows, as will be shown below, the implementations of velocity and temperature boundary conditions, at the level of the distribution functions, could be coupled. Source terms could also affect the implementation details. Such fine points are not fully realized in the literature. Below we shall explore the relations between the components of the distribution functions (typically the distribution functions between two opposite particle velocity directions after the particle velocity space is discretized).

By using the relation $\boldsymbol{c} = \boldsymbol{\xi} - \boldsymbol{u}$, the expression for $G_1(\boldsymbol{\xi})$, $G_2(\boldsymbol{\xi})$, $G_3(\boldsymbol{\xi})$ and $\Phi_1(\boldsymbol{\xi})$ in Eqs. (24a) – (24c) and (26) can be rewritten in terms of the particle velocity $\boldsymbol{\xi}$.

$$G_1(\boldsymbol{\xi}) = G_{11}(\boldsymbol{\xi}) + G_{12}(\boldsymbol{\xi}), \tag{68a}$$

where

$$G_{11}(\boldsymbol{\xi}) = \left(\frac{\xi^2\boldsymbol{\xi}}{2RT} - \frac{D+2}{2}\boldsymbol{\xi} + \frac{\boldsymbol{\xi}\cdot\boldsymbol{u}\boldsymbol{u}}{RT} + \frac{u^2\boldsymbol{\xi}}{2RT}\right)\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right), \tag{68b}$$

$$G_{12}(\boldsymbol{\xi}) = \left(-\frac{u^2\boldsymbol{u}}{2RT} + \frac{D+2}{2}\boldsymbol{u} - \frac{\boldsymbol{u}\cdot\boldsymbol{\xi}\boldsymbol{\xi}}{RT} - \frac{\xi^2\boldsymbol{u}}{2RT}\right)\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right). \tag{68c}$$

$$G_2(\boldsymbol{\xi}) = G_{21}(\boldsymbol{\xi}) + G_{22}(\boldsymbol{\xi}), \tag{69a}$$

where

$$G_{21}(\boldsymbol{\xi}) = 2\left(-\frac{\boldsymbol{\xi}\cdot\boldsymbol{S}\cdot\boldsymbol{u}}{RT} + \frac{1}{K+3}\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT}\boldsymbol{\nabla}\cdot\boldsymbol{u}\right), \tag{69b}$$

$$G_{22}(\boldsymbol{\xi}) = \frac{\boldsymbol{\xi}\cdot\boldsymbol{S}\cdot\boldsymbol{\xi}}{RT} + \frac{\boldsymbol{u}\cdot\boldsymbol{S}\cdot\boldsymbol{u}}{RT} - \frac{1}{K+3}\left(\frac{\xi^2+u^2}{RT} + 3 - D + K\right)\boldsymbol{\nabla}\cdot\boldsymbol{u}. \tag{69c}$$

$$G_3(\boldsymbol{\xi}) = G_{31}(\boldsymbol{\xi}) + G_{32}(\boldsymbol{\xi}), \tag{70a}$$

where

$$G_{31}(\boldsymbol{\xi}) = \frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT}\frac{\Lambda}{C_v T}, \tag{70b}$$

$$G_{32}(\boldsymbol{\xi}) = \left(-\frac{\xi^2+u^2}{2RT}+\frac{D}{2}\right)\frac{\Lambda}{C_v T}. \tag{70c}$$

$$\Phi_1(\boldsymbol{\xi}) = \Phi_{11}(\boldsymbol{\xi}) + \Phi_{12}(\boldsymbol{\xi}), \tag{71a}$$

where

$$\Phi_{11}(\boldsymbol{\xi}) = \boldsymbol{\xi}\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right), \tag{71b}$$

$$\Phi_{12}(\boldsymbol{\xi}) = -\boldsymbol{u}\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right) - \frac{2}{K+3}\boldsymbol{\nabla}\cdot\boldsymbol{u} - \frac{\Lambda}{C_v T}. \tag{71c}$$

Obviously, we have $G_{i1}(\boldsymbol{\xi}) = -G_{i1}(-\boldsymbol{\xi})$, $G_{i2}(\boldsymbol{\xi}) = G_{i2}(-\boldsymbol{\xi})$ and $\Phi_{11}(\boldsymbol{\xi}) = -\Phi_{11}(-\boldsymbol{\xi})$, $\Phi_{12}(\boldsymbol{\xi}) = \Phi_{12}(-\boldsymbol{\xi})$, $(i = 1, 2, 3)$.

From Eqs. (27a) and (27b), we have

$$\phi(\boldsymbol{\xi}) = (A_\phi(\boldsymbol{\xi}) - B_\phi(\boldsymbol{\xi}))\phi^{eq}(\boldsymbol{\xi}) + \tau S_\phi(\boldsymbol{\xi}) + O(\tau^2), \tag{72a}$$

$$\phi(-\boldsymbol{\xi}) = (A_\phi(\boldsymbol{\xi}) + B_\phi(\boldsymbol{\xi}))\phi^{eq}(-\boldsymbol{\xi}) + \tau S_\phi(-\boldsymbol{\xi}) + O(\tau^2), \tag{72b}$$

where $\phi = g$ or h. Obviously, the coefficients satisfy the relations $A_\phi(\boldsymbol{\xi}) = A_\phi(-\boldsymbol{\xi})$ and $B_\phi(\boldsymbol{\xi}) = -B_\phi(-\boldsymbol{\xi})$. They can be expressed explicitly as follows,

$$A_g(\boldsymbol{\xi}) = 1 - \tau G_{12}(\boldsymbol{\xi}) - \tau G_{22}(\boldsymbol{\xi}) - \tau G_{32}(\boldsymbol{\xi}), \tag{73a}$$

$$B_g(\boldsymbol{\xi}) = \tau G_{11}(\boldsymbol{\xi}) + \tau G_{21}(\boldsymbol{\xi}) + \tau G_{31}(\boldsymbol{\xi}), \tag{73b}$$

$$A_h(\boldsymbol{\xi}) = 1 - \tau G_{12}(\boldsymbol{\xi}) - \tau G_{22}(\boldsymbol{\xi}) - \tau G_{32}(\boldsymbol{\xi}) - \tau \Phi_{12}(\boldsymbol{\xi}), \tag{73c}$$

$$B_h(\boldsymbol{\xi}) = \tau G_{11}(\boldsymbol{\xi}) + \tau G_{21}(\boldsymbol{\xi}) + \tau G_{31}(\boldsymbol{\xi}) + \tau \Phi_{11}(\boldsymbol{\xi}). \tag{73d}$$

If the particle distribution function $\phi(-\boldsymbol{\xi})$ is already known, then the particle distribution function $\phi(\boldsymbol{\xi})$ in the opposite direction can be obtained in the following way. From Eqs. (72a) and (72b), we obtain a generalized bounce back scheme

$$\begin{aligned} &\phi(\boldsymbol{\xi}) - \beta\phi(-\boldsymbol{\xi}) \\ &= A_\phi(\boldsymbol{\xi})(\phi^{eq}(\boldsymbol{\xi}) - \beta\phi^{eq}(-\boldsymbol{\xi})) - B_\phi(\boldsymbol{\xi})(\phi^{eq}(\boldsymbol{\xi}) + \beta\phi^{eq}(-\boldsymbol{\xi})) \\ &+\tau(S_\phi(\boldsymbol{\xi}) - \beta S_\phi(-\boldsymbol{\xi})) + O(\tau^2), \end{aligned} \tag{74}$$

where β is a coefficient to be determined. Specially, we can choose $\beta = 1$ or $\beta = -1$ in real implementation. For this purpose, we have to evaluate the sum or difference of the equilibriums and source terms.

From the Hermite expansion of the equilibrium distribution functions given in Appendix A, we have

$$\begin{aligned} &g^{eq}(\boldsymbol{\xi}) + g^{eq}(-\boldsymbol{\xi}) = 2\rho\omega(\boldsymbol{\xi}, T_0) \times \\ &\left\{ \begin{aligned} &1 + \frac{1}{2}\left[\left(\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^2 - \frac{u^2}{RT_0} + (\theta-1)\left(\frac{\xi^2}{RT_0} - D\right)\right] \\ &+ \frac{1}{24}\left[\begin{aligned} &\left(\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^4 - 6\frac{u^2}{RT_0}\left(\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^2 + 3\left(\frac{u^2}{RT_0}\right)^2 \\ &+ 6(\theta-1)\left[\left(\frac{\xi^2}{RT_0} - D - 4\right)\left(\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^2 + \frac{u^2}{RT_0}\left(D + 2 - \frac{\xi^2}{RT_0}\right)\right] \\ &+ 3(\theta-1)^2\left[\left(\frac{\xi^2}{RT_0}\right)^2 - 2(D+2)\frac{\xi^2}{RT_0} + D(D+2)\right] \end{aligned} \right] \end{aligned} \right\} \\ &+\text{high order terms}, \end{aligned} \tag{75a}$$

$$
\begin{aligned}
&g^{eq}(\boldsymbol{\xi}) - g^{eq}(-\boldsymbol{\xi}) = 2\rho\omega(\boldsymbol{\xi}, T_0) \times \\
&\left\{\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0} + \frac{1}{6}\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\left[\left(\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^2 - 3\frac{u^2}{RT_0} + 3(\theta-1)\left(\frac{\xi^2}{RT_0} - D - 2\right)\right]\right\} \\
&+\text{high order terms.}
\end{aligned} \tag{75b}
$$

$$
\begin{aligned}
&h^{eq}(\boldsymbol{\xi}) + h^{eq}(-\boldsymbol{\xi}) \\
&= 2\omega(\boldsymbol{\xi}, T_0)(3 - D + K)\rho RT \times \\
&\left\{1 + \frac{1}{2}\left[\left(\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^2 - \frac{u^2}{RT_0} + (\theta-1)\left(\frac{\xi^2}{RT_0} - D\right)\right]\right\} \\
&+\text{high order terms,}
\end{aligned} \tag{75c}
$$

$$
\begin{aligned}
&h^{eq}(\boldsymbol{\xi}) - h^{eq}(-\boldsymbol{\xi}) \\
&= 2\omega(\boldsymbol{\xi}, T_0)(3 - D + K)\rho RT\left(\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right) + \text{high order terms,}
\end{aligned} \tag{75d}
$$

where $\theta = T/T_0$ represents the temperature normalized by a reference temperature T_0.

