Reduced kinetic model of polyatomic gases

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Kinetic models of polyatomic gas typically account for the internal degrees of freedom at the level of the two-particle distribution function. However, close to the hydrodynamic limit, the internal (rotational) degrees of freedom tend to be well represented just by rotational kinetic energy density. We account for the rotational energy by augmenting the Ellipsoidal-statistical BGK (ES–BGK) model, an extension of the Bhatnagar–Gross–Krook (BGK) model, at the level of the single-particle distribution function with an advection-diffusion-relaxation equation for the rotational energy. This reduced model respects the $H$ theorem and recovers the compressible hydrodynamics for polyatomic gases as its macroscopic limit. As required for a polyatomic gas model, this extension of the ES–BGK model has not only correct specific heat ratio but also allows for three independent tunable transport coefficients: thermal conductivity, shear viscosity, and bulk viscosity. We illustrate the effectiveness of the model via a lattice Boltzmann method implementation.

1. Introduction

The dynamics of a dilute monoatomic gas in terms of the single-particle distribution function is described by the Boltzmann equation (Chapman & Cowling 1970; Cercignani 1988). Unlike the continuum Navier–Stokes–Fourier hydrodynamics equation, the Boltzmann equation is a valid description even at highly non-equilibrium states (Mott-Smith 1951; Liepmann et al. 1962; Cercignani 1988), encountered in the presence of strong shock waves at high Mach number (ratio of flow speed to sound speed) and in a highly rarefied flow characterized by a large Knudsen number (ratio of the mean free path to characteristic length scale) (Oh et al. 1997; Struchtrup 2004; Ansumali et al. 2007b). However, any analysis of the integro-differential Boltzmann equation is a formidable task even for the simplest problems. Thus, one often models the Boltzmann dynamics via a simplified collision term that converts the evolution equation to a partial differential equation (Bhatnagar et al. 1954; Lebowitz et al. 1960; Holway Jr 1966; Shakhov 1968; Gorbà & Karlin 1994; Levermore 1996; Andries et al. 2000; Ansumali et al. 2007a; Lebowitz et al. 1960; Singh & Ansumali 2015; Agrawal et al. 2020). An important example is the BGK model (Bhatnagar et al. 1954), which states that the relaxation of the distribution function towards the Maxwell–Boltzmann (MB) form happens in a time scale corresponding to the mean free time $\tau$ with the assumption that every moment of the distribution function relaxes at the same rate. The BGK model is quite successful in replicating qualitative features of the Boltzmann dynamics (collisional invariants, the zero of the collision, $H$-theorem, conservation laws, etc). However, the BGK model predicts the Prandtl number of the fluid to be unity, while the value predicted by the Boltzmann equation for monoatomic gas is $2/3$. Thus, several other variations of the collision model such as ES–BGK model (Holway Jr 1966; Andries et al. 2000), the quasi-equilibrium models (Gorbà & Karlin 1994; Levermore 1996), the Shakhov model

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(Shakhov 1968), and the Fokker-Plank model (Singh & Ansumali 2015; Singh et al. 2016) are used as kinetic models with tunable Prandtl number. The ES–BGK model (Holway Jr 1966; Andries et al. 2000) is an elegant but simple improvement over the BGK model. This model assumes that the distribution function relaxes to an anisotropic Gaussian distribution within mean free time $\tau$. The anisotropic Gaussian in itself evolves towards the MB distribution with a second time scale. The presence of a second time scale as free parameter ensures that the time scales related to momentum and thermal diffusivity are independent and thus permits one to vary the Prandtl number in the range of $2/3$ to $\infty$.

Despite their success, the Boltzmann collision kernel and its aforementioned simplifications are limited to monoatomic gases as they do not account for the internal molecular structure. However, many real gases such as nitrogen, oxygen, or methane are polyatomic. At the macroscopic level, the internal molecular structure predominantly manifests in terms of modified specific heat ratio $\gamma$ and bulk viscosity $\eta_B$, which is crucial for a number of aerodynamic and turbomachinery engineering applications (von Backstrom 2008; Wu et al. 2015). The specific heat ratio predicted by the Boltzmann equation is that of a monoatomic gas ($\gamma = 5/3$), whereas that of a diatomic gas is 7/5.

Two-particle kinetic theory as an extension of the Boltzmann equation as expected correctly predicts the specific heat ratio for polyatomic gases along with heat conductivity and the bulk viscosity (Wang-Chang & Uhlenbeck 1951; Wu et al. 2015; Chapman & Cowling 1970). However, it is often not feasible to do any analysis on the Boltzmann-type equation for polyatomic gases. Therefore, several simplifications to model polyatomic gases have also been proposed. They essentially incorporate the rotational kinetic energy by decomposing the two-particle distribution function into two independent single-particle distribution functions (Morse 1964; Andries et al. 2000; Tsutahara et al. 2008; Kataoka & Tsutahara 2004; Watari 2007; Nje et al. 2008; Larina & Rykov 2010; Wu et al. 2015; Wang et al. 2017; Bernard et al. 2019). Furthermore, a thermodynamic framework and extensions thereof were developed for modelling highly nonequilibrium phenomena in dense and rarefied polyatomic gases where the Navier–Stokes–Fourier theory is no longer valid (Müller & Ruggeri 2013; Ruggeri & Sugiyama 2015; Arima et al. 2012). A few BGK like models have also been proposed for polyatomic gases which accept the Prandtl number as a tunable parameter (Andries et al. 2000; Brull & Schneider 2009).

Hydrodynamic simulations for a realistic system require the development of reduced-order models to account for rotational degrees of freedom ideally without increasing the phase-space dimensionality. Indeed, the standard approach is to demonstrate that the two-particle distribution function describing the translational and rotational degree of freedom can be approximated by considering two single-particle distribution functions (one each for the translational and rotational degree of freedom) whose dynamics are coupled to each other (Andries et al. 2000). However, recently it was pointed out that a simplified description in terms of single-particle distribution function for the translational degree of freedom and a scalar field variable for rotational kinetic energy is sufficient for modelling the change in specific heat ratio for a dilute diatomic gas in the hydrodynamic limit (Kolluru et al. 2020a). This model supplemented the standard Boltzmann BGK equation with an advection-relaxation equation for the evolution of rotational energy. It preserved the correct conservation laws for diatomic gases in the hydrodynamic limit and satisfied the $H$ theorem. However, the model was restricted to diatomic gases and a Prandtl number 7/5, limiting its application for heat transfer problems.

We propose a kinetic model of polyatomic gases to tune Prandtl number, specific heat ratio, and bulk viscosity in a physically transparent fashion. To do so, we write a new collision kernel which is a linear combination of the ES–BGK and BGK kernels.
that are locally relaxing to different temperatures at different times scales. The ratio of the two relaxation timescales is used to tune the Prandtl number. We couple the evolution of the single-particle distribution function (with this modified collision kernel) via an advection-diffusion-relaxation equation for the rotational energy. The rotational contribution to the internal energy alters the specific heat ratio to that of a polyatomic gas and allows to model bulk viscosity contribution arising out of the rotational degree of freedom. Such an extension of the ES–BGK model indeed reproduces the hydrodynamic behaviour of a polyatomic gas and also has a valid $H$ theorem. These minimal extensions of the ES–BGK model of monoatomic gas are constructed at a single-particle level for polyatomic gases and are phenomenological by construction. It is commensurate with the top-down modelling approach as developed in the context of the lattice Boltzmann models and aim to be analytically and numerically tractable (Succi 2001, Ansumali et al. 2007b, Atif et al. 2017). The present model which requires only the solution of an advection-diffusion-relaxation equation along with the Boltzmann ES–BGK equation adds only a minor complexity over analogous monoatomic gas ES–BGK model and can be implemented in the mesoscale framework such as lattice Boltzmann (LB) method quite easily. This approach is distinctly different and is more detailed than the existing approach in the LB models where the effect of rotational degree of freedom is further coarse-grained and the correction needed to model specific heat ratio is directly added as a force term in the BGK collision model (Kataoka & Tsutahara 2004, Nie et al. 2008, Chen et al. 2010, Huang et al. 2020). In contrast, this model of polyatomic gas enlarges the set of microscopic degrees of freedom and models dynamics of rotational energy in an explicit manner.

The manuscript is organized as follows: A brief kinetic description of monoatomic and polyatomic gases is given in Sections 2 and 3 respectively. In Section 4 we propose an extension to the ES–BGK model for polyatomic gases. The lattice Boltzmann formulation is described in Section 5. The proposed model is numerically validated in Section 6.

2. Kinetic description of a monoatomic gas

The dynamics of dilute monoatomic gases is well-described by the Boltzmann equation in terms of the evolution of the single-particle distribution function $f$, where $f(x, c, t) \, dx \, dc$ is the probability of finding a particle within $(x, x + dx)$, possessing a velocity in the range $(c, c + dc)$ at a time $t$. The hydrodynamic variables are density $\rho(x, t)$, velocity $u(x, t)$ and total energy $E(x, t) = (\rho u^2 + 3\rho k_B T/m)/2$. Here onwards, we use a scaled temperature $\theta$ defined in terms of Boltzmann constant $k_B$ and mass of the particle $m$ as $\theta = k_B T/m$. The thermodynamic pressure $p$ and the scaled temperature $\theta$ are related via the ideal gas equation of state as $p = \rho \theta$. These hydrodynamic variables are computed as the moments of the single-particle distribution function

$$\{\rho, \rho u, E\} = \left\langle \left\{1, c, \frac{c^2}{2}\right\}, f \right\rangle,$$

(2.1)

where we define the averaging operator $\left\langle \phi_1(c), \phi_2(c)\right\rangle = \int_{-\infty}^{\infty} \phi_1(c)\phi_2(c) dc$. In the comoving reference frame with fluctuating velocity $\xi = c - u$, the stress tensor $\sigma_{\alpha\beta}$ is traceless part of the flux of the momentum tensor $\Theta_{ij} \equiv \sigma_{\alpha\beta} + \rho \theta \delta_{\alpha\beta}$ and the heat flux $q_\alpha$ is the flux of the energy. Thus,

$$\Theta_{ij} \equiv \left\langle \xi_i\xi_j, f \right\rangle, \quad \sigma_{\alpha\beta} = \left\langle \xi_\alpha\xi_\beta, f \right\rangle, \quad q_\alpha = \left\langle \xi_\alpha\frac{\xi^2}{2}, f \right\rangle,$$

