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REFINED NAVIER-STOKES-FOURIER EQUATIONS FOR RAREFIED POLYATOMIC GASES

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ABSTRACT

A macroscopic model for the description of rarefied polyatomic gas flows is introduced. Grad's moment method is used to construct a closed set of equations for 36 primary moments. The order of magnitude method is then applied to acquire optimized moment definitions. The appropriate sets of equations corresponding to the desired order of accuracy in the Knudsen number are derived by reducing the equations. A refined version of the Navier-Stokes-Fourier (NSF) equations is obtained where the dynamic temperature is an additional independent variable.

INTRODUCTION

The Navier-Stokes-Fourier (NSF) equations of hydrodynamics for gases can be derived from the Boltzmann equation by means of the Chapman-Enskog (CE) method [1–3]. The CE method relies on an expansion in the Knudsen number, which must be sufficiently small for the NSF equations to be valid. The Knudsen number is the ratio between the mean free path of the gas particles (i.e., the average distance between collisions) and a macroscopically relevant lengthscale,

$$\mathrm{Kn} = \frac{\lambda}{L_0} = \frac{\tau}{\tau_0}, \tag{1}$$

where L_0 is the characteristic length scale of the process, τ_0 is a typical characteristic time of the process, and λ and τ are the mean free path and mean free time. Accordingly, the NSF equations are valid only for lengthscales that are sufficiently larger than the mean free path.

A closer examination shows that for monatomic gases there is only a single mean free path. For polyatomic gases, however, even the simplest realistic microscopic model includes at least two different mean free paths, since different types of collisions occur [2, 4]. Indeed, as two gas particles meet, they can either exchange only translational kinetic energy, or they can exchange translational energy and energy stored in their internal degrees of freedom (rotational and vibrational energies). These exchange processes occur on different characteristic time scales, hence there are two different relaxation times, τ_{tr} and τ_{int}, and two distinct Knudsen numbers, $\mathrm{Kn}_{tr} = \frac{\tau_{tr}}{\tau_0}$ and $\mathrm{Kn}_{int} = \frac{\tau_{int}}{\tau_0}$, where $\mathrm{Kn}_{int} > \mathrm{Kn}_{tr}$; depending on the conditions, the ratio between both can be several orders of magnitude in size.

The standard NSF equations are derived from the CE method by accounting for terms of first order in both Knudsen numbers. However, due to the large ratio possible between the Knudsen numbers, the underlying multiscale problem might require more than a simple accounting of first order terms only. For instance, when $\mathrm{Kn}_{int}^2 \simeq \mathrm{Kn}_{tr}$, proper accounting to first order in Kn_{tr} might require consideration of *different* orders in the CE expansion: expansion to first order in Kn_{tr}, but to second order in Kn_{int}.

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It is well known that the CE expansion to higher than first order leads to unstable equations. Hence, with polyatomic gases we face two problems: (a) How to properly account for largely different Knudsen numbers. (b) How to derive stable macroscopic equations from the microscopic description. Both problems are intertwined.

Indeed, we aim for macroscopic equations at higher than first order, hence the CE expansion cannot be used. Instead we use the order of magnitude method [3, 6], which mixes elements of the CE method [1] with elements of Grad's moment method [3,5] to derive stable sets of moment equations which are directly tied to orders in the Knudsen numbers. Previously, this method was used only for monatomic gases, where it yields the Euler and NSF equations at zeroth and first order, respectively, Grad's 13 moment equations (G13) at second order, and the regularized 13 moment equations (R13) at third order [3, 6–8]. The application of the method is particularly transparent when the underlying microscopic model is either the Boltzmann equation for Maxwell molecules, or the BGK model. The generalization to other molecular models, e.g., hard sphere molecules, is possible, but adds a high level of complexity [9].

For this first treatment of polyatomic gases, we decided to base the order of magnitude method on a simple yet meaningful microscopic description by means of a two-term BGK model, and a continuous parameter to describe the internal (i.e., rotational and vibrational) particle energies. The two terms in the BGK model describe collisions in which translational energy only, and translational and internal energies are exchanged between the colliding particles [4]. Each term is attached to its own mean free time, thus the model introduces two Knudsen numbers as discussed above.

The order of magnitude works, in short, as follows. In the first step, a larger set of moment equations is obtained from the underlying kinetic equation (here the two-term BGK model). The moment system is then closed by the Grad method; this gives a Grad-type moment system for 36 moments (G36). This number is chosen so that the model will produce higher order sets of equations, particularly those at third order, which will be presented elsewhere. The second step uses the Chapman-Enskog method to determine the leading order in terms of the two Knudsen numbers for all moments. With the orders established, new moments are introduced by linear combination of the original moments such that the number of moments at each order in the Knudsen numbers is as small as possible. The moment equations are rewritten as equations for the newly introduced moments. In the final step, all Knudsen number scales of all moments are introduced into the moment equations. Then, starting from the lowest order, a hierarchy of sets of equations is build, by adding terms with higher and higher orders.

