

## Capturing non-equilibrium phenomena in rarefied polyatomic gases: A high-order macroscopic model

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A high-order macroscopic model for the accurate description of rarefied polyatomic gas flows is introduced based on a kinetic equation of Bhatnagar-Gross-Krook (BGK)-type, where the different energy exchange processes are accounted for by two collision terms. The order of magnitude method is applied to the primary moment equations to acquire the optimized moment definitions and the final scaled set of Grad's 36 moment equations for polyatomic gases. The two Knudsen numbers of the system are used for model reduction in terms of their powers, which yields a wide range of different reduced systems, a total of 13 different orders. These include, at lower order, a modification of the Navier-Stokes-Fourier (NSF) equations which shows considerable extended range of validity in comparison to the classical NSF equations. The highest order of accuracy considered gives a set of 18 regularized partial differential equations (PDEs) (R18). Attenuation and speed of linear waves are studied as the first application of the many sets of equations. For frequencies where the internal degrees of freedom are effectively frozen, the equations reproduce the behavior of monatomic gases. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4873577>]

### I. INTRODUCTION

Conventional hydrodynamics fails in the description of rarefied gas flows, where the Knudsen number is not too small. The Knudsen number is a measure illustrating the degree of non-equilibrium and rarefaction in a gas and is used to characterize the processes in kinetic theory. In the following we shall consider models of extended hydrodynamics for polyatomic gases that extend the validity of the macroscopic description towards larger Knudsen numbers. These models close the gap between classical fluid dynamics, as described by the Navier-Stokes-Fourier (NSF) equations, and kinetic theory, that is, they aim at a good description in the transition regime.

The NSF equations result from applying the Chapman-Enskog method<sup>1-3</sup> to the Boltzmann equation to first order in the Knudsen number. However, the Chapman-Enskog method at higher order, even for modified models,<sup>4-7</sup> usually yields unstable equations.<sup>8-10</sup> Alternatively, to obtain a stable set of equations at higher order, Grad's moment method<sup>11,12</sup> with different numbers of moments was proposed, with, e.g., 13 moments,<sup>13</sup> 14 moments,<sup>14,15</sup> and 17 moments.<sup>16,17</sup> However, in the cited literature, no clear reasons for the choice and number of moments are given. We will address this issue in this paper by a rational approach to derive a hierarchy of moment equations based on orders in the Knudsen numbers.

For the monatomic case, we had good success with regularized moment equations<sup>18</sup> which were derived by means of the order of magnitude method.<sup>19,20</sup> This model gives smooth shocks even at higher Mach numbers<sup>10</sup> and captures Knudsen boundary layers.<sup>21</sup> One major advantage of the order of magnitude method is that it uses the Knudsen number of the flow to define the order of the moments, and to identify the equations required at a given order.

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The present paper aims at introducing a rigorous macroscopic model for rarefied polyatomic gases. In order to meet this goal we develop a model based on meeting these requirements:

1. be stable,
2. provide a clear definition of moments,
3. identify the field variables to be considered for different levels of accuracy based on the Knudsen number,
4. have high order of accuracy; specifically, higher than the existing first order (NSF) and second order (14 moments) theories,
5. model the exchange processes in particle collisions based on their characteristic microscopic time scales, and
6. have a nice, firm, and simple mathematical structure.

The first item in the list eliminates the use of Chapman-Enskog method and brings the stable Grad's moment method into attention. However, in Grad's method the choice of moments is unclear (item 2) and not linked to the Knudsen number (item 3). This implies the need of a more genuine model which satisfies all requirements. Here, we suggest the order of magnitude method, which will be applied and generalized to polyatomic gases. The order of magnitude method specifically aims at identifying the order of moments in terms of the Knudsen number, and the set of moments that needs to be considered for a given order of accuracy (items 2, 3, and 4). We model the exchange processes with two different microscopic time scales, using a collision operator with two terms (item 5).

For this first attempt to apply the order of magnitude method to polyatomic gases, we chose a continuous internal energy parameter to model the internal degrees of freedom, instead of having discrete internal energy levels. For the same reason we chose a two-term Bhatnagar-Gross-Krook (BGK) collision model<sup>22</sup> to describe different collision processes. This gives a fast access to a complete hierarchy of moment equations. The resulting sets of macroscopic equations for various orders in the Knudsen number have all desired properties (items 6 and 1).

The order of magnitude method<sup>19,23–25</sup> is used to derive the regularized set of equations. We briefly describe the procedure of this method which consists of the following steps:

1. Constructing an infinite set of equations: A system of moment equations using Grad's moment method with arbitrary choice of definition and number of moments is constructed.
2. Reconstructing moments: The Chapman-Enskog expansion is applied to the moment equations, and their leading order terms are determined. New moments are defined using linear combinations of the original moments, in order to have the minimal number of moments at each order of magnitude.
3. Full set of equations: The set of equations for the new moments is constructed from the equations of the original moments. The Chapman-Enskog expansion is applied to the new moments to determine their leading order.
4. Model reduction: The full set of equations is rescaled considering the obtained orders of the new moments. Then, the model is reduced to the desired orders of accuracy.

The remainder of the paper is structured as follows. In Sect. II, the foundation of the kinetic theory of polyatomic gases is presented. The two term collision operator is discussed and the BGK model is introduced. In Sec. III, the general moment equation for polyatomic gases is introduced and the system of Grad's 36 moment equations is constructed, which is step 1 in the order of magnitude method. In Sec. IV, the Chapman-Enskog method is applied, the leading order terms of all moments are determined, and the new set of moments is constructed (step 2). The full set of new moment equations is obtained in Sec. V (step 3). Step 4, the model reduction, is performed in Sec. VI, which also presents the reduced equations for different orders of accuracy. To get some insight into the various sets of equations, as a first application of the equations damping and attenuation of linear waves are computed and compared in Sec. VII. Finally, some concluding remarks are given in Sec. VIII.

## II. KINETIC MODEL

In 1872, Boltzmann<sup>26</sup> proposed a transport equation which models the velocity distribution function over time, known as Boltzmann equation. A first attempt into considering the effects of internal degrees of freedom (DoF) on the behavior of molecules was made by Eucken in 1913.<sup>27</sup> Afterward, Wang Chang and Uhlenbeck considered excitation of internal degrees of freedom and presented the generalized Boltzmann equation.<sup>28,29</sup> Bourgat *et al.* introduced a model which uses just one additional continuous internal parameter to represent the internal degrees of freedom of the polyatomic gas.<sup>30</sup>

Dealing with the collision term of the Boltzmann equation is an intricate task due to its complicated and non-linear structure. Often, for simplification, the linearized Boltzmann equation is considered.<sup>31</sup> Bird<sup>32</sup> introduced the direct simulation monte carlo (DSMC) method for solving the Boltzmann equation by means of particle-based statistical simulations. However, due to statistical noise, the need for large sample size and higher number of collisions in transition regime, DSMC is computationally expensive and extremely time consuming method in the transition flow regime. Macroscopic methods offer an alternative to the Boltzmann equation in the transition regime, since they offer high computational speed, although their accuracy is limited based on the Knudsen number.

The best known approaches to obtain macroscopic models from the Boltzmann equation are the Chapman-Enskog method and the method of moments of Grad. First attempts to deal with the Wang Chang and Uhlenbeck equation were made using the Chapman-Enskog method. Monchick *et al.*<sup>33-35</sup> and Morse *et al.*<sup>36,37</sup> obtained the relations for shear and bulk viscosity and heat conductivity as functions of the relaxation times. Recently, Kustova, Nagnibeda, and co-workers<sup>38</sup> studied the strong vibrational non-equilibrium in reacting mixtures of polyatomic gases for different cases with regards to the characteristic time of the microscopic processes. They used the Chapman-Enskog method up to the first order to tackle the problem.<sup>38</sup>

First attempts for solving the Wang Chang and Uhlenbeck equation using the moment equations were made in Refs. 13, 39, and 40. Kogan used entropy maximization to obtain a generalization of Grad's 13 moment equations.<sup>13</sup> The generalized 17-moment equations for polyatomic gases were derived independently by Zhdanov<sup>16</sup> and McCormack<sup>17</sup> to cover a wider range of physical problems; the latter derived expressions for slip velocity and temperature jump. Also, Mallinger<sup>14</sup> generalized Grad's method and derived the 14 moment equations based on Bourgat's model.