The sum and difference of the source terms depend on the specific form used. For S_g given in Eq. (34) and S_h given in Eq. (39), we have

$$
\begin{aligned}
&S_g(\boldsymbol{\xi}) + S_g(-\boldsymbol{\xi}) \\
&= -2\omega(\boldsymbol{\xi}, T_0)\left[\left(\chi - \frac{2(3-D+K)}{D(K+3)}\right)\frac{p\nabla\cdot\boldsymbol{u}}{2RT_0} + \frac{p}{2RT_0}\frac{\Lambda}{C_v T}\right]\left(\frac{\xi^2}{RT_0} - D\right),
\end{aligned} \tag{76a}
$$

$$
S_g(\boldsymbol{\xi}) - S_g(-\boldsymbol{\xi}) = 0, \tag{76b}
$$

$$
\begin{aligned}
&S_h(\boldsymbol{\xi}) + S_h(-\boldsymbol{\xi}) \\
&= \omega(\boldsymbol{\xi}, T_0)\left[2D\left(\chi - \frac{2(3-D+K)}{D(K+3)}\right)p\boldsymbol{\nabla}\cdot\boldsymbol{u} - \frac{4(3-D+K)}{K+3}\rho\Lambda\right],
\end{aligned} \tag{76c}
$$

$$
\begin{aligned}
&S_h(\boldsymbol{\xi}) - S_h(-\boldsymbol{\xi}) \\
&= \omega(\boldsymbol{\xi}, T_0) \begin{bmatrix} \dfrac{4(1-Pr)\boldsymbol{q}^{(NS)} \cdot \boldsymbol{\xi}}{\tau R T_0} - 4\dfrac{\boldsymbol{\xi} \cdot \boldsymbol{u}}{RT_0} \left(\chi - \dfrac{2(3-D+K)}{D(K+3)} \right) p \boldsymbol{\nabla} \cdot \boldsymbol{u} \\ - 4\dfrac{K+5}{K+3} \dfrac{\boldsymbol{\xi} \cdot \boldsymbol{u}}{RT_0} \rho \Lambda \end{bmatrix}. \quad (76d)
\end{aligned}
$$

Consider the three-dimensional ($D = 3$) isothermal flow in the incompressible limit with constant temperature T_0. The internal degree of freedom is $K = 0$ and the bulk viscosity is $\mu_V = 0$. No thermal cooling function is applied, *i.e.* $\Lambda = 0$. The source term $S_g = 0$. Then the Eq. (74) with $\phi = g$ and $\beta = 1$ can be simplified as

$$
\begin{aligned}
&g(\boldsymbol{\xi}) - g(-\boldsymbol{\xi}) \\
&= 2\omega(\boldsymbol{\xi}, T_0)\rho \left(\frac{\boldsymbol{\xi} \cdot \boldsymbol{u}}{RT_0} \right) + \frac{1}{3}\omega(\boldsymbol{\xi}, T_0)\rho \left(\frac{\boldsymbol{\xi} \cdot \boldsymbol{u}}{RT_0} \right) \left[\left(\frac{\boldsymbol{\xi} \cdot \boldsymbol{u}}{RT_0} \right)^2 - 3\frac{u^2}{RT_0} \right] \\
&+4\omega(\boldsymbol{\xi}, T_0)\rho \frac{\boldsymbol{u} \cdot (\tau \boldsymbol{S}) \cdot \boldsymbol{\xi}}{RT_0} - 2\omega(\boldsymbol{\xi}, T_0)\rho \left(\frac{\boldsymbol{\xi} \cdot \boldsymbol{u}}{RT_0} \right) \frac{\boldsymbol{\xi} \cdot (\tau \boldsymbol{S}) \cdot \boldsymbol{\xi}}{RT_0} \\
&+2\omega(\boldsymbol{\xi}, T_0)\rho\tau (\nabla \cdot \boldsymbol{u}) \left(\frac{\boldsymbol{\xi} \cdot \boldsymbol{u}}{RT_0} \right) \\
&+O(\tau Ma^4) + O(Ma^4) + O(\tau^2) + O(\tau^2 Ma^2). \qquad (77)
\end{aligned}
$$

In the lattice Boltzmann method [17], we first introduce a transformation as

$$
\tilde{g}(\boldsymbol{x}, \boldsymbol{\xi}, t) = g(\boldsymbol{x}, \boldsymbol{\xi}, t) + \frac{\Delta t}{2\tau} \left(g(\boldsymbol{x}, \boldsymbol{\xi}, t) - g^{eq}(\boldsymbol{x}, \boldsymbol{\xi}, t) \right) - \frac{\Delta t}{2} \frac{\boldsymbol{a} \cdot \boldsymbol{c}}{RT_0} g^{eq}(\boldsymbol{x}, \boldsymbol{\xi}, t), \quad (78)
$$

where Δt is the time step.

Next, in order to use the Gauss-Hermite quadrature for the evaluation of the integrals, we introduce another transformation as,

$$
\tilde{g}\left(\boldsymbol{x}, \boldsymbol{\xi}_\alpha, t\right) = \frac{W(\boldsymbol{\xi}_\alpha)}{\omega(\boldsymbol{\xi}_\alpha, T_0)} \tilde{g}\left(\boldsymbol{x}, \boldsymbol{\xi}_\alpha, t\right), \quad (79)
$$

where α denotes the directions of the discrete velocities $\boldsymbol{\xi}_\alpha$ and W_α denotes the corresponding weight.

After some reorganization, the final result is

$$\begin{aligned}
&\tilde{g}\left(\boldsymbol{x}, \boldsymbol{\xi}_{\alpha}, t\right)-\tilde{g}\left(\boldsymbol{x},-\boldsymbol{\xi}_{\alpha}, t\right) \\
&=2 \rho W_{\alpha} \frac{\left(\boldsymbol{u}-\frac{\Delta t}{2} \boldsymbol{a}\right) \cdot \boldsymbol{\xi}_{\alpha}}{R T_{0}}+\frac{1}{3} \rho W_{\alpha}\left(\frac{\boldsymbol{\xi}_{\alpha} \cdot \boldsymbol{u}}{R T_{0}}\right)\left[\left(\frac{\boldsymbol{\xi}_{\alpha} \cdot \boldsymbol{u}}{R T_{0}}\right)^{2}-3 \frac{u^{2}}{R T_{0}}\right] \\
&+\frac{2 \tau+\Delta t}{2 \tau} \rho W_{\alpha}\left[\begin{array}{l}
4 \frac{\boldsymbol{u} \cdot(\tau \boldsymbol{S}) \cdot \boldsymbol{\xi}_{\alpha}}{R T_{0}}-2\left(\frac{\boldsymbol{\xi}_{\alpha} \cdot \boldsymbol{u}}{R T_{0}}\right) \frac{\boldsymbol{\xi}_{\alpha} \cdot(\tau \boldsymbol{S}) \cdot \boldsymbol{\xi}_{\alpha}}{R T_{0}} \\
+2 \tau(\boldsymbol{\nabla} \cdot \boldsymbol{u})\left(\frac{\boldsymbol{\xi}_{\alpha} \cdot \boldsymbol{u}}{R T_{0}}\right)
\end{array}\right] \\
&-\frac{\Delta t}{2} \rho W_{\alpha} \frac{\boldsymbol{a} \cdot \boldsymbol{\xi}_{\alpha}}{R T_{0}}\left[\left(\frac{\boldsymbol{\xi}_{\alpha} \cdot \boldsymbol{u}}{R T_{0}}\right)^{2}-\frac{u^{2}}{R T_{0}}\right]+\Delta t \rho W_{\alpha} \frac{\boldsymbol{a} \cdot \boldsymbol{u}}{R T_{0}} \frac{\boldsymbol{\xi}_{\alpha} \cdot \boldsymbol{u}}{R T_{0}} \\
&+O\left(\tau M a^{4}\right)+O\left(M a^{4}\right)+O\left(\tau^{2}\right)+O\left(\tau^{2} M a^{2}\right).
\end{aligned} \tag{80}$$

If we only keep the first term in Eq. (80), we can obtain

$$\tilde{g}\left(\boldsymbol{x}, \boldsymbol{\xi}_{\alpha}, t\right)-\tilde{g}\left(\boldsymbol{x},-\boldsymbol{\xi}_{\alpha}, t\right)=2 \rho W_{\alpha} \frac{\left(\boldsymbol{u}-\frac{\Delta t}{2} \boldsymbol{a}\right) \cdot \boldsymbol{\xi}_{\alpha}}{R T_{0}}+O\left(\tau^{2}, \tau M a, M a^{2}\right). \tag{81}$$

We note that the body force enters the implementation of the bounce-back scheme, which is not well documented in the literature. Furthermore, it must be cautioned that Eq. (81) is not fully consistent with the Chapman-Enskog expansion of the NSF system as the $O(\tau)$ terms in Eq. (80) are not included. Luckily, in the special case of no-slip boundary $\boldsymbol{u}=\mathbf{0}$, the $O(\tau)$ terms in Eq. (80) will disappear. Note that the source term and velocity could all enter the implementation of the thermal boundary conditions.

9 High-order structure of the distribution functions

The NSF equations, which are based on the continuum hypothesis, have been widely used in understanding flow behaviors in many natural and engineering problems. However, in some cases such as microchannel flows [27], compressible turbulence [28] and space vehicles in low earth orbits [29], the local Knudsen number may be finite such that the flow may lie in the continuum-transition regime locally. Therefore, the NSF equations are not adequate to capture the finite Knudsen number effect while the Boltzmann equation can describe the flows in all Kn number regimes.

In order to quantitatively estimate the departure from the local thermodynamic equilibrium and study the extended hydrodynamics, the second-order Chapman-

Enskog expansion of the particle distribution function is desired, which results in the so-called "Burnett equations" [30]. The Burnett equations have been derived from the original Boltzmann equation by applying the Chapman-Enskog expansion [1] or the Grad's 13 momentum equations [31] by the iteration approach [32]. However, these theoretical results are seldom compared with those using the single-relaxation-time BGK model. In addition, detailed derivations are less reported or the final results are not presented in a general form. In this section, we will derive the structure of the distribution functions up to the order $O(\tau^2)$. Then, the complete analytical expressions for the viscous stress tensor and the heat flux are obtained in the subsequent sections. Furthermore, by comparing our results with those from Grad's 13 momentum equations, it is found that the mathematical form of the viscous stress tensor and the heat flux can be fully determined in the single-relaxation-time BGK model. The difference from the literature in the coefficients could be attributed to different relaxation rates to the local equilibrium for different moments used in the literature.

By using the Eqs. (29a), (29b) and (30), we obtain the expression for Dg^{eq}/Dt and Dh^{eq}/Dt to the order of $O(\tau)$,

$$\frac{Dg^{eq}}{Dt} = (G + L)\, g^{eq} + O(\tau^2),\ \frac{Dh^{eq}}{Dt} = (G + \Phi_1 + L + \Phi_2)\, h^{eq} + O(\tau^2), \quad (82)$$

where G and Φ_1 have been given above, L and Φ_2 are given as

$$L = \frac{\boldsymbol{c}}{\rho RT} \cdot (\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}^{(NS)}) + \left(\frac{c^2}{2RT} - \frac{D}{2}\right) \frac{1}{\rho C_v T} \left(\boldsymbol{\sigma}^{(NS)} : \boldsymbol{S} - \boldsymbol{\nabla} \cdot \boldsymbol{q}^{(NS)}\right), \quad (83a)$$

$$\Phi_2 = \frac{1}{\rho C_v T} \left(\boldsymbol{\sigma}^{(NS)} : \boldsymbol{S} - \boldsymbol{\nabla} \cdot \boldsymbol{q}^{(NS)}\right). \quad (83b)$$

By applying the Chapman-Enskog expansion, we can obtain the structure of the particle distribution function as

$$
\begin{aligned}
g &= g^{eq} - \tau\frac{Dg^{eq}}{Dt} + \tau\frac{D}{Dt}\left(\tau\frac{Dg^{eq}}{Dt}\right) + \tau S_g - \tau\frac{D(\tau S_g)}{Dt} + O(\tau^3) \\
&= (1-\tau G)g^{eq} + \tau S_g \\
&\quad + \left(-\tau L + \tau\frac{D(\tau G)}{Dt} + \tau^2 G^2\right) g^{eq} - \tau\frac{D(\tau S_g)}{Dt} + O(\tau^3),
\end{aligned} \tag{84a}
$$

$$
\begin{aligned}
h &= h^{eq} - \tau\frac{Dh^{eq}}{Dt} + \tau\frac{D}{Dt}\left(\tau\frac{Dh^{eq}}{Dt}\right) + \tau S_h - \tau\frac{D(\tau S_h)}{Dt} + O(\tau^3) \\
&= \left(1-\tau G - \tau\Phi_1\right) h^{eq} + \tau S_h - \tau(L+\Phi_2)h^{eq} + \tau\frac{D\left[\tau\left(G+\Phi_1\right)\right]}{Dt}h^{eq} \\
&\quad + \tau^2\left(G+\Phi_1\right)^2 h^{eq} - \tau\frac{D(\tau S_h)}{Dt} + O(\tau^3).
\end{aligned} \tag{84b}
$$

The explicit expressions for some terms in Eqs. (84a) and (84b) are included in Appendix C.