In the context of the BGK model for polyatomic gases, the order of magnitude method yields, among other sets of equations, the Euler and NSF equations, as well as Grad-type moment equations for 14 moments (G14) and their regularization (R14). However, due to the occurrence of two relevant Knudsen numbers, the ordering of terms by magnitude is not straightforward, since it depends on the relative size of the Knudsen numbers. Anticipating some of our later notation, we write $\mathrm{Kn}_{tr} = \varepsilon$ and $\mathrm{Kn}_{int} = \varepsilon^{\alpha}$ where $\alpha < 1$. Depending on the value of α, the powers of ε must be ordered differently. For instance, when $\alpha < \frac{1}{3}$, the terms actually occurring in the G36 equations are, by increasing order, $\left\{\varepsilon^{\alpha}, \varepsilon^{2\alpha}, \varepsilon, \varepsilon^{1+\alpha}, \varepsilon^{1+2\alpha}, \varepsilon^{2-\alpha}, \varepsilon^{2}, \varepsilon^{2+\alpha}, \varepsilon^{3}\right\}$. However, when $\frac{1}{3} < \alpha < \frac{1}{2}$ the same terms must be ordered as $\left\{\varepsilon^{\alpha}, \varepsilon^{2\alpha}, \varepsilon, \varepsilon^{1+\alpha}, \varepsilon^{2-\alpha}, \varepsilon^{1+2\alpha}, \varepsilon^{2}, \varepsilon^{2+\alpha}, \varepsilon^{3}\right\}$. Other orders of the terms occur when $\frac{1}{2} < \alpha < \frac{2}{3}$, where $\left\{\varepsilon^{\alpha}, \varepsilon, \varepsilon^{2\alpha}, \varepsilon^{2-\alpha}, \varepsilon^{1+\alpha}, \varepsilon^{2}, \varepsilon^{1+2\alpha}, \varepsilon^{2+\alpha}, \varepsilon^{3}\right\}$, and when $\frac{2}{3} < \alpha < 1$, where $\left\{\varepsilon^{\alpha}, \varepsilon, \varepsilon^{2-\alpha}, \varepsilon^{2\alpha}, \varepsilon^{1+\alpha}, \varepsilon^{2}, \varepsilon^{1+2\alpha}, \varepsilon^{2+\alpha}, \varepsilon^{3}\right\}$.

The classical NSF equations have only the leading order terms in Kn_{int} and Kn_{tr}, corresponding to $\{\varepsilon^{\alpha}, \varepsilon\}$. From the above lists follows immediately that validity of classical NSF for polyatomic gases requires $\alpha > \frac{1}{2}$, so that $\varepsilon^{2\alpha} < \varepsilon$ which is equivalent to $\mathrm{Kn}_{int} = \varepsilon^{\alpha} < \frac{\tau_{tr}}{\tau_{int}}$. Here τ_{tr} and τ_{int} are the two relaxation times of the BGK model, respectively; their ratio is equal to the ratio of shear and bulk viscosities. With the ratio of relaxation times rather small, down to the order of 10^{-3} in some cases, this restricts the validity of the NSF equations to rather small Knudsen numbers Kn_{int}. Note that $\mathrm{Kn}_{tr} = \mathrm{Kn}_{int} \frac{\tau_{tr}}{\tau_{int}}$, hence both Knudsen numbers must be small.

A full account of the application of the order of magnitude method to polyatomic gases would widely exceed the space available. Hence, here we concentrate on only one aspect of the method, which is the correction of the Navier-Stokes-Fourier equations by a full balance law for what we call the dynamic temperature, i.e., the dynamic pressure divided by mass density. Results for speed of sound and damping of sound waves show that a relatively small correction gives drastically improved predictions, in the sense of agreement to more refined moment systems.

The remainder of the paper is structured as follows. In the next section, the foundation of the kinetic theory of polyatomic gases is presented. The two term collision operator for the BGK model is introduced. In Sec. 3, the system of moment equations is discussed, and Sec. 4, presents the construction of optimized moments. The model reduction is performed in Sec. 5, which presents the reduced equations for first order of accuracy in Kn_{tr}. The equations are tested for speed and damping of sound. Finally, some concluding remarks are given in Sec. 6.

A rather detailed paper on the ideas introduced here is in preparation and will be published elsewhere.

KINETIC THEORY OF POLYATOMIC GASES

Microscopic model

In the model we shall pursue, at time t, the gas particles are described by their position, x_i, velocity, c_i, and their internal energy parameter, $I \geq 0$, in a 7-dimensional space known as phase space. We assume that the spectrum of the internal energy is continuous and the internal energy of a particle is given by [10, 11]

$$e_{int} = I^{\frac{2}{\delta}} \ , \tag{2}$$

where δ is the number of non-translational degrees of freedom of the gas. The velocity distribution function $f(\mathbf{x},\mathbf{c},I,t)$ is defined such that the number of molecules in a phase space element $d\mathbf{x}d\mathbf{c}dI$ is

$$f(\mathbf{x},\mathbf{c},I,t)\,d\mathbf{x}d\mathbf{c}dI \ . \tag{3}$$

In the absence of external forces, the evolution of the distribution function is determined by the Boltzmann equation. Kinetic models, such as the BGK model [12] used below, replace the Boltzmann collision term by simpler models that preserve the basic relaxation properties and give the transport coefficients at correct order, while loosing some of the detailed accuracy. We use a two term collision operator, where the first term describes collisions in which only the translational energy is exchanged, and the second term describes collisions in which internal and translational energies are exchanged [4]. The resulting BGK equation reads

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = -\frac{1}{\tau_{tr}}\left(f - f_{tr}\right) - \frac{1}{\tau_{int}}\left(f - f_{int}\right) . \tag{4}$$