In the past two years Ruggeri, Sugiyama, and co-workers used the framework of extended thermodynamics to develop a generalized 14 field theory for polyatomic gases, for both dense and rarefied gases. Their theory is consistent with Mallinger's model,<sup>14</sup> in the rarefied gas limit.<sup>15</sup> They studied the dispersion relation for sound and showed that their results have a good consistency with experimental data up to the non-dimensional frequency of 0.1.<sup>41</sup> Moreover, they showed the equivalency between extended thermodynamics and maximization of entropy,<sup>42</sup> and recovered the monatomic gas model as a singular limit of their model.<sup>43</sup>

The order of magnitude method bridges between the Chapman-Enskog and Grad method by using Knudsen number orders in the Chapman-Enskog sense to identify the appropriate moments and moment equations required for a given order. So far, the method was only applied to monatomic gases,<sup>19,20,25,44</sup> where it gives the regularized 13 moment equations (R13). The R13 equations were solved for a wide variety of one- and two-dimensional problems, where – within their range of validity – they are able to reproduce all interesting rarefaction phenomena in good agreement to solutions of the Boltzmann equation.<sup>45-48</sup> The extension of the method towards higher order suggests the regularized 26 moment equations, which indeed yields accurate results up to higher Knudsen numbers.<sup>49-51</sup> The application of the order of magnitude method to polyatomic gases is the topic of this paper.

### A. Kinetic theory of polyatomic gases

A gas particle has three translational degrees of freedom associated with its motion, and additional degrees of freedom due to rotation and vibration. All degrees of freedom, translational and internal, contribute to the energy of the molecule due to the laws of quantum mechanics. At room temperature, the vibrational degrees of freedom are usually frozen.<sup>52</sup>

The energetic state of a molecule changes due to the interaction with other molecules, i.e., collisions. While total energy and momentum are conserved, the colliding particles exchange different energy forms. 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 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 a simplified model where all internal degrees of freedom are either fully developed or frozen. Then, the spectrum of the internal energy is continuous, and the internal energy of a particle is given by<sup>53,54</sup>

$$e_{int} = I^{\frac{2}{\delta}}, \quad (1)$$

where  $\delta$  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

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

In the absence of external forces, the evolution of the distribution function is determined by the Boltzmann equation, which is a nonlinear integro-differential equation written as

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = S(f, f). \quad (2)$$

The left and right-hand sides take into account the effects of the particle's free flight and collisions, respectively. Depending on the accuracy of description, the quadratic collision term,  $S(f, f)$ , assumes different complex forms, which might require lengthy and expensive computations. Kinetic models, such as the BGK model used below, replace the Boltzmann collision term by simpler models that preserve the basic relaxation properties and give the correct transport coefficients, while losing some of the detailed accuracy.

## B. Macroscopic quantities

Macroscopic properties such as mass density  $\rho$ , momentum  $\rho v_i$ , energy  $u$ , pressure  $p$ , stress tensor  $\sigma_{ij}$ , and heat flux vector  $q_i$  are moments of the phase density. Based on the definition of general trace free central moments,

$$u_{i_1 \dots i_n}^{\zeta, A} = m \int \int (I^{2/\delta})^A C^{2\zeta} C_{<i_1} C_{i_2} \dots C_{i_n} f d\mathbf{c}dI, \quad (3)$$

the important moments can be expressed as

$$\text{Density } \rho = m \int \int f d\mathbf{c}dI = \int \rho_I dI = u^{0,0}, \quad (4a)$$

$$\text{Velocity } \rho v_i = m \int \int c_i f d\mathbf{c}dI \text{ or } 0 = m \int \int C_i f d\mathbf{c}dI = u_i^{0,0}, \quad (4b)$$

$$\text{Stress } \sigma_{ij} = m \int \int C_{<i} C_{j>} f d\mathbf{c}dI = u_{ij}^{0,0}, \quad (4c)$$

$$\text{Translational energy } \rho u_{tr} = \frac{3}{2} p = m \int \int \frac{C^2}{2} f d\mathbf{c}dI = \frac{1}{2} u^{1,0}, \quad (4d)$$

$$\text{Internal energy } \rho u_{int} = m \int \int I^{2/\delta} f d\mathbf{c}dI = \int I^{2/\delta} \rho_I dI = u^{0,1}, \quad (4e)$$

$$\text{Translational heat flux } q_{i,tr} = m \int \int C_i \frac{C^2}{2} f d\mathbf{c} dI = \frac{1}{2} u_i^{1,0}, \quad (4f)$$

$$\text{Internal heat flux } q_{i,int} = m \int \int C_i I^{2/\delta} f d\mathbf{c} dI = u_i^{0,1}. \quad (4g)$$

Here,  $c_i$  is the microscopic velocity,  $C_i = c_i - v_i$  is the peculiar particle velocity,  $\rho_I = m \int f d\mathbf{c}$  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 particle, where  $\theta = \frac{k_b}{m} T$  is temperature in specific energy units. Thus in equilibrium, the translational and internal energies are

$$u_{tr|E} = \frac{3}{2}\theta \quad \text{and} \quad u_{int|E} = \frac{\delta}{2}\theta. \quad (5)$$

We extend the definition of temperatures to non-equilibrium, by defining the translational temperature  $\theta_{tr}$  and the internal temperature  $\theta_{int}$  through the energies as

$$u_{tr} = \frac{3}{2}\theta_{tr} \quad \text{and} \quad u_{int} = \frac{\delta}{2}\theta_{int}. \quad (6)$$

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  $\theta$  as

$$u = \frac{3}{2}\theta_{tr} + \frac{\delta}{2}\theta_{int} = \left(\frac{3}{2} + \frac{\delta}{2}\right)\theta. \quad (7)$$

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

### C. BGK model

For monatomic gases, the BGK model<sup>22</sup> describes relaxation towards the equilibrium distribution as

$$S = \frac{1}{\tau} (\mathcal{M} - f), \quad (8)$$

where the Maxwellian  $\mathcal{M}$  is the distribution function in local equilibrium, and  $\tau$  is the characteristic relaxation time (mean free time or microscopic time scale).

Morse<sup>36</sup> introduced a BGK-type model with two collision terms to replace the Wang Chang and Uhlenbeck equation and tackled it using the Chapman-Enskog method. Andries *et al.* introduced the ellipsoidal Gaussian BGK model for polyatomic gases considering the additional continuous internal parameter and proved the H-theorem.<sup>53</sup> Brull *et al.* used maximization of entropy to obtain the model of Andries *et al.*<sup>54</sup>

As discussed earlier, in a polyatomic gas, translational energy is exchanged in all molecular collisions, but internal energy of the molecules is exchanged only in some collisions. Hence, the characteristic microscopic time for internal energy is larger than that for the translational energy exchange. To describe this in a BGK model, we use a two term collision operator, where the first term describes only the translational energy exchange during the collisions and the second term models the exchange of the internal and translational energies.<sup>55</sup> The resulting BGK equation reads

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = -\frac{1}{\tau_{tr}} (f - f_{tr}) - \frac{1}{\tau_{int}} (f - f_{int}). \quad (9)$$

Here,  $\tau_{tr}$  and  $\tau_{int}$  are the corresponding mean free times that we assume to depend only on the macroscopic equilibrium variables  $(\rho, \theta)$ . 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 we obtained them using entropy maximization<sup>56,57</sup> as Maxwellian functions,

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

$$f_{int} = \frac{\rho}{m} \frac{1}{(2\pi)^{\frac{3}{2}} \theta^{(\delta+3)/2}} \frac{1}{\Gamma(1 + \frac{\delta}{2})} \exp \left[ -\frac{1}{\theta} \left( \frac{C^2}{2} + I^{2/\delta} \right) \right]. \quad (10b)$$

Processes in kinetic theory are characterized by the Knudsen number,

$$\text{Kn} = \frac{\lambda}{L_0} = \frac{\tau}{\tau_0}, \quad (11)$$

where  $L_0$  is the characteristic length scale of the process,  $\tau_0$  is a typical characteristic time of the process, and  $\lambda$  is the mean free path. The typical reference time scale  $\tau_0$  is defined as  $L_0/\sqrt{\theta_0}$ .