(2.2)
where the symmetrized traceless part $A_{\alpha \beta}$ for any second-order tensor $A_{\alpha \beta}$ is $A_{\alpha \beta} = (A_{\alpha \beta} + A_{\beta \alpha} - 2A_{\gamma \delta} \delta_{\alpha \beta}/3)/2$. The stress tensor and heat flux tensor are related to the pressure tensor $P_{\alpha \beta} = \langle c_c c_\beta, f \rangle$ and energy flux $\langle c^2 c_\alpha / 2, f \rangle$ respectively as

$$\sigma_{\alpha \beta} = P_{\alpha \beta} - \rho u_\alpha u_\beta - \rho \theta \delta_{\alpha \beta}, \quad q_\alpha = \left\langle \frac{c^2 c_\alpha}{2}, f \right\rangle - u_\alpha (E + \rho \theta) - u_\beta \sigma_{\alpha \beta}. \quad (2.3)$$

We also define third-order moment $Q_{\alpha \beta \gamma}$, with the traceless part $Q_{\alpha \beta \gamma}$ and the fourth-order moments divided into contracted part $R_{\alpha \beta}$ and the trace $R$

$$Q_{\alpha \beta \gamma} = \langle \xi_\alpha \xi_\beta \xi_\gamma, f \rangle, \quad Q_{\alpha \beta \gamma} = Q_{\alpha \beta \gamma} - \frac{2}{3} (q_\alpha \delta_{\beta \gamma} + q_\beta \delta_{\alpha \gamma} + q_\gamma \delta_{\alpha \beta}), \quad (2.4)$$

$$R_{\alpha \beta} = \langle \xi^2 \xi_\alpha \xi_\beta, f \rangle, \quad R = \langle \xi^4, f \rangle. \quad (2.5)$$

In the dilute gas limit, the time evolution of the distribution function is a sequence of free-flight and binary collisions well described by the Boltzmann equation

$$\partial_t f + c_\alpha \partial_\alpha f = \Omega(f, f), \quad (2.6)$$

where the collision kernel $\Omega(f, f)$ models the binary collisions between particles under the assumptions of molecular chaos (Chapman & Cowling 1970; Cercignani 1988, McQuarrie 2000). The nonlinear integro-differential Boltzmann collision kernel is often replaced by simpler models that should recover the following essential features (Cercignani 1988):

(a) **Conservation Laws:** As the mass, momentum, and energy density of the particles are conserved during the elastic collision, any collision model must satisfy

$$\langle \Omega(f, f), \{1, c, c^2\} \rangle = \{0, 0, 0\}. \quad (2.7)$$

Thus, the macroscopic conservation laws obtained by taking appropriate moments (with respect to $\{1, c, c^2\}$) of the Boltzmann equation

$$\partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0, \quad \partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta + \rho \theta \delta_{\alpha \beta} + \sigma_{\alpha \beta}) = 0, \quad \partial_t E + \partial_\alpha [(E + p) u_\alpha + q_\alpha + \sigma_{\alpha \beta} u_\beta] = 0, \quad (2.8)$$

are the same as those of the compressible hydrodynamics.

(b) **Zero of collision:** The collision term is zero if and only if the distribution function attains Maxwell–Boltzmann form, i.e.,

$$\Omega(f, f) = 0 \iff f = f^{MB}, \quad (2.9)$$

where the Maxwell–Boltzmann distribution $f^{MB}$ is

$$f^{MB}(\rho(f), u(f), \theta(f)) = \rho \left( \frac{1}{2\pi \theta} \right)^{3/2} \exp \left( -\frac{(c - u)^2}{2 \theta} \right), \quad (2.10)$$

which ensures that the dynamics is consistent with the equilibrium thermodynamics.

(c) **The H Theorem:** The Boltzmann equation generalizes the second law of thermodynamics to nonequilibrium situations. Boltzmann defined a nonequilibrium generalization of the entropy known as the $H$ function (Cercignani 1988)

$$H[f] = \int (f \ln f - f) dc. \quad (2.11)$$
At equilibrium, the thermodynamic entropy is calculated as \( S_{\text{eq}} = -k_B H[f^\text{MB}] = -\rho k_B \left[ \ln \frac{\rho}{(2\pi\theta)^{3/2}} - \frac{5}{2} \right] \). (2.12)

The evolution of this \( H \) function is

\[
\partial_t H + \partial_\alpha J^H_\alpha = \langle \Omega(f,f), \ln f \rangle \Sigma \leq 0, \tag{2.13}
\]

where \( J^H_\alpha \) is the entropy flux and \( \Sigma \) is the negative of the entropy generation. Boltzmann demonstrated that the entropy generation is positive, hence, the \( H \) function is nonincreasing in time (Cercignani 1988). Thus, any consistent approximation for the Boltzmann collision kernel should also satisfy the same condition.

We briefly describe the two most widely used models, the BGK collision model and the ES–BGK model. The Bhatnagar–Gross–Krook (BGK) model, perhaps the simplest and most widely-used model of the Boltzmann collision kernel models the collision as a relaxation of the distribution function towards the equilibrium \( f^\text{MB} \) (Bhatnagar et al. 1954) as

\[
\Omega_{\text{BGK}} = \frac{1}{\tau} (f^\text{MB}(\rho, u, \theta) - f). \tag{2.14}
\]

This assumes that the process occurs at a single time scale \( \tau \) corresponding to the mean free time. It is trivial to see that this model has the same collisional invariants as the Boltzmann kernel, hence, recovers the same conservation laws (Bhatnagar et al. 1954). The entropy production \( \Sigma_{\text{BGK}} \) due to the BGK model is written as

\[
\Sigma_{\text{BGK}} = \langle \Omega_{\text{BGK}}, \ln f \rangle = \frac{1}{\tau} \int (f^\text{MB}(\rho, u, \theta) - f) \ln \left( \frac{f}{f^\text{MB}(\rho, u, \theta)} \right) dc \leq 0. \tag{2.15}
\]

Thus, like the Boltzmann equation, the BGK model also satisfies the \( H \) theorem. By taking appropriate moments of the Boltzmann BGK equation, we can also see that the evolution of the stress and the heat flux are (Liboff 2003)

\[
\begin{align*}
\partial_t \sigma_{\alpha\beta} + \partial_\gamma (\sigma_{\alpha\beta}u_\gamma) + \partial_\gamma Q_{\alpha\beta\gamma} + 2\sigma_{\gamma\beta} \partial_\gamma u_\alpha + 2p \partial_\gamma u_\alpha + \frac{4}{5} \partial_\beta q_\alpha &= -\frac{1}{\tau} \sigma_{\alpha\beta}, \\
\partial_t q_\alpha + \frac{1}{2} \partial_\beta \left( R_{\alpha\beta} + \frac{1}{3}\delta_{\alpha\beta} \right) + Q_{\alpha\beta\gamma} \partial_\gamma u_\beta + \partial_\beta (q_\alpha u_\beta) + \frac{7}{5} q_\beta \partial_\beta u_\alpha &= 0. \tag{2.16}
\end{align*}
\]

The form of relaxation dynamics shows that the time-scales for the momentum diffusivity and thermal diffusivity are equal for the BGK model. These equations show that, like any equation of Boltzmann type, the dynamics of \( M^{th} \) order moment involves \((M + 1)^{th}\) moment and thus form an infinite order moment chain. The hydrodynamic limit is typically analysed via Chapman–Enskog expansion which allows evaluating the dynamic viscosity \( \mu \) and thermal conductivity \( \kappa \) for the model with the specific heat \( C_p \) for a monoatomic ideal gas as \( 5/2 \) is (Chapman & Cowling 1970)

\[
\mu = \rho \tau, \quad \kappa = \frac{5}{2} \rho \tau \quad \implies \Pr = \frac{\mu C_p}{\kappa} = 1. \tag{2.17}
\]

Despite this defect of \( \Pr = 1 \), the BGK model is extremely successful both as a numerical and an analytical tool for analysis. The ES–BGK model (Holway Jr 1965) also describes
the collision as simple relaxation process but unlike the BGK model, it overcomes
the restriction on the Prandtl number. The extra ingredient for ES–BGK model is
 quasi-equilibrium form of distribution derived by minimizing the $H$–function (Eq. (2.11))
under the constraints of an additional condition of fixed stresses, which implies absolute
minimization of

$$
\Xi[f] = \int df \left[ (f \ln f - f) + \alpha f + \beta_j c_j f + \gamma_{ij} c_i c_j f \right].
$$

(2.18)

The solution to this minimization problem is an anisotropic Gaussian

$$
f^{\text{Quasi}}(\rho, \mathbf{u}, \Theta_{ij}) = \frac{\rho}{\sqrt{\det[2\pi \Theta_{ij}]}} \exp \left( -\frac{1}{2} \xi_i \Theta_{ij}^{-1} \xi_j \right).
$$

(2.19)

Like the MB distribution, this has the same conserved moments as that of the single-
particle distribution function but this also treats $\Theta_{ij}(f)$ as a conserved variable (Kogan
1969) i.e.,

$$
\{\rho(f^{\text{Quasi}}), u_\alpha(f^{\text{Quasi}}), \theta(f^{\text{Quasi}}), \Theta_{ij}(f^{\text{Quasi}})\} = \{\rho(f), u_\alpha(f), \theta(f), \Theta_{ij}(f)\}.
$$

(2.20)

On this quasi-equilibrium manifold with stress as variable when the $H$ is minimum we have

$$
H[f^{\text{Quasi}}(\rho, \mathbf{u}, \Theta_{ij})] = \rho \ln \left( \frac{\rho}{\sqrt{\det[2\pi \Theta_{ij}]}} \right) - \frac{5}{2} \rho.
$$