10 Viscous stress tensor up to $O(\tau^2)$

When the local Knudsen number becomes finite, additional contributions from the non-equilibrium part of the distribution function result in the high-order components of the viscous stress tensor. Agarwal *et al.* [32] and Struchtrup [33] derived the viscous stress tensor up to the second-order for Maxwell molecules from the Grad's 13 moment equations by the series expansion in terms of the shear viscosity. Chen *et al.* [4] obtained the expression of viscous stress tensor up to the second-order based on the single-relaxation-time BGK model. However, they mainly focus on the incompressible limit and the terms proportional to the density gradient, the temperature gradient and the velocity divergence have been neglected in their derivation. By making an analogy between the turbulent fluctuations and microscale thermal fluctuations, they show that the Reynolds stress obtained by the BGK-Boltzmann equation has model coefficients similar to some existing turbulence models. They also claimed that the turbulence phenomenon such as the secondary flow structures and rapid distortion processes [34] can be better understood according to the kinetic theory. As an extension of Chen's work, the complete form of the viscous stress tensor will be derived up to $\boldsymbol{O}(\tau^2)$ using the single-relaxation-time BGK model considering the internal degree of freedom of molecules. Moreover, this new result will be compared to that obtained by Agarwal et al. [32] for Maxwell molecules.

The general expression of the viscous stress tensor is given as follows.

$$\begin{aligned}\boldsymbol{\sigma} &= -\int \boldsymbol{cc}\left(g - g^{eq}\right) d\boldsymbol{\xi} \\ &= \tau \int \boldsymbol{cc} G g^{eq} d\boldsymbol{\xi} - \tau \int \boldsymbol{cc} S_g d\boldsymbol{\xi} \\ &\quad + \tau \int \boldsymbol{cc} L g^{eq} \boldsymbol{\xi} - \tau \int \boldsymbol{cc} \frac{D(\tau G)}{Dt} g^{eq} d\boldsymbol{\xi} - \int \boldsymbol{cc} \tau^2 G^2 g^{eq} d\boldsymbol{\xi} \\ &\quad + \tau \int \boldsymbol{cc} \frac{D(\tau S_g)}{Dt} d\boldsymbol{\xi} + \boldsymbol{O}(\tau^3). \end{aligned} \tag{85}$$

The first two terms in Eq. (85) will yield the Newtonian constitutive relation:

$$\tau \int \boldsymbol{cc} G g^{eq} d\boldsymbol{\xi} - \tau \int \boldsymbol{cc} S_g d\boldsymbol{\xi} = \boldsymbol{\sigma}^{(NS)}. \tag{86}$$

The third term in Eq. (85) can be evaluated as

$$\begin{aligned}&\tau \int \boldsymbol{cc} L g^{eq} d\boldsymbol{\xi} \\ &= \frac{2\tau}{K+3} \left(\boldsymbol{\sigma}^{(NS)} : \boldsymbol{S} - \boldsymbol{\nabla} \cdot \boldsymbol{q}^{(NS)} \right) \boldsymbol{I} \\ &= \frac{4\mu\tau}{K+3} \left(\boldsymbol{S} : \boldsymbol{S} \right) \boldsymbol{I} + \frac{2\mu\tau}{K+3} \left(\chi - \frac{2}{D} \right) \left(\boldsymbol{\nabla} \cdot \boldsymbol{u} \right)^2 \boldsymbol{I} \\ &\quad - \frac{2\tau}{K+3} (\boldsymbol{\nabla} \cdot \boldsymbol{q}^{(NS)}) \boldsymbol{I}. \end{aligned} \tag{87}$$

The fourth term in Eq. (85) can be written as the sum of the following two integrals.

$$\begin{aligned}&-\tau \int \boldsymbol{cc} \frac{D\tau}{Dt} G g^{eq} d\boldsymbol{\xi} \\ &= -\tau^2 pRT \left\{ \begin{aligned} &\left(\frac{1}{\tau} \boldsymbol{\nabla} \tau \right) \left(\frac{1}{T} \boldsymbol{\nabla} T \right) + \left(\frac{1}{T} \boldsymbol{\nabla} T \right) \left(\frac{1}{\tau} \boldsymbol{\nabla} \tau \right) \\ &+ \left(\frac{1}{T} \boldsymbol{\nabla} T \right) \cdot \left(\frac{1}{\tau} \boldsymbol{\nabla} \tau \right) \boldsymbol{I} \end{aligned} \right\} \\ &\quad - 2\tau \frac{d\tau}{dt} p \boldsymbol{S} + \frac{2}{K+3} \tau \frac{d\tau}{dt} p (\boldsymbol{\nabla} \cdot \boldsymbol{u}) \boldsymbol{I} + \tau \frac{d\tau}{dt} \frac{\Lambda}{C_v T} p \boldsymbol{I}, \end{aligned} \tag{88a}$$

$$
\begin{aligned}
&-\int \boldsymbol{c}\boldsymbol{c}\tau^2\frac{DG}{Dt}g^{eq}d\boldsymbol{\xi}\\
&=-\tau^2 pRT\left\{\begin{array}{l}
\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\boldsymbol{I}\\
+\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right)+\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\\
-\frac{D+4}{2}\left|\frac{1}{T}\boldsymbol{\nabla}T\right|^2\boldsymbol{I}-(D+4)\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\\
+\left(\frac{1}{T}\boldsymbol{\nabla}^2T\right)\boldsymbol{I}+2\left(\frac{1}{T}\boldsymbol{\nabla}\boldsymbol{\nabla}T\right)
\end{array}\right\}\\
&\quad+\left\{\begin{array}{l}
2\tau^2p\left[(\boldsymbol{S}:\boldsymbol{S})\boldsymbol{I}+2\boldsymbol{S}\cdot\boldsymbol{S}-\boldsymbol{\Omega}\cdot\boldsymbol{S}+\boldsymbol{S}\cdot\boldsymbol{\Omega}\right]\\
-2\tau^2p\frac{d\boldsymbol{S}}{dt}+\frac{2\tau^2p}{K+3}\frac{d(\boldsymbol{\nabla}\cdot\boldsymbol{u})}{dt}\boldsymbol{I}\\
-\frac{8}{K+3}\tau^2p(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{S}+\frac{2}{K+3}\left(\frac{D+2}{K+3}-2\right)\tau^2p(\boldsymbol{\nabla}\cdot\boldsymbol{u})^2\boldsymbol{I}
\end{array}\right\}\\
&\quad+\left\{\begin{array}{l}
-4\tau^2p\frac{\Lambda}{C_vT}\boldsymbol{S}+2\left(\frac{D+2}{K+3}-1\right)\tau^2p\frac{\Lambda}{C_vT}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\\
+\frac{D+2}{2}\tau^2p\left(\frac{\Lambda}{C_vT}\right)^2\boldsymbol{I}+\tau^2p\frac{d}{dt}\left(\frac{\Lambda}{C_vT}\right)\boldsymbol{I}
\end{array}\right\}+\boldsymbol{O}(\tau^3). \qquad (88b)
\end{aligned}
$$

The fifth term in Eq. (85) is

$$
\begin{aligned}
&-\int \boldsymbol{c}\boldsymbol{c}\tau^2G^2g^{eq}d\boldsymbol{\xi}\\
&=-\frac{D+6}{2}\tau^2pRT\left\{\left|\frac{1}{T}\boldsymbol{\nabla}T\right|^2\boldsymbol{I}+2\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\right\}\\
&\quad-\tau^2p\left\{\begin{array}{l}
2(\boldsymbol{S}:\boldsymbol{S})\boldsymbol{I}+8\boldsymbol{S}\cdot\boldsymbol{S}\\
+\frac{2(D-2-2K)}{(K+3)^2}(\boldsymbol{\nabla}\cdot\boldsymbol{u})^2\boldsymbol{I}-\frac{16}{K+3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{S}
\end{array}\right\}\\
&\quad+\tau^2p\left\{8\boldsymbol{S}-\frac{2(D+1-K)}{K+3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right\}\frac{\Lambda}{C_vT}\\
&\quad-\frac{D+4}{2}\tau^2p\left(\frac{\Lambda}{C_vT}\right)^2\boldsymbol{I}. \qquad (89)
\end{aligned}
$$

Finally, we obtain the expression for the viscous stress tensor $\boldsymbol{\sigma}$ as

$$
\begin{aligned}
\boldsymbol{\sigma} = \boldsymbol{\sigma}^{(NS)} - \frac{2\tau}{K+3}\left(\boldsymbol{\nabla}\cdot\boldsymbol{q}^{(NS)}\right)\boldsymbol{I} \\
-\tau^2 pRT \left\{ \begin{aligned} &\left(\frac{1}{\tau}\boldsymbol{\nabla}\tau\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right) + \left(\frac{1}{T}\boldsymbol{\nabla}T\right)\left(\frac{1}{\tau}\boldsymbol{\nabla}\tau\right) \\ &+ \left(\frac{1}{T}\boldsymbol{\nabla}T\right)\cdot\left(\frac{1}{\tau}\boldsymbol{\nabla}\tau\right)\boldsymbol{I} + \left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right) \\ &+ \left(\frac{1}{T}\boldsymbol{\nabla}T\right)\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right) + \left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\boldsymbol{I} \\ &+ \left|\frac{1}{T}\boldsymbol{\nabla}T\right|^2\boldsymbol{I} + 2\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right) \\ &+ \left(\frac{1}{T}\boldsymbol{\nabla}^2T\right)\boldsymbol{I} + 2\left(\frac{1}{T}\boldsymbol{\nabla}\boldsymbol{\nabla}T\right) \end{aligned} \right\} \\
+\tau^2 p \left\{ \begin{aligned} &-2\left(\frac{1}{\tau}\frac{d\tau}{dt}\right)\boldsymbol{S} + \frac{2}{K+3}\left(\frac{1}{\tau}\frac{d\tau}{dt}\right)(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I} \\ &+ \frac{2}{K+3}\left[\left(\chi - \frac{2}{D}\right) - \frac{2}{K+3}\right](\boldsymbol{\nabla}\cdot\boldsymbol{u})^2\boldsymbol{I} \\ &+ \frac{8}{K+3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{S} - 2\frac{d\boldsymbol{S}}{dt} + \frac{2}{K+3}\frac{d(\boldsymbol{\nabla}\cdot\boldsymbol{u})}{dt}\boldsymbol{I} \\ &+ \frac{4}{K+3}(\boldsymbol{S}:\boldsymbol{S})\boldsymbol{I} - 4\boldsymbol{S}\cdot\boldsymbol{S} + 2\left(\boldsymbol{S}\cdot\boldsymbol{\Omega} - \boldsymbol{\Omega}\cdot\boldsymbol{S}\right) \end{aligned} \right\} \\
+\tau^2 p \left\{ \begin{aligned} &4\frac{\Lambda}{C_vT}\boldsymbol{S} + \frac{d}{dt}\left(\frac{\Lambda}{C_vT}\right)\boldsymbol{I} + \left(\frac{1}{\tau}\frac{d\tau}{dt}\right)\frac{\Lambda}{C_vT}\boldsymbol{I} \\ &- \frac{4}{K+3}\frac{\Lambda}{C_vT}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I} - \left(\frac{\Lambda}{C_vT}\right)^2\boldsymbol{I} \end{aligned} \right\} \\
+\tau\int \boldsymbol{c}\boldsymbol{c}\frac{D(\tau S_g)}{Dt}d\boldsymbol{\xi} + \boldsymbol{O}(\tau^3), \qquad (90)
\end{aligned}
$$

where the material derivative of the strain rate tensor $d\boldsymbol{S}/dt$ can be derived from the Euler equations, which reads

$$
\begin{aligned}
\frac{d\boldsymbol{S}}{dt} &= -\left(\boldsymbol{S}\cdot\boldsymbol{S} + \boldsymbol{\Omega}\cdot\boldsymbol{\Omega}\right) \\
&+RT\left[\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right) + \frac{1}{2}\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right) + \frac{1}{2}\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\right] \\
&-\frac{1}{\rho}\boldsymbol{\nabla}\boldsymbol{\nabla}p + \frac{1}{2}\left(\boldsymbol{\nabla}\boldsymbol{a} + \boldsymbol{\nabla}\boldsymbol{a}^T\right) + \boldsymbol{O}(\tau). \qquad (91)
\end{aligned}
$$

