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Kinetic Model and Moment Method for Polyatomic Gases

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Abstract. A model kinetic equation for accurate description of rarefied polyatomic gases is introduced. The collisions of polyatomic gas particles are modeled by a two term collision operator, one modeling only exchange of translational energy and the other modeling exchange of both translational and internal energies. The proposed kinetic model, which is an extension of the Rykov and Shakov models, predicts correct relaxation of higher moments and delivers the accurate Prandtl (Pr) number. Also, the model has a non-linear H-theorem. The model is used to construct a system of 36 moment equations, which is closed by the generalized Grad method for polyatomic gases.

Keywords: rarefied gas flows, microflows, polyatomic gases, moment equations, Grad's 36 equations, S-Model
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INTRODUCTION

Recently we developed a high order macroscopic model for description of rarefied polyatomic gases [1, 2]. The proposed model consists of a hierarchy of thirteen different sets of equations for different order of accuracies in the Knudsen number. This model is obtained using a two term BGK collision model, which is known to give incorrect Pr number and relaxation time for higher moments. Here we introduce a sophisticated generalized two term model for polyatomic gases. The model can be be seen as an extension to the the Rykov and Shakov model [3, 4], and like these is gurantees the correct Prandtl number (Pr). Due to additional terms in the equation, our extended model gurantees also proper relaxation times for higher moments. Using the proposed collision model, the full set of 36 moment equations are written and are closed by a generalized form of the Grad's phase density [1, 5, 6].

The Knudsen number, defined as the ratio of molecular mean free path to the characteristic length of the system $\left(Kn = \frac{\lambda}{L_0} = \frac{\tau}{\tau_0}\right)$, measures the degree of rarefaction of a gas flow. At the low Knudsen range $(Kn < 0.01)$, the flow is in the continuum regime and the classical Navier-Stokes-Fourier equations are valid. However, in the transition flow regime, i.e., at intermediate Kn numbers, the conventional hydrodynamics fails in the description of the gas behavior. Typically, gas flows in microelectromechanical systems are in the transition regime [7, 8]. The Boltzmann equation offers accurate description of the gas flow for all Kn numbers through modeling the evolution of velocity distribution function. However, solving the Boltzmann equation or related kinetic equation directly, deterministically or stochastically, is expensive and time consuming. As an alternative to the Boltzmann equation, kinetic theory provides macroscopic models for not too large Knudsen numbers [9]. These models offer high computational speed and explicit equations for macroscopic variables, which are helpful for understanding and analyzing the flow behavior [10].

A close examination shows that even for a simple realistic microscopic model for polyatomic gases, there are at least two distinct mean free path in contrast to the one mean free path of monatomic gases [1, 2]. The exchange processes of colliding particles of a polyatomic gases could either exchange just translational (kinetic) energy or exchange both translational and internal energy which are characterized by the mean free times τ_{tr} and τ_{int}, respectively. Therefore, there are two distinct Knudsen numbers associated with above mean free times, Kn_{tr} and Kn_{int}; depending on the physics of the problem their ratio can be several order of magnitude in size .

Compared to the BGK, Shakov and Rykov model, in the model proposed here the number of free parameters is increased to allow proper ect Pr number and moment relaxation times.

The rest of the paper is organized as follows: In the next section, the foundation of the kinetic theory of polyatomic gases is presented. In Section 3, the two term collision operator is discussed and the generalized S-model is introduced along with the derivation of the required equilibrium distribution functions. In Section 4, the general moment equation for polyatomic gases is discussed and the system of Grad's 36 moment equations is constructed and closed. The Prandtl number and thermophysical properties are obtained in Section 5. Finally, some concluding remarks are given in Section 6.

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KINETIC MODEL

A gas particle has three translational degrees of freedom associated with its motion, and additional degrees of freedom due to its rotation and vibration energies. All degrees of freedom, translational and internal, contribute to the energy of the molecule due to the laws of quantum mechanics. The molecule is at ground state if it is at lowest energy level possible, e.g., any molecular structure at absolute zero temperature is at ground state. A molecule is excited when it has higher energy level than ground state. Temperature increase will result in faster movement of the molecules and, in average, higher translational energy. This increase also thermally excites the molecule to higher internal energy levels. In the following, we consider continuous energy levels for translational and rotational energies, and frozen vibrational degrees of freedom [11, 1].

The energetic state of a molecule changes due to the interaction with other molecules, i.e., collisions; we ignore radiative processes. While total energy and momentum are conserved, the colliding particles exchange different energy forms, where the various exchange processes occur on different characteristic time scales. In all collisions, translational energy is exchanged between particles, but internal energy is exchanged only in some of the collisions. Hence, the characteristic time scale for equilibration of translational energy is faster than that for the equilibration of internal energy.

In the model we are presenting, at time t, the gas particles are described by their position x_i, velocity c_i, and their internal energy parameter, $I \succeq 0$, which form a 7-dimensional phase space. The internal energy of a particle is defined by assuming continuous internal spectrum as $e_{int} = I^{\frac{2}{\delta}}$, where δ is the number of excited non-translational degrees of freedom. The number of particles in a phase space element, $d\mathbf{x}d\mathbf{c}dI$, is defined through the velocity distribution function, $f(\mathbf{x},\mathbf{c},I,t)$, as $fd\mathbf{x}d\mathbf{c}dI$. The evolution of the distribution function is determined by the Boltzmann equation, which is a nonlinear integro-differential equation [12].