(2.21)

The ES–BGK model uses the anisotropic Gaussian distribution $f^{\text{ES}} \equiv f^{\text{Quasi}}(\rho, \mathbf{u}, \lambda_{ij})$

$$
f^{\text{ES}}(\rho, \mathbf{u}, \lambda_{ij}) = \frac{\rho}{\sqrt{\det[2\pi \lambda_{ij}]}} \exp \left( -\frac{1}{2} \xi_i \lambda_{ij}^{-1} \xi_j \right),
$$

(2.22)

where instead of pressure tensor a positive definite matrix $\lambda_{ij}$

$$
\lambda_{ij} = (1 - b) \delta_{ij} + b \Theta_{ij} \equiv \theta \delta_{ij} + b \sigma_{ij},
$$

(2.23)

is used with $-1/2 \leq b \leq 1$ as a free parameter, the range of $b$ is dictated by the positive
definiteness of $\lambda_{ij}^{-1}$. For $0 \leq b \leq 1$, $\lambda_{ij}$ is trivially positive as it is a convex combination of
two positive definite matrices. The non-trivial range $-1/2 \leq b < 0$ is better understood from the eigenvalue analysis of $\lambda_{ij}$ (Andries et al. 2000). Let the eigenvalues of $\lambda_{ij}$ be $\Lambda_i$
and that of positive definite matrix $\Theta_{ij}$ be $\phi_i$ and thus $\phi_1 + \phi_2 + \phi_3 = \Lambda_1 + \Lambda_2 + \Lambda_3 = 3\theta$. In terms of these eigenvalues, the matrix $\lambda$ after suitable rotation can be rewritten as

$$
\lambda = \begin{pmatrix}
(1 - b)\theta + b\phi_1 & 0 & 0 \\
0 & (1 - b)\theta + b\phi_2 & 0 \\
0 & 0 & (1 - b)\theta + b\phi_3
\end{pmatrix},
$$

(2.24)

which is a convex combination of diagonal matrices $\Psi_1, \Psi_2$ and $\Psi_3$ as

$$
\lambda = \left( \frac{1 + 2b}{3} \right) \begin{pmatrix}
\phi_1 & 0 & 0 \\
0 & \phi_2 & 0 \\
0 & 0 & \phi_3
\end{pmatrix}_{\Psi_1} + \left( \frac{1 - b}{3} \right) \begin{pmatrix}
\phi_2 & 0 & 0 \\
0 & \phi_3 & 0 \\
0 & 0 & \phi_1
\end{pmatrix}_{\Psi_2} + \left( \frac{1 - b}{3} \right) \begin{pmatrix}
\phi_3 & 0 & 0 \\
0 & \phi_1 & 0 \\
0 & 0 & \phi_2
\end{pmatrix}_{\Psi_3}.
$$

(2.25)

As in the diagonal representation, the non-zero components are the eigenvalues and one
obtains the relationship between $\phi_i$ and $\Lambda_i$ as

$$ A_i = \left( \frac{1 + 2b}{3} \right) \phi_i + \left( \frac{1 - b}{3} \right) \sum_{i \neq j} \phi_j. \quad (2.26) $$

Thus, the eigenvalues of $\lambda_{ij}$ are non-negative if the range of $b$ is restricted to $-1/2 \leq b \leq 1$ as we also know that $\phi_i \geq 0$. In the ES–BGK model, the collisional relaxation is towards this anisotropic Gaussian distribution $f^{ES}$ which itself attains the form of the Maxwellian at the equilibrium. The collision kernel in explicit form is

$$ \Omega_{ESBGK} = \frac{1}{\tau} \left( f^{ES} (\rho, u, \lambda_{ij}) - f \right), \quad (2.27) $$

where it is evident that $b = 0$ corresponds to the limit of the BGK equation and $b = 1$ would imply that stress is conserved. For $b \neq 1$, the model has the same set of conservation laws as the BGK equation. As the stress and heat flux tensors follow the relation

$$ \sigma_{\alpha\beta} (f^{ES}) = b \sigma_{\alpha\beta} (f), \quad \langle \xi_\alpha \xi_\beta^2, f^{ES} \rangle = 0, \quad (2.28) $$

thus, the evolution equations for stress tensor and heat flux are

$$ \partial_t \sigma_{\alpha\beta} + \partial_\gamma (u_\gamma \sigma_{\alpha\beta}) + \partial_\gamma Q_{\alpha\beta\gamma} + 2p \partial_\beta \sigma_{\alpha\beta} + \frac{4}{5} \partial_\beta q_\alpha = - \left( \frac{1 - b}{\tau} \right) \sigma_{\alpha\beta}, $$

$$ \partial_t q_\alpha + \frac{1}{2} \partial_\beta \left( R_{\alpha\beta} + \frac{1}{3} R \sigma_{\alpha\beta} \right) + \frac{Q_{\alpha\beta\gamma}}{5} \partial_\gamma u_\beta + \partial_\beta (q_\alpha u_\beta) + \frac{7}{5} q_\beta \partial_\beta u_\alpha + \frac{2}{5} q_\alpha \partial_\beta \sigma_{\alpha\beta} - \frac{2}{5} p \partial_\beta \sigma_{\alpha\beta} - \frac{2}{5} p \partial_\beta \sigma_{\alpha\beta} = - \frac{q_\alpha}{\tau}, \quad (2.29) $$

which shows that the momentum and thermal diffusivities are different in an ES–BGK model and the Prandtl number $Pr = \mu c_p/\kappa$ is a free parameter. In particular, the Chapman-Enskog analysis of this model yields

$$ \mu = \frac{p \tau}{1 - b}, \quad \kappa = \frac{5}{2} p \tau \quad \Rightarrow \quad Pr = \frac{1}{1 - b}. \quad (2.30) $$

Thus, the free parameter $b$ in the anisotropic Gaussian allows one to vary the Prandtl number from $2/3$ to infinity. At $b = -1/2$, the Prandtl number predicted by the ES–BGK model is $2/3$, which matches with the value obtained from the Boltzmann equation, and when $b = 0$, the model is equivalent to the BGK model. The thermal conductivity is fixed only by $\tau$ while the viscosity can be tuned via $b$ to obtain the required Prandtl number.

The $H$ theorem for this model was first proved by [Andries & Perthame (2001)] by showing that the entropy production $\Sigma^{ESBGK}$ is non-positive. We briefly review the proof of the $H$ theorem for the ES-BGK model. The expression for the entropy production is

$$ \Sigma^{ESBGK} = \langle \Omega_{ESBGK}, \ln f \rangle = \frac{1}{\tau} \left\langle \left( f^{ES} (\rho, u, \lambda_{ij}) - f \right), \frac{\partial H}{\partial f} \right\rangle. \quad (2.31) $$

The proof is built on the property of an arbitrary convex function $G(x)$ that

$$ \frac{\partial G}{\partial x} (y - x) \leq G(y) - G(x) \quad (2.32) $$

using which we can write

$$ \Sigma^{ESBGK} \leq \frac{1}{\tau} \left( H \left[ f^{ES} (\rho, u, \lambda_{ij}) \right] - H \left[ f^{Quasi} (\rho, u, \Theta_{ij}) \right] \right) + \frac{1}{\tau} \Delta H^{Quasi}, \quad (2.33) $$
with the last term as $\Delta H^{\text{Quasi}} = H[f^{\text{ES}}(\rho, u, \Theta_{ij})] - H[f]$ in the above equation is non-positive as $f^{\text{Quasi}}(\rho, u, \Theta_{ij})$ is by construction the minima of $H$. To prove that $H[f^{\text{ES}}(\rho, u, \lambda_{ij})] - H[f^{\text{Quasi}}(\rho, u, \Theta_{ij})] \leq 0$, using Eq. (2.21) we have

$$H[f^{\text{ES}}(\rho, u, \lambda_{ij})] - H[f^{\text{Quasi}}(\rho, u, \Theta_{ij})] = \frac{1}{2} \rho \ln \left( \frac{\det[\Theta_{ij}]}{\det[\lambda_{ij}]} \right). \hspace{1cm} (2.34)$$

Starting from the Brunn-Minkowsky inequality

$$\det[aA + (1-a)B] \geq (\det[A])^a (\det[B])^{1-a}, \hspace{1cm} (2.35)$$

relating the determinants of two positive matrices $A$ and $B$ and their convex combinations, we can show that $\det[\lambda_{ij}] \geq \det[\Theta_{ij}]$ (Horn & Johnson 2012). This inequality along with Eq. (2.25) allows us to write

$$\det[\lambda_{ij}] \geq (\det[\Psi_1])^{\frac{1+2b}{4}} (\det[\Psi_2])^{\frac{1+b}{4}} (\det[\Psi_3])^{\frac{1+b}{4}}. \hspace{1cm} (2.36)$$

However, from the definitions of $\Psi_1, \Psi_2, \text{and} \Psi_3$ one can see that

$$\det[\Psi_1] = \det[\Psi_2] = \det[\Psi_3] = \phi_1 \phi_2 \phi_3 = \det[\Theta_{ij}]. \hspace{1cm} (2.37)$$

Hence, the total entropy production is non-positive, i.e., $\Sigma^{\text{ESBGK}} \leq 0$.