The last term in Eq. (85) depends on the choice of the source term. For example, for S_g given in Eq. (34), it can be evaluated as

$$
\tau\int \boldsymbol{c}\boldsymbol{c}\frac{D(\tau S_g)}{Dt}d\boldsymbol{\xi} = -2\tau RT_0\frac{\partial(\tau A_0)}{\partial t}\boldsymbol{I} + 2\tau RT_0\left[\boldsymbol{u}\boldsymbol{\nabla}(\tau A_0) + \boldsymbol{\nabla}(\tau A_0)\boldsymbol{u}\right], \quad (92)
$$

where A_0 is

$$A_0 = \left(\chi - \frac{2(3-D+K)}{D(K+3)}\right)\frac{p\boldsymbol{\nabla}\cdot\boldsymbol{u}}{2RT_0} + \frac{p}{2RT_0}\frac{\Lambda}{C_vT}. \tag{93}$$

Furthermore, by setting $D = 3,\ K = 0,\ \chi = 0,\ \Lambda = 0$ and neglecting all the terms proportional to the velocity divergence $\boldsymbol{\nabla}\cdot\boldsymbol{u}$, the density gradient $\boldsymbol{\nabla}\rho$ and the temperature gradient $\boldsymbol{\nabla}T$, it is found that $S_g = 0$ and the following approximate result obtained by Chen et al. [4] can be reproduced from the Eq. (90), namely,

$$\boldsymbol{\sigma} \approx 2\mu\boldsymbol{S} + \frac{4\mu\tau}{3}\boldsymbol{S}:\boldsymbol{S}\boldsymbol{I} - 4\tau^2 p\boldsymbol{S}\cdot\boldsymbol{S} + 2\tau^2 p\left(\boldsymbol{S}\cdot\boldsymbol{\Omega} - \boldsymbol{\Omega}\cdot\boldsymbol{S}\right) - 2\tau p\frac{d(\tau\boldsymbol{S})}{dt}. \tag{94}$$

For Maxwell molecules of which the shear viscosity is linearly proportional to the temperature, we have $d\mu/dT = \mu/T$. Therefore, the relations $(1/\tau)\boldsymbol{\nabla}\tau = -(1/\rho)\boldsymbol{\nabla}\rho$ and $(1/\tau)d\tau/dt = -(1/\rho)d\rho/dt$ hold. Using the continuity equation, it follows that $(1/\tau)d\tau/dt = \boldsymbol{\nabla}\cdot\boldsymbol{u}$. Then, using our notations, the results obtained by Agarwal *et al.* [32] can be rewritten as

$$\begin{aligned}
\boldsymbol{\sigma} &= 2\mu\left(\boldsymbol{S} - \frac{1}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right) - \frac{10}{9}\frac{\mu^2}{p}(\boldsymbol{\nabla}\cdot\boldsymbol{u})^2\boldsymbol{I} + \frac{2}{3}\frac{\mu^2}{p}\boldsymbol{S}(\boldsymbol{\nabla}\cdot\boldsymbol{u}) \\
&+4\frac{\mu^2}{p}(\boldsymbol{S}:\boldsymbol{S})\boldsymbol{I} - 4\frac{\mu^2}{p}\boldsymbol{S}\cdot\boldsymbol{S} + 2\frac{\mu^2}{p}(\boldsymbol{S}\cdot\boldsymbol{\Omega} - \boldsymbol{\Omega}\cdot\boldsymbol{S}) - 2\frac{\mu^2}{p}\frac{d}{dt}\left(\boldsymbol{S} - \frac{1}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right) \\
&+\frac{\mu^2}{\rho T^2}|\boldsymbol{\nabla}T|^2\boldsymbol{I} - 3\frac{\mu^2}{\rho T^2}\left(\boldsymbol{\nabla}T\right)\left(\boldsymbol{\nabla}T\right) + \frac{\mu^2}{\rho T}(\nabla^2 T)\boldsymbol{I} - 3\frac{\mu^2}{\rho T}\boldsymbol{\nabla}\boldsymbol{\nabla}T + \boldsymbol{O}(\tau^3).
\end{aligned} \tag{95}$$

Moreover, Eq. (90) can be simplified as

$$\begin{aligned}
\boldsymbol{\sigma} &= 2\mu\left(\boldsymbol{S} - \frac{1}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right) - \frac{2}{9}\frac{\mu^2}{p}(\boldsymbol{\nabla}\cdot\boldsymbol{u})^2\boldsymbol{I} + \frac{2}{3}\frac{\mu^2}{p}\boldsymbol{S}(\boldsymbol{\nabla}\cdot\boldsymbol{u}) \\
&+\frac{4}{3}\frac{\mu^2}{p}(\boldsymbol{S}:\boldsymbol{S})\boldsymbol{I} - 4\frac{\mu^2}{p}\boldsymbol{S}\cdot\boldsymbol{S} + 2\frac{\mu^2}{p}(\boldsymbol{S}\cdot\boldsymbol{\Omega} - \boldsymbol{\Omega}\cdot\boldsymbol{S}) - 2\frac{\mu^2}{p}\frac{d}{dt}\left(\boldsymbol{S} - \frac{1}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right) \\
&+\frac{3}{2}\frac{\mu^2}{\rho T^2}|\boldsymbol{\nabla}T|^2\boldsymbol{I} - 2\frac{\mu^2}{\rho T^2}\left(\boldsymbol{\nabla}T\right)\left(\boldsymbol{\nabla}T\right) + \frac{3}{2}\frac{\mu^2}{\rho T}(\nabla^2 T)\boldsymbol{I} - 2\frac{\mu^2}{\rho T}\boldsymbol{\nabla}\boldsymbol{\nabla}T + \boldsymbol{O}(\tau^3).
\end{aligned} \tag{96}$$

From Eqs. (95) and (96), we observe that these two expressions share identical mathematical form up to the order $\boldsymbol{O}(\tau^2)$ except for values of some coefficients. It is observed that the nonlinear terms $\boldsymbol{S}\cdot\boldsymbol{S}$, $\boldsymbol{S}\cdot\boldsymbol{\Omega} - \boldsymbol{\Omega}\cdot\boldsymbol{S}$ and $\boldsymbol{S}(\boldsymbol{\nabla}\cdot\boldsymbol{u})$ are exactly identical. Besides, the material derivative term $d(\boldsymbol{S} - (\boldsymbol{\nabla}\cdot\boldsymbol{u})/3\boldsymbol{I})/dt$ is also the same and the terms related to the temperature gradient and temperature diffusion are also very close to each other. The sign of corresponding coefficients is also the same, which implies that the negative or positive contribution to the viscous stress tensor can be qualitatively determined based on the BGK collision model. Moreover, it is found that the viscous stress tensor can be changed by the body force effect included in the material derivative term $d(\boldsymbol{S}-(\boldsymbol{\nabla}\cdot\boldsymbol{u})/3\boldsymbol{I})/dt$ at the second-order expansion but not at the first-order. Therefore, we conclude that although the BGK model only use single relaxation time to characterize the relaxation process to the local equilibrium without considering rigorous collision interaction details, all the dominant terms in the viscous stress tensor can be recovered compared to those obtained from the Grad's 13 momentum equations.

11 Heat flux up to $O(\tau^2)$

Based on the second-order Chapman-Enskog expansion of the distribution functions, the analytical expression for the heat flux $\boldsymbol{q}$ is given by

$$
\begin{aligned}
\boldsymbol{q} &= \frac{1}{2}\int \boldsymbol{c}\left(c^2 g + h\right) d\boldsymbol{\xi} \\
&= \frac{1}{2}\int \boldsymbol{c}c^2\left[g^{eq} - \tau G g^{eq} + \tau S_g\right] d\boldsymbol{\xi} + \frac{1}{2}\int \boldsymbol{c}\left[h^{eq} - \tau(G+\Phi_1)h^{eq} + \tau S_h\right] d\boldsymbol{\xi} \\
&+ \frac{1}{2}\int \boldsymbol{c}c^2\left[-\tau L g^{eq} + \tau\frac{D(\tau G)}{Dt}g^{eq} + \tau^2 G^2 g^{eq} - \tau\frac{D\left(\tau S_g\right)}{Dt}\right] d\boldsymbol{\xi} \\
&+ \frac{1}{2}\int \boldsymbol{c}\left\{\begin{array}{l} -\tau(L+\Phi_2)h^{eq} + \tau\dfrac{D(\tau G)}{Dt}h^{eq} + \tau^2(G+\Phi_1)^2 h^{eq} \\ +\tau\dfrac{D(\tau\Phi_1)}{Dt}h^{eq} - \tau\dfrac{D(\tau S_h)}{Dt}\end{array}\right\} d\boldsymbol{\xi} + \boldsymbol{O}(\tau^3). \qquad (97)
\end{aligned}
$$

Noticing Eqs. (28a)–(28e) and Eqs. (24a), (24b), (24c), (26), (83a), (83b), all the integrals in Eq. (97) can be evaluated term by term. After some reorganization, we obtain

$$
\begin{aligned}
&\boldsymbol{q}=\boldsymbol{q}^{(NS)}-\frac{1}{2}(K+5)\tau RT\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}^{(NS)}\\
&+\tau^2\rho(RT)^2\left\{\begin{aligned}&\frac{1}{2}(K+5)\left(\frac{1}{\tau}\frac{d\tau}{dt}\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\\&+(K+7)\boldsymbol{S}\cdot\left(\frac{1}{\tau}\boldsymbol{\nabla}\tau\right)-\frac{K+7}{K+3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\left(\frac{1}{\tau}\boldsymbol{\nabla}\tau\right)\end{aligned}\right\}\\
&+\tau^2\rho(RT)^2\left\{\begin{aligned}&2(K+7)\boldsymbol{S}\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right)-\frac{3K+19}{K+3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\\&+(K+5)\boldsymbol{S}\cdot\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)-\frac{K+5}{K+3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\\&+(K+7)\boldsymbol{\nabla}\cdot\boldsymbol{S}-2\frac{K+6}{K+3}\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{u})+(K+5)\boldsymbol{\Omega}\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\end{aligned}\right\}\\
&+\tau^2\rho(RT)^2\left\{\begin{aligned}&-\frac{3}{2}(K+5)\boldsymbol{\nabla}\left(\frac{\Lambda}{C_vT}\right)-(K+5)\left(\frac{1}{\tau}\boldsymbol{\nabla}\tau\right)\frac{\Lambda}{C_vT}\\&-\frac{1}{2}(K+5)\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\frac{\Lambda}{C_vT}-\frac{5}{2}(K+5)\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\frac{\Lambda}{C_vT}\end{aligned}\right\}\\
&-\frac{1}{2}\int\boldsymbol{c}c^2\tau\frac{D}{Dt}(\tau S_g)d\boldsymbol{\xi}-\frac{1}{2}\int\boldsymbol{c}\tau\frac{D}{Dt}(\tau S_h)\,d\boldsymbol{\xi}+\boldsymbol{O}(\tau^3),
\end{aligned}
\tag{98}
$$

where the time and spatial derivatives of the relaxation time are given by

$$
\begin{aligned}
\frac{1}{\tau}\frac{d\tau}{dt}&=\left(\gamma-\frac{2}{K+3}\frac{T}{\mu}\frac{d\mu}{dT}\right)(\boldsymbol{\nabla}\cdot\boldsymbol{u})+\left(1-\frac{T}{\mu}\frac{d\mu}{dT}\right)\frac{\Lambda}{C_vT}+O(\tau),\\
\frac{1}{\tau}\boldsymbol{\nabla}\tau&=-\left(1-\frac{T}{\mu}\frac{d\mu}{dT}\right)\frac{1}{T}\boldsymbol{\nabla}T-\frac{1}{\rho}\boldsymbol{\nabla}\rho.
\end{aligned}
\tag{99}
$$

The results in Eq. (98) are briefly discussed here. The first term is the Fourier's law. The second term is determined by the divergence of the viscous stress tensor. The third term is caused by the variation of the particle relaxation time in both space and time. The fourth term is composed of the coupling terms between the strain rate, rotation rate, temperature gradient and density gradient as well as the divergence of the strain rate. The fourth term represents the contributions from the terms relevant to the thermal energy source. The last two integrals depend on the specific form of the source terms S_g and S_h used in different models.