Macroscopic quantities are moments of the phase density. We define the general trace free moment as

$$u^{\varsigma,A}_{i_1\ldots i_n} = m\int\int (I^{2/\delta})^A C^{2\varsigma} C_{<i_1}C_{i_2}\ldots C_{i_n>} f d\mathbf{c} dI \,, \tag{1}$$

where the indices between angular brackets indicate the symmetric and trace-free part of a tensor. The moments which have physical definitions are

$$\text{mass density } \ \rho = m\int\int f d\mathbf{c} dI = \int \rho_I dI = u^{0,0} \,, \ \text{velocity } \ \rho v_i = m\int\int c_i f d\mathbf{c} dI \,, \tag{2a}$$

$$\text{stress } \ \sigma_{ij} = m\int\int C_{<i}C_{j>} f d\mathbf{c} dI = u^{0,0}_{ij} \,, \ \text{trans. energy } \ \rho u_{tr} = \frac{3}{2}p = m\int\int \frac{C^2}{2} f d\mathbf{c} dI = \frac{1}{2}u^{1,0} \,, \tag{2b}$$

$$\text{int. energy } \ \rho u_{int} = m\int\int I^{2/\delta} f d\mathbf{c} dI = u^{0,1} \,, \ \text{trans. heat flux } \ q_{i,tr} = m\int\int C_i \frac{C^2}{2} f d\mathbf{c} dI = \frac{1}{2}u^{1,0}_i \,, \tag{2c}$$

$$\text{int. heat flux } \ q_{i,int} = m\int\int C_i I^{2/\delta} f d\mathbf{c} dI = u^{0,1}_i \,. \tag{2d}$$

Here, c_i is the microscopic velocity, $C_i = c_i - v_i$, is the peculiar particle velocity, and $\rho_I = m\int f d\mathbf{c}$ is the density of molecules with the same internal energy parameter I. Moreover, u_{tr} and u_{int} are the translational energy and the energy of the internal degrees of freedom, respectively, while $q_{i,tr}$ and $q_{i,int}$ are the translational and internal heat flux vectors.

The classical equipartition theorem states that in thermal equilibrium each degree of freedom contributes an energy of $\frac{1}{2}\theta$ to the energy of a particle, where $\theta = \frac{k_b}{m}T$ is temperature in specific energy units. Thus, in equilibrium the translational and internal energies are

$$u_{tr|E} = \frac{3}{2}\theta \ \text{ and } \ u_{int|E} = \frac{\delta}{2}\theta \,. \tag{3}$$

We extend the definition of temperatures to non-equilibrium, by defining the translational temperature θ_{tr} and the internal temperature θ_{int} through the energies as $u_{tr} = \frac{3}{2}\theta_{tr}$ and $u_{int} = \frac{\delta}{2}\theta_{int}$. The ideal gas law in non-equilibrium using these definitions is $p = \rho\theta_{tr}$. The total thermal energy, $u = u_{int} + u_{tr}$, is defined as the sum of the internal and translational energies, and we use the equipartition theorem to define the overall temperature θ as

$$u = \frac{3}{2}\theta_{tr} + \frac{\delta}{2}\theta_{int} = \left(\frac{3}{2} + \frac{\delta}{2}\right)\theta \,. \tag{4}$$

In equilibrium, the three temperatures agree, $\theta_{tr|E} = \theta_{int|E} = \theta$, while in non-equilibrium they will differ.

S-MODEL

Kinetic models such as BGK type models [13, 3, 4], which are used here, replace the collision term of the Boltlzmann equation with the simpler terms. We use a two term collision operator, where the first term only models the translational exchange processes and the second term models translational and internal exchange processes,

$$\frac{\partial f}{\partial t}+c_k\frac{\partial f}{\partial x_k}=-\frac{1}{\tau_{tr}}\left(f-f_{tr}\right)-\frac{1}{\tau_{int}}\left(f-f_{int}\right). \tag{5}$$

Here, τ_{tr} and τ_{int} are the corresponding mean free times that we assume to depend only on the macroscopic equilibrium variables (ρ,θ). In the original BGK model [1, 13] f_{tr} and f_{int} are the Maxwellian equilibrium distribution functions corresponding to different collision types which could not predict correct relaxation of the higher moments and the Prandtl number. In order to overcome these defects we introduce a generalized and modified S-model for polyatomic gases. The relaxation times of Boltzmann collision term for Maxwell molecules in the case of monatomic gases for some higher moments are presented in Table 1.