Here, τ_{tr} and τ_{int} are the corresponding mean free times that we assume to depend only on the macroscopic equilibrium variables, i.e., mass density ρ and temperature θ (in energy units). Moreover, f_{tr} and f_{int} are equilibrium distribution functions that describe the different equilibria to which the distribution function will relax due to the collisions. They depend on the collisional invariants and are obtained from the maximum entropy principle as

$$\begin{aligned} f_{tr} &= \frac{\rho_I}{m}\left(\frac{1}{2\pi\theta_{tr}}\right)^{\frac{3}{2}} \exp\left[-\frac{1}{2\theta_{tr}}C^2\right] , \\ f_{int} &= \frac{\rho}{m}\frac{1}{(2\pi)^{\frac{3}{2}}\,\theta^{(\delta+3)/2}}\frac{1}{\Gamma\left(1+\frac{\delta}{2}\right)} \exp\left[-\frac{1}{\theta}\left(\frac{C^2}{2}+I^{2/\delta}\right)\right] \end{aligned} \tag{5}$$

The definitions for the densities ρ and ρ_I, and the temperatures θ_{tr} and θ will be shown in the next section.

Macroscopic quantities

Macroscopic quantities such as mass density ρ, momentum ρv_i, energy u, pressure p, stress tensor σ_{ij}, and heat flux vector q_i are moments of the phase density. General trace free central moments are defined as

$$u^{\varsigma,A}_{i_1\ldots i_n} = m\int\int \left(I^{2/\delta}\right)^A C^{2\varsigma} C_{<i_1}C_{i_2}\ldots C_{i_n>} f\,d\mathbf{c}dI \ , \tag{6}$$

where indices between angular brackets indicated the symmetric and trace-free part of a tensor. Particular moments that will be important in the sequel are

$$\begin{aligned} \text{mass density} \ \ \rho &= m\int\int f\,d\mathbf{c}dI = \int \rho_I dI = u^{0,0} \ , \\ \text{velocity} \ \ \rho v_i &= m\int\int c_i f\,d\mathbf{c}dI \ , \\ \text{stress} \ \ \sigma_{ij} &= m\int\int C_{<i}C_{j>} f\,d\mathbf{c}dI = u^{0,0}_{ij} \ , \\ \text{transl. energy} \ \ \rho u_{tr} &= \frac{3}{2}p = m\int\int \frac{C^2}{2} f\,d\mathbf{c}dI = \frac{1}{2}u^{1,0} \ , \\ \text{int. energy} \ \ \rho u_{int} &= m\int\int I^{2/\delta} f\,d\mathbf{c}dI = u^{0,1} \ , \\ \text{transl. heat flux} \ \ q_{i,tr} &= m\int\int C_i \frac{C^2}{2} f\,d\mathbf{c}dI = \frac{1}{2}u^{1,0}_i \ , \\ \text{int. heat flux} \ \ q_{i,int} &= m\int\int C_i I^{2/\delta} f\,d\mathbf{c}dI = u^{0,1}_i \ . \end{aligned} \tag{7}$$

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 mass 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 the gas, where $\theta = RT$ is temperature in energy units (R is the gas constant). Thus in equilibrium (E), the translational and internal energies are

$$u_{tr|E} = \frac{3}{2}\theta \quad \text{and} \quad u_{int|E} = \frac{\delta}{2}\theta \ . \tag{8}$$

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

$$u_{tr} = \frac{3}{2}\theta_{tr} \quad \text{and} \quad u_{int} = \frac{\delta}{2}\theta_{int} \ . \tag{9}$$

With these definitions, the ideal gas law in non-equilibrium reads $p = \rho\theta_{tr}$. 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

$$u = u_{tr} + u_{int} = \frac{3}{2}\theta_{tr} + \frac{\delta}{2}\theta_{int} = \left(\frac{3}{2} + \frac{\delta}{2}\right)\theta \ . \tag{10}$$

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

Moment equations

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 (4) with $m(I^{2/\delta})^A C^{2\varsigma} C_{<i_1} C_{i_2} \ldots C_{i_n>}$, and subsequent integration over velocity space and internal energy parameter gives the general moment equation as (with the convective derivative $\frac{D}{Dt} = \frac{\partial}{\partial t} + v_k \frac{\partial}{\partial x_k}$)