Similar to what we have done for the viscous stress tensor, by setting $D=3,\ K=0,\ \chi=0,\ \Lambda=0$ and $S_g=0$, a comparison would also be performed for heat flux for Maxwell molecules. The result obtained by Agarwal *et al.* [32] can be reformulated as

$$\boldsymbol{q} = -\frac{15}{4}\mu R\boldsymbol{\nabla}T + 15\frac{\mu^2}{\rho}\boldsymbol{S}\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right) - 3\frac{\mu^2}{\rho}\boldsymbol{S}\cdot\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)$$
$$-\frac{25}{8}\frac{\mu^2}{\rho}\left(\boldsymbol{\nabla}\cdot\boldsymbol{u}\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right) + \frac{\mu^2}{\rho}\left(\boldsymbol{\nabla}\cdot\boldsymbol{u}\right)\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)$$
$$+3\frac{\mu^2}{\rho}\boldsymbol{\nabla}\cdot\boldsymbol{S} - \frac{19}{4}\frac{\mu^2}{\rho}\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{u}) + \frac{45}{4}\frac{\mu^2}{\rho}\boldsymbol{\Omega}\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right) + \boldsymbol{O}(\tau^3). \tag{100}$$

Correspondingly, Eq. (98) can be simplified as

$$\boldsymbol{q} = -\frac{15}{4}\mu R\boldsymbol{\nabla}T + 9\frac{\mu^2}{\rho}\boldsymbol{S}\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right) - 2\frac{\mu^2}{\rho}\boldsymbol{S}\cdot\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)$$
$$-\frac{13}{6}\frac{\mu^2}{\rho}\left(\boldsymbol{\nabla}\cdot\boldsymbol{u}\right)\left(\frac{1}{T}\boldsymbol{\nabla}T\right) + \frac{2}{3}\frac{\mu^2}{\rho}\left(\boldsymbol{\nabla}\cdot\boldsymbol{u}\right)\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)$$
$$+2\frac{\mu^2}{\rho}\boldsymbol{\nabla}\cdot\boldsymbol{S} - \frac{7}{3}\frac{\mu^2}{\rho}\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{u}) + 5\frac{\mu^2}{\rho}\boldsymbol{\Omega}\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right)$$
$$-\frac{1}{2}\int \boldsymbol{c}\tau\frac{D(\tau S_h)}{Dt}d\boldsymbol{\xi} + \boldsymbol{O}(\tau^3). \tag{101}$$

Again, Eqs. (100) and (101) share the same mathematical form and the same sign for each contribution up to the order $\boldsymbol{O}(\tau^2)$. In our model, S_h is mainly designed to modify the Prandtl number and thermal energy source. Note that we keep the term relevant to S_h in Eq. (101) but it can be evaluated once the specific form of S_h is given.

12 Conclusions

In this paper, a general framework for the inverse design of mesoscopic models has been presented. The design began with a model Boltzmann equation in a high dimensional phase space and with an undetermined source term. Then two reduced model Boltzmann equations in a lower-dimensional phase space (of dimension 2D) are introduced, each containing a source term. First, it is found that there are many possible ways to design the source terms in order to recover the NSF system in the continuum limit, as long as five newly-derived requirements for the two source terms are met. These source terms allow for flexible Prandtl number, bulk-to-shear viscosity ratio, and a thermal energy source/sink term.

Second, based on the Hermite expansion, we have provided one design for the two source terms. This newly introduced model has been utilized to simulate decaying compressible isotropic turbulence [35] and forced compressible isotropic turbulence [36], achieving results in excellent agreement with those based on solving the NSF system [28].

Third, three existing models, namely, the Shakhov model, the total energy double-distribution-function model, and the Rykov model, have been shown to be special designs of the two source terms under the same five constraints. This indicates that the source terms can be designed from different physical considerations and numerical implementation requirements.

Furthermore, by applying the first-order Chapman-Enskog expansion to the distribution functions, we discuss the structures of the distribution functions and the implementation of bounce back boundary conditions. These results can be used to improve the implementation of hydrodynamic boundary conditions in terms of the distribution functions, namely, constructing the missing distributions from the known distribution near a solid boundary, in both laminar and turbulent flows.

Finally, we have obtained the complete analytical expressions for the viscous stress tensor and the heat flux based on the second-order Chapman-Enskog expansion of the distribution functions, generalizing the previous results in the incompressible limit. These new results have been compared with those obtained from Grad's 13 momentum equations, which demonstrates that the final structure of the viscous stress tensor and heat flux can be fully determined by the single-relaxation-time BGK model except for differences in the values of some coefficients. We expect that the incorrect values of the coefficients can also be corrected by adding higher-order source terms, just like we did for heat flux and bulk viscosity; although the design of such higher order source terms involves more sophisticated derivations. It would be desirable to explore underlying physics associated with the second-order terms especially in compressible turbulence, in the future using DNS data. The second-order terms may also provide a way to assess the difference between NSF flows and the flows governed by the model Boltzmann equation.

Appendix A: Hermite polynomials and Hermite expansion

In D-dimensional Cartesian coordinate system, the n-th order Hermite polynomials is defined by [37, 38].

$$\mathscr{H}^{(n)}(\boldsymbol{\xi}, T_0) \equiv \left(\sqrt{RT_0}\right)^n \frac{(-1)^n}{\omega(\boldsymbol{\xi}, T_0)} \nabla^n \omega(\boldsymbol{\xi}, T_0), \tag{102}$$

where $\nabla^n = \nabla_{\boldsymbol{\xi}} \nabla_{\boldsymbol{\xi}} \cdots \nabla_{\boldsymbol{\xi}}$ implies that $\mathscr{H}^{(n)}(\boldsymbol{\xi}, T_0)$ is a symmetrical tensor of rank-n. The weighting function is $\omega\left(\boldsymbol{\xi}, T_0\right) = \frac{1}{(2\pi RT_0)^{D/2}} \exp\left(-\frac{\xi^2}{2RT_0}\right)$.

The zeroth- to the third-order Hermite polynomials are expressed as

$$\mathscr{H}^{(0)}(\boldsymbol{\xi}, T_0) = 1,\ \mathscr{H}^{(1)}(\boldsymbol{\xi}, T_0) = \frac{\boldsymbol{\xi}}{\sqrt{RT_0}}, \tag{103a}$$

$$\mathscr{H}^{(2)}(\boldsymbol{\xi}, T_0) = \frac{\boldsymbol{\xi}}{\sqrt{RT_0}} \frac{\boldsymbol{\xi}}{\sqrt{RT_0}} - \boldsymbol{I}, \tag{103b}$$

$$\mathscr{H}^{(3)}(\boldsymbol{\xi}, T_0) = \frac{\boldsymbol{\xi}}{\sqrt{RT_0}} \frac{\boldsymbol{\xi}}{\sqrt{RT_0}} \frac{\boldsymbol{\xi}}{\sqrt{RT_0}} - \frac{[\boldsymbol{\xi}\boldsymbol{\delta}]}{\sqrt{RT_0}}, \tag{103c}$$

where $[\boldsymbol{\xi}\boldsymbol{\delta}]_{ijk} = \xi_i \delta_{jk} + \xi_j \delta_{ki} + \xi_k \delta_{ij}$. It should be noted that Hermite polynomials of different orders are orthonogal to each other in the following sense.

$$\int \omega(\boldsymbol{\xi}, T_0) \mathscr{H}_{\boldsymbol{i}}^m(\boldsymbol{\xi}, T_0) \mathscr{H}_{\boldsymbol{j}}^n(\boldsymbol{\xi}, T_0) d\boldsymbol{\xi} = \delta_{mn} \boldsymbol{\delta}_{\boldsymbol{ij}}^n, \tag{104}$$

where $\boldsymbol{i}$ represents an abbreviation of $i_1 i_2 \cdots i_n$ and $\boldsymbol{\delta}_{\boldsymbol{ij}}^n$ is equal to one if and only if $\boldsymbol{i}$ is a permutation of $\boldsymbol{j}$.

Similarly, we can define another three sets of Hermite polynomials $\mathscr{H}^{(n)}\left(\boldsymbol{\xi}, T\right)$, $\mathscr{H}^{(n)}\left(\boldsymbol{c}, T_0\right)$ and $\mathscr{H}^{(n)}\left(\boldsymbol{c}, T\right)$ and the corresponding weighting functions $\omega(\boldsymbol{\xi}, T)$, $\omega(\boldsymbol{c}, T_0)$ and $\omega(\boldsymbol{c}, T)$.

For any square integrable function $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$, it can be expressed in terms of Hermite polynomials as follows:

$$f(\boldsymbol{x}, \boldsymbol{\xi}, t) = \omega\left(\boldsymbol{\xi}\right) \sum_{n=0}^{\infty} \frac{1}{n!} \boldsymbol{a}^{(n)}\left(\boldsymbol{x}, t\right) : \mathscr{H}^{(n)}(\boldsymbol{\xi}), \tag{105}$$

where the coefficients $\boldsymbol{a}^{(n)}(\boldsymbol{x}, t) = \int f(\boldsymbol{x}, \boldsymbol{\xi}, t) \mathscr{H}^{(n)}(\boldsymbol{\xi}) d\xi$. In the inverse design process of the source terms, the weighting function $\omega(\boldsymbol{\xi})$ can be chosen as one of

$\omega(\boldsymbol{\xi}, T_0)$, $\omega(\boldsymbol{\xi}, T)$, $\omega(\boldsymbol{c}, T_0)$ and $\omega(\boldsymbol{c}, T)$. Correspondingly, the Hermite polynomials $\mathscr{H}^{(n)}(\boldsymbol{\xi})$ can be chosen as $\mathscr{H}^{(n)}(\boldsymbol{\xi}, T_0)$, $\mathscr{H}^{(n)}(\boldsymbol{\xi}, T)$, $\mathscr{H}^{(n)}(\boldsymbol{c}, T_0)$, or $\mathscr{H}^{(n)}(\boldsymbol{c}, T)$.

The Hermite expansion of the particle equilibrium distribution g^{eq} function can be written as

$$
\begin{aligned}
&g^{eq}(\boldsymbol{x}, \boldsymbol{\xi}, t) = \rho\omega(\boldsymbol{\xi}, T_0) \times \\
&\left\{
\begin{array}{l}
1 + \dfrac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0} + \dfrac{1}{2}\left[\left(\dfrac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^2 - \dfrac{u^2}{RT_0} + (\theta-1)\left(\dfrac{\xi^2}{RT_0} - D\right)\right] \\
+ \dfrac{1}{6}\left(\dfrac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)\left[\left(\dfrac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^2 - 3\dfrac{u^2}{RT_0} + 3(\theta-1)\left(\dfrac{\xi^2}{RT_0} - D - 2\right)\right] \\
+ \dfrac{1}{24}\left\{
\begin{array}{l}
\left(\dfrac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^4 - 6\left(\dfrac{u^2}{RT_0}\right)\left(\dfrac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^2 + 3\left(\dfrac{u^2}{RT_0}\right)^2 \\
+ 6(\theta-1)\left[\begin{array}{l}\left(\dfrac{\xi^2}{RT_0} - D - 4\right)\left(\dfrac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{RT_0}\right)^2 \\ + \dfrac{u^2}{RT_0}\left(D + 2 - \dfrac{\xi^2}{RT_0}\right)\end{array}\right] \\
+ 3(\theta-1)^2\left[\left(\dfrac{\xi^2}{RT_0}\right)^2 - 2(D+2)\dfrac{\xi^2}{RT_0} + D(D+2)\right]
\end{array}
\right\}
\end{array}
\right\} \\
&+\text{high order terms,}
\end{aligned}
\tag{106a}
$$

where the normalized temperature $\theta = T/T_0$.