The relaxation time for all higher moments in the original BGK model are the same as stress tensor. The relaxation time of $u_{ij}^{1,0}$ is close to the relaxation time of σ_{ij}, but for other moments the differences are considerable and should not be ignored. Therefore, we introduce a model which correctly predictd the Pr number and the relaxation of these higher moments and their internal moment counterparts $\left\{q_{i,tr},\,q_{i,int},\,\sigma_{ij},\,u^{2,0},\,u^{1,1}\right\}$. Based on the definition of these higher moments, we introduce relaxation translational and internal distribution functions by expansion about the equilibrium Maxwellian functions in corresponding polynomials in specular velocity and particle's internal energy as

$$f_{tr}=f_{tr_0}\left[1+\left(a^{0,0}+a_i^{0,0}C_i+a^{1,0}C^2+a_{ij}^{0,0}C_{<i}C_{j>}+a_i^{1,0}C_iC^2+a_i^{0,1}C_iI^{2/\delta}+a^{2,0}C^2C^2+a^{1,1}C^2I^{2/\delta}\right)\right], \tag{6a}$$

$$f_{int}=f_{int_0}\left[1+\left(b^{0,0}+b_i^{0,0}C_i+b^{1+1}\left(C^2+I^{2/\delta}\right)+b_{ij}^{0,0}C_{<i}C_{j>}+b_i^{1,0}C_iC^2+b_i^{0,1}C_iI^{2/\delta}+b^{2,0}C^2C^2+b^{1,1}C^2I^{2/\delta}\right)\right]. \tag{6b}$$

Here, f_{tr_0} and f_{int_0} are equilibrium distribution functions that describe the different equilibria to which the distribution function will finally relax due to the collisions; they depend on the collisional invariants. The maximum entropy principle will be used to obtain these equilibrium distribution functions. The unknown coefficients in f_{tr} and f_{int} are obtained based on the conditions that the proposed two term collision model predicts correct relaxation for higher moments by introducing four free parameters $\mathrm{Pr}_{q_{tr}}$, $\mathrm{Pr}_{q_{int}}$, $\mathrm{Pr}_{u^{2,0}}$, $\mathrm{Pr}_{u^{1,1}}$ as shown in Table 2. These conditions along with the collision invariants result in coefficients for the translational distribution function as,

$$a^{0,0}=\frac{\left(1-\mathrm{Pr}_{u^{2,0}}\right)\left(u^{2,0}-15\rho\theta_{tr}^2\right)}{8\rho\theta_{tr}^2}\quad,\quad a_i^{0,0}=-\left[\frac{\left(1-\mathrm{Pr}_{q_{tr}}\right)q_{i,tr}+\left(1-\mathrm{Pr}_{q_{int}}\right)q_{i,int}\frac{2\delta\theta_{tr}\theta_{int}}{4u^{0,2}-\delta^2\rho\theta_{int}^2}}{\rho\theta_{tr}^2}\right], \tag{7a}$$

$$a^{1,0}=\frac{5\left[4\frac{u^{0,2}}{\rho}-\delta^2\theta_{int}\theta_{int}\right]\left(1-\mathrm{Pr}_{u^{2,0}}\right)\left(u^{2,0}-15\rho\theta_{tr}^2\right)+8\delta\theta_{tr}\theta_{int}\left(1-\mathrm{Pr}_{u^{1,1}}\right)\left(u^{1,1}-\frac{3}{2}\delta\rho\theta_{tr}\theta_{int}\right)}{60\rho\theta_{tr}^3\left(-4u^{0,2}+\delta^2\theta_{int}^2\right)}, \tag{7b}$$

$$a_{ij}^{0,0}=0\quad,\quad a_i^{1,0}=\frac{\left(1-\mathrm{Pr}_{q_{tr}}\right)q_{i,tr}}{5\rho\theta_{tr}^3}\quad,\quad a_i^{0,1}=\frac{4\left(1-\mathrm{Pr}_{q_{int}}\right)q_{i,int}}{4u^{0,2}\theta_{tr}-\delta^2\rho\theta_{int}^2\theta_{tr}}, \tag{7c}$$

$$a^{1,1}=\frac{4\left(1-\mathrm{Pr}_{u^{1,1}}\right)\left(u^{1,1}-\frac{3}{2}\delta\rho\theta_{tr}\theta_{int}\right)}{15\theta_{tr}^2\left[4u^{0,2}-\delta^2\rho\theta_{int}^2\right]}\quad,\quad a^{2,0}=\frac{\left(1-\mathrm{Pr}_{u^{2,0}}\right)\left(u^{2,0}-15\rho\theta_{tr}^2\right)}{120\rho\theta_{tr}^4}, \tag{7d}$$

TABLE 1. Maxwell molecules's relaxation times [14, 9].

σ_{ij}	q_i	$u^{2,0}$	$u_{ij}^{1,0}$
τ	$\mathrm{Pr}\,\tau$	$\frac{2}{3}\tau$	$\frac{7}{6}\tau$

TABLE 2. Correct relaxation times for higher moments based on four new free parameters.

σ_{ij}	$q_{i,tr}$	$q_{i,int}$	$u^{2,0}$	$u^{1,1}$
$\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}$	$\mathrm{Pr}_{q_{tr}}\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]$	$\mathrm{Pr}_{q_{int}}\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]$	$\mathrm{Pr}_{u^{2,0}}\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]$	$\mathrm{Pr}_{u^{1,1}}\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]$

and internal distribution function as,

$$b^{0,0}=(6+\delta)\,\frac{28\,(1-\mathrm{Pr}_{u^{1,1}})\left[u^{1,1}-\frac{3}{2}\delta\rho\theta^2\right]+(5-\delta)\,(1-\mathrm{Pr}_{u^{2,0}})\left[u^{2,0}-15\rho\theta^2\right]}{8\rho\theta^2\,(30+\delta\,(3+\delta))}\,, \tag{8a}$$