3. Kinetic description of a polyatomic gas

The rotational degrees of freedom of a polyatomic gas manifest themselves at the continuum level in terms of change in specific heat ratio $\gamma$ and a non-zero bulk viscosity due to interaction among the translational component $E_T = \rho u^2/2 + 3\rho \theta_T/2$ and rotational component $E_R$ of energy. Thus, the rotational degrees of freedom need to be explicitly accounted for in any microscopic or kinetic description. Indeed, typically the kinetic descriptions are in terms of a two-particle distribution function $F(x, c, t, I)$ which defines the probability of finding a molecule with a position in the range $(x, x + dx)$ possessing a velocity in the range $(c, c + dc)$ with an internal energy $(I, I + dI)$ due to the additional degrees of freedom (Morse 1964; Rykov 1975; Kusćet 1989). For a polyatomic gas with $\delta$ additional rotational degrees of freedom, the moments of this distribution function give the density, momentum, and total energy (with $\delta = 0$ corresponding to a monoatomic gas)

$$\{\rho, \rho u, E_T + E_R\} = \left\langle \left\{ \frac{1}{2} c^2 + I^2/\delta \right\}, F \right\rangle, \hspace{1cm} (3.1)$$

like its monoatomic counterpart and the operator $\langle \langle \cdot, \cdot \rangle \rangle$ is defined as

$$\langle \langle \phi_1(c, I), \phi_2(c, I) \rangle \rangle = \int \int \phi_1(c, I) \phi_2(c, I) dcdI. \hspace{1cm} (3.2)$$

For the reduced-order modeling, the distribution function $F(x, c, t, I)$ is often split into two coupled distribution functions $f_1(x, c, t)$ and $f_2(x, c, t)$ defined as

$$f_1(x, c, t) = \int F(x, c, I, t) dI, \hspace{1cm} f_2(x, c, t) = \int F(x, c, I, t) I^{2/\delta} dI, \hspace{1cm} (3.3)$$

where $f_1$ is related to the translational energy and $f_2$ with the rotational energy dynamics (Rykov 1975; Andries et al., 2000). The moments of reduced distribution $f_1(x, c, t)$ are then same as the moments of single-particle distribution function

$$\{\rho, \rho u, E_T\} = \left\langle \left\{ \frac{1}{2} c^2 \right\}, f_1 \right\rangle. \hspace{1cm} (3.4)$$
By construction, we have the zeroth moment of $f_2(x, c, t)$ as the rotational energy

$$E_R = \left\langle \frac{\langle c^2 \rangle}{2} + I^{2/\delta}, F \right\rangle - \left\langle \frac{\langle c_1^2 \rangle}{2} \right\rangle = \left\langle \left\langle F, I^{2/\delta} \right\rangle \right\rangle \equiv \left\langle f_2, 1 \right\rangle = \frac{\delta}{2} \rho \theta R. \tag{3.5}$$

In other words, the temperature $\theta$ consists of contributions from the translational and rotational temperatures, and they follow the relation

$$\theta = \left( \frac{3}{3 + \delta} \right) \theta_T + \left( \frac{\delta}{3 + \delta} \right) \theta_R, \tag{3.6}$$

and in thermodynamic equilibrium the equipartition of energy requires $\theta_R = \theta_T$. The heat flux for a polyatomic gas is $q_\alpha = q_\alpha^T + q_\alpha^R$ where $q_\alpha^T$ is the translational heat flux and $q_\alpha^R$ is an additional heat flux due rotational energy. The rotational heat flux and a stress like quantity (second moment) are defined as

$$q_\alpha^R = \int d\xi f_2 \xi_\alpha, \quad \sigma_{\alpha\beta}^R = \int d\xi f_2 \xi_\alpha \xi_\beta - \rho \theta^2 \delta_{\alpha\beta}. \tag{3.7}$$

Like the monoatomic gas, the evolution equation for this distribution function $F(x, c, t, I)$ with collisional kernel $\Omega(F, F)$ in the Boltzmann form is

$$\partial_t F + c_\alpha \partial_\alpha F = \Omega(F, F), \tag{3.8}$$

which is consistent with the equipartition of energy at equilibrium \cite{Pullin1978, Kusscher1989}. Similar to the monoatomic gas, one defines the BGK collision kernel in terms of the two-particle distribution function for a polyatomic gas as \cite{Brull&Schneider2009}

$$\Omega_{\text{BGK}} = \frac{1}{\tau} \left( F_{\text{MB}}(\rho, u, \theta, I) - F \right), \tag{3.9}$$

with normalisation factor $A_\delta = \int \exp \left( -\frac{1}{2} I^{2/\delta} \right) dI$. Equation \eqref{3.8} with $\Omega_{\text{BGK}}$ is written as two kinetic equations for the reduced distributions $f_1(x, c, t)$ and $f_2(x, c, t)$ by multiplying with 1 and $I^{2/\delta}$ and then integrating over the internal energy variable as

$$\partial_t f_1 + c_\alpha \partial_\alpha f_1 = \frac{1}{\tau} \left( f_{1 \text{MB}}(\rho, u, \theta) - f_1 \right),$$

$$\partial_t f_2 + c_\alpha \partial_\alpha f_2 = \frac{1}{\tau} \left( \frac{\delta}{2} f_{1 \text{MB}}(\rho, u, \theta) - f_2 \right). \tag{3.10}$$

This approach, where two reduced distributions are weakly coupled via temperature, recovers all the features of Eq.\eqref{3.9} and is widely adopted for polyatomic gases. \cite{Andries2000} extended this approach via an extended ES–BGK collision kernel as

$$\Omega_{\text{ESBGK}}(F) = \frac{Z_{\text{ES}}}{\tau} \left( F_{\text{ES}}(\rho, u, \lambda_{ij}, \theta_{\text{rel}}) - F \right), \tag{3.11}$$

where $\lambda_{ij} = (1 - \alpha) [(1 - b) \theta_T \delta_{ij} + b \Theta_{ij}] + \alpha \theta \delta_{ij}$ with a generalized Gaussian $F_{\text{ES}}$

$$F_{\text{ES}}(\rho, u, \lambda_{ij}, \theta_{\text{rel}}) = \frac{\rho A_\delta}{\theta_{\text{rel}}^{3/2} \sqrt{\det[2\pi \lambda_{ij}]}} \exp \left( -\frac{1}{2} \xi_i \lambda_{ij}^{-1} \xi_j - \frac{I^{2/\delta}}{\theta_{\text{rel}}} \right), \tag{3.12}$$

with $\theta_{\text{rel}} = \alpha \theta + (1 - \alpha) \theta_R$ and $Z_{\text{ES}} = 1/(1 - b + b\alpha)$. Similar to the monoatomic ES–BGK model, the parameter $b$ is used to tune the Prandtl number, while parameter $\alpha$ is
used to tune the bulk viscosity coefficient independently. The reduced description which generalizes the ES–BGK model in terms of the $f_1$ and $f_2$ is

$$
\frac{\partial}{\partial t} f_1 + c_\alpha \partial_\alpha f_1 = \frac{Z_{\text{ES}}}{\tau} \left( f_{\text{ES}}^{\rho,\lambda}(\rho, u, \lambda_{ij}) - f_1 \right),
$$

$$
\frac{\partial}{\partial t} f_2 + c_\alpha \partial_\alpha f_2 = \frac{Z_{\text{ES}}}{\tau} \left( \frac{\delta}{2} \theta_{\text{rel}} f_{\text{ES}}^{\rho,\lambda}(\rho, u, \lambda_{ij}) - f_2 \right). 
$$

(3.13)

A common feature between Eqs. (3.10) and (3.13) is that the kinetic equation for translation distribution function $f_1$ is coupled with the kinetic equation for the rotational distribution function $f_2$ via rotational temperature $\theta_R$ only. At this point, it might be instructive to analyse the moment chains of the BGK and ES–BGK systems. As both the collision kernels conserve mass and momentum, the evolution equations for density and momentum are of the same form as that of monoatomic gas. In particular

$$
\frac{\partial}{\partial t} \rho + \partial_\alpha (\rho u_\alpha) = 0,
$$

$$
\frac{\partial}{\partial t} (\rho u_\alpha) + \partial_\alpha (\rho u_\alpha u_\beta + \rho \theta \delta_{\alpha\beta} + \sigma_{\alpha\beta}) = 0,
$$

(3.14)

where $\sigma_{\alpha\gamma} = \sigma_{\alpha\gamma} + \rho (\theta_T - \theta) \delta_{\alpha\gamma}$ is the modified stress tensor and the velocity evolution is

$$
\frac{\partial}{\partial t} u_\alpha + u_\beta \partial_\beta u_\alpha + \frac{1}{\rho} \partial_\alpha (\rho \theta \delta_{\alpha\beta} + \sigma_{\alpha\beta}) = 0.
$$

(3.15)

For polyatomic gases, the energy equation gets an additional contribution from the rotational energy. In both the BGK and ES–BGK models, the evolution equation for translational part of the energy and the rotational part of the energy $E_R = \delta \rho \theta_R / 2$ are of the form

$$
\frac{\partial}{\partial t} E_T + \partial_\alpha \left[ (E_T + \rho \theta) u_\alpha + q_T^\alpha + u_\gamma \sigma_{\alpha\gamma} \right] = \frac{Z_E}{\tau} \frac{3\rho}{2} (\theta - \theta_T),
$$

$$
\frac{\partial}{\partial t} E_R + \partial_\alpha \left( E_R u_\alpha + q_R^\alpha \right) = \frac{Z_E}{\tau} \frac{\delta \rho}{2} (\theta - \theta_R),
$$

(3.16)

with $Z_E = 1$ for the BGK model and $Z_E = \alpha Z_{\text{ES}}$ for the ES–BGK model. The evolution equation for the total energy is written as the sum of Eqs. (3.16) as

$$
\frac{\partial}{\partial t} (E_T + E_R) + \partial_\alpha \left[ (E_T + E_R + \rho \theta) u_\alpha + q_\alpha + u_\gamma \sigma_{\alpha\gamma} \right] = 0,
$$