Appendix B: The models for thermal cooling function and shear viscosity

In a compressible turbulence, the kinetic energy input at large scales is converted into the internal energy at small scales. This can be removed by large-scale thermal cooling function to prevent the internal energy from increasing.

The cooling function typicallys take a power law form [28].

$$\Lambda_1 = \sigma_1 T^0,\ \Lambda_2 = \sigma_2 T^2,\ \Lambda_3 = \sigma_3 T^4. \tag{107}$$

The shear viscosity is determined by the intermolecular interactions and molecular thermal motions. For air, the shear viscosity increases with temperature, which introduces an additional effect of thermal field on the hydrodynamic velocity field. Two well-known models are briefly discussed here. The first one is called hard-sphere

(HS) model [21, 25], namely,

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{\omega}, \tag{108}$$

where T_0 is a reference temperature, $\mu_0 = \mu(T_0)$ is the reference shear viscosity at the reference temperature and the constant exponent ω depends on the intermolecular interaction model. The second one is called the Sutherland's law [28, 39], which can be written as

$$\frac{\mu}{\mu_0} = \frac{1.4042\,(T/T_0)^{1.5}}{(T/T_0) + 0.40417}. \tag{109}$$

It has been verified from the experimental data that the HS model has a maximum relative error of about 5% for extreme cases of $T \to 0.55$ and $T \to 3$ while the Sutherland's law has a maximum relative error of 2.0% at $T = 3$ and less than 0.52% at $T = 0.55$.

Appendix C: Chapman-Enskog expansion of the particle distribution function

The explicit expressions of some terms in Eqs. (84a) and (84b) are given in this Appendix.

$$\tau^2 \frac{DG_1}{Dt} = \tilde{A}_1 + \tilde{A}_2 + \tilde{A}_3 + \tilde{A}_4, \tag{110}$$

where the terms $\tilde{A}_1, \tilde{A}_2, \tilde{A}_3$ and $\tilde{A}_4$ are expressed as

$$\begin{aligned}
\tilde{A}_1 &= \tau^2 \frac{1}{2RT^2} \boldsymbol{\nabla} T \cdot \frac{D(c^2 \boldsymbol{c})}{Dt} \\
&= -\tau^2 \frac{\boldsymbol{c} \cdot \boldsymbol{S} \cdot \boldsymbol{c}}{RT} \boldsymbol{c} \cdot \left(\frac{1}{T} \boldsymbol{\nabla} T\right) - \tau^2 \frac{c^2}{2RT} \boldsymbol{c} \cdot \boldsymbol{\nabla} \boldsymbol{u} \cdot \left(\frac{1}{T} \boldsymbol{\nabla} T\right) \\
&+ \tau^2 \boldsymbol{cc} : \left(\frac{1}{\rho} \boldsymbol{\nabla} \rho\right) \left(\frac{1}{T} \boldsymbol{\nabla} T\right) + \tau^2 \boldsymbol{cc} : \left(\frac{1}{T} \boldsymbol{\nabla} T\right) \left(\frac{1}{T} \boldsymbol{\nabla} T\right) \\
&+ \frac{1}{2} \tau^2 c^2 \left(\frac{1}{\rho} \boldsymbol{\nabla} \rho\right) \cdot \left(\frac{1}{T} \boldsymbol{\nabla} T\right) + \frac{1}{2} \tau^2 c^2 \left|\frac{1}{T} \boldsymbol{\nabla} T\right|^2 + O(\tau^3),
\end{aligned} \tag{111a}$$

$$
\begin{aligned}
\tilde{A}_2 &= \tau^2 c^2 \boldsymbol{c} \cdot \frac{D}{Dt}\left(\frac{1}{2RT^2}\boldsymbol{\nabla} T\right) \\
&= -\tau^2 \frac{c^2}{RT}\boldsymbol{cc} : \left(\frac{1}{T}\boldsymbol{\nabla} T\right)\left(\frac{1}{T}\boldsymbol{\nabla} T\right) + \frac{1}{K+3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\tau^2 \frac{c^2}{RT}\boldsymbol{c}\cdot\left(\frac{1}{T}\boldsymbol{\nabla} T\right) \\
&+\tau^2 \frac{c^2}{RT}\boldsymbol{c}\cdot\left(\frac{1}{T}\boldsymbol{\nabla} T\right)\frac{\Lambda}{C_v T} - \tau^2 \frac{c^2}{2RT}\boldsymbol{c}\cdot\boldsymbol{\nabla}\boldsymbol{u}\cdot\left(\frac{1}{T}\boldsymbol{\nabla} T\right) \\
&+\tau^2 \frac{c^2}{2RT}\boldsymbol{cc} : \left(\frac{1}{T}\boldsymbol{\nabla}\boldsymbol{\nabla} T\right) \\
&-\frac{1}{K+3}\tau^2 \frac{c^2}{RT}\boldsymbol{c}\cdot\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{u}) - \tau^2 \frac{c^2}{2RT}\frac{1}{C_v T}\boldsymbol{c}\cdot\boldsymbol{\nabla}\Lambda + O(\tau^3),
\end{aligned}
\tag{111b}
$$

$$
\begin{aligned}
\tilde{A}_3 &= -\tau^2 \frac{D+2}{2}\frac{D}{Dt}\left(\frac{1}{T}\boldsymbol{\nabla} T\right)\cdot\boldsymbol{c} \\
&= \frac{D+2}{2}\tau^2 \boldsymbol{cc} : \left(\frac{1}{T}\boldsymbol{\nabla} T\right)\left(\frac{1}{T}\boldsymbol{\nabla} T\right) - \frac{D+2}{2}\tau^2 \boldsymbol{cc} : \left(\frac{1}{T}\boldsymbol{\nabla}\boldsymbol{\nabla} T\right) \\
&+\frac{D+2}{2}\tau^2 \boldsymbol{c}\cdot\boldsymbol{\nabla}\boldsymbol{u}\cdot\left(\frac{1}{T}\boldsymbol{\nabla} T\right) + \frac{D+2}{K+3}\tau^2 \boldsymbol{c}\cdot\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{u}) \\
&+\frac{D+2}{2}\tau^2 \boldsymbol{c}\cdot\boldsymbol{\nabla}\left(\frac{\Lambda}{C_v T}\right) + O(\tau^3),
\end{aligned}
\tag{111c}
$$

$$
\begin{aligned}
\tilde{A}_4 &= -\tau^2 \frac{D+2}{2}\left(\frac{1}{T}\boldsymbol{\nabla} T\right)\cdot\frac{D\boldsymbol{c}}{Dt} \\
&= \frac{D+2}{2}\tau^2 \boldsymbol{c}\cdot\boldsymbol{\nabla}\boldsymbol{u}\cdot\left(\frac{1}{T}\boldsymbol{\nabla} T\right) - \frac{D+2}{2}\tau^2 RT\left(\frac{1}{T}\boldsymbol{\nabla} T\right)\cdot\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right) \\
&-\frac{D+2}{2}\tau^2 RT\left|\frac{1}{T}\boldsymbol{\nabla} T\right|^2 + O(\tau^3).
\end{aligned}
\tag{111d}
$$

$$
\begin{aligned}
&\tau^2 \frac{DG_2}{Dt} = \\
&-2\tau^2 \frac{\boldsymbol{cc}}{RT} : (\boldsymbol{\nabla u} \cdot \boldsymbol{S}) + 2\tau^2 \boldsymbol{c} \cdot \boldsymbol{S} \cdot \left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right) + 2\tau^2 \boldsymbol{c} \cdot \boldsymbol{S} \cdot \left(\frac{1}{T}\boldsymbol{\nabla}T\right) \\
&-\tau^2 \frac{\boldsymbol{c} \cdot \boldsymbol{S} \cdot \boldsymbol{c}}{RT} \boldsymbol{c} \cdot \left(\frac{1}{T}\boldsymbol{\nabla}T\right) + \frac{4}{K+3}\tau^2 \frac{\boldsymbol{c} \cdot \boldsymbol{S} \cdot \boldsymbol{c}}{RT} \boldsymbol{\nabla} \cdot \boldsymbol{u} + \tau^2 \frac{\boldsymbol{c} \cdot \boldsymbol{S} \cdot \boldsymbol{c}}{RT} \frac{\Lambda}{C_v T} \\
&-\frac{2}{K+3}\tau^2 \boldsymbol{c} \cdot \left(\frac{1}{\rho}\nabla\rho\right) \boldsymbol{\nabla} \cdot \boldsymbol{u} - \frac{2}{K+3}\tau^2 \boldsymbol{c} \cdot \left(\frac{1}{T}\boldsymbol{\nabla}T\right) \boldsymbol{\nabla} \cdot \boldsymbol{u} \\
&+\frac{1}{K+3}\tau^2 \frac{c^2}{RT} \boldsymbol{c} \cdot \left(\frac{1}{T}\boldsymbol{\nabla}T\right) \boldsymbol{\nabla} \cdot \boldsymbol{u} - \frac{2}{(K+3)^2}\tau^2 \frac{c^2}{RT} (\boldsymbol{\nabla} \cdot \boldsymbol{u})^2 \\
&-\frac{1}{K+3}\tau^2 \frac{c^2}{RT} (\boldsymbol{\nabla} \cdot \boldsymbol{u}) \frac{\Lambda}{C_v T} \\
&+\tau^2 \left[\frac{\boldsymbol{cc}}{RT} - \frac{1}{K+3}\left(\frac{c^2}{RT} + 3 - D + K\right)\boldsymbol{I}\right] : \frac{D\boldsymbol{S}}{Dt} + O(\tau^3). \qquad (112)
\end{aligned}
$$

$$
\tau^2 \frac{DG_3}{Dt} = \tilde{B}_1 + \tilde{B}_2 + \tilde{B}_3, \qquad (113)
$$

where $\tilde{B}_1$, $\tilde{B}_2$ and $\tilde{B}_3$ are

$$
\begin{aligned}
\tilde{B}_1 &= -\tau^2 \frac{\boldsymbol{c}}{RT} \cdot \frac{D\boldsymbol{c}}{Dt} \frac{\Lambda}{C_v T} \\
&= \tau^2 \frac{\boldsymbol{c} \cdot \boldsymbol{S} \cdot \boldsymbol{c}}{RT} \frac{\Lambda}{C_v T} - \tau^2 \boldsymbol{c} \cdot \left(\frac{1}{\rho}\boldsymbol{\nabla}\rho + \frac{1}{T}\boldsymbol{\nabla}T\right) \frac{\Lambda}{C_v T} + O(\tau^3), \qquad (114a)
\end{aligned}
$$

$$
\begin{aligned}
\tilde{B}_2 &= \tau^2 \frac{c^2}{2RT^2} \frac{DT}{Dt} \frac{\Lambda}{C_v T} \\
&= \tau^2 \frac{c^2}{2RT} \boldsymbol{c} \cdot \left(\frac{1}{T}\boldsymbol{\nabla}T\right) \frac{\Lambda}{C_v T} - \frac{2}{K+3}\tau^2 \frac{c^2}{2RT} (\boldsymbol{\nabla} \cdot \boldsymbol{u}) \frac{\Lambda}{C_v T} \\
&-\tau^2 \frac{c^2}{2RT} \left(\frac{\Lambda}{C_v T}\right)^2 + O(\tau^3), \qquad (114b)
\end{aligned}
$$