$$b_i^{0,0}=-\left[\frac{(1-\mathrm{Pr}_{q_{tr}})\,q_{i,tr}+(1-\mathrm{Pr}_{q_{int}})\,q_{i,int}}{\rho\theta^2}\right]\,, \tag{8b}$$

$$b^{1+1}=\frac{-28\,(1-\mathrm{Pr}_{u^{1,1}})\left[u^{1,1}-\frac{3}{2}\delta\rho\theta^2\right]-(5-\delta)\,(1-\mathrm{Pr}_{u^{2,0}})\left[u^{2,0}-15\rho\theta^2\right]}{2\rho\theta^3\,(30+\delta\,(3+\delta))}\,, \tag{8c}$$

$$b_{ij}^{0,0}=0\quad,\quad b_i^{1,0}=\frac{(1-\mathrm{Pr}_{q_{tr}})\,q_{i,tr}}{5\rho\theta^3}\quad,\quad b_i^{0,1}=\frac{2\,(1-\mathrm{Pr}_{q_{int}})\,q_{i,int}}{\delta\rho\theta^3}\,, \tag{8d}$$

$$b^{2,0}=\frac{20\,(6-\delta)\,(1-\mathrm{Pr}_{u^{1,1}})\left[u^{1,1}-\frac{3}{2}\delta\rho\theta^2\right]+(30-\delta\,(7-\delta))\,(1-\mathrm{Pr}_{u^{2,0}})\left[u^{2,0}-15\rho\theta^2\right]}{120\rho\theta^4\,(30+\delta\,(3+\delta))}\,, \tag{8e}$$

$$b^{1,1}=\frac{24\,(1+\delta)\,(1-\mathrm{Pr}_{u^{1,1}})\left[u^{1,1}-\frac{3}{2}\delta\rho\theta^2\right]+\delta\,(3-\delta)\,(1-\mathrm{Pr}_{u^{2,0}})\left[u^{2,0}-15\rho\theta^2\right]}{6\delta\rho\theta^4\,(30+\delta\,(3+\delta))}\,. \tag{8f}$$

Equilibrium Distribution Functions

The energy of internal states of molecules does not change during translational collisions. So, the number of molecules with the same internal energy level is an invariant for this type of collisions. However, in internal processes due to exchange of the internal energy, only the total number of the molecules is an invariant. Also, momentum is conserved in all the collisions. Conservation of the energy for the translational processes consists of two parts as the translational and internal energies do not convert to one another. Only the total energy is conserved for the internal processes.

The problem of finding the equilibrium distribution function which maximizes the entropy,

$$\rho s=-k_b\int\int f\ln\frac{f}{y}d\mathbf{c}dI\,, \tag{9}$$

under the collision invariants constraints is solved using the Lagrange multipliers method [9]. This method is based on the fact that finding the extremum of a function, L, under constraints $G_i=0$, is the same as finding the extremum of $L-\sum_i\lambda_iG_i$, where λ is the Lagrange multiplier. The unknown multipliers are obtained using the constraints. Substituting the multipliers back into the distribution function and using the definition of the translational temperature, $u_{tr}=\frac{3}{2}\theta_{tr}$, the equilibrium distribution function of the translational processes is obtained to be a Maxwellian distribution function,

$$f_{tr_0}=\frac{\rho_I}{m}\left(\frac{1}{2\pi\theta_{tr}}\right)^{\frac{3}{2}}\exp\left[-\frac{1}{2\theta_{tr}}C^2\right]\,. \tag{10}$$

A similar procedure gives the internal processes equilibrium distribution function. The final result is also a Maxwellian like function,

$$f_{int_0} = \frac{\rho}{m}\frac{1}{(2\pi)^{\frac{3}{2}}\,\theta^{(\delta+3)/2}}\frac{1}{\Gamma\left(1+\frac{\delta}{2}\right)}\exp\left[-\frac{1}{\theta}\left(\frac{C^2}{2}+I^{2/\delta}\right)\right]\ . \tag{11}$$

Important Properties of the Proposed Model

Now we examine some important properties of our proposed model. We consider equilibrium first. In equilibrium we have zero collision term and all moments of the collision term must vanish, e.g., $q_{i,tr} = q_{i,int} = 0$. Using the Maxwellian distribution functions, we get

$$u^{1,1}_{|E,tr} \;=\; m\int\int C^2 I^{2/\delta} f_{tr_0} d\mathbf{c}dI = \frac{3}{2}\delta\rho\theta_{int}\theta_{tr} \quad \text{and} \quad u^{2,0}_{|E,tr} = m\int\int C^4 f_{tr_0} d\mathbf{c}dI = 15\rho\theta^2_{tr}\ , \tag{12a}$$

$$u^{1,1}_{|E,int} \;=\; m\int\int C^2 I^{2/\delta} f_{int_0} d\mathbf{c}dI = \frac{3}{2}\delta\rho\theta^2 \qquad \text{and} \quad u^{2,0}_{|E,int} = m\int\int C^4 f_{int_0} d\mathbf{c}dI = 15\rho\theta^2\ . \tag{12b}$$

Therefore, we will get $f = f_{tr} = f_{tr_0}$ when we have equilibrium in translational processes *only*, and $f = f_{int} = f_{int_0}$ when we have equilibrium in both internal *and* translational processes.