(3.17)

where the relationship between translational, rotational temperatures (Eq. (3.6)) is used to show that energy is collisional invariant. From Eqs. (3.10) and (3.13), the stress evolution and the translational heat flux evolution equations in explicit form are

$$
\frac{\partial}{\partial t} \sigma_{\alpha\beta} + \partial_\gamma (u_\gamma \sigma_{\alpha\beta}) + \frac{1}{5} \partial_\beta q_T^{\alpha\beta} + 2 \rho \theta_T \partial_\beta u_\alpha + 2 \partial_\gamma u_\alpha \sigma_{\alpha\gamma} = \frac{1}{\tau} \sigma_{\alpha\beta},
$$

$$
\frac{\partial}{\partial t} q_T^{\alpha\beta} + \partial_\beta \left( u_\beta q_T^{\alpha\beta} \right) + \frac{1}{\tau} \partial_\beta R_{\alpha\beta} + \frac{7}{5} q_T^{\alpha\beta} \partial_\beta u_\alpha + \frac{2}{\tau} q_T^{\alpha\beta} \partial_\gamma u_\gamma + \frac{2}{\tau} q_T^{\alpha\beta} \partial_\beta u_\beta
$$

$$
- \frac{5}{2} \theta_T \partial_\alpha (\rho \theta_T) - \frac{\sigma_{\alpha\beta}}{\rho} \partial_\beta (\rho \theta_T) - \frac{5}{2} \theta_T \partial_\kappa \sigma_{\kappa\alpha} - \frac{\sigma_{\alpha\beta}}{\rho} \partial_\kappa \sigma_{\kappa\beta} = -Z_q q_T^{\alpha\beta},
$$

(3.18)

with $Z_q = 1$ for BGK and $Z_q = Z_{\text{ES}}$ for the ES–BGK model. Multiplying rotational energy equation from Eq. (3.16) with $u_\alpha$ and using Eq. (3.15) we have

$$
\frac{\partial}{\partial t} (E_R u_\alpha) + \partial_\beta \left( E_R u_\alpha u_\beta + q_R^\alpha \right) + \frac{E_R}{\rho} \partial_\beta (\rho \theta \delta_{\alpha\beta} + \sigma_{\alpha\beta}) = \frac{Z_E}{\tau} \frac{\delta}{2 \rho} u_\alpha (\theta - \theta_R),
$$

(3.19)
using which the rotational heat flux evolution obtained as first moment of $f_2$ dynamics is

$$\partial_t q^R_{\alpha} + \partial_\beta (u_\beta q^R_{\alpha}) + q^R_{\beta} \partial_\beta u_{\alpha} + \partial_\beta \sigma^R_{\alpha\beta} + \partial_\alpha \left( \frac{\delta}{2} \rho \theta^2 \right) - \frac{\delta}{2} \theta_R \partial_\beta (\rho \theta \delta_{\alpha\beta} + \delta_{\alpha\beta}) = -\frac{Z_q}{\tau} q^R_{\alpha},$$

(3.20)

where $\sigma^R_{\alpha\beta} = \int f_2 \xi_\alpha \xi_\beta$. The Eqs. (3.14) and (3.17) form the compressible Navier–Stokes–Fourier equations for a polyatomic gas. A Chapman-Enskog analysis shows that the Eq. (3.14) can be written in familiar compressible Navier–Stokes equation form as

$$\partial_t (\rho u_{\alpha}) + \partial_\beta (\rho u_\beta u_\alpha) + \partial_\alpha \rho - \partial_\beta (2\eta \partial_\beta u_\alpha + \eta_\theta \partial_\alpha \theta) = 0$$

(3.21)

with the shear and bulk viscosities

$$\eta = \rho \tau, \quad \eta_\theta = \frac{2\delta}{3(3 + \delta) Z E}.$$  

(3.22)

Similarly, an analysis of the translational and rotational heat flux dynamics at $O(\text{Kn})$ leads to $q^T_{\alpha} = -\kappa \tau \partial_\alpha \theta$, $q^R_{\alpha} = -\kappa R \partial_\alpha \theta$, with the translational and rotational thermal conductivities $\kappa_T = 5\rho \tau/(2Z_q)$, $\kappa_R = \delta \rho \tau/(2Z_q)$ respectively. The effective thermal conductivity $\kappa = \kappa_T + \kappa_R = (5 + \delta)\rho \tau/(2Z_q)$ thus, the Prandtl number is $Pr = Z_q i.e., Pr = 1$ for BGK model and $Pr = 1/(1 - b + b\alpha)$ for the ES–BGK model.

4. Reduced ES–BGK model for polyatomic gases

In the kinetic theory of gases, one often builds an extended moment system in terms of physically relevant lower-order moments (Grad 1958). In this spirit of Grad’s moment method, one may ask whether a reduced description for rotational degrees of freedom is feasible. It should be noted that the evolution equation of $f_1$ is only weakly coupled with the evolution of $f_2$ via $\theta_R$. An appropriate choice in the current context is a reduced description in terms of lower-order moments of second distribution $f_2$. For example, the rotational component can be modelled by the evolution of two scalars – rotational energy and its flux (which are the zeroth and the first moment of $f_2$). Such a class of reduced-order kinetic models might be better suited for large-scale hydrodynamic simulations. An extended BGK model for diatomic gases was formulated by Kolluru et al (2020a) wherein the BGK collision model was coupled with the rotational part of energy (zeroth moment of $f_2$) which in itself follows an advection-relaxation equation.

We extend this approach by a generalized ES-BGK model for polyatomic gases with tunable Prandtl numbers where the collision term is a linear combination of ES–BGK and the BGK collision kernels. In this model, the ES–BGK term describes relaxation to a temperature $\theta_T$ over a time $\tau$ whereas the BGK collision kernel describes relaxation to a temperature $\theta$ over a time $\tau_1$. The kinetic equation of the unified model along with the evolution equation for the rotational energy is

$$\partial_t f_1 + c_\alpha \partial_\alpha f_1 = \frac{1}{\tau} (f^{\text{ES}}(\rho, u, \theta_T \delta_{\alpha\beta} + b \sigma_{\alpha\beta}) - f_1) + \frac{1}{\tau_1} (f^{\text{MB}}(\rho, u, \theta) - f_1),$$

$$\partial_t (E_R) + \partial_\alpha (E_R u_\alpha + q^R_{\alpha}) = \frac{1}{\tau_1} \left( \frac{\delta}{2} \rho \theta - E_R \right),$$

(4.1)

with the form of heat flux due to internal degrees of freedom as

$$q^R_{\alpha} = -\kappa R \partial_\alpha \theta R.$$  

(4.2)

This model is a minimal extension of the monoatomic ES–BGK model needed for
modeling polyatomic gases which also recovers all important features such as the positivity, macroscopic limit, and the $H$ theorem. Here, the Prandtl number is a tunable parameter due to the presence of two relaxation time scales, whereas the rotational part of the internal energy alters the specific heat ratio to that of a polyatomic gas. The model satisfies the $H$ theorem, thus ensuring convergence to a unique equilibrium state. A few important characteristic of the present model are as follows:

- **Conservation Laws:** The mass and momentum conservation equations for the proposed model are obtained by taking the zeroth and first moments of $f_1$ evolution (Eq. (4.1)). The second moment signifying translational energy evolution equation is

  \[
  \partial_t E_T + \partial_\beta \left[ (E_T + \rho \theta_T) u_\beta + \sigma_{\beta\gamma} u_\gamma + q_\beta \right] = \frac{\rho}{\tau_1} \left[ \frac{3}{2} \theta - \frac{3}{2} \theta_T \right],
  \]

  which when combined with the rotational energy equation shows that the total energy is conserved. This implies that the evolution equation for slow moments

  \[
  M_{\text{slow}} = \left\{ \rho, \rho u_\alpha, \frac{1}{2} \rho u^2 + \left( \frac{3 + \delta}{2} \right) \rho \theta \right\},
  \]

  mass density, momentum density, and total energy density are

  \[
  \partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0, \\
  \partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta + \rho \delta \alpha \beta + \hat{\sigma} \alpha \beta) = 0, \\
  \partial_t (E_T + E_R) + \partial_\beta \left[ (E_T + E_R + \rho \theta) u_\beta + \hat{\sigma} \beta \gamma u_\gamma + q_\beta \right] = 0.
  \]

  Thus, the conservation laws have correct macroscopic form.

- **$H$–Theorem:** For polyatomic gases, a part of entropy production should be due to rotational degrees of freedom. In the current model, as internal degrees of freedom are accounted for in a mean-field manner, similar to the Enskog equation one would expect that entropy contribution should only depend on rotational energy (Resibois 1978). Thus, we write generalized $H$ function for polyatomic gas $H_1$ in Sackur–Tetrode form as a sum of Boltzmann part for monoatomic contribution and rotational part $k \rho \ln \theta_R$ (Huang 2009)

  \[
  H_1 = H + k \rho \ln \theta_R,
  \]

  with $k$ being an unknown scale factor to be fixed later. On multiplying Eq. (4.1) with $\ln f$, and integrating over the velocity space we obtain the evolution of $H$ as

  \[
  \partial_t H + \partial_\alpha J_H^\alpha = \Sigma^{\text{ESBGK}} + \frac{\tau}{\tau_1} \Sigma^{\text{BGK}} \left( f^{\text{MB}}(\rho, u, \theta) \right) - \frac{3 \rho}{2 \tau_1} \frac{\theta - \theta_T}{\theta},
  \]

  where $J_H^\alpha$ is related to the entropy flux with $\Sigma^{\text{ESBGK}}, \Sigma^{\text{BGK}}$ being the entropy production due to the ES–BGK and the BGK terms respectively. The evolution of the rotational energy (second equation in Eq. (4.1)) can be rewritten as

  \[
  \partial_t \ln \theta_R + u_\alpha \partial_\alpha \ln \theta_R + \frac{2}{\delta \rho \theta_R} \partial_\alpha q_R^\alpha = \frac{\theta - \theta_R}{\tau_1 \theta_R}.
  \]

  Multiplying the above equation with $\rho$ and exploiting continuity we obtain

  \[
  \partial_t (\rho \ln \theta_R) + \partial_\alpha \left( \rho u_\alpha \ln \theta_R + \frac{2}{\delta} q_R^\alpha \right) = \frac{\rho}{\tau_1} \frac{\theta - \theta_R}{\theta_R} - \frac{2}{\delta} q_R^\alpha \partial_\alpha \theta_R.
  \]

  Thereby, adding Eq. (4.7) and Eq. (4.9) and using the form of $q_R^\alpha$ from Eq. (4.2) the
evolution of $H_1$ is obtained as
\[
\partial_t H_1 + \partial_\alpha \left( J^H_\alpha + k\rho u_\alpha \ln \theta_R + k^2 \frac{q_R}{\delta \theta_R} \right) = \Sigma^{\text{ESBGK}} + \Sigma^{\text{BGK}} + \hat{\Sigma},
\]
where the right hand side is the net entropy production with contributions from the ES–BGK collision, the BGK collision, and the rotational component of the model. Here,
\[
\hat{\Sigma} = -\frac{3\rho \theta - \theta_T}{2\tau_1} + \frac{k\rho \theta - \theta_R}{\tau_1} + k^2 \frac{\delta}{\delta \theta_R} \left( \frac{\partial_\alpha \theta_R}{\theta_R} \right)^2.
\]
Similarly to the standard BGK or ES–BGK case [Andries et al. 2000], the entropy production $\hat{\Sigma}$ in this model is non-positive too. This is achieved by choosing $k = -\delta/2$ and exploiting the relation Eq.(3.6) to rewrite $\hat{\Sigma}$ as
\[
\hat{\Sigma} = -\frac{\delta}{2} \rho \frac{(\theta - \theta_R)^2}{\theta \theta_R} - \kappa_R \left( \frac{\partial_\alpha \theta_R}{\theta_R} \right)^2 \leq 0.
\]
Hence, the proposed model satisfies the $H$ theorem.