For the polyatomic BGK model (9) we have two different relaxation times, corresponding to two different mean free paths, and two distinct Knudsen numbers,  $\text{Kn}_{tr} = \frac{\tau_{tr}}{\tau_0}$  and  $\text{Kn}_{int} = \frac{\tau_{int}}{\tau_0}$ . The Knudsen numbers will be used for model reduction.

### III. 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. Also, increasing the number of moments typically leads to a better approximation.<sup>58</sup>

#### A. General moment equation

The moment equations are obtained by taking weighted averages of the kinetic equation. Multiplying the kinetic equation (9) with  $m(I^{2/\delta})^A C^{2\zeta} C_{<i_1} C_{i_2} \dots C_{i_n}>$ , and subsequent integration over velocity space and internal energy parameter gives the general moment equation as

$$\begin{aligned} \frac{Du_{i_1 \dots i_n}^{\zeta, A}}{Dt} + 2\zeta u_{i_1 \dots i_n k}^{\zeta-1, A} \frac{Dv_k}{Dt} + 2\zeta u_{i_1 \dots i_n k j}^{\zeta-1, A} \frac{\partial v_j}{\partial x_k} + \frac{n}{2n+1} 2\zeta u_{j <i_1 \dots i_{n-1}>}^{\zeta, A} \frac{\partial v_j}{\partial x_{i_n}} + \frac{\partial u_{i_1 \dots i_n k}^{\zeta, A}}{\partial x_k} \\ + \frac{n}{2n+1} \frac{\partial u_{<i_1 \dots i_{n-1}>}^{\zeta+1, A}}{\partial x_{i_n}} + 2\zeta \frac{n}{2n+1} u_{<i_1 \dots i_{n-1}>}^{\zeta, A} \frac{Dv_{i_n}}{Dt} + 2\zeta \frac{n+1}{2n+3} u_{<i_1 \dots i_n>}^{\zeta, A} \frac{\partial v_k}{\partial x_k} \\ + \frac{n-1}{2n-1} n u_{<i_1 \dots i_{n-2}>}^{\zeta+1, A} \frac{\partial v_{i_{n-1}}}{\partial x_{i_n}} + n u_{<i_1 \dots i_{n-1}>}^{\zeta, A} \frac{Dv_{i_n}}{Dt} + u_{i_1 \dots i_n}^{\zeta, A} \frac{\partial v_k}{\partial x_k} + \frac{n}{2n+1} \frac{n-1}{2n-1} 2\zeta u_{<i_1 \dots i_{n-2}>}^{\zeta+1, A} \frac{\partial v_{i_{n-1}}}{\partial x_{i_n}} \\ + n u_{k <i_1 \dots i_{n-1}>}^{\zeta, A} \frac{\partial v_{i_n}}{\partial x_k} = \frac{1}{\tau_{tr}} \left[ u_{i_1 \dots i_n | E, tr}^{\zeta, A} - u_{i_1 \dots i_n}^{\zeta, A} \right] + \frac{1}{\tau_{int}} \left[ u_{i_1 \dots i_n | E, int}^{\zeta, A} - u_{i_1 \dots i_n}^{\zeta, A} \right]. \end{aligned} \quad (12)$$

Here, the relation  $u_{<i_1 \dots i_n>k}^{\zeta, A} = u_{i_1 \dots i_n k}^{\zeta, A} + \frac{n}{2n+1} u_{<i_1 \dots i_{n-1}>}^{\zeta+1, A} \delta_{i_n > k}$  is used.<sup>20</sup> The right hand side of the equation describes the change of the moment  $u_{i_1 \dots i_n}^{\zeta, A}$  due to collisions, which relax the moment toward its value according to the equilibrium distributions,

$$u_{|E, int}^{\zeta, A} = \frac{(2\zeta+1)!!}{\Gamma(\frac{\delta}{2})} \rho \theta^{\zeta+A} \Gamma\left(A + \frac{\delta}{2}\right), \quad (13a)$$

$$u_{|E, tr}^{\zeta, A} = (2\zeta+1)!! \theta_{tr}^{\zeta} \int (I^{2/\delta})^A \rho_I dI, \quad (13b)$$

$$u_{i_1 \dots i_n | E}^{\zeta, A} = 0 \quad n \neq 0, \quad (13c)$$

where  $(2\zeta+1)!! = \prod_{s=1}^{\zeta} (2s+1)$  and  $\rho_I = m \int f d\mathbf{c}$ .

## B. Conservation laws

Conservation laws for mass ( $\zeta = A = n = 0$ ), momentum ( $\zeta = A = 0, n = 1$ ), and total energy are obtained from the general moment equation (12) as

$$\frac{D\rho}{Dt} + \rho \frac{\partial v_i}{\partial x_i} = 0, \quad (14a)$$

$$\frac{Dv_i}{Dt} + \frac{1}{\rho} \frac{\partial \sigma_{ij}}{\partial x_j} + \frac{\partial \theta_{tr}}{\partial x_i} + \frac{\theta_{tr}}{\rho} \frac{\partial \rho}{\partial x_i} = 0, \quad (14b)$$

$$\rho \frac{3 + \delta}{2} \frac{D\theta}{Dt} + \frac{\partial q_{i,int}}{\partial x_i} + \frac{\partial q_{i,tr}}{\partial x_i} + \sigma_{ij} \frac{\partial v_j}{\partial x_i} + \rho \theta_{tr} \frac{\partial v_i}{\partial x_i} = 0. \quad (14c)$$

The conservation of the total energy results from summation of the balance laws for translational ( $\zeta = 1, A = n = 0$ ) and internal ( $\zeta = 0, A = 1, n = 0$ ) energies. The balance law for translational energy reads

$$\rho \frac{3}{2} \frac{D\theta_{tr}}{Dt} + \frac{\partial q_{i,tr}}{\partial x_i} + \sigma_{ij} \frac{\partial v_j}{\partial x_i} + \rho \theta_{tr} \frac{\partial v_i}{\partial x_i} = \frac{3\rho}{\tau_{int}} \frac{(\theta - \theta_{tr})}{2}. \quad (15)$$

Later, we will replace the translational temperature  $\theta_{tr}$  as variable by its non-equilibrium part  $\Delta\theta = \theta - \theta_{tr}$ , named dynamic temperature.

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 are present in the conservation laws, are obtained from the general moment equation (12) by appropriate choice of ( $\zeta, A, n$ ). These equations contain 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 can be obtained from Eq. (12). Choosing all moments mentioned so far as variables will construct a 36 moments set,

$$\left\{ \rho, v_i, \theta_{tr}, \theta_{int}, \sigma_{ij}, q_{i,tr}, q_{i,int}, u_{ij}^{1,0}, u^{2,0}, u_{ij}^{0,1}, u^{1,1}, u_{ijk}^{0,0} \right\}. \quad (16)$$

The equations for these 36 moments contain higher moments  $u_{ijk}^{1,0}, u_i^{2,0}, u_{ijkl}^{0,0}, u_{ijk}^{0,1}$ , and  $u_i^{1,1}$ . To close the system of 36 equations, Grad's distribution function will be used next to obtain expressions for these higher moments in terms of the 36 variables.

## C. Grad closure: 36 moments

Grad<sup>11,12</sup> proposed a distribution function based on the expansion of the Maxwellian into a series of Hermite polynomials. It is convenient to consider the expansion with the trace free moments instead of regular moments, so that the generalized Grad distribution function based on the 36 variables is written as

$$f_{|36} = f_{int} \left( \lambda^{0,0} + \lambda_i^{0,0} C_i + \lambda^{1,0} C^2 + \lambda_{\langle ij \rangle}^{0,0} C_{\langle i} C_{j \rangle} + \lambda^{0,1} I^{2/\delta} + \lambda_i^{1,0} C_i C^2 + \lambda_i^{0,1} C_i I^{2/\delta} \right. \\ \left. + \lambda_{\langle ij \rangle}^{1,0} C^2 C_{\langle i} C_{j \rangle} + \lambda^{2,0} C^4 + \lambda_{\langle ijk \rangle}^{0,0} C_{\langle i} C_j C_{k \rangle} + \lambda_{\langle ij \rangle}^{0,1} C_{\langle i} C_{j \rangle} I^{2/\delta} + \lambda^{1,1} C^2 I^{2/\delta} \right), \quad (17)$$

where  $\lambda_{(i_1 i_2 \dots i_n)}^{\zeta, A}$  are expansion coefficients. Grad's 36 distribution function should reproduce the set of 36 moments, this is done by choosing the coefficients  $\lambda$  based on the definition of moments, Eq. (A2). The obtained coefficients are presented in Subsection A 1 of the Appendix. Using Grad's distribution function (17), the constitutive equations are obtained as

$$u_{ijk}^{1,0} = 9\theta u_{ijk}^{0,0}, \quad u_i^{2,0} = 28\theta q_{i,tr}, \quad u_{ijkl}^{0,0} = 0, \\ u_{ijk}^{0,1} = \frac{\delta}{2} \theta u_{ijk}^{0,0}, \quad u_i^{1,1} = (5q_{i,int} + \delta q_{i,tr}) \theta. \quad (18)$$

Substituting these equations into the 36 balance laws gives the closed set of equations. Due to lack of space, the full set of equations will be shown only later.