Next we consider conservation of moments: For the translational exchange processes the mass of particles with the same internal energy level, I, should be conserved. Internal exchange processes conserves the total mass. Both internal and translational exchange processes conserve the momentum. The total energy is conserved in the internal exchange processes, where the translational processes conserves the translational and internal energies separately. The above conditions imply that the three phase densities, f, f_{tr} and f_{int}, have the moments in common,

$$\rho_I = m\int f_{tr} d\mathbf{c} = m\int f d\mathbf{c}\ \text{ and }\ 0 = m\int\int C_i f_{tr} d\mathbf{c}dI = m\int\int C_i f d\mathbf{c}dI\ ,$$
$$\frac{3}{2}\rho\theta_{tr} = \frac{m}{2}\int\int C^2 f_{tr} d\mathbf{c}dI = \frac{m}{2}\int\int C^2 f d\mathbf{c}dI\ . \tag{13a}$$

$$\rho = m\int\int f_{int} d\mathbf{c}dI = m\int\int f d\mathbf{c}dI\ \text{ and }\ 0 = m\int\int C_i f_{int} d\mathbf{c}dI = m\int\int C_i f d\mathbf{c}dI\ ,$$
$$\left(\frac{3}{2}+\frac{\delta}{2}\right)\rho\theta = m\int\int\left(\frac{C^2}{2}+I^{2/\delta}\right) f_{int} d\mathbf{c}dI = m\int\int\left(\frac{C^2}{2}+I^{2/\delta}\right) f d\mathbf{c}dI\ . \tag{13b}$$

Therefore, the conservation of mass, momentum and energy is guaranteed by using the proposed model

The full non-linear H-theorem for the model was proved too, however, due to the lack of space this will be presented elsewhere.

MOMENT METHOD

Moment methods replace the kinetic equation by a finite set of differential equations for the moments of the distribution function. The set of moment equations approximates the kinetic equation and can be used to describe rarefied gas flows. The moment equations are obtained by taking weighted averages of the kinetic equation. Multiplying the kinetic equation (5) with $m(I^{2/\delta})^A C^{2\varsigma} C_{<i_1} C_{i_2} ... C_{i_n>}$, and subsequent integration over velocity space and internal energy parameter gives the general moment equation. We will construct an explicit set of moment equations for the first 36 moments $\left\{\rho, v_i, \theta_{tr}, \theta_{int}, \sigma_{ij}, q_{i,tr}, q_{i,int}, u^{1,0}_{ij}, u^{2,0}, u^{0,1}_{ij}, u^{1,1}, u^{0,0}_{ijk}\right\}$.

The generalized version of the Grad's phase density for polyatomic gases and 36 moments is used to obtain constitutive equations and close the set of equations [1]. There appear higher moments, $\left\{u^{1,0}_{ijk}, u^{2,0}_{i}, u^{0,0}_{ijkl}, u^{0,1}_{ijk}, u^{1,1}_{i}\right\}$, in the set of moment equations and their constitutive equations are obtained as

$$u^{1,0}_{ijk} = 9\theta u^{0,0}_{ijk}\ ,\ u^{2,0}_{i} = 28\theta q_{i,tr}\ ,\ u^{0,0}_{ijkl} = 0\ ,\ u^{0,1}_{ijk} = \frac{\delta}{2}\theta u^{0,0}_{ijk}\ ,\ u^{1,1}_{i} = (5q_{i,int} + \delta q_{i,tr})\,\theta\ . \tag{14}$$

Using these equations and the definitions of total and dynamic temperatures $\left(\theta = \frac{\delta\theta_{int}+3\theta_{tr}}{3+\delta} \text{ and } \Delta\theta = \theta - \theta_{tr}\right)$, we write the full set of closed 36 moment equations for accurate description of polyatomic gases. The conservation laws for mass ($\varsigma = A = n = 0$), momentum ($\varsigma = A = 0$, $n = 1$), and the balance laws for translational ($\varsigma = 1$, $A = n = 0$) and internal ($\varsigma = 0$, $A = 1$, $n = 0$) energies are obtained by the appropriate choice of ς, A, and n from the general moment equation. The conservation of the total energy results from summation of the laws for internal and translational energies. The conservations laws and the equation for dynamic temperature read

$$\frac{D\rho}{Dt} + \rho \frac{\partial v_i}{\partial x_i} = 0 \,, \tag{15a}$$

$$\frac{Dv_i}{Dt} + \frac{1}{\rho}\frac{\partial \sigma_{ij}}{\partial x_j} + \frac{\partial \theta}{\partial x_i} - \frac{\partial \Delta\theta}{\partial x_i} + \frac{[\theta - \Delta\theta]}{\rho}\frac{\partial \rho}{\partial x_i} = 0 \,, \tag{15b}$$

$$\rho\left(\frac{3+\delta}{2}\right)\frac{D\theta}{Dt} + \frac{\partial q_{i,tr}}{\partial x_i} + \frac{\partial q_{i,int}}{\partial x_i} + \sigma_{ij}\frac{\partial v_j}{\partial x_i} + \rho\,[\theta - \Delta\theta]\frac{\partial v_i}{\partial x_i} = 0 \,, \tag{15c}$$

$$\frac{3}{2}\rho\frac{D\Delta\theta}{Dt} - \frac{\delta}{3+\delta}\frac{\partial q_{i,tr}}{\partial x_i} + \frac{3}{2}\left(\frac{2}{3+\delta}\right)\frac{\partial q_{i,int}}{\partial x_i} - \frac{\delta}{3+\delta}\sigma_{ij}\frac{\partial v_j}{\partial x_i} - \frac{\delta}{3+\delta}\rho\,[\theta - \Delta\theta]\frac{\partial v_i}{\partial x_i} = -\frac{3\rho}{\tau_{int}}\frac{\Delta\theta}{2} \,. \tag{15d}$$