**Hydrodynamics**: In order to derive the hydrodynamic limit and the transport coefficients, the moments are typically categorized into fast $M^{\text{fast}}$ and slow moments $M^{\text{slow}}$. The stress tensor and the heat flux constitutes the relevant set of fast moments along with the translational and rotational temperatures as they are not conserved
\[
M^{\text{fast}} = \{\theta_T, \theta_R, \sigma_{\alpha\beta}, q_\alpha\}.
\]
The base state is obtained from zero of collision from Eq.(4.1) as
\[
f = f^{MB} \implies \theta = \theta_T \quad \text{and} \quad \theta = \theta_R.
\]
Thus, the fast moment can be expanded around their equilibrium values in a series as
\[
M^{\text{fast}} = M^{\text{fast}} \left(f^{MB}\right) + \tau M^{(1)}_{\text{fast}} + \cdots.
\]
In Chapman–Enskog expansion, the time derivative of any quantity $\phi$ is expanded as
\[
\partial_t \phi = \partial_t^{(0)} \phi + \tau \partial_t^{(1)} \phi + \mathcal{O}(\tau^2).
\]
The set of conservation laws (Eqs.(4.5)) upon substituting the expansion of time derivative provide the definition of time derivative at $\mathcal{O}(1)$ of slow variables as Euler equations
\[
\partial_t^{(0)} \rho + \partial_\alpha (\rho u_\alpha) = 0,
\]
\[
\partial_t^{(0)} (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta + \rho \theta \delta_{\alpha\beta}) = 0,
\]
\[
\partial_t^{(0)} E + \partial_\beta (E u_\beta + \rho \theta u_\beta) = 0.
\]
Thus, pressure evolution at $\mathcal{O}(1)$ satisfies the adiabatic condition for a polyatomic gas
\[
\left( \partial_t^{(0)} + u_\beta \partial_\beta \right) \left( \frac{p}{\rho^\gamma} \right) = 0, \quad \text{where} \quad \gamma = \frac{5 + \delta}{3 + \delta}.
\]
Similarly, at order $\mathcal{O}(\tau)$ we have
\[
\partial_t^{(1)} \rho = 0,
\]
\[
\partial_t^{(1)} (\rho u_\alpha) + \partial_\alpha (\rho \theta_T^{(1)}) + \partial_\beta \sigma_{\alpha\beta}^{(1)} = 0,
\]
\[
\partial_t^{(1)} E + \partial_\beta \left( \sigma_{\alpha\beta}^{(1)} u_\alpha + \rho \theta_T^{(1)} u_\beta + q_\beta^{(1)} \right) = 0.
\]
The expressions for $\rho \theta^{(1)}_T$ and $\sigma^{(1)}_{\alpha \beta}$ can be obtained from the evolution equations of translational temperature (Eq. (A7)) and stress tensor (Eq. (A9)) respectively as [Details of derivations in Appendix A]

$$\rho \theta^{(1)}_T = -\frac{2 \delta}{3(3 + \delta)} \tau p \partial_{\gamma} u_{\gamma}, \quad \sigma^{(1)}_{\alpha \beta} = -\frac{2 \rho \partial_{\beta} u_{\alpha}}{B - b},$$  \hspace{1cm} (4.20)

where $B = 1 + \tau / \tau_1$. Substituting the above expressions in momentum conservation equation, $O(\tau)$ hydrodynamics with shear viscosity $\eta$ and bulk viscosity $\eta_b$ is

$$\eta = \frac{p \tau}{B - b}, \quad \text{and} \quad \eta_b = \frac{2 \delta}{3(3 + \delta)} p \tau_1.$$  \hspace{1cm} (4.21)

Similarly, translational thermal conductivity for the model is obtained from the translational heat flux evolution (Eq. (A10)). A Chapman–Enskog expansion of Eq. (A10) by substituting $q_T^{(1)} = (q_T^{(1)})_{MB} + \tau (q_T^{(1)})_{O(2)} + O(1)$ at $O(1)$ yields

$$\left(1 + \frac{\tau}{\tau_1}\right) (q_T^{(1)}) = -\frac{5}{2} \rho \theta \partial_{\alpha} \theta.$$  \hspace{1cm} (4.22)

Thus, the translational thermal conductivity is $\kappa_T = 5p \tau/(2B)$ which means the total thermal conductivity $\kappa = \kappa_T + \kappa_R$ with $k_r = \kappa_R / \kappa_T$ is $\kappa = 5p \tau/(2B) (1 + k_r)$. Hence,

$$\text{Pr} = \frac{\eta C_p}{\kappa} = \left(\frac{B}{B - b}\right) \left(1 + \frac{\delta}{5}\right) \left(\frac{1}{1 + k_r}\right).$$  \hspace{1cm} (4.23)

The relaxation times $\tau$ and $\tau_1$ are fixed based on the shear and bulk viscosities respectively and the free parameters $b$ and $k_r$ can be adjusted to obtain a target Prandtl number.

5. Discretizing via lattice Boltzmann Method

In this section, we formulate a lattice Boltzmann scheme for solving the proposed model. Firstly, the velocity space is discretized into a discrete velocity set $c = \{c_i, i = 1 \cdots N\}$ consisting of $N$ vectors. These vectors form the links of a lattice that should satisfy appropriate isotropy conditions (Succi 2001; Atif et al. 2018). In particular, we validate the proposed kinetic model using a 41-velocity crystallographic lattice from Kolluru et al. (2020b), which uses a body-centered cubic (bcc) arrangement of grid points. The bcc lattice contains two simple cubic lattices offset by half the length of grid spacing in all directions for better spatial discretization (Namburi et al. 2016). The discrete velocities and their corresponding weights for this RD3Q41 model are given in Table 1. The kinetic equation (Eq. (4.1)) in discrete in velocity space for populations $f_{1i}$ is

$$\partial_t f_{1i}(x, c, t) + c_i \partial_{c_i} f_{1i}(x, c, t) = \Omega_i(x, t),$$  \hspace{1cm} (5.1)

where

$$\Omega_i(x, t) = \frac{1}{\tau} \left[f_{1i}^\text{ES}(\rho, u, \theta_T \delta_{\alpha \beta} + b \sigma_{\alpha \beta}) - f_{1i}\right] + \frac{1}{\tau_1} \left[f_{1i}^\text{Eq}(\rho, u, \theta) - f_{1i}\right],$$  \hspace{1cm} (5.2)

with moments of the discrete populations $f_{1i}$ defined as

$$\rho(f_i) = \sum_i f_{1i}, \quad \rho u_{\alpha}(f_i) = \sum_i f_{1i} c_{i\alpha}, \quad \theta_T(f_i) = \frac{1}{3\rho(f_i)} \left(\sum_i f_{1i} c_i^2 - \rho u^2\right).$$  \hspace{1cm} (5.3)

To have a numerically efficient scheme for the $N$ coupled partial differential equations of
The MacCormack scheme (MacCormack 2003), which uses forward and backward relation in Eq. (3.6) to obtain is first solved using the backward Euler method for a half-time step along with the trapezoid rule, we obtain the implicit relation along the characteristics and approximating the integral related to collision term via differences for spatial derivatives in the predictor and corrector steps respectively, is
\[ X = 3\Delta t/(2\tau_1(3 + \delta)). \]

Tab. 1: Velocities and their corresponding weights for the RD3Q41 model with \( \theta_0 = 0.2948964908710633 \)

| Discrete Velocities \( (c_i) \) | Weight \( (w_i) \) |
|-------------------------------|-----------------|
| \((0, 0, 0)\)                | \((52 - 323\theta_0 + 921\theta_0^2 - 1036\theta_0^3)\)/52 |
| \((\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1)\) | \(\theta_0 \frac{12 - 38\theta_0 + 63\theta_0^2}{39}\) |
| \((\pm 2, 0, 0), (0, \pm 2, 0), (0, 0, \pm 2)\) | \(\theta_0 \frac{3 - 29\theta_0 + 84\theta_0^2}{312}\) |
| \((\pm 1, \pm 1, 0), (\pm 1, 0, \pm 1), (0, \pm 1, \pm 1)\) | \(\theta_0 \frac{45\theta_0 - 6 - 77\theta_0^2}{26}\) |
| \((\pm 1, \pm 1, \pm 1)\) | \(\theta_0 \frac{20 - 163\theta_0 + 378\theta_0^2}{312}\) |
| \((\pm 0.5, \pm 0.5, \pm 0.5)\) | \(\theta_0 \frac{4 - 17\theta_0 + 21\theta_0^2}{39}\) |