$$\begin{aligned}
&\frac{Du^{\varsigma,A}_{i_1\ldots i_n}}{Dt} + 2\varsigma u^{\varsigma-1,A}_{i_1\ldots i_n k}\frac{Dv_k}{Dt} + 2\varsigma u^{\varsigma-1,A}_{i_1\ldots i_n kj}\frac{\partial v_j}{\partial x_k} \\
&\quad + \frac{n}{2n+1} 2\varsigma u^{\varsigma,A}_{j<i_1\ldots i_{n-1}}\frac{\partial v_j}{\partial x_{i_n>}} + \frac{\partial u^{\varsigma,A}_{i_1\ldots i_n k}}{\partial x_k} \\
&\quad + \frac{n}{2n+1}\frac{\partial u^{\varsigma+1,A}_{<i_1\ldots i_{n-1}}}{\partial x_{i_n>}} + 2\varsigma\frac{n}{2n+1} u^{\varsigma,A}_{<i_1\ldots i_{n-1}}\frac{Dv_{i_n>}}{Dt} \\
&\quad + 2\varsigma\frac{n+1}{2n+3} u^{\varsigma,A}_{<i_1\ldots i_n}\frac{\partial v_{k>}}{\partial x_k} + \frac{n-1}{2n-1} n u^{\varsigma+1,A}_{<i_1\ldots i_{n-2}}\frac{\partial v_{i_{n-1}}}{\partial x_{i_n>}} \\
&\quad + n u^{\varsigma,A}_{<i_1\ldots i_{n-1}}\frac{Dv_{i_n>}}{Dt} + u^{\varsigma,A}_{i_1\ldots i_n}\frac{\partial v_k}{\partial x_k} \\
&\quad + \frac{n}{2n+1}\frac{n-1}{2n-1} 2\varsigma u^{\varsigma+1,A}_{<i_1\ldots i_{n-2}}\frac{\partial v_{i_{n-1}}}{\partial x_{i_n>}} + n u^{\varsigma,A}_{k<i_1\ldots i_{n-1}}\frac{\partial v_{i_n>}}{\partial x_k} \\
&= \frac{1}{\tau_{tr}}\left[u^{\varsigma,A}_{i_1\ldots i_n|E,tr} - u^{\varsigma,A}_{i_1\ldots i_n}\right] + \frac{1}{\tau_{int}}\left[u^{\varsigma,A}_{i_1\ldots i_n|E,int} - u^{\varsigma,A}_{i_1\ldots i_n}\right] \ .
\end{aligned} \tag{11}$$

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. The conservation of the total energy results from summation of the laws for internal and translational energies.

Later, we will replace the translational temperature θ_{tr} as variable by its non-equilibrium part $\Delta\theta = \theta - \theta_{tr}$, which we denote as dynamic temperature. Then, instead of the balances of translational and internal energies, we shall consider the conservation law for total energy, and the equation for dynamic temperature.

The moment equations for stress tensor, $\sigma_{ij} = u^{0,0}_{ij}$, translational heat flux, $q_{i,tr} = \frac{1}{2}u^{1,0}_i$, and internal heat flux, $u^{0,1}_i = q_{i,int}$, which all are present in the conservation laws, are obtained from the general moment equation by the appropriate choice of ς, A, and n. These equations contain the higher moments $u^{1,0}_{ij}$, $u^{2,0}$, $u^{0,0}_{ijk}$, $u^{0,1}_{ij}$ and $u^{1,1}$ for which full moment equations can be obtained. Choosing all moments mentioned so far as variables will construct a set of 36 moments,

$$\left\{\rho, v_i, \theta_{tr}, \theta_{int}, \sigma_{ij}, q_{i,tr}, q_{i,int}, u^{1,0}_{ij}, u^{2,0}, u^{0,1}_{ij}, u^{1,1}, u^{0,0}_{ijk}\right\} \ . \tag{12}$$

The equations for these 36 moments contain the higher moments

$$\left\{u^{1,0}_{ijk}, u^{2,0}_i, u^{0,0}_{ijkl}, u^{0,1}_{ijk}, u^{1,1}_i\right\} \ , \tag{13}$$

hence the 36-moment system is not closed a priori. To close the system of 36 equations, we used the appropriate from of Grad's distribution function [5] for 36 moments. Here, we show only the results which are

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

Substituting these equations into the 36 balance laws gives the closed set of equations for the 36 variables (12). We shall not show the rather lengthy equations here, to save some space.

RECONSTRUCTING MOMENTS

Smallness parameters

The expansion parameter in the Chapman-Enskog method is the Knudsen number, of which we have two, Kn_{tr} and Kn_{int}, to account for translational and internal energy exchange. Kn_{tr} should be less than Kn_{int}, since internal energies are exchanged only in a smaller portion of collisions and $\tau_{int} > \tau_{tr}$. Considering both Knudsen numbers to be less than unity, we define

$$\mathrm{Kn}_{tr} = \varepsilon \quad \text{and} \quad \mathrm{Kn}_{int} = \varepsilon^{\alpha} \ . \tag{15}$$

With this, the two Knudsen numbers are replaced by a single smallness parameter, ε, and a magnifying parameter, α, with $0 < \alpha < 1$. The lower limit of the internal smallness parameter is recovered when $\alpha = 1$ and the upper limit is reached when $\alpha = 0$. Particularly for higher Knudsen numbers, mostly values of α less than $\frac{1}{2}$ are relevant.

Chapman-Enskog expansion

The Chapman-Enskog expansion on the moment equations must be performed for both Knudsen numbers, that is for all powers of ε and ε^{α}. The variables related to conservation laws, i.e., mass density, velocity and total temperature, have equilibrium values and hence are of zeroth order in the Knudsen number. The remaining variables are expanded in the smallness parameters ε and ε^{α} as

$$\begin{aligned}\psi = \varepsilon^{0\alpha}&\left[\varepsilon^0\psi^{(0,0)}+\varepsilon^1\psi^{(0,1)}+\varepsilon^2\psi^{(0,2)}+\varepsilon^3\psi^{(0,3)}+\cdots\right]\\ &+\varepsilon^{1\alpha}\left[\varepsilon^0\psi^{(1,0)}+\varepsilon^1\psi^{(1,1)}+\varepsilon^2\psi^{(1,2)}+\varepsilon^3\psi^{(1,3)}+\cdots\right]\\ &+\varepsilon^{2\alpha}\left[\varepsilon^0\psi^{(2,0)}+\varepsilon^1\psi^{(2,1)}+\varepsilon^2\psi^{(2,2)}+\varepsilon^3\psi^{(2,3)}+\cdots\right]+\cdots\end{aligned} \tag{16}$$

Here, ψ stands for any of the variables that must be expanded, and $\psi^{(i,j)}$ is the contribution at order $\varepsilon^{(i\alpha+j)}$. The $\psi^{(i,j)}$ are found by inserting the above expansion into the closed moment equations, and equating terms that are of the same order. The leading order terms of the moments are found as the first non-vanishing terms in their expansion. For instance, ψ is of order $\varepsilon^{(k+l\alpha)}$ if $\psi^{(i,j)}=0$ for $i<k$, $l<j$ and $\psi^{(k,l)}\neq 0$.