The moment equations for stress tensor, $\sigma_{ij} = u_{ij}^{0,0}$, translational heat flux, $q_{i,tr} = \frac{1}{2}u_i^{1,0}$, and internal heat flux, $u_i^{0,1} = q_{i,int}$, which all are present in the conservation laws, are obtained from the general moment equation by the appropriate choice of ς, A, and n, as

$$\begin{aligned}
&\frac{Dq_{i,tr}}{Dt} - \frac{5}{2}\rho\,[\theta_t - \Delta\theta]\frac{\partial \theta_t}{\partial x_{i_1}} - \sigma_{i_1k}\frac{\partial \theta_t}{\partial x_k} + \frac{5}{2}\rho\,[\theta_t - \Delta\theta]\frac{\partial \Delta\theta}{\partial x_{i_1}} \\
&\quad + \sigma_{i_1k}\frac{\partial \Delta\theta}{\partial x_k} - \frac{1}{\rho}\sigma_{i_1k}\frac{\partial \sigma_{kj}}{\partial x_j} - \frac{5}{2}[\theta_t - \Delta\theta]\frac{\partial \sigma_{i_1j}}{\partial x_j} + \frac{1}{2}\frac{\partial u_{i_1k}^{1,0}}{\partial x_k} + \frac{1}{6}\frac{\partial u^{2,0}}{\partial x_{i_1}} + u_{i_1jk}^{0,0}\frac{\partial v_j}{\partial x_k} \\
&\quad + \frac{7}{5}q_{i_1,tr}\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_{k,tr}\frac{\partial v_{i_1}}{\partial x_k} + \frac{2}{5}q_{j,tr}\frac{\partial v_j}{\partial x_{i_1}} - \frac{5}{2}\left[\theta_t^2 - 2\theta_t\Delta\theta + \Delta\theta^2\right]\frac{\partial \rho}{\partial x_{i_1}} \\
&\quad - \sigma_{i_1k}[\theta_t - \Delta\theta]\frac{\partial \ln\rho}{\partial x_k} = -\underset{q_{tr}}{\mathrm{Pr}}\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]q_{i,tr} \,,
\end{aligned} \tag{15e}$$

$$\begin{aligned}
&\frac{Dq_{i,int}}{Dt} - \frac{\delta}{2}\left[\theta + \frac{3}{\delta}\Delta\theta\right]\frac{\partial \sigma_{ij}}{\partial x_j} - \frac{\delta}{2}\rho\left[\theta + \frac{3}{\delta}\Delta\theta\right]\frac{\partial \theta}{\partial x_i} + \frac{\delta}{2}\rho\left[\theta + \frac{3}{\delta}\Delta\theta\right]\frac{\partial \Delta\theta}{\partial x_i} + \frac{1}{3}\frac{\partial u^{1,1}}{\partial x_i} \\
&\quad - \frac{\delta}{2}\rho\,[\theta - \Delta\theta]\left[\theta + \frac{3}{\delta}\Delta\theta\right]\frac{\partial \ln\rho}{\partial x_{i_1}} + \frac{\partial u_{ik}^{0,1}}{\partial x_k} + q_{k,int}\frac{\partial v_i}{\partial x_k} + q_{i,int}\frac{\partial v_k}{\partial x_k} = -\underset{q_{int}}{\mathrm{Pr}}\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]q_{i,int} \,,
\end{aligned} \tag{15f}$$

$$\frac{D\sigma_{ij}}{Dt} + \frac{\partial u_{ijk}^{0,0}}{\partial x_k} + \frac{4}{5}\frac{\partial q_{<i,tr}}{\partial x_{j>}} + 2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k} + 2\rho\,[\theta - \Delta\theta]\frac{\partial v_{<i}}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\sigma_{ij} \,. \tag{15g}$$

These equations contain the higher moments $u_{ij}^{1,0}$, $u^{2,0}$, $u_{ijk}^{0,0}$, $u_{ij}^{0,1}$ and $u^{1,1}$ for which full moment equations are obtained as