Eq. (5.1), it is desirable to have large time steps, i.e., \( \Delta t \gg \tau \). Upon integrating Eq. (5.1) along the characteristics and approximating the integral related to collision term via trapezoidal rule, we obtain the implicit relation
\[
 f_{1i}(x + c\Delta t, t + \Delta t) = f_{1i}(x, t) + \frac{\Delta t}{2}[\Omega_i(x, t) + \Omega_i(x + ct, t + \Delta t)], \tag{5.4}
\]
which is made explicit by a transformation to an auxiliary population \( g_{1i}(x, c, t) = f_{1i}(x, c, t) - (\Delta t/2)\Omega_i(x, c, t) \). This implies the evolution equation for \( g_{1i} \) as
\[
 g_{1i}(x + c, \Delta t, t + \Delta t) = g_{1i}(x, t)(1 - 2\beta^*) + 2\tau^*\beta^*\Omega_i(x, c, t), \tag{5.5}
\]
with \( 1/\tau^* = 1/\tau + 1/\tau_1 \) and \( \beta^* = \Delta t/(2\tau^* + \Delta t) \). The moments of the auxiliary distribution \( g_1 \) are related to the moments of discrete populations \( f_1 \) as
\[
 \rho(g_1) = \rho(f_1), \quad u(g_1) = u(f_1), \quad \theta_T(g_1) = \theta_T(f_1) + \left( \frac{\delta \Delta t}{2\tau_1(3 + \delta)} \right)(\theta_T(f_1) - \theta_R),
\]
\[
 \sigma_{\alpha\beta}(g_1) = \sigma_{\alpha\beta}(f_1) \left( 1 + \frac{\Delta t}{2\tau^*} - \frac{\Delta t}{2\tau} \right).
\]

To solve the second part of Eq. (4.1) that represents the internal energy, we write
\[
 \frac{\partial\theta_{\text{Rot}}}{\partial t} + u_{\alpha} \frac{\partial\theta_{\text{Rot}}}{\partial x_{\alpha}} = \frac{1}{\tau_1}(\theta - \theta_{\text{Rot}}) + \frac{2}{\rho^2} \kappa R \nabla^2 \theta_{\text{Rot}}, \tag{5.7}
\]
by exploiting the Eqs. (3.6), (4.2), and the continuity equation. The above equation is an advection-relaxation-diffusion equation that is solved by the steps detailed below:

(i) The relaxation equation
\[
 \frac{\partial\theta_{\text{Rot}}}{\partial t} = \frac{1}{\tau_1}(\theta - \theta_{\text{Rot}}), \tag{5.8}
\]
is first solved using the backward Euler method for a half-time step along with the relation in Eq. (3.6) to obtain
\[
 \theta_{\text{Rot}}^{t + \Delta t/2} = \frac{1}{1 + X}\theta_{\text{Rot}}^{t} + \frac{X}{1 + X}\theta_T(f_1), \tag{5.9}
\]
used to solve the advection equation

\[
\frac{\partial \theta_{\text{Rot}}}{\partial t} + u_\alpha \frac{\partial \theta_{\text{Rot}}}{\partial x_\alpha} = 0.
\]  

(5.10)

(iii) The diffusion equation

\[
\frac{\partial \theta_{\text{Rot}}}{\partial t} = \frac{2}{\rho_0} \kappa_R \nabla^2 \theta_{\text{Rot}},
\]  

(5.11)

is then solved using the standard forward time centered space (FTCS) scheme to get \( \theta_{\text{Rot}}^{\text{diff}} \).

(iv) Finally, the second part of relaxation is completed by an advance of \( \theta_{\text{Rot}}^{\text{diff}} \) by another half time-step \( \Delta t/2 \) leading to the final solution at \( t + \Delta t \) as

\[
\theta_{\text{Rot}}^{t+\Delta t} = \frac{1}{1 + X} \theta_{\text{Rot}}^{\text{diff}} + \frac{X}{1 + X} \theta_T(f_1).
\]  

(5.12)

Note that the choice of the solver for the evolution equation of rotational energy is independent of the lattice Boltzmann solver used for solving \( f_1 \). In the next section, we validate the proposed numerical model by simulating a few benchmark problems related to acoustics, hydrodynamics, and heat transfer such as propagation of an acoustic pulse, startup of a simple shear flow, thermal conduction, and viscous heat dissipation.

6. Validation

In this section, we validate the model by contrasting simulation result with various benchmark results. As a first example, we consider a periodic domain \([-\pi, \pi]\) with \(128 \times 4 \times 4\) lattice points to verify numerical sound speed. We initialize the domain with a pressure fluctuation of the form \( p(x, t = 0) = p_0(1.0 + \epsilon \cos(x)) \) with \( p_0 = \theta_0 \). The pressure pulse is expected to reach the same state as the initial condition after one acoustic time period \( (t_a) \). The \( L_2 \)-norm of the pressure fluctuation is computed using the current state and initial state which is expected to be minimum when the waves are in-phase. The number of time-steps taken to achieve the least \( L_2 \)-norm is used to compute \( t_a \) and the speed of sound as \( c_s = L/t_a \) where \( L \) is the domain length. The \( \gamma = c_s^2/\theta_0 \) is thus computed from the speed of sound and the lattice temperature. Here, we demonstrate the versatility of the model by simulating several real fluids by imposing the effective rotational degrees of freedom \( \delta \) as given in Table 2. We show in Figure 1 that our model accurately recovers the specific heat ratio for various polyatomic gases, even for fractional (effective) rotational degrees of freedom. The proposed model remains accurate even for fractional rotational degrees of freedom, thereby achieving any target specific heat ratio values. In Figure 2 we perform a grid convergence study for air and observe a second order convergence. We perform additional validation studies by restricting our attention to diatomic gases with variable Prandtl number.

Next, we study the absorption of sound in a dissipative compressible medium. The presence of both viscosity and thermal conductivity leads to the dissipation of energy in the sound waves. For an emitted wave, the pressure perturbations \( p' \) far away from the source decays during a finite time is \( \text{[Landau & Lifshitz 1987]} \)

\[
p'(r, t) \propto (La r L)^{-1/2} \exp \left( -\frac{(r - c_s t)^2}{2La r L} \right),
\]  

(6.1)
Table 2: Specific heat ratios of real fluids (Green & Southard 2019) and their effective rotational degrees of freedom

| Fluid          | \( \gamma \) | Effective-\( \delta \) |
|----------------|--------------|------------------------|
| Argon, Helium  | 1.66         | 0.03                   |
| Air            | 1.403        | 1.96                   |
| Nitrogen       | 1.404        | 1.95                   |
| Steam          | 1.33         | 3.06                   |
| Methane        | 1.31         | 3.45                   |
| Ethane         | 1.22         | 6.09                   |
| Ethyl alcohol  | 1.13         | 12.38                  |
| Benzene        | 1.1          | 17                     |
| n-Pentane      | 1.086        | 20.26                  |
| Hexane         | 1.08         | 22                     |
| Methylal       | 1.06         | 30.33                  |

Figure 1: Specific heat ratio in simulating sound propagation in different gases. The line represents the reference value with \( \delta \) the number of effective rotational degrees of freedom for various gases as listed in Table 2.

Figure 2: Percentage error of speed of sound \((|1 - \frac{c_s^{\text{simulation}}}{c_s^{\text{expected}}}| \times 100)\) versus grid sizes showing a second order convergence for air.
where the dimensionless Landau number $La$ is (Ansumali et al. 2005)

$$La = Kn \left( \frac{4}{3} + \lambda \right) + \frac{Kn}{Pr} (\gamma - 1). \quad (6.2)$$

Here, $\lambda$ is the ratio of bulk to shear viscosities and $Kn$ is the Knudsen number. The form of pressure perturbation shows that the wave profile is Gaussian-like at large distances and the width of the wave is proportional to $\sqrt{La}$ for a fixed domain length $L$.

To demonstrate the effectiveness of the LB scheme, we perform a simulation at a fixed Kn value of $10^{-3}$ on a domain of size $400 \times 400$ at Prandtl numbers $1.4$, $2.0$, $5.0$, and $10.0$. We initialize the domain with a normal density perturbation of amplitude $0.001$ at the center of the fluid of uniform density $1.0$ at rest. From Eq. (4.21) and setting $\tau = (3/5)\tau_1$ one obtains $\lambda = 224/(225 \text{Pr})$. Using this above relation and $\gamma = 7/5$ the Landau number $La$ is calculated as

$$La = Kn \left( \frac{4}{3} + \frac{314}{225 \text{Pr}} \right). \quad (6.3)$$

The Landau numbers for the chosen set of parameters are listed in Table 3. It is evident that $La$ is inversely proportional to $Pr$ which suggests that the width of the Gaussian increases with a decrease in Pr number. The pressure fluctuations far from the source of perturbation after $t = 0.2t_a$ for various Prandtl numbers are plotted in Figure 3 where $t_a = L/c_s$ is the acoustic time scale. It is evident that as expected the width of the wave is inversely proportional to the Prandtl number.

Next, we investigate the propagation of an acoustic pulse in a diatomic gas with $\gamma = 7/5$ where the isentropic speed of sound is $c_s = \sqrt{\gamma \theta}$. An axisymmetric pressure pulse is initialized at the centre of a domain of size $[-1, 1]$ with $256 \times 256 \times 4$ grid points. The acoustic pulse is of the form

$$p(x, y, t = 0) = p_0 \left( 1.0 + e^{\alpha r^2} \right), \quad (6.4)$$
with $p_0 = \theta_0$, $\epsilon = 0.001$, $b = 0.1$, $\alpha = \ln(2)/b^2$, and $r = \sqrt{x^2 + y^2}$. For low amplitudes of pressure fluctuations and low viscosity, the exact form of the pressure fluctuation is known as the solution of the linearized Euler equations as (Tam & Webb 1993)

$$p'(x, y, t) = p_0 \times \epsilon^2 \frac{\alpha}{2} \int_0^\infty \exp\left(-\frac{\xi^2}{4\alpha}\right) \cos(c_\alpha \xi t) J_0(\xi r) \xi d\xi,$$

(6.5)

where $J_0$ is the Bessel function of the first kind of zero-order (Abramowitz & Stegun 1965). Figure 4 shows that the pressure fluctuations from the simulation and the exact solution along the centerline of $y$-axis are in agreement.