Grad's distribution function implies a relation between the internal state density,  $\rho_I$ , the total density,  $\rho$ , and the temperatures,  $\theta$  and  $\Delta\theta = \theta - \theta_{tr}$ , viz.

$$\rho_I = \frac{\rho}{\theta^{1+\delta/2}\Gamma(1+\frac{\delta}{2})} \left[ I^{2/\delta} \left( 1 - \left( 1 - \frac{3}{\delta} \right) \frac{\Delta\theta}{\theta} \right) + \theta - \frac{3}{2}\Delta\theta \right] \exp\left(-\frac{1}{\theta}I^{2/\delta}\right). \quad (19)$$

#### IV. RECONSTRUCTING MOMENTS

##### A. Smallness parameters

Applying the order of magnitude method to the set of 36 moment equations will ensure that the minimum number of variables are used for any wanted order of accuracy in terms of power of the Knudsen numbers. This method first applies the Chapman-Enskog expansion on the moments to find their leading order terms. Then, new moments are constructed such that only those which are linearly independent have the same order of accuracy. This will give the minimum number of moments at a certain order of accuracy.

The expansion parameter in the Chapman-Enskog method is the Knudsen number, of which we have two,  $\text{Kn}_{tr}$  and  $\text{Kn}_{int}$ , to account for translational and internal energy exchange. We rescale the microscopic time scales as

$$\tau_{tr} = \text{Kn}_{tr} \tilde{\tau}_{tr} \quad \text{and} \quad \tau_{int} = \text{Kn}_{int} \tilde{\tau}_{int}. \quad (20)$$

Here,  $\tilde{\tau}_{tr}$  and  $\tilde{\tau}_{int}$  are of the order of the macroscopic time scale  $\tau_0$ . The notation used is chosen since it always indicates the type of collision (translational or internal) that gives rise to a term occurring in the equations below. After the expansion is done, the Knudsen numbers will be substituted back to the microscopic time scales and the original equations will be recovered.

$\text{Kn}_{tr}$  should be less than  $\text{Kn}_{int}$ , because 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 the internal smallness parameter  $\epsilon$  as

$$\text{Kn}_{tr} = \epsilon \quad \text{and} \quad \text{Kn}_{int} = \epsilon^\alpha. \quad (21)$$

With this, the two Knudsen numbers are replaced by a single smallness parameter,  $\epsilon$ , and a magnifying parameter,  $\alpha$ , with  $0 < \alpha < 1$ . The lower limit of the internal smallness parameter is recovered when  $\alpha = 1$  and the upper limit is reached when  $\alpha = 0$ . From the above we find

$$\alpha = 1 - \frac{\ln \frac{\tau_{tr}}{\tau_{int}}}{\ln \text{Kn}_{tr}} = \left( 1 + \frac{\ln \frac{\tau_{tr}}{\tau_{int}}}{\ln \text{Kn}_{int}} \right)^{-1}. \quad (22)$$

While the ratio of relaxation times  $\frac{\tau_{tr}}{\tau_{int}}$  depends on the state of the gas, the ratio  $\frac{\tau_{tr}}{\tau_0} = \epsilon = \text{Kn}_{tr}$  depends on the relevant macroscopic time scale  $\tau_0$ . Accordingly, the values of both,  $\alpha$  and  $\epsilon = \text{Kn}_{tr}$ , depend on the chosen scale. To show some examples of the translational and internal relaxation times and their ratios, we used the experimental data on shear viscosity<sup>59</sup> and fitting data on bulk viscosity<sup>41</sup> of normal hydrogen and deuterium. As will be shown later, shear and bulk viscosity (42) in the linear case with ground state  $\{\rho_0, \theta_0, \Delta\theta_0 = 0\}$  are

$$\mu = \tau_{tr} \rho_0 \theta_0 = \tau_{tr} p_0 \quad \text{and} \quad v = \tau_{int} \frac{2\delta(\rho_0 \theta_0)}{3(3+\delta)} = \tau_{int} \frac{2\delta(p_0)}{3(3+\delta)}. \quad (23)$$

Values for the translational and internal relaxation times of normal hydrogen and deuterium for reference pressure of  $10^3$  Pa and reference temperature of 77.3 and 293 (K) are listed in Table I. Bulk viscosity values are obtained by assuming different values for specific heat based on the temperature, which are converted to corresponding values of  $\delta$ . The obtained relaxation times and their ratio,  $\tau_{tr}/\tau_{int} = \text{Kn}_{tr}/\text{Kn}_{int}$ , is at order of  $10^{-2}$  and  $10^{-3}$ .

Different values of  $\alpha$  correspond to different values of internal or translational Knudsen number and ratios of the relaxation times,  $\tau_{tr}/\tau_{int} = \text{Kn}_{tr}/\text{Kn}_{int}$ , as shown in Fig. 1. For higher Knudsen numbers  $\text{Kn}_{int}$ , particularly near unity, mostly values of  $\alpha$  less than 0.5 are relevant. The ratio of the



TABLE I. Shear, bulk viscosity, and specific heat values<sup>41,59</sup> of hydrogen and deuterium for two temperature values and reference pressure of  $10^3$  Pa. Obtained values of relaxation times and their ratios.

Gas	$T_0(K)$	$\mu$ (Pa s) $\times 10^7$	$\nu$ (Pa s) $\times 10^6$	$C_v = \frac{3+\delta}{2}$	$\tau_{tr}$ (s)	$\tau_{int}$ (s)	$\tau_{tr}/\tau_{int}$
H <sub>2</sub>	77.3	35.0	98	1.57	$3.50 \times 10^{-9}$	$3.30 \times 10^{-6}$	$1.06 \times 10^{-3}$
	293	88.2	326	2.45	$8.82 \times 10^{-9}$	$1.26 \times 10^{-6}$	$7 \times 10^{-3}$
D <sub>2</sub>	77.3	48.2	174	2.54	$4.82 \times 10^{-9}$	$6.37 \times 10^{-7}$	$7.57 \times 10^{-3}$
	293	123	271	2.50	$1.23 \times 10^{-8}$	$1.01 \times 10^{-6}$	0.012

relaxation times considered here covers both extreme cases,  $\tau_{tr} \approx \tau_{int}$  ( $\tau_{tr}/\tau_{int} = 0.5$ ) and  $\tau_{tr} \ll \tau_{int}$  ( $\tau_{tr}/\tau_{int} = 10^{-7}$ ), and the values in between.

Different problems may encounter different relaxation times and different Knudsen numbers. A vacuum system with pressure of 20 Pa, temperature of 293 K, and macroscopic length scale of 5 cm with deuterium has the following characteristics:  $\text{Kn}_{tr} = 0.00956$ ,  $\text{Kn}_{int} = 0.797$ ,  $\alpha = 0.0488$ . However, if the pressure and length scale increase to 100 Pa and 8 cm, the values become  $\text{Kn}_{tr} = 0.00119$ ,  $\text{Kn}_{int} = 0.0996$ ,  $\alpha = 0.343$ . As another example, a microsystem at atmospheric pressure, temperature of 293 K, and macroscopic length scale of  $20 \mu\text{m}$  with hydrogen has the following characteristics:  $\text{Kn}_{tr} = 0.0067$ ,  $\text{Kn}_{int} = 0.954$ ,  $\alpha = 0.0094$ . If the characteristic length increases to  $150 \mu\text{m}$ , we have  $\text{Kn}_{tr} = 0.00089$ ,  $\text{Kn}_{int} = 0.1272$ ,  $\alpha = 0.294$ .