It turns out that to leading order the heat fluxes, $q_{i,tr}^{(0,1)}$ and $q_{i,int}^{(0,1)}$, are proportional to the temperature gradient, and hence to each other. In the order of magnitude method we aim at having the smallest number of moments at each order [3,6]. The vectors $q_{i,tr}$ and $q_{i,int}$, which are of first order, can be combined into one first order vector, the total heat flux,

$$q_i = q_{i,tr}+q_{i,int}\ , \tag{17}$$

and one unique higher order variable, the heat flux difference,

$$\Delta q_i = q_{i,tr}-\frac{5}{\delta}q_{i,int}\ . \tag{18}$$

With this, the two first order vectors $\{q_{i,tr},q_{i,int}\}$ are replaced by the equivalent quantities $\{q_i,\Delta q_i\}$, where only one (the smallest possible number) is of first order.

The same idea of using linear combinations of original variables to create a set of variables, so that the number of variables at each order is as small as possible, is applied to all variables. After going through several rounds at increasing orders, this cumbersome procedure creates a unique set of optimized variables, which are linear combinations of the original 36 variables (12).

The final balance laws, which are the closed form of the 36 moment equations, are obtained from the original moment equations by the appropriate linear combinations based on the definitions of the optimized moments. The leading order of all (optimized) moments occurring in these final equations can now be used for model reduction.

MODEL REDUCTION

Scaled equations

While the expansion series (16) contains all mixed powers of ε and ε^{α}, not all orders of magnitude occur in the 36 moment equations for the optimized variables. For this short account of the approach, we are interested in the subset of equations that is accurate up to order ε^1. We shall differentiate between the cases where α is below and above $\frac{1}{2}$. For the case $\alpha<\frac{1}{2}$, the subsequent orders up to ε^1 are $\left\{\varepsilon^0,\varepsilon^{\alpha},\varepsilon^{2\alpha},\varepsilon^1\right\}$, while for the case $\alpha>\frac{1}{2}$ the orders are $\left\{\varepsilon^0,\varepsilon^{\alpha},\varepsilon^1\right\}$

For the model reduction by orders, it is required to clearly assign the orders of magnitude of all terms in the equations considered. For this, we write the conservation laws and the equation for dynamic temperature $\Delta\theta$ in a notation that indicates the relative order of magnitude of the occurring terms by underlining:

$$\begin{gathered}\frac{D\rho}{Dt}+\rho\frac{\partial v_i}{\partial x_i}=0\ ,\\ \rho\frac{Dv_i}{Dt}+\frac{\partial(\rho\theta)}{\partial x_i}-\underline{\frac{\partial(\rho\Delta\theta)}{\partial x_i}}+\underline{\underline{\frac{\partial\sigma_{ij}}{\partial x_j}}}=0\ ,\\ \frac{3+\delta}{2}\rho\frac{D\theta}{Dt}+\rho\theta\frac{\partial v_i}{\partial x_i}-\underline{\rho\Delta\theta\frac{\partial v_i}{\partial x_i}}+\underline{\underline{\frac{\partial q_i}{\partial x_i}}}+\underline{\underline{\sigma_{ij}\frac{\partial v_j}{\partial x_i}}}=0\ .\end{gathered} \tag{19}$$

$$\begin{aligned}&\underline{\rho\frac{D\Delta\theta}{Dt}}+\underline{\frac{2}{3}\frac{\delta}{3+\delta}\rho\Delta\theta\frac{\partial v_i}{\partial x_i}}\\ &\qquad\underline{\underline{-\frac{2}{3}\frac{\delta}{3+\delta}\left(\frac{2}{5+\delta}\frac{\partial q_i}{\partial x_i}+\sigma_{ij}\frac{\partial v_j}{\partial x_i}\right)}}\\ &\qquad\underbrace{-\frac{2}{3}\frac{\delta}{5+\delta}\frac{\partial\Delta q_i}{\partial x_i}}_{}\\ &\qquad\qquad=\frac{2}{3}\frac{\delta}{3+\delta}\rho\theta\frac{\partial v_i}{\partial x_i}-\frac{\rho}{\tau_{int}}\Delta\theta\ .\end{aligned} \tag{20}$$

Here, all terms that are *not* underlined are of zeroth order in ε, *single* underlined terms are of order ε^{α}, *double* underlined terms are of order ε, and the term underlined by a *curly bracket* is of order $\varepsilon^{1+\alpha}$. The order of all terms in the moment equations for higher moments (σ_{ij}, q_i, Δq_i, etc) can be identified and indicated in a similar fashion. The following subsections will show how the recognized orders are used for model reduction.