Next, we simulate the transient hydrodynamics in the startup of a simple shear flow between two flat plates separated by a distance $L$ on a grid of size $128 \times 64 \times 8$ with diffusive wall boundary condition (Ansumali & Karlin 2002) and periodicity in the other two directions. Here, the top plate is suddenly started with a velocity $u_w$ while the bottom plate remains stationary. The viscous effects play an important role in the development of the flow which is driven by momentum diffusion. Figure 5 contrasts the solutions at various diffusion times $t^* = t/(L^2/\nu)$ obtained from our simulations with the known analytical solution for the velocity (Pozrikidis & Jankowski 1997)

$$u^* = \frac{u}{u_w} = \frac{y}{L} - 2 \pi \sum_{k=1}^\infty \frac{1}{k} \exp\left(-k^2 \pi^2 \frac{\nu t}{L^2}\right) \sin \left(k \pi \left(1 - \frac{y}{L}\right)\right).$$

(6.6)

As expected, the simulation recovers the analytical solution with good accuracy.

Next, we investigate the effects of thermal conduction by considering a setup consisting of fluid confined in a square cavity of size $[L, L]$ with $128 \times 128$ points and stationary walls. The top wall maintained at a higher temperature $T_1$, while the other three walls are maintained at a temperature $T_0(< T_1)$. Diffusive wall boundary conditions are applied in both directions. The analytical solution for the temperature profile at steady state is (Leal 2007)

$$\frac{T - T_0}{T_1 - T_0} = 2 \pi \sum_{n=1}^\infty \frac{(-1)^{n+1} + 1}{n} \sin(n \pi x) \frac{\sinh(n \pi y)}{\sinh(n \pi)}.$$

(6.7)

Figure 6 shows that the simulated temperature profiles along lines $x = 0.1L$, $0.2L$, and
0.5L and along y = 0.25L, 0.5L, and 0.75L for a temperature difference of 0.1θ₀ matches well with the analytical solution.

Next, we validate our model for a thermal Couette flow problem to evaluate its capability in simulating viscous heat dissipation at various Prandtl numbers. We study the steady-state of a flow induced by a wall at y = H moving with a constant horizontal velocity U₀ and maintained at a constant elevated temperature T₁. The lower wall at y = 0 is kept stationary at a constant temperature T₀ (T₁ > T₀). The analytical solution for the temperature profile for this setup is (Bird et al. 2015)

\[
\frac{T - T₀}{∆T} = \frac{y}{H} + \frac{Pr Ec}{2} \frac{y}{H} \left(1 - \frac{y}{H}\right),
\]

where ∆T = T₁ - T₀ is the temperature difference between the two walls and Ec = U₀²/(cₚ∆T) is the Eckert number that represents the ratio of viscous dissipation to heat conduction with cₚ = 7/2 as the specific heat at constant pressure for a diatomic gas.

Simulations were performed for Pr = 0.75, 2.5, 5.0, 7.5, and 10 at Eckert number fixed at unity on a domain with 128 grid points. The walls were maintained at temperatures θ₀ + 0.5Δθ and θ₀ - 0.5Δθ and plate velocity U₀ is chosen corresponding to a Mach number of 0.1. Figure 7 compares the temperature profiles obtained analytically and via simulations and they are found to be in good agreement.

7. Outlook

We have proposed a kinetic model for polyatomic gases with a tunable Prandtl number. This model is based on the ES–BGK model and recovers the compressible hydrodynamic equations of polyatomic gases as its macroscopic limit. It was shown that the transport
coefficients of the model can be tuned for simulation of flows at different Prandtl numbers and specific heat ratios. This framework is general enough to deal with a more complex model of internal structures. We also demonstrated that the model respects the $H$ theorem. The simplicity of the model makes it suitable for LB and other numerical implementations.

**Appendix A. Evolution equations**

We derive the evolution equations for kinetic energy, internal energy, pressure, stress, heat flux, translational, and rotational temperatures for the proposed model. Using the momentum evolution equation Eq.(4.5), we obtain the evolution equation for $\rho u_\alpha u_\beta$ as

$$\partial_t (\rho u_\alpha u_\beta) + \partial_\gamma (\rho u_\alpha u_\beta u_\gamma) + u_\alpha \partial_\gamma (\rho \theta_T \delta_{\beta\gamma} + \sigma_{\beta\gamma}) + u_\beta \partial_\gamma (\rho \theta_T \delta_{\alpha\gamma} + \sigma_{\alpha\gamma}) = 0. \quad (A 1)$$

Evolution of kinetic energy obtained by taking the trace of the above equation is

$$\partial_t \left( \frac{1}{2} \rho u^2 \right) + \partial_\gamma \left( \frac{1}{2} \rho u^2 u_\gamma \right) + u_\beta \partial_\gamma (\rho \theta_T \delta_{\beta\gamma} + \sigma_{\beta\gamma}) = 0. \quad (A 2)$$

Subtracting the above equation from the evolution equation of total energy from Eq.(4.5), gives the evolution equation for internal energy $e = (3 + \delta)\rho \theta/2$ as

$$\partial_t e + \partial_\beta (\rho u_\beta) + \partial_\beta q_\beta + \sigma_{\beta\gamma} \partial_\gamma u_\beta + \rho \theta_T \partial_\gamma u_\gamma = 0, \quad (A 3)$$

and the evolution equation of pressure $p = \rho \theta$ as

$$\partial_t p + \partial_\beta (\rho u_\beta) + \left( \frac{2}{3 + \delta} \right) (\partial_\beta q_\beta + \sigma_{\beta\gamma} \partial_\gamma u_\beta + \rho \theta_T \partial_\gamma u_\gamma) = 0. \quad (A 4)$$

Using the pressure and continuity equation, the evolution equation for temperature $\theta$ is

$$\partial_t \theta + u_\beta \partial_\beta \theta + \left( \frac{2}{(3 + \delta)\rho} \right) (\partial_\beta q_\beta + \sigma_{\beta\gamma} \partial_\gamma u_\beta + \rho \theta_T \partial_\gamma u_\gamma) = 0. \quad (A 5)$$

From the evolution of kinetic energy (Eq.(A2)) and the translational temperature (Eq.(4.3)), the evolution for translational energy can be evaluated as

$$\partial_t \left( \frac{3\rho \theta_T}{2} \right) + \partial_\beta \left( \frac{3\rho \theta_T}{2} u_\beta \right) + \rho \theta_T \partial_\beta u_\beta + \sigma_{\beta\gamma} \partial_\gamma u_\beta + \partial_\beta q_\beta = \frac{\rho}{\tau_1} \left( \frac{3}{2} \theta - \frac{3}{2} \theta_T \right). \quad (A 6)$$
Using the continuity equation, the evolution for translational temperature $\theta_T$ is
\[
\partial_t \theta_T + u_\beta \partial_\beta \theta_T + \frac{2}{3} \theta_T \partial_\beta u_\beta + \frac{2}{3 \rho} \sigma_{\beta \gamma} \partial_\beta u_\gamma + \frac{2}{3 \rho} \partial_\beta q^T_\beta = \frac{1}{\tau_1} (\theta - \theta_T). \tag{A 7}
\]

For the evolution of the stress tensor $\sigma_{\alpha \beta}$, we multiply the kinetic equation (Eq. (4.1)) with $\xi_\alpha \xi_\beta$ and integrate over the velocity space to obtain
\[
\partial_t (\rho \theta_T \delta_{\alpha \beta} + \sigma_{\alpha \beta}) + \partial_\kappa Q^T_{\alpha \beta \kappa} + \partial_\kappa (u_\kappa (\rho \theta_T \delta_{\alpha \beta} + \sigma_{\alpha \beta})) + (\rho \theta_T \delta_{\alpha \beta} + \sigma_{\alpha \beta}) \partial_\kappa u_\alpha
\]
\[
+ \rho \theta_T \delta_{\kappa \alpha} + \sigma_{\kappa \alpha}) \partial_\kappa u_\beta = \frac{1}{\tau} (b - 1) \sigma_{\alpha \beta} + \frac{1}{\tau_1} (\rho \theta_T \delta_{\alpha \beta} - \rho \theta_T \delta_{\alpha \beta} - \sigma_{\alpha \beta}). \tag{A 8}
\]

Thereafter, multiplying Eq. (A 6) with $\delta_{\alpha \beta}$ and subtracting from the above equation one obtains evolution of stress tensor as
\[
\partial_t (\sigma_{\alpha \beta}) + \partial_\gamma (u_\gamma \sigma_{\alpha \beta}) + \partial_\gamma Q^T_{\alpha \beta \gamma} + \frac{4}{5} \partial_\kappa q^T_\alpha + 2 \rho \theta_T \partial_\beta u_\alpha + 2 \partial_\gamma u_\alpha \sigma_{\gamma \beta} = \left( \frac{1}{\tau} (b - 1) - \frac{1}{\tau_1} \right) \sigma_{\alpha \beta}. \tag{A 9}
\]

Similarly, the evolution equation for translational heat flux is obtained by multiplying the kinetic equation (Eq. (4.1)) with $\xi^2 \xi_\alpha$ to obtain
\[
\partial_t q^T_\alpha + \partial_\beta (u_\beta q^T_\alpha) + Q^T_\alpha + \frac{1}{2} \partial_\beta R_{\alpha \beta} + \frac{7}{5} q^T_\alpha \partial_\beta u_\alpha + \frac{2}{5} q^T_\alpha \partial_\kappa u_\alpha + \frac{2}{5} q^T_\alpha \partial_\kappa u_\beta
\]
\[
- \frac{5}{2} \theta_T \partial_\alpha (\rho \theta_T) - \frac{\sigma_{\alpha \beta}}{\rho} \partial_\beta (\rho \theta_T) - \frac{5}{2} \theta_T \partial_\kappa \sigma_{\alpha \kappa} - \frac{\sigma_{\alpha \beta}}{\rho} \partial_\kappa \sigma_{\alpha \kappa} = - \left( \frac{1}{\tau} + \frac{1}{\tau_1} \right) q^T_\alpha. \tag{A 10}
\]

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