Based on the values of  $\alpha$ , different set of equations in various required order of accuracy will be obtained in Sec. VI. Therefore, the particular problem under consideration determines which set of equations should be used.

## B. Chapman-Enskog expansion

The Chapman-Enskog expansion on the moment equations must be performed for both Knudsen numbers, that is, for all powers of  $\epsilon$  and  $\epsilon^\alpha$ . Due to the large ratio possible between the Knudsen numbers, the underlying multiscale problem might require more than a simple accounting of terms with the same order only. For instance, when  $\text{Kn}_{int}^2 \simeq \text{Kn}_{tr}$ , proper accounting to first order in  $\text{Kn}_{tr}$  might require consideration of *different* orders in the CE expansion: expansion to first order in  $\text{Kn}_{tr}$ , but to second order in  $\text{Kn}_{int}$ . The conserved variables, density, velocity, and total temperature,

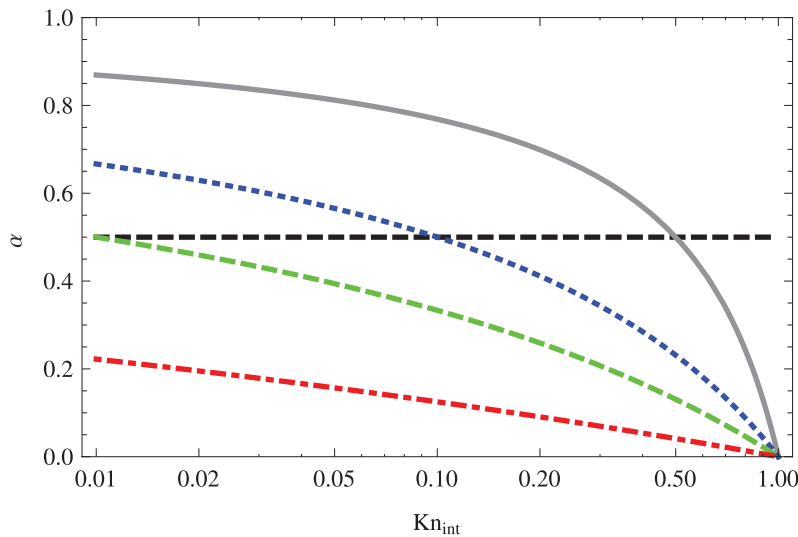


FIG. 1. Values of  $\alpha$  for a range of internal Knudsen number and four relaxation times ratio,  $\tau_{tr}/\tau_{int} = 0.5$  (gray solid line),  $\tau_{tr}/\tau_{int} = 10^{-1}$  (blue dots),  $\tau_{tr}/\tau_{int} = 10^{-2}$  (green dashed line), and  $\tau_{tr}/\tau_{int} = 10^{-7}$  (red dotted-dashed line). The limit of  $\alpha = 0.5$  is shown with black dashed line.

have equilibrium values and hence are at zero order. The remaining variables are expanded in the smallness parameter as

$$\psi = \epsilon^{0\alpha} [\epsilon^0 \psi^{(0,0)} + \epsilon^1 \psi^{(0,1)} + \epsilon^2 \psi^{(0,2)} + \epsilon^3 \psi^{(0,3)} + \dots] + \epsilon^{1\alpha} [\epsilon^0 \psi^{(1,0)} + \epsilon^1 \psi^{(1,1)} + \epsilon^2 \psi^{(1,2)} + \dots] + \epsilon^{2\alpha} [\epsilon^0 \psi^{(2,0)} + \epsilon^1 \psi^{(2,1)} + \dots] + \dots, \quad (24)$$

where for the 36 moment system,  $\psi = \{\Delta\theta, \sigma_{ij}, q_{i,tr}, q_{i,int}, u_{ij}^{1,0}, u^{2,0}, u_{ij}^{0,1}, u^{1,1}, u_{ijk}^{0,0}\}$ .

The leading order terms of the moments are found as the first nonvanishing term in their expansion; one finds

$$\mathcal{O}(\epsilon^0): u^{2,0(0,0)} = 15\rho\theta^2, \quad u^{1,1(0,0)} = \frac{3}{2}\rho\delta\theta^2, \quad (25a)$$

$$\mathcal{O}(\epsilon^\alpha): \Delta\theta^{(1,0)} = \tilde{\tau}_{int} \frac{2\delta}{3(3+\delta)} \theta \frac{\partial v_i}{\partial x_i}, \quad (25b)$$

$$\mathcal{O}(\epsilon^1): q_{i,tr}^{(0,1)} = -\tilde{\tau}_{tr} \frac{5}{2} \rho \theta \frac{\partial \theta}{\partial x_i}, \quad u_{ij}^{1,0(0,1)} = -\tilde{\tau}_{tr} 14 \rho \theta^2 \frac{\partial v_{<i}}{\partial x_{>}}, \quad (25c)$$

$$\mathcal{O}(\epsilon^1): \sigma_{ij}^{(0,1)} = -\tilde{\tau}_{tr} 2 \rho \theta \frac{\partial v_{<i}}{\partial x_{>}}, \quad q_{i,int}^{(0,1)} = -\tilde{\tau}_{tr} \frac{\delta}{2} \rho \theta \frac{\partial \theta}{\partial x_i}, \quad u_{ij}^{0,1(0,1)} = -\tilde{\tau}_{tr} \rho \delta \theta^2 \frac{\partial v_{<i}}{\partial x_{>}}, \quad (25d)$$

$$\mathcal{O}(\epsilon^2): u_{ijk}^{0,0(0,2)} = -\tilde{\tau}_{tr} \left( \frac{3}{7} \frac{\partial u_{<ij}^{1,0}}{\partial x_{>}} - 3\sigma_{<ij} \frac{\partial \theta}{\partial x_{>}} - 3\theta \sigma_{<ij} \frac{\partial \ln \rho}{\partial x_{>}} + \frac{12}{5} q_{<i,tr} \frac{\partial v_{>}}{\partial x_{>}} \right). \quad (25e)$$

To leading order, the two scalar moments,  $u^{2,0(0,0)}$  and  $u^{1,1(0,0)}$ , are proportional to the total temperature and density. The heat fluxes,  $q_{i,tr}^{(0,1)}$  and  $q_{i,int}^{(0,1)}$ , are proportional to each other, and also the three tensorial moments,  $\sigma_{ij}^{(0,1)}$ ,  $u_{ij}^{0,1(0,1)}$ , and  $u_{ij}^{1,0(0,1)}$ , are proportional to each other.

We aim at having the smallest number of moments at each order. Higher order replacements for the scalars  $u^{2,0}$  and  $u^{1,1}$  are obtained by subtracting their leading order terms to define new variables as

$$w^{2,0} = u^{2,0} - 15\rho\theta^2 \quad \text{and} \quad w^{1,1} = u^{1,1} - \rho \frac{3}{2} \delta \theta^2. \quad (26)$$

The dynamic temperature,  $\Delta\theta = \theta - \theta_{tr}$ , is the only variable at order  $\alpha$ .

The linear dependent 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,

$$q_i = q_{i,tr} + q_{i,int}, \quad (27a)$$

and one unique higher order variable, heat flux difference,

$$\Delta q_i = q_{i,tr} - \frac{5}{8} q_{i,int}. \quad (27b)$$

Similarly, the 2-tensors can be combined such that only the stress tensor  $\sigma_{ij}$  is of first order, while the moments  $u_{ij}^{1,0}$  and  $u_{ij}^{0,1}$  are replaced by higher order moments as,

$$u_{ij}^- = u_{ij}^{1,0} - \frac{14}{\delta} u_{ij}^{0,1} \quad \text{and} \quad u_{ij}^+ = u_{ij}^{1,0} + u_{ij}^{0,1} - \frac{(14+\delta)\theta}{2} \sigma_{ij}. \quad (28)$$

The second order moment  $u_{ijk}^{0,0}$  is the only 3-tensor in the equations and thus remains unchanged.