$$\begin{aligned}
&\frac{Du_{i_1i_2}^{1,0}}{Dt} - 2u_{i_1i_2k}^{0,0}[\theta_t - \Delta\theta]\frac{\partial \ln\rho}{\partial x_k} - \frac{28}{5}[\theta_t - \Delta\theta]\,q_{<i_1,tr}\frac{\partial \ln\rho}{\partial x_{i_2>}} + 2u_{i_1i_2k}^{0,0}\frac{\partial \Delta\theta}{\partial x_k} + \frac{28}{5}q_{<i_1,tr}\frac{\partial \Delta\theta}{\partial x_{i_2>}} \\
&\quad + 7u_{i_1i_2k}^{0,0}\frac{\partial \theta_t}{\partial x_k} + \frac{28}{5}q_{<i_1,tr}\frac{\partial \theta_t}{\partial x_{i_2>}} + 9\theta_t\frac{\partial u_{i_1i_2k}^{0,0}}{\partial x_k} + \frac{2}{5}28\theta_t\frac{\partial q_{<i_1,tr}}{\partial x_{i_2>}} + \frac{6}{7}u_{<i_1i_2}^{1,0}\frac{\partial v_{k>}}{\partial x_k} \\
&\quad + \frac{4}{5}u_{j<i_1}^{1,0}\frac{\partial v_j}{\partial x_{i_2>}} + 2u_{k<i_1}^{1,0}\frac{\partial v_{i_2>}}{\partial x_k} + u_{i_1i_2}^{1,0}\frac{\partial v_k}{\partial x_k} + \frac{14}{15}u^{2,0}\frac{\partial v_{<i_1}}{\partial x_{i_2>}} \\
&\quad - 2\frac{1}{\rho}u_{i_1i_2k}^{0,0}\frac{\partial \sigma_{kj}}{\partial x_j} - \frac{28}{5}\frac{1}{\rho}q_{<i_1,tr}\frac{\partial \sigma_{i_2>j}}{\partial x_j} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]u_{i_1i_2}^{1,0} \,,
\end{aligned} \tag{15h}$$

$$
\begin{aligned}
&\frac{Du^{2,0}}{Dt} - 8q_{k,tr}\left[\theta_t - \Delta\theta\right]\frac{\partial \ln\rho}{\partial x_k} + 28\theta_t\frac{\partial q_{k,tr}}{\partial x_k} - 8\frac{q_{k,tr}}{\rho}\frac{\partial \sigma_{kj}}{\partial x_j} + 20q_{k,tr}\frac{\partial \theta_t}{\partial x_k} + 8q_{k,tr}\frac{\partial \Delta\theta}{\partial x_k} \\
&\qquad + 4u^{1,0}_{kj}\frac{\partial v_j}{\partial x_k} + \frac{7}{3}u^{2,0}\frac{\partial v_k}{\partial x_k} = \frac{\mathrm{Pr}_{u^{2,0}}}{\tau_{tr}}\left[\left(15\rho\left[\theta-\Delta\theta\right]^2\right) - u^{2,0}\right] + \frac{\mathrm{Pr}_{u^{2,0}}}{\tau_{int}}\left[\left(15\rho\theta^2\right) - u^{2,0}\right] ,
\end{aligned}
\tag{15i}
$$

$$
\begin{aligned}
&\frac{Du^{0,0}_{ijk}}{Dt} - 3\sigma_{<ij}\frac{1}{\rho}\frac{\partial \sigma_{k>l}}{\partial x_l} + \frac{3}{7}\frac{\partial u^{1,0}_{<ij}}{\partial x_{k>}} - 3\sigma_{<ij}\frac{\partial \theta}{\partial x_{k>}} + 3\sigma_{<ij}\frac{\partial \Delta\theta}{\partial x_{k>}} \\
&\qquad - 3\sigma_{<ij}\left[\theta-\Delta\theta\right]\frac{\partial \ln\rho}{\partial x_{k>}} + 3u^{0,0}_{l<ij}\frac{\partial v_{k>}}{\partial x_l} + u^{0,0}_{ijk}\frac{\partial v_l}{\partial x_l} + \frac{12}{5}q_{<i,tr}\frac{\partial v_j}{\partial x_{k>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]u^{0,0}_{ijk} ,
\end{aligned}
\tag{15j}
$$

$$
\begin{aligned}
&\frac{Du^{0,1}_{i_1 i_2}}{Dt} - 2\frac{1}{\rho}q_{<i_1,int}\frac{\partial \sigma_{i_2>j}}{\partial x_j} - 2\frac{\left[\theta_t-\Delta\theta\right]}{\rho}q_{<i_1,int}\frac{\partial \rho}{\partial x_{i_2>}} + \frac{\delta}{2}\theta_t\frac{\partial u^{0,0}_{i_1 i_2 k}}{\partial x_k} + \frac{\delta}{2}u^{0,0}_{i_1 i_2 k}\frac{\partial \theta_t}{\partial x_k} \\
&\qquad + \frac{2}{5}\delta q_{<i_1,tr}\frac{\partial \theta_t}{\partial x_{i_2>}} + 2q_{<i_1,int}\frac{\partial \Delta\theta}{\partial x_{i_2>}} + 2\theta_t\frac{\partial q_{<i_1,int}}{\partial x_{i_2>}} + \frac{2}{5}\delta\theta_t\frac{\partial q_{<i_1,tr}}{\partial x_{i_2>}} \\
&\qquad\qquad + 2u^{0,1}_{k<i_1}\frac{\partial v_{i_2>}}{\partial x_k} + u^{0,1}_{i_1 i_2}\frac{\partial v_k}{\partial x_k} + \frac{2}{3}u^{1,1}\frac{\partial v_{<i_1}}{\partial x_{i_2>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]u^{0,1}_{i_1 i_2} ,
\end{aligned}
\tag{15k}
$$