Zeroth order, ε^0 : Euler equations

If we are interested in zeroth order contributions only, we need to consider only the un-underlined terms in the conservation laws (19). This gives the Euler equations in their typical form for polyatomic gases with constant specific heat $c_v = \frac{3+\delta}{2}R$:

$$\begin{aligned} \frac{D\rho}{Dt} + \rho\frac{\partial v_i}{\partial x_i} &= 0\,, \\ \rho\frac{Dv_i}{Dt} + \frac{\partial(\rho\theta)}{\partial x_i} &= 0\,, \\ \frac{3+\delta}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_i}{\partial x_i} &= 0\,. \end{aligned} \tag{21}$$

The Euler equations are a closed set of equations for the variables $\{\rho, v_i, \theta\}$. The equations for higher moments are not needed at this order, they only contribute at higher order.

Order ε^α : Dynamic temperature

Since $\alpha < 1$ and $\varepsilon < 1$, we have $\varepsilon^\alpha > \varepsilon$. Accordingly, if we want to consider the first correction to the Euler equations, we have to add the terms that are of order ε^α. Considering the conservation laws (19) with the single underlined terms only, we find

$$\begin{aligned} \frac{D\rho}{Dt} + \rho\frac{\partial v_i}{\partial x_i} &= 0\,, \\ \rho\frac{Dv_i}{Dt} + \frac{\partial(\rho\theta)}{\partial x_i} - \frac{\partial(\rho\Delta\theta)}{\partial x_i} &= 0\,, \\ \frac{3+\delta}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_i}{\partial x_i} - \rho\Delta\theta\frac{\partial v_i}{\partial x_i} &= 0\,. \end{aligned} \tag{22}$$

These equations contain the dynamic temperature $\Delta\theta$, and the appropriate expression for closure comes from the leading contribution of equation (20), i.e., the un-underlined terms,

$$\Delta\theta = \frac{2}{3}\frac{\delta}{3+\delta}\tau_{int}\theta\frac{\partial v_i}{\partial x_i}\,. \tag{23}$$

In the literature one often finds the dynamic pressure $\pi = -\rho\Delta\theta$ used instead of the dynamic temperature [2, 14]. Here, we find the dynamic pressure as

$$\pi = -\rho\Delta\theta = -\nu\frac{\partial v_i}{\partial x_i}\,. \tag{24}$$

with the bulk viscosity

$$\nu = \frac{2}{3}\frac{\delta}{3+\delta}\tau_{int}\rho\theta\,. \tag{25}$$

Order $\varepsilon^{2\alpha}$ $(\alpha < \frac{1}{2})$: Refined dynamic temperature

For $\alpha < \frac{1}{2}$, the next correction is to consider terms of order $\varepsilon^{2\alpha}$. The conservation laws do not contain terms of that order, hence they are unchanged from the previous case (order ε^α). The equation for dynamic temperature (20) provides corrections to $\Delta\theta$. The un-underlined terms, which are of order ε^0, give the leading contribution to $\Delta\theta$, which itself is of order ε^α. The single underlined terms, which are of order ε^α, therefore give contributions to $\Delta\theta$ of order $\varepsilon^{2\alpha}$, which are the single underlined terms—these must be considered. All other terms in (20) contribute to $\Delta\theta$ at higher orders and must be discarded.

Thus, the relevant equations at this order are the conservation laws in the form (22) with a full balance equation for the dynamic temperature,

$$\frac{D\Delta\theta}{Dt} + \frac{2}{3}\frac{\delta}{3+\delta}(\Delta\theta - \theta)\frac{\partial v_i}{\partial x_i} = -\frac{\Delta\theta}{\tau_{int}}\,. \tag{26}$$

This set of equations was used by Arima et al. [13] to study polyatomic gases as an extension of Meixner's theory, in which they defined their pressure as the equilibrium pressure, $p = \rho\theta$.

Order ε^1 $(\alpha < \frac{1}{2})$: Refined Navier-Stokes-Fourier

To account for first order terms (ε^1) in the conservation laws, the double underlined terms in (19) must be considered, that is now we need the full conservation laws,

$$\begin{aligned} \frac{D\rho}{Dt} + \rho\frac{\partial v_i}{\partial x_i} &= 0\,, \\ \rho\frac{Dv_i}{Dt} + \frac{\partial(\rho\theta)}{\partial x_i} - \frac{\partial(\rho\Delta\theta)}{\partial x_i} + \frac{\partial\sigma_{ij}}{\partial x_j} &= 0\,, \\ \frac{3+\delta}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_i}{\partial x_i} - \rho\Delta\theta\frac{\partial v_i}{\partial x_i} + \frac{\partial q_i}{\partial x_i} + \sigma_{ij}\frac{\partial v_j}{\partial x_i} &= 0\,. \end{aligned} \tag{27}$$

The appropriate equation for dynamic temperature is again extracted from (20). Following up on the discussion of this equation in the previous subsection, we see that the double underlined terms, which are of order ε, contribute corrections to $\Delta\theta$ of order $\varepsilon^{1+\alpha}$, while the terms with the curly bracket underneath contribute to order $\varepsilon^{1+2\alpha}$. Accordingly, at first order, and $\alpha < \frac{1}{2}$, we need to use the same reduced balance law for $\Delta\theta$ as before,

$$\frac{D\Delta\theta}{Dt} + \frac{2}{3}\frac{\delta}{3+\delta}(\Delta\theta - \theta)\frac{\partial v_i}{\partial x_i} = -\frac{\Delta\theta}{\tau_{int}}\,. \tag{28}$$

Finally, for closure at first order, the leading terms of the stress tensor and total heat flux are required, which are found from their respective moment equations which were not shown above.