After this first round of the reconstructing moments, we replaced the original 36 variables by the alternative set

$$\left\{ \rho, v_i, \theta, \Delta\theta, \sigma_{ij}, q_i, \Delta q_i, w^{2,0}, w^{1,1}, u_{ij}^-, u_{ij}^+, u_{ijk}^{0,0} \right\}.$$

Here,  $\left\{ \rho, v_i, \theta, q_i, \sigma_{ij}, u_{ijk}^{0,0} \right\}$  have linear independent leading order terms, thus, there will be no further change for these variables. The other variables are treated with the same procedure, i.e.,

rewriting the moment equations with the new moment definitions, and applying the Chapman-Enskog expansion to obtain the leading order terms as

$$\begin{aligned} \mathcal{O}(\epsilon^\alpha) : w^{2,0(1,0)} &= -30\rho\theta\Delta\theta, \quad w^{1,1(1,0)} = \frac{3}{2}[3-\delta]\rho\theta\Delta\theta, \\ \mathcal{O}(\epsilon^{1+\alpha}) : u_{ij}^{-(1,1)} &= \tilde{\tau}_{ir}14\frac{[3+\delta]}{\delta}\rho\theta\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}, \quad u_{ij}^{+(1,1)} = \tilde{\tau}_{ir}11\rho\theta\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}. \end{aligned} \quad (29)$$

Now the leading order terms of the scalars  $\{\Delta\theta, w^{2,0}, w^{1,1}\}$  are linearly dependent, also the leading order terms of the 2-tensors  $\{u_{ij}^-, u_{ij}^+\}$  are linearly dependent. Therefore, we construct new moments to have linearly independent moments in all the orders; the results are four new moments which substitute  $\{w^{2,0}, w^{1,1}, u_{ij}^+, u_{ij}^-\}$  by

$$z^{2,0} = w^{2,0} + 30\rho\theta\Delta\theta, \quad z^{1,1} = w^{1,1} - \frac{3}{2}[3-\delta]\rho\theta\Delta\theta, \quad (30a)$$

$$B_{ij}^- = u_{ij}^+ - \frac{11}{14}\frac{\delta}{\delta+3}u_{ij}^-, \quad B_{ij}^+ = u_{ij}^+ + u_{ij}^-. \quad (30b)$$

There will be no further change for  $B_{ij}^-$  and  $B_{ij}^+$ , since they have linearly independent leading order terms. Applying again the Chapman-Enskog expansion, the leading order terms for  $z^{2,0}$  and  $z^{1,1}$  are

$$z^{1,1(2,0)} = -\frac{9}{2}\rho\Delta\theta^2 \quad \text{and} \quad z^{2,0(2,0)} = 15\rho\Delta\theta^2. \quad (31)$$

The linear dependent scalars  $z^{1,1}$  and  $z^{2,0}$ , which are of  $2\alpha$  order, can be combined into one  $2\alpha$  order scalar,  $B^+$ , and one unique higher order scalar,  $B^-$ , as

$$B^+ = z^{1,1} - z^{2,0} \quad \text{and} \quad B^- = z^{1,1} + \frac{3}{10}z^{2,0}. \quad (32)$$

After this set of operations, we have the final set of 36 moments,

$$\left\{ \rho, v_i, \theta, \Delta\theta, \sigma_{ij}, q_i, \Delta q_i, B_{ij}^+, B^+, B_{ij}^-, B^-, u_{ijk}^{0,0} \right\}.$$

By construction, these variables are linearly independent in their leading orders.

### C. Orders and leading terms of moments

The leading order contributions of all non-equilibrium variables are obtained from Chapman-Enskog expansion for proper accounting of the magnitude and later use of the expressions. For the model reduction, we require the explicit order of all terms be clearly visible in the equations, hence we rewrite the variables as

$$\Psi = \epsilon^\xi \tilde{\Psi}, \quad (33)$$

$$\Psi = \left\{ \Delta\theta, B^+, \sigma_{ij}, q_i, \Delta q_i, B_{ij}^+, B^-, B_{ij}^-, u_{ijk}^{0,0} \right\},$$

$$\xi = \left\{ \alpha, 2\alpha, 1, 1, 1 + \alpha, 1 + \alpha, \left\{ \begin{array}{ll} 1 + 2\alpha & 0 < \alpha < 0.5 \\ 2 & 0.5 < \alpha < 1 \end{array} \right\}, 2, 2 \right\}.$$

Quantities with a tilde are considered to be of zeroth order, while the orders are made explicit with  $\epsilon$  and  $\epsilon^\alpha$ . The leading orders of the above variables are not affected by the value of  $\alpha$ , except for  $B^-$  where we find

$$\mathcal{O}(\epsilon^{1+2\alpha}) : B^{-(2,1)} = \tilde{\tau}_{ir} \left[ \frac{2}{13}B^+ + 3\rho\Delta\theta^2 \right] \frac{\partial v_i}{\partial x_i} \quad \text{for} \quad 0 < \alpha < 0.5, \quad (34a)$$

or

$$\begin{aligned} \mathcal{O}(\epsilon^2) : B^{-(0,2)} = \tilde{\tau}_{tr} \left[ \frac{2(6+\delta)}{5+\delta} q_k \theta \frac{\partial \ln \rho}{\partial x_k} - \left( 8 - \frac{10}{5+\delta} \right) q_k \frac{\partial \theta}{\partial x_k} \right. \\ \left. - \frac{12}{5} \theta \sigma_{kj} \frac{\partial v_j}{\partial x_k} - \frac{(24-\delta)}{2(5+\delta)} \theta \frac{\partial q_i}{\partial x_i} \right] \quad \text{for } 0.5 < \alpha < 1. \end{aligned} \quad (34b)$$

Note that for  $\alpha \simeq 0.5$  both contributions have the same order and their sum must be considered.

## V. GRAD'S 36 MOMENT EQUATIONS IN OPTIMIZED VARIABLES

We identified the final variables in Sec. IV. Their balance laws, which are the final closed form of the 36 moment equations, are obtained from the original moment equations by the appropriate linear combinations. Here, we only show the equations for the first 18 moments, the equations for the remaining 18 moments are presented in Subsection A 2 of the Appendix. The introduced notation allows us to arrange all terms by their explicit  $\epsilon$ -orders. In particular we have the following.

The conservation laws for mass, momentum, and energy

$$\frac{D\rho}{Dt} + \rho \frac{\partial v_i}{\partial x_i} = 0, \quad (35a)$$

$$\left[ \frac{Dv_i}{Dt} + \theta \frac{\partial \ln \rho}{\partial x_i} + \frac{\partial \theta}{\partial x_i} \right] - \epsilon^\alpha \left[ \frac{\partial \Delta \tilde{\theta}}{\partial x_i} + \Delta \tilde{\theta} \frac{\partial \ln \rho}{\partial x_i} \right] + \epsilon^1 \left[ \frac{1}{\rho} \frac{\partial \tilde{\sigma}_{ij}}{\partial x_j} \right] = 0, \quad (35b)$$

$$\left[ \rho \frac{D\theta}{Dt} + \frac{2}{3+\delta} \rho \theta \frac{\partial v_i}{\partial x_i} \right] - \epsilon^\alpha \left[ \frac{2}{3+\delta} \rho \Delta \tilde{\theta} \frac{\partial v_i}{\partial x_i} \right] + \epsilon^1 \left[ \frac{2}{3+\delta} \left( \frac{\partial \tilde{q}_i}{\partial x_i} + \tilde{\sigma}_{ij} \frac{\partial v_j}{\partial x_i} \right) \right] = 0; \quad (35c)$$

the balance laws for dynamic temperature  $\Delta\theta$ , stress tensor  $\sigma_{ij}$ , overall heat flux  $q_i$ , heat flux difference  $\Delta q_i$ , and higher moment  $B^+$ :

$$\begin{aligned} \epsilon^\alpha \left[ \rho \frac{D\Delta \tilde{\theta}}{Dt} + \frac{2}{3} \frac{\delta}{3+\delta} \rho \Delta \tilde{\theta} \frac{\partial v_i}{\partial x_i} \right] - \epsilon^1 \left[ \frac{2}{3} \frac{\delta}{3+\delta} \left( \frac{2}{5+\delta} \frac{\partial \tilde{q}_i}{\partial x_i} + \tilde{\sigma}_{ij} \frac{\partial v_j}{\partial x_i} \right) \right] \\ - \epsilon^{1+\alpha} \left[ \frac{2}{3} \frac{\delta}{5+\delta} \frac{\partial \Delta \tilde{q}_i}{\partial x_i} \right] = \frac{2}{3} \frac{\delta}{3+\delta} \rho \theta \frac{\partial v_i}{\partial x_i} - \frac{\rho}{\tilde{\tau}_{int}} \Delta \tilde{\theta}, \end{aligned} \quad (35d)$$