$$
\begin{aligned}
&\frac{Du^{1,1}}{Dt} - 2\frac{1}{\rho}q_{k,int}\frac{\partial \sigma_{kj}}{\partial x_j} - 2q_{k,int}\left[\theta_t-\Delta\theta\right]\frac{\partial \ln\rho}{\partial x_k} - 2q_{k,int}\frac{\partial \theta_t}{\partial x_k} + 2q_{k,int}\frac{\partial \Delta\theta}{\partial x_k} \\
&\qquad + \left(5q_{k,int} + \delta q_{k,tr}\right)\frac{\partial \theta_t}{\partial x_k} + 5\theta_t\frac{\partial q_{k,int}}{\partial x_k} + \delta\theta_t\frac{\partial q_{k,tr}}{\partial x_k} \\
&+ 2u^{0,1}_{kj}\frac{\partial v_j}{\partial x_k} + \frac{5}{3}u^{1,1}\frac{\partial v_k}{\partial x_k} = \frac{\mathrm{Pr}_{u^{1,1}}}{\tau_{tr}}\left[\rho\frac{3}{2}\left[\delta\theta^2 + (3-\delta)\,\theta\Delta\theta - 3\Delta\theta^2\right] - u^{1,1}\right] + \frac{\mathrm{Pr}_{u^{1,1}}}{\tau_{int}}\left[\left(\rho\frac{3}{2}\delta\theta^2\right) - u^{1,1}\right] .
\end{aligned}
\tag{15l}
$$

THE PRANDTL NUMBER

The Prandtl number is defined as the dimensionless ratio of shear viscosity and heat conductivity,

$$
\mathrm{Pr} = \frac{5+\delta}{2}\frac{\mu}{k}. \tag{16}
$$

This is a measure of the importance of momentum over thermal diffusivity. We applied the Chapman-Enskog expansion on the heat fluxes and stress tensor equations and obtained their leading order terms as

$$
\begin{aligned}
q^{(1)}_{i,tr} &= -\frac{5}{2\left[\frac{\mathrm{Pr}_{q_{tr}}}{\tau_{tr}}\right]}\rho\theta\frac{\partial \theta}{\partial x_i} \quad \text{and} \quad q^{(1)}_{i,int} = -\frac{\delta}{2\left[\frac{\mathrm{Pr}_{q_{int}}}{\tau_{tr}}\right]}\rho\theta\frac{\partial \theta}{\partial x_i} , \\
\sigma^{(1)}_{ij} &= -\tau_{tr}2\rho\theta\frac{\partial v_{<i}}{\partial x_{j>}} \quad \text{and} \quad \Delta\theta^{(1)} = \tau_{int}\frac{2\delta}{3\left(3+\delta\right)}\theta\frac{\partial v_i}{\partial x_i} .
\end{aligned}
\tag{17}
$$

Therefore, the shear viscosity μ, bulk viscosity v and heat conductivity k are

$$
k = \left(\frac{5}{\mathrm{Pr}_{q_{tr}}} + \frac{\delta}{\mathrm{Pr}_{q_{int}}}\right)\frac{\tau_{tr}}{2}\rho\theta \ , \quad \mu = \tau_{tr}\rho\theta \quad \text{and} \quad v = \tau_{int}\frac{2\delta}{3\left(3+\delta\right)}\rho\theta \ . \tag{18}
$$

The calculated Prandtl number using our model is

$$
\mathrm{Pr} = \frac{5+\delta}{\left(\frac{5}{\mathrm{Pr}_{q_{tr}}} + \frac{\delta}{\mathrm{Pr}_{q_{int}}}\right)} \ . \tag{19}
$$

The values of the modelling parameters $\mathrm{Pr}_{q_{tr}}$, $\mathrm{Pr}_{q_{int}}$ thus are restricted by the Prandtl number. Therefore the model provides the freedom to fit three paramteres ($\mathrm{Pr}_{u^{2,0}}$, $\mathrm{Pr}_{u^{1,1}}$ and $\mathrm{Pr}_{q_{tr}}$ or $\mathrm{Pr}_{q_{int}}$). These values can be found from fitting to experimental or numerical data for rarefied flows, such as damping of ultrasound, light scattering experiments, or shockwave structure.

CONCLUSION AND OUTLOOK

Our general goal is the derivation and examination of an extended system of moment equations for polyatomic gases, i.e., the generalization of the G26 equations [9]. The present paper gave a brief overview over the ideas behind that derivation, but the details and full development of the extended moment system will be presented elsewhere. Above, we have based the method on a system of 36 moment equations, which is closed by the generalized Grad method. Polyatomic gases are governed by at least two distinct time scales, the mean free times for processes that exchange only translational energy, or translational and internal energies. We introduced a generalized S-model which have the ability to predict correct relaxation of higher moments. The correct relaxation of the model towards equilibrium phase density is shown. Also, we showed that the model conserves the collision invariants and allows to predict the correct Prandtl number. The proof of the H-theorem is omitted due to the lack of space. The next important steps in this research program are: (a) the development of extended moment equations based on the ordering of Knudsen numbers [1], (b) development of suitable boundary conditions for the equations, (c) analytical and numerical solutions of the equations, and a careful evaluation of their merits.

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