$$
\begin{aligned}
\tilde{B}_3 &= -\tau^2 \left(\frac{c^2}{2RT} - \frac{D}{2}\right) \frac{D}{Dt}\left(\frac{\Lambda}{C_v T}\right) \\
&= -\tau^2 \left(\frac{c^2}{2RT} - \frac{D}{2}\right) \left(\frac{d}{dt}\left(\frac{\Lambda}{C_v T}\right) + \boldsymbol{c} \cdot \boldsymbol{\nabla}\left(\frac{\Lambda}{C_v T}\right)\right) + O(\tau^3). \qquad (114c)
\end{aligned}
$$

$$
\tau^2 \frac{D\Phi_1}{Dt}
= \tau^2 \left\{ \begin{array}{l}
-\boldsymbol{c}\cdot\boldsymbol{\nabla}\boldsymbol{u}\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right) + RT\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\cdot\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\\
+RT\left|\frac{1}{T}\boldsymbol{\nabla}T\right|^2 + \boldsymbol{c}\cdot\frac{d}{dt}\left(\frac{1}{T}\boldsymbol{\nabla}T\right) + \boldsymbol{c}\cdot\boldsymbol{\nabla}\left(\frac{1}{T}\boldsymbol{\nabla}T\right)\cdot\boldsymbol{c}\\
-\frac{d}{dt}\left(\frac{2}{K+3}\boldsymbol{\nabla}\cdot\boldsymbol{u} + \frac{\Lambda}{C_v T}\right)\\
-\boldsymbol{c}\cdot\boldsymbol{\nabla}\left(\frac{2}{K+3}\boldsymbol{\nabla}\cdot\boldsymbol{u} + \frac{\Lambda}{C_v T}\right)
\end{array}\right\} + O(\tau^3). \quad (115)
$$

Appendix D: Derivations of the requirements for the source terms

The Euler equations can be obtained by assuming that $g = g^{eq} + O(\tau)$ when evaluating the viscous stress and the heat flux. This leads to $\boldsymbol{\sigma} \sim \boldsymbol{O}(\tau)$ and $\boldsymbol{q} \sim \boldsymbol{O}(\tau)$. Therefore, the Euler equations are

$$
\begin{aligned}
&\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{u}) = 0,\\
&\rho\left(\frac{\partial\boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u}\right) = -\boldsymbol{\nabla}p + \rho\boldsymbol{a} + \boldsymbol{O}(\tau),\\
&\rho C_v \frac{dT}{dt} = -p\boldsymbol{\nabla}\cdot\boldsymbol{u} - \rho\Lambda + O(\tau).
\end{aligned} \quad (116)
$$

Taking the first order moments of Eq. (11a) gives

$$
\frac{\partial}{\partial t}\left(\int \boldsymbol{\xi} g d\boldsymbol{\xi}\right) + \boldsymbol{\nabla}\cdot\left(\int \boldsymbol{\xi}\boldsymbol{\xi} g d\boldsymbol{\xi}\right) = \rho\boldsymbol{a} + \int \boldsymbol{\xi} S_g d\boldsymbol{\xi}. \quad (117)
$$

The first term in Eq. (117) can be evaluated as

$$
\frac{\partial}{\partial t}\left(\int \boldsymbol{\xi} g d\boldsymbol{\xi}\right) = \frac{\partial}{\partial t}(\rho\boldsymbol{u}). \quad (118)
$$

The second term in Eq. (117) can be evaluated as

$$
\begin{aligned}
&\int \boldsymbol{\xi}\boldsymbol{\xi} g d\boldsymbol{\xi} = \int \boldsymbol{c}\boldsymbol{c}\left(g - g^{eq}\right) d\boldsymbol{\xi} + \int \boldsymbol{c}\boldsymbol{c} g^{eq} d\boldsymbol{\xi} + \rho\boldsymbol{u}\boldsymbol{u}\\
&= -\boldsymbol{\sigma} + p\boldsymbol{I} + \rho\boldsymbol{u}\boldsymbol{u}.
\end{aligned} \quad (119)
$$

By substituting of Eqs. (118) and (119) into Eq. (117), we have

$$\frac{\partial(\rho\boldsymbol{u})}{\partial t}+\boldsymbol{\nabla}\cdot(\rho\boldsymbol{u}\boldsymbol{u})=-\boldsymbol{\nabla}p+\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}+\rho\boldsymbol{a}+\int\boldsymbol{\xi}S_g d\boldsymbol{\xi}. \tag{120}$$

Therefore, the Eq. (28b) is derived.

Noticing that $\boldsymbol{c}=\boldsymbol{\xi}-\boldsymbol{u}$ and $\boldsymbol{\xi}\boldsymbol{\xi}=\boldsymbol{c}\boldsymbol{c}+\boldsymbol{u}\boldsymbol{c}+\boldsymbol{c}\boldsymbol{u}+\boldsymbol{u}\boldsymbol{u}$, we have

$$\int\boldsymbol{c}S_g d\boldsymbol{\xi}=\boldsymbol{0},\ \int\boldsymbol{\xi}\boldsymbol{\xi}S_g d\boldsymbol{\xi}=\int\boldsymbol{c}\boldsymbol{c}S_g d\boldsymbol{\xi}. \tag{121}$$

By using the Eq. (27a), we can make a closure of the viscous stress,

$$\begin{aligned}\boldsymbol{\sigma}&=-\int\boldsymbol{c}\boldsymbol{c}\left(g-g^{eq}\right)d\boldsymbol{\xi}=-\int\boldsymbol{c}\boldsymbol{c}\left(-\tau\frac{Dg^{eq}}{Dt}+\tau S_g\right)d\boldsymbol{\xi}+\boldsymbol{O}(\tau^2)\\&=\tau\int\boldsymbol{c}\boldsymbol{c}G_1g^{eq}d\boldsymbol{\xi}+\tau\int\boldsymbol{c}\boldsymbol{c}G_2g^{eq}d\boldsymbol{\xi}\\&+\tau\int\boldsymbol{c}\boldsymbol{c}G_3g^{eq}d\boldsymbol{\xi}-\tau\int\boldsymbol{c}\boldsymbol{c}S_g d\boldsymbol{\xi}+\boldsymbol{O}(\tau^2).\end{aligned} \tag{122}$$

All the integrals in the RHS of Eq. (122) can be evaluated term by term.

$$\tau\int\boldsymbol{c}\boldsymbol{c}G_1g^{eq}d\boldsymbol{\xi}=\boldsymbol{0}, \tag{123a}$$

$$\tau\int\boldsymbol{c}\boldsymbol{c}G_2g^{eq}d\boldsymbol{\xi}=\tau p\left[2\boldsymbol{S}-\frac{2}{K+3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right], \tag{123b}$$

$$\tau\int\boldsymbol{c}\boldsymbol{c}G_3g^{eq}d\boldsymbol{\xi}=-\frac{p\tau\Lambda}{C_vT}\boldsymbol{I}. \tag{123c}$$

Substitution of Eq. (123a) to Eq. (123c) into Eq. (122) yields

$$\begin{aligned}\boldsymbol{\sigma}&=2\mu\left(\boldsymbol{S}-\frac{1}{D}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right)+\mu_V(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\\&-\left(\chi-\frac{2(3-D+K)}{D(K+3)}\right)\mu(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}-\frac{\tau p\Lambda}{C_vT}\boldsymbol{I}-\tau\int\boldsymbol{c}\boldsymbol{c}S_g d\boldsymbol{\xi}+\boldsymbol{O}(\tau^2).\end{aligned} \tag{124}$$

Hence, in order to recover the Newtonian constitutive law (see Eq. (21)), the Eq. (28c) must be satisfied. The resulting momentum equation is the Eq. (29b).

Similarly, combining the second-order moment of Eq. (11a) and the zeroth-order moment of the Eq. (11b) yields the following equation,

$$\frac{\partial(\rho E)}{\partial t} + \frac{1}{2}\boldsymbol{\nabla}\cdot\left(\int \boldsymbol{\xi}\left(\xi^2 g + h\right) d\boldsymbol{\xi}\right) = \rho\boldsymbol{a}\cdot\boldsymbol{u} + \frac{1}{2}\int\left(\xi^2 S_g + S_h\right) d\boldsymbol{\xi}. \tag{125}$$

The integral in the second term of Eq. (125) is

$$\begin{aligned}
&\frac{1}{2}\int \boldsymbol{\xi}\left(\xi^2 g + h\right) d\boldsymbol{\xi} \\
&= \frac{1}{2}\int \boldsymbol{c}\left(c^2 g + h\right) d\boldsymbol{\xi} + \boldsymbol{u}\cdot\int \boldsymbol{cc}g^{eq} d\boldsymbol{\xi} + \boldsymbol{u}\cdot\int \boldsymbol{cc}\left(g - g^{eq}\right) d\boldsymbol{\xi} + \boldsymbol{u}\frac{1}{2}\int\left(\xi^2 g + h\right) d\boldsymbol{\xi} \\
&= \boldsymbol{q} + \rho E\boldsymbol{u} + p\boldsymbol{u} - \boldsymbol{\sigma}\cdot\boldsymbol{u}.
\end{aligned} \tag{126}$$

Therefore, substituting Eqs. (28d) and (126) into Eq. (125) gives the energy equation (see Eq. (29c)).

By using the Eqs. (27a) and (27b) , we can make a closure of the heat flux term,

$$\begin{aligned}
\boldsymbol{q} &= \frac{1}{2}\int \boldsymbol{c}\left(c^2 g + h\right) d\boldsymbol{\xi} \\
&= \frac{1}{2}\int \boldsymbol{c}c^2\left(g^{eq} - \tau\frac{Dg^{eq}}{Dt} + \tau S_g\right) d\boldsymbol{\xi} + \frac{1}{2}\int \boldsymbol{c}\left(h^{eq} - \tau\frac{Dh^{eq}}{Dt} + \tau S_h\right) d\boldsymbol{\xi} + \boldsymbol{O}(\tau^2) \\
&= -\frac{1}{2}\tau\int \boldsymbol{c}c^2 G g^{eq} d\boldsymbol{\xi} - \frac{1}{2}\tau\int \boldsymbol{c}G h^{eq} d\boldsymbol{\xi} - \frac{1}{2}\tau\int \boldsymbol{c}\Phi_1 h^{eq} d\boldsymbol{\xi} \\
&\quad + \frac{1}{2}\tau\int \boldsymbol{c}c^2 S_g d\boldsymbol{\xi} + \frac{1}{2}\tau\int \boldsymbol{c}S_h d\boldsymbol{\xi} + \boldsymbol{O}(\tau^2).
\end{aligned} \tag{127}$$

Because of

$$\int \boldsymbol{c}c^2 G_1 g^{eq} d\boldsymbol{\xi} = (D+2)\,\rho\,(RT)^2\left(\frac{1}{T}\boldsymbol{\nabla}T\right), \tag{128a}$$

$$\int \boldsymbol{c}c^2 G_2 g^{eq} d\boldsymbol{\xi} = \boldsymbol{0}, \tag{128b}$$

$$\int \boldsymbol{c}c^2 G_3 g^{eq} d\boldsymbol{\xi} = \boldsymbol{0}, \tag{128c}$$

we obtain

$$-\frac{1}{2}\tau\int \boldsymbol{c}c^2Gg^{eq}d\boldsymbol{\xi}=-\frac{1}{2}\tau\left(D+2\right)\rho\left(RT\right)^2\left(\frac{1}{T}\boldsymbol{\nabla}T\right). \tag{129}$$