$$\begin{aligned} \epsilon^1 \left[ \frac{D\tilde{\sigma}_{ij}}{Dt} + \frac{4}{5+\delta} \frac{\partial \tilde{q}_{<i}}{\partial x_{j>}} + 2\tilde{\sigma}_{k<i} \frac{\partial v_{j>}}{\partial x_k} + \tilde{\sigma}_{ij} \frac{\partial v_k}{\partial x_k} \right] - \epsilon^\alpha \left[ 2\rho \Delta \tilde{\theta} \frac{\partial v_{<i}}{\partial x_{j>}} \right] \\ + \epsilon^{1+\alpha} \left[ \frac{4}{5} \frac{\delta}{5+\delta} \frac{\partial \Delta \tilde{q}_{<i}}{\partial x_{j>}} \right] + \epsilon^2 \left[ \frac{\partial \tilde{u}_{ijk}^{0,0}}{\partial x_k} \right] = -2\rho \theta \frac{\partial v_{<i}}{\partial x_{j>}} - \left( \frac{1}{\tilde{\tau}_{tr}} + \frac{\epsilon^{1-\alpha}}{\tilde{\tau}_{int}} \right) \tilde{\sigma}_{ij}, \end{aligned} \quad (35e)$$

$$\begin{aligned} \epsilon^1 \left[ \frac{D\tilde{q}_i}{Dt} + \frac{1}{5+\delta} \left( (7+\delta) \left( \tilde{q}_k \frac{\partial v_i}{\partial x_k} + \tilde{q}_i \frac{\partial v_k}{\partial x_k} \right) + 2\tilde{q}_j \frac{\partial v_j}{\partial x_i} \right) + \tilde{\sigma}_{ij} \left( \frac{5+\delta}{2} \frac{\partial \theta}{\partial x_j} - \theta \frac{\partial \ln \rho}{\partial x_j} \right) + \theta \frac{\partial \tilde{\sigma}_{ij}}{\partial x_j} \right] \\ - \epsilon^\alpha \left[ \rho \theta \frac{\partial \Delta \tilde{\theta}}{\partial x_i} + \frac{(\delta+5)}{2} \rho \Delta \tilde{\theta} \frac{\partial \theta}{\partial x_i} \right] - \epsilon^{2\alpha} \left[ \rho \Delta \tilde{\theta} \frac{\partial \Delta \tilde{\theta}}{\partial x_i} + \Delta \tilde{\theta}^2 \frac{\partial \rho}{\partial x_i} + \frac{2}{39} \frac{\partial \tilde{B}^+}{\partial x_i} \right] + \epsilon^{1+\alpha} \left[ \frac{4\delta}{25\delta+42} \frac{\partial \tilde{B}_{ik}^+}{\partial x_k} \right] \\ + \epsilon^{1+\alpha} \left[ \frac{\delta}{5+\delta} \left( \Delta \tilde{q}_k \frac{\partial v_i}{\partial x_k} + \Delta \tilde{q}_i \frac{\partial v_k}{\partial x_k} + \frac{2}{5} \Delta \tilde{q}_j \frac{\partial v_j}{\partial x_i} \right) + \tilde{\sigma}_{ij} \left( \Delta \tilde{\theta} \frac{\partial \ln \rho}{\partial x_j} + \frac{\partial \Delta \tilde{\theta}}{\partial x_j} \right) + \Delta \tilde{\theta} \frac{\partial \tilde{\sigma}_{ij}}{\partial x_j} \right] \\ + \left\{ \frac{\epsilon^{1+2\alpha}}{\epsilon^2} \right\} \left[ \frac{5}{13} \frac{\partial \tilde{B}^-}{\partial x_i} \right] + \epsilon^2 \left[ \frac{14+3\delta}{14+\delta} \frac{7(\delta+3)}{25\delta+42} \frac{\partial \tilde{B}_{ik}^-}{\partial x_k} - \frac{\tilde{\sigma}_{ik}}{\rho} \frac{\partial \tilde{\sigma}_{kj}}{\partial x_j} + \tilde{u}_{ijk}^{0,0} \frac{\partial v_j}{\partial x_k} \right] \\ = -\frac{(\delta+5)}{2} \rho \theta \frac{\partial \theta}{\partial x_i} - \tilde{q}_i \left( \frac{1}{\tilde{\tau}_{tr}} + \frac{\epsilon^{1-\alpha}}{\tilde{\tau}_{int}} \right), \end{aligned} \quad (35f)$$

$$\begin{aligned}
& \epsilon^1 \left[ \frac{D\Delta\tilde{q}_i}{Dt} + \frac{25+7\delta}{5(5+\delta)} \Delta\tilde{q}_k \frac{\partial v_i}{\partial x_k} + \frac{5}{2} \frac{3+\delta}{\delta} \Delta\tilde{\theta} \frac{\partial \tilde{\sigma}_{ij}}{\partial x_j} + \tilde{\sigma}_{ik} \Delta\tilde{\theta} \frac{\partial \ln \rho}{\partial x_k} + \tilde{\sigma}_{ik} \frac{\partial \Delta\tilde{\theta}}{\partial x_k} \right] \\
& + \epsilon^1 \left[ \frac{1}{5(5+\delta)} \left( (25+7\delta) \Delta\tilde{q}_i \frac{\partial v_k}{\partial x_k} + 2\delta \Delta\tilde{q}_k \frac{\partial v_i}{\partial x_k} \right) + \frac{15+7\delta}{42+25\delta} \frac{\partial \tilde{B}_{ik}^+}{\partial x_k} \right] \\
& - \epsilon^\alpha \left[ \frac{5(3+\delta)}{2\delta} \rho \Delta\tilde{\theta} \frac{\partial \Delta\tilde{\theta}}{\partial x_i} + \frac{5}{2} \frac{3+\delta}{\delta} \Delta\tilde{\theta}^2 \frac{\partial \rho}{\partial x_i} + \frac{5(\delta+3)}{39\delta} \frac{\partial \tilde{B}^+}{\partial x_i} \right] \\
& + \epsilon^{1-\alpha} \left[ \frac{2}{5+\delta} \left( \tilde{q}_i \frac{\partial v_k}{\partial x_k} + \tilde{q}_k \frac{\partial v_i}{\partial x_k} + \tilde{q}_j \frac{\partial v_j}{\partial x_i} \right) + \theta \left( \frac{\partial \tilde{\sigma}_{ij}}{\partial x_j} - \tilde{\sigma}_{ik} \frac{\partial \ln \rho}{\partial x_k} \right) \right] + \left\{ \begin{array}{l} \epsilon^{1+\alpha} \\ \epsilon^{2-\alpha} \end{array} \right\} \frac{5(\delta-10)}{39\delta} \frac{\partial \tilde{B}^-}{\partial x_i} \\
& + \epsilon^{2-\alpha} \left[ \tilde{u}_{ijk}^{0,0} \frac{\partial v_j}{\partial x_k} - \frac{\tilde{\sigma}_{ik}}{\rho} \frac{\partial \tilde{\sigma}_{kj}}{\partial x_j} - 7 \frac{3+\delta}{14+\delta} \frac{\delta+6}{42+25\delta} \frac{\partial \tilde{B}_{ik}^-}{\partial x_k} \right] = \frac{5(3+\delta)}{2\delta} \rho \theta \frac{\partial \Delta\tilde{\theta}}{\partial x_i} - \left( \frac{1}{\tilde{\tau}_{tr}} + \frac{\epsilon^{1-\alpha}}{\tilde{\tau}_{int}} \right) \Delta\tilde{q}_i, \tag{35g}
\end{aligned}$$