These first order equations for σ_{ij} and q_i are the classical Navier–Stokes-Fourier (NSF) equations, which relate the stress deviator and heat flux to the gradients of velocity and temperature,

$$\sigma_{ij} = -2\tau_{tr}\rho\theta\frac{\partial v_{<i}}{\partial x_{j>}} \ , \ q_i = -\frac{5+\delta}{2}\tau_{tr}\rho\theta\frac{\partial\theta}{\partial x_i} \ . \tag{29}$$

We identify the shear viscosity μ and the heat conductivity κ as

$$\mu = \tau_{tr}\rho\theta \ , \ \kappa = \frac{5+\delta}{2}\tau_{tr}\rho\theta \ . \tag{30}$$

Order ε^1 $(\alpha > \frac{1}{2})$: Classical Navier-Stokes-Fourier

The classical Navier-Stokes-Fourier equations arise for $\frac{1}{2} < \alpha < 1$. In this case, the correction to dynamic temperature of order $\varepsilon^{2\alpha}$ can be discarded, i.e., the proper first order equation for dynamic temperature is (23) instead of (28),

$$\Delta\theta = \frac{2}{3}\frac{\delta}{3+\delta}\tau_{int}\theta\frac{\partial v_i}{\partial x_i} \ , \tag{31}$$

The classical NSF equations is a five variables model for $\{\rho, v_i, \theta\}$. However, the refined NSF equations obtained have six independent field variables, $\{\rho, v_i, \theta, \Delta\theta\}$.

PHASE VELOCITY AND DAMPING

The kinetic model (4), and hence the macroscopic equations, contain the two relaxation times τ_{int} and τ_{tr}. In the Navier-Stokes-Fourier equations, the relaxation times directly determine the bulk and shear viscosities ν and μ, and the heat conductivity κ. These coefficients are accessible to measurements: shear viscosity μ can be measured in Couette flows, and heat conductivity κ can be measured in simple heat transfer experiments. The dimensionless ratio between both is known as the Prandtl number, $\mathrm{Pr} = \frac{c_p\mu}{\kappa}$, where $c_p = \frac{5+\delta}{2}$ is the specific heat at constant pressure. The BGK model used above yields $\mathrm{Pr} = 1$, which is above the proper value of ~ 0.7 for polyatomic gases; this inaccuracy is inherent in the BGK model [2]. Hence, there will be discrepancy to measurements and the presented model. At present, our main goal is to understand the principles of modeling and model reduction for polyatomic gases, and for this the BGK model provides a solid base, that is relatively easy to use.

The best way to measure bulk viscosity is through speed and attenuation of sound waves. Here, due to the inaccuracy of the underlying BGK model, we do not aim to adjust the above equations to measurements, but to increase the understanding of the influence of the relaxation time τ_{int}, which describes the exchange of internal and translational energies in collisions, and is directly related to bulk viscosity. In particular, we shall compare the standard Navier-Stokes-Fourier model, where the dynamic temperature is proportional to the divergence of velocity, Eq. (31), to the refined equations, where the dynamic temperature is determined by the full balance equation (28). Attenuation and damping for both cases are compared to the predictions of the full Grad 36 moment equations, which serve as the benchmark case.

To be specific, we consider the one-dimensional propagation of plane waves of low amplitude. Hence, we have to solve the linearized, one-dimensional equations. These can be brought into the general form

$$A_{AB}\frac{\partial u_B}{\partial t} + C_{AB}\frac{\partial u_B}{\partial x} = L_{AB}u_B \ , \tag{32}$$

with the appropriate choice of the coefficients matrices A_{AB}, C_{AB} and L_{AB} corresponding to the equations, and the variables $u_A = \left\{\rho, v_i, \theta, \Delta\theta, \sigma_{ij}, q_i\right\}$. Making the harmonic wave ansatz,

$$u_A(x,t) = \breve{u}_A \exp[i(\omega t - kx)] \ , \tag{33}$$

with the complex amplitude $\breve{u}_A$, real frequency ω and complex wave number $k = k_r + ik_i$, and inserting the harmonic wave into the general form of the equations results in an algebraic equation,

$$[i\omega A_{AB} - ikC_{AB} - L_{AB}]\,\breve{u}_B = 0 \ . \tag{34}$$

Non-trivial solutions are obtained when the determinant of the complex matrix inside the bracket vanishes, which gives the dispersion relation $k(\omega)$. For different set of equations, the dispersion relation has different numbers of branches, and we consider only the branch corresponding to the lowest damping—this is the sound wave [15]. Phase velocity and damping factor are defined as

$$v_{ph} = \frac{\omega}{k_r} \quad \text{and} \quad \phi = -k_i \ . \tag{35}$$

The speed of sound in the low frequency limit, where the damping vanishes, is $a = \sqrt{\frac{5+\delta}{3+\delta}RT_0}$, T_0 is the reference state equilibrium temperature. Figures 1 and 2 show, in dimensionless form, the ratio a/v_{ph} and the reduced damping ϕ/ω as functions of the dimensionless inverse frequency $1/(\omega\tau_{int})$. Hence, the limit of low frequency undamped sound is toward the right of the plots, while higher frequencies are to the left. The figures show results for two ratios of Knudsen numbers, or relaxation times, $\mathrm{Kn}_{tr}/\mathrm{Kn}_{int} = \tau_{tr}/\tau_{int} = \{0.001, 0.01\}$. Comparing the results