Because of

$$\int \boldsymbol{c}G_1g^{eq}d\boldsymbol{\xi}=\int \boldsymbol{c}G_2g^{eq}d\boldsymbol{\xi}=\int \boldsymbol{c}G_3g^{eq}d\boldsymbol{\xi}=\boldsymbol{0}, \tag{130a}$$

we have

$$-\frac{1}{2}\tau\int \boldsymbol{c}Gh^{eq}d\boldsymbol{\xi}=\boldsymbol{0}. \tag{131}$$

Further, we have

$$-\frac{1}{2}\tau\int \boldsymbol{c}\Phi_1h^{eq}d\boldsymbol{\xi}=-\frac{1}{2}\tau\left(3-D+K\right)\rho\left(RT\right)^2\left(\frac{1}{T}\boldsymbol{\nabla}T\right). \tag{132}$$

By substituting of Eqs. (129), (131) and (132) into Eq. (127), we obtain

$$\begin{aligned}\boldsymbol{q}&=-\frac{(K+5)R}{2}p\tau\boldsymbol{\nabla}T+\frac{1}{2}\tau\int \boldsymbol{c}c^2S_gd\boldsymbol{\xi}+\frac{1}{2}\tau\int \boldsymbol{c}S_hd\boldsymbol{\xi}+\boldsymbol{O}(\tau^2)\\&=\boldsymbol{q}^{(NS)}-\left(1-Pr\right)\boldsymbol{q}^{(NS)}+\frac{1}{2}\tau\int \boldsymbol{c}c^2S_gd\boldsymbol{\xi}+\frac{1}{2}\tau\int \boldsymbol{c}S_hd\boldsymbol{\xi}+\boldsymbol{O}(\tau^2).\end{aligned} \tag{133}$$

Therefore, we have derived the fifth requirement for the source term in Eq. (28e) and the resulting energy equation is given in Eq. (29c).

Appendix E: Details in the derivations of the Rykov model

Here we prove that the two source terms in Eq. (65) should satisfy the five general requirements.

From the Euler equations for the Rykov model, the time derivative for the translational temperature T_t and rotational temperature T_r are

$$\frac{\partial T_t}{\partial t}=-\boldsymbol{u}\cdot\boldsymbol{\nabla}T_t-\frac{2}{3}T_t\boldsymbol{\nabla}\cdot\boldsymbol{u}+\frac{1}{\tau Z}\left(T-T_t\right)+O(\tau), \tag{134}$$

$$\frac{\partial T_r}{\partial t} = -\boldsymbol{u} \cdot \boldsymbol{\nabla} T_r + \frac{1}{\tau Z}\left(T - T_r\right) + O(\tau). \tag{135}$$

The first requirement for the source term is satisfied because of

$$\begin{aligned}\int S_g d\boldsymbol{\xi} &= \frac{1}{\tau}\left[\frac{1}{Z}\int f_0^r d\boldsymbol{\xi} + \left(1 - \frac{1}{Z}\right)\int f_0^t d\boldsymbol{\xi} - \int f_M(T) d\boldsymbol{\xi}\right] \\ &= \frac{1}{\tau}\left[\rho - \rho\right] = 0. \end{aligned}\tag{136}$$

The second requirement for the source term is satisfied because of

$$\int \boldsymbol{\xi} S_g d\boldsymbol{\xi} = \frac{1}{\tau}\left[\frac{1}{Z}\int \boldsymbol{c} f_0^r d\boldsymbol{\xi} + \left(1 - \frac{1}{Z}\right)\int \boldsymbol{c} f_0^t d\boldsymbol{\xi} - \int \boldsymbol{c} f_M(T) d\boldsymbol{\xi}\right] = \boldsymbol{0}. \tag{137}$$

According to Eqs. (136) and (137), we have

$$\int \boldsymbol{\xi\xi} S_g d\boldsymbol{\xi} = \int \boldsymbol{cc} S_g d\boldsymbol{\xi}. \tag{138}$$

Since

$$\int \boldsymbol{cc} f_0^r d\boldsymbol{\xi} = p\boldsymbol{I}, \int \boldsymbol{cc} f_0^t d\boldsymbol{\xi} = p_t\boldsymbol{I}, \int \boldsymbol{cc} f_M(T) d\boldsymbol{\xi} = p\boldsymbol{I}, \tag{139}$$

therefore,

$$\int \boldsymbol{cc} S_g d\boldsymbol{\xi} = \frac{1}{\tau}\left[\frac{1}{Z}p\boldsymbol{I} + \left(1 - \frac{1}{Z}\right)p_t\boldsymbol{I} - p\boldsymbol{I}\right] = -\frac{1}{\tau}\left(1 - \frac{1}{Z}\right)\left(p - p_t\right)\boldsymbol{I}. \tag{140}$$

From Eqs. (134) and (135), we have

$$\begin{aligned} T - T_t &= \frac{2}{5}\left(T_r - T_t\right) \\ &= \frac{4}{15}\tau Z T_t \boldsymbol{\nabla} \cdot \boldsymbol{u} + O(\tau^2) \\ &= \frac{4}{15}\tau Z T \boldsymbol{\nabla} \cdot \boldsymbol{u} + O(\tau^2). \end{aligned}\tag{141}$$

Therefore, we obtain

$$
\begin{aligned}
p - p_t &= \rho R(T - T_t) \\
&= \frac{4}{15} Z \mu_t \boldsymbol{\nabla} \cdot \boldsymbol{u} + O(\tau^2) \\
&= \frac{4}{15} Z \mu \boldsymbol{\nabla} \cdot \boldsymbol{u} + O(\tau^2).
\end{aligned} \tag{142}
$$

Substituting Eq. (142) into (140), we have

$$
\int \boldsymbol{\xi\xi} S_g d\boldsymbol{\xi} = \int \boldsymbol{cc} S_g d\boldsymbol{\xi} = -\left(\frac{4}{15} Z - \frac{4}{15}\right) p \left(\nabla \cdot \boldsymbol{u}\right) \boldsymbol{I} + O(\tau). \tag{143}
$$

Therefore, the third requirement for the source term is proved. The ratio of bulk to shear viscosity is proportional to the collision ratio, *i.e.*, $\chi = 4Z/15$.

From Eq. (140), we have

$$
\int \xi^2 S_g d\boldsymbol{\xi} = \int c^2 S_g d\boldsymbol{\xi} = -\frac{3}{\tau}\left(1 - \frac{1}{Z}\right)\left(p - p_t\right). \tag{144}
$$

From the definition of S_h in Eq. (65), we have

$$
\begin{aligned}
&\int S_h d\boldsymbol{\xi} = \frac{2}{\tau}\left[\frac{1}{Z}\int f_1^r d\boldsymbol{\xi} + \left(1 - \frac{1}{Z}\right)\int f_1^t d\boldsymbol{\xi} - RT \int f_M(T) d\boldsymbol{\xi}\right] \\
&= \frac{2}{\tau}\left[\frac{1}{Z} p + \left(1 - \frac{1}{Z}\right) p_r - p\right] = -\frac{2}{\tau}\left(1 - \frac{1}{Z}\right)\left(p - p_r\right).
\end{aligned} \tag{145}
$$

Because of

$$
p - p_r = -\frac{3}{2}\left(p - p_t\right), \tag{146}
$$

we arrive at

$$
\int S_h d\boldsymbol{\xi} = \frac{3}{\tau}\left(1 - \frac{1}{Z}\right)\left(p - p_t\right). \tag{147}
$$

From Eqs. (144) and (147), the fourth requirement is satisfied.

We note that the following integrals can be carried out directly.

$$\int \boldsymbol{c} f_1^t d\boldsymbol{\xi} = (1-\delta)\, \boldsymbol{q}^r, \ \int \boldsymbol{c} f_1^r d\boldsymbol{\xi} = \omega_1 (1-\delta) \boldsymbol{q}^r, \ \int \boldsymbol{c} f_M(T) d\boldsymbol{\xi} = \boldsymbol{0},$$
$$\int \boldsymbol{c} c^2 f_0^t d\boldsymbol{\xi} = \frac{2}{3} \boldsymbol{q}^t, \ \int \boldsymbol{c} c^2 f_0^r d\boldsymbol{\xi} = \frac{2}{3} \omega_0 \boldsymbol{q}^t, \ \int \boldsymbol{c} c^2 f_M(T) d\boldsymbol{\xi} = \boldsymbol{0}. \tag{148}$$

Hence, we have

$$\int \boldsymbol{c} S_h d\boldsymbol{\xi} = \frac{2}{\tau} \left[\boldsymbol{q}^r - \left(\delta + \frac{1}{Z} (1-\omega_1)(1-\delta) \right) \boldsymbol{q}^r \right], \tag{149}$$

and

$$\int \boldsymbol{c} c^2 S_g d\boldsymbol{\xi} = \frac{2}{\tau} \left[\boldsymbol{q}^t - \frac{2}{3} \left(1 + 0.5 \frac{1-\omega_0}{Z} \right) \boldsymbol{q}^t \right]. \tag{150}$$

By applying the Chapman-Enskog expansion, we can prove that the heat fluxes are given by

$$\begin{aligned} \boldsymbol{q}^t &= -\kappa^t \boldsymbol{\nabla} T_t + O(\tau^2) = -\kappa^t \boldsymbol{\nabla} T + \boldsymbol{O}(\tau^2), \\ \boldsymbol{q}^r &= -\kappa^r \boldsymbol{\nabla} T_r + O(\tau^2) = -\kappa^r \boldsymbol{\nabla} T + \boldsymbol{O}(\tau^2), \\ \boldsymbol{q} &= -\kappa \boldsymbol{\nabla} T + \boldsymbol{O}(\tau^2), \end{aligned} \tag{151}$$

where the transport coefficients κ^t, κ^r and κ are given in Eq. (67).

Combining Eqs. (149), (150) and (151) gives

$$\int \boldsymbol{c} S_h d\boldsymbol{\xi} + \int \boldsymbol{c} c^2 S_g d\boldsymbol{\xi} = \frac{2}{\tau} (1 - Pr)\, \boldsymbol{q} + \boldsymbol{O}(\tau), \tag{152}$$

where the Prandtl number is $Pr = \mu C_p / \kappa = 7R\mu / 2\kappa$. Therefore, the fifth requirement is satisfied.

Abbreviations

NSF: Navier-Stokes-Fourier; CFD: Computational fluid dynamics; BGK: Bhatnagar-Gross-Krook; SH: Shakhov; ES: Ellipsoidal statistical; IEDDF: Internal energy double-distribution-function; TEDDF: Total energy double-distribution-function; R: Rykov; LBM: Lattice Boltzmann method; GKS: Gas kinetic scheme; UGKS: Unified gas kinetic scheme; DUGKS: Discrete unified gas kinetic scheme; EOS: Equation of state; DNS: Direct numerical simulation

Acknowledgements

Computing resources are provided by the Center for Computational Science and Engineering of Southern University of Science and Technology and by National Center for Atmospheric Research (CISL-UDEL0001).

Author's contributions

Tao Chen developed the derivations, drafted and edited the manuscript. Lian-Ping Wang conceptualized the methodology and reviewed the derivations, edited the manuscript, provided suggestions for improving the manuscript, acquired funding for this research, and served as the corresponding author. Jun Lai checked the derivations. Shiyi Chen participated in funding acquisition and supervised this research. All authors read and approved the final manuscript.

Funding

This work has been supported by the U.S. National Science Foundation (CNS-1513031, CBET-1706130), the National Natural Science Foundation of China (91852205, 91741101 & 11961131006), the National Numerical Wind Tunnel program, Guangdong Provincial Key Laboratory of Turbulence Research and Applications (2019B21203001), and Shenzhen Science & Technology Program (Grant No. KQTD20180411143441009).

Availability of data and materials

Not applicable.

Competing interests

The authors declare that they have no competing interests.

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