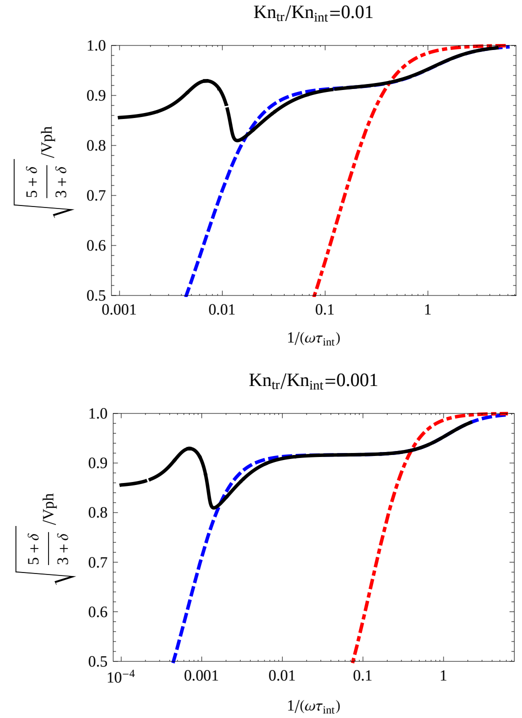

FIGURE 1. Inverse dimensionless phase velocity $\sqrt{(5+\delta)/(3+\delta)}/v_{ph}$ as functions of inverse frequency $1/(\omega\tau_{int})$ for two Knudsen number ratios and different sets of equations: G36 (black continuous), classical NSF (red dash-dotted), modified NSF (blue dashed).

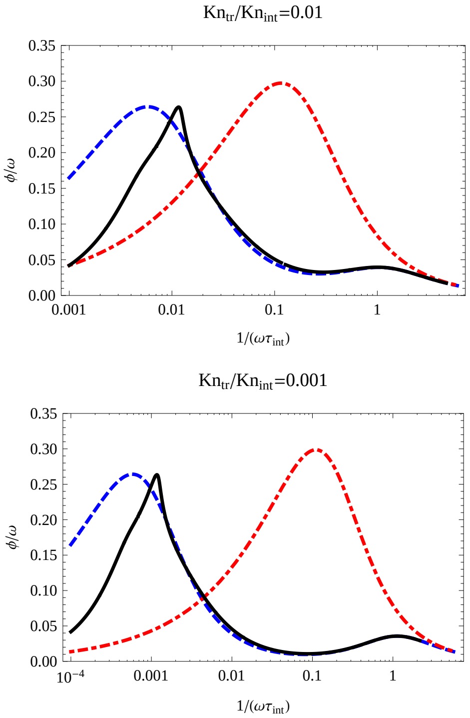

FIGURE 2. Reduced damping ϕ/ω as functions of inverse frequency $1/(\omega\tau_{int})$ for two Knudsen number ratios and different sets of equations: G36 (black continuous), classical NSF (red dash-dotted), modified NSF (blue dashed).

of original NSF (red dash-dotted) to the refined NSF equations (blue dashed) and the G36 equations (black continuous) shows marked deviation of original NSF from the other two models. Original NSF deviates from G36 for almost all frequencies plotted, while refined NSF agrees to G36 for dimensionless inverse frequencies $1/(\omega\tau_{int})$ down to the values of $\mathrm{Kn}_{tr}/\mathrm{Kn}_{int}$. This marked agreement is solely due to the time derivative $\frac{D\Delta\theta}{Dt}$ which appears in the refined NSF model (28), but not in the classical NSF model (31).

Considering the refined version of the NSF equations, instead of the classical one, will extend the range of validity of the NSF equations considerably.

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 R13 equations, which so far are available only for mon-atomic gases [3]. 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. The extended moment equations are obtained from the order of magnitude method, which reduces a large moment system to only those contributions that are relevant up to a certain order in the Knudsen number. Above, we have based the method on a system of 36 moment equations—closed by the Grad method—and have reduced it to the Navier-Stokes-Fourier (NSF) order. 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. Our analysis has shown that the classical NSF equations must be refined, if the respective Knudsen numbers fulfill the condition $\mathrm{Kn}_{\mathrm{int}}^2 < \mathrm{Kn}_{\mathrm{tr}}$. In this case, it is not sufficient to use the usual NSF expression for dynamic temperature (or dynamic pressure), which describes bulk viscosity effects, but a full balance law for dynamic temperature has to be used instead. We emphasize that this refinement will be needed in particular at somewhat larger, but still small enough, Knudsen numbers. We also point out that bulk viscosity effects do not play a role in many classical flows, e.g., Couette and Poiseuille flows, and quasi-incompressible flows. Therefore, the full balance law for dynamic temperature might not be needed for some flow configurations. As an example where it plays an important role, we showed speed and attenuation of sound waves, where the refinement leads to significant improvements. The next important steps in this research program are: (a) the development of extended moment equations based on the ordering of Knudsen numbers, (b) development of suitable boundary conditions for the equations, including boundary conditions for the refined NSF model, (c) analytical and numerical solutions of the equations, and a careful evaluation of their merits. Finally, it must be noted that the equations considered here were based on the BGK model. Re-derivation of the basic moment equations based on more accurate kinetic equations will be required in the future, to obtain better matching of transport coefficients (e.g., the Prandtl number).

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