$$\begin{aligned}
& \epsilon^1 \left[ \frac{D\tilde{B}^+}{Dt} + \frac{85}{39} \tilde{B}^+ \frac{\partial v_k}{\partial x_k} + \frac{(23-\delta)}{3+\delta} 3\rho \Delta\tilde{\theta}^2 \frac{\partial v_k}{\partial x_k} \right] + \epsilon^{1-\alpha} \left[ \frac{26\delta}{3+\delta} \rho \theta \Delta\tilde{\theta} \frac{\partial v_k}{\partial x_k} \right] \\
& + \epsilon^{2-\alpha} \left[ 3 \frac{23-\delta}{3+\delta} \Delta\tilde{\theta} \tilde{\sigma}_{kj} \frac{\partial v_j}{\partial x_k} + 3 \frac{\delta-23}{3+\delta} \Delta\tilde{\theta} \frac{\partial \tilde{q}_i}{\partial x_i} - \frac{\delta(\delta-23)}{5+\delta} \Delta\tilde{q}_k \frac{\partial \theta}{\partial x_k} \right] \\
& + \epsilon^{2-\alpha} \left[ \frac{10\delta}{5+\delta} \theta \left( -\frac{\partial \Delta\tilde{q}_k}{\partial x_k} + \Delta\tilde{q}_k \frac{\partial \ln \rho}{\partial x_k} \right) - \frac{20-\delta}{5+\delta} 2\tilde{q}_k \left( \frac{\partial \Delta\tilde{\theta}}{\partial x_k} + \Delta\tilde{\theta} \frac{\partial \ln \rho}{\partial x_k} \right) - \frac{62\delta}{25\delta+42} \tilde{B}_{kj}^+ \frac{\partial v_j}{\partial x_k} \right] \\
& - \epsilon^{2-2\alpha} \left[ \frac{240-\delta(47-\delta)}{2(3+\delta)(5+\delta)} \theta \frac{\partial \tilde{q}_i}{\partial x_i} + \frac{2}{5+\delta} \tilde{q}_k \left( \frac{100-8\delta}{2} \frac{\partial \theta}{\partial x_k} - (20-\delta) \theta \frac{\partial \ln \rho}{\partial x_k} \right) + 8\theta \tilde{\sigma}_{kj} \frac{\partial v_j}{\partial x_k} \right] \\
& + \epsilon^2 \left[ -\frac{10\delta}{5+\delta} \Delta\tilde{q}_k \left[ \frac{\partial \Delta\tilde{\theta}}{\partial x_k} + \Delta\tilde{\theta} \frac{\partial \ln \rho}{\partial x_k} \right] \right] + \epsilon^{3-\alpha} \left[ \frac{10\delta}{5+\delta} \frac{\Delta\tilde{q}_k}{\rho} \frac{\partial \tilde{\sigma}_{kj}}{\partial x_j} \right] - \left\{ \begin{array}{l} \epsilon^2 \\ \epsilon^{3-2\alpha} \end{array} \right\} \frac{20}{39} \tilde{B}^- \frac{\partial v_k}{\partial x_k} \\
& + \epsilon^{3-2\alpha} \left[ -\frac{112(7-\delta)(3+\delta)}{(14+\delta)(42+25\delta)} \tilde{B}_{kj}^- \frac{\partial v_j}{\partial x_k} + \frac{2(20-\delta)}{5+\delta} \frac{\tilde{q}_k}{\rho} \frac{\partial \tilde{\sigma}_{kj}}{\partial x_j} \right] = -\frac{39}{2} \frac{\rho \Delta\tilde{\theta}^2}{\tilde{\tau}_{tr}} - \left( \frac{1}{\tilde{\tau}_{tr}} + \frac{\epsilon^{1-\alpha}}{\tilde{\tau}_{int}} \right) \tilde{B}^+. \tag{35h}
\end{aligned}$$

The order of terms with  $\tilde{B}^-$  are shown with two powers of  $\epsilon$  in braces; the upper one corresponds to  $0 < \alpha < 0.5$  and the lower one corresponds to  $0.5 < \alpha < 1$ .

## VI. MODEL REDUCTION

The explicit orders can be used for model reduction such that in each order under consideration only terms up to corresponding power of  $\epsilon$  are kept, while all other terms can be ignored.

As it was discussed earlier, for rarefied gas flows values of  $\alpha$  less than 0.5 are relevant and will be considered from now on, unless stated otherwise. While the expansion series (24) contains all mixed powers of  $\epsilon$  and  $\epsilon^\alpha$ , the final equations ((35a)–(35h) and (A3a)–(A3d)) only contain some terms. In the following, we are interested in terms up to  $\epsilon^3$ , and find only the following powers:

$$\{ \epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \epsilon^{1+2\alpha}, \epsilon^{1+3\alpha}, \epsilon^{2-\alpha}, \epsilon^2, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^{2+3\alpha}, \epsilon^{2+4\alpha}, \epsilon^3 \}.$$

Their order depends on the value of  $\alpha$ . For values of  $\alpha$  below 0.5 the different sequences of orders are (up to  $\epsilon^3$ )

$$\begin{aligned}
0 < \alpha < 0.25 : & \{ \epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \epsilon^{1+2\alpha}, \epsilon^{1+3\alpha}, \epsilon^{2-\alpha}, \epsilon^2, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^{2+3\alpha}, \epsilon^3 \}, \\
0.25 < \alpha < 0.33 : & \{ \epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \epsilon^{1+2\alpha}, \underline{\epsilon^{2-\alpha}}, \underline{\epsilon^{1+3\alpha}}, \epsilon^2, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^{2+3\alpha}, \epsilon^3 \}, \tag{36} \\
0.33 < \alpha < 0.5 : & \{ \epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \underline{\epsilon^{2-\alpha}}, \underline{\epsilon^{1+2\alpha}}, \underline{\epsilon^2}, \underline{\epsilon^{1+3\alpha}}, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^3 \}.
\end{aligned}$$

Here, only the underlined terms are changing location between different values of  $\alpha$ .

### A. Zeroth order, $\epsilon^0$ : Euler equations

As we proceed, we will identify relevant terms in the equations as written for the scaled variables  $\{\Delta\tilde{\theta}, \tilde{\sigma}_{ij}, \tilde{q}_i, \dots\}$ , but we will write the final equations for the unscaled variables  $\{\Delta\theta, \sigma_{ij}, q_i, \dots\}$ .

We begin the reduction process with the conservation laws, which are required at all orders of accuracy. Their details, however, depend on the order considered. We write the full equations as

$$\begin{aligned} \frac{D\rho}{Dt} + \rho \frac{\partial v_i}{\partial x_i} &= 0, \\ \rho \frac{Dv_i}{Dt} + \frac{\partial(\rho\theta)}{\partial x_i} - \left[ \frac{\partial(\rho\Delta\theta)}{\partial x_i} \right] + \left[ \left[ \frac{\partial\sigma_{ij}}{\partial x_j} \right] \right] &= 0, \\ \frac{3+\delta}{2} \rho \frac{D\theta}{Dt} + \rho\theta \frac{\partial v_i}{\partial x_i} - \left[ \rho\Delta\theta \frac{\partial v_i}{\partial x_i} \right] + \left[ \left[ \frac{\partial q_i}{\partial x_i} + \sigma_{ij} \frac{\partial v_j}{\partial x_i} \right] \right] &= 0. \end{aligned} \quad (37)$$

Comparing with (35a) we see that the terms in single brackets are of order  $\mathcal{O}(\epsilon^\alpha)$ , while the terms in double brackets are of order  $\mathcal{O}(\epsilon^1)$ .

Accordingly, to zeroth order ( $\epsilon^0$ ), all terms with brackets will vanish. Then, the conservation laws reduce simply to the Euler equations in their typical form for polyatomic gases with constant specific heat  $c_v = \frac{3+\delta}{2}R$ , which corresponds to setting  $\Delta\theta = \sigma_{ij} = q_i = 0$ . The Euler equations are a closed set of equations for the variables  $\{\rho, v_i, \theta\}$ .

For higher orders, however, the terms with brackets must be considered. Since these contain the variables  $\Delta\theta$ ,  $\sigma_{ij}$ , and  $q_i$ , additional equations for these are required, which must be carefully extracted from the full set of equations.

Subsections VI B–VI J will discuss this based on the desired order of accuracy in the powers of  $\epsilon$ , and the different values of the exponent  $\alpha$ , which determines the relative importance of contributions. For this, we will consider the increasing orders as laid out in (36).

### B. Order $\epsilon^\alpha$ : Dynamic temperature

The first non-equilibrium correction appears for  $\alpha$  order, where the terms in single brackets in the conservation laws (37) must be considered, but not the terms in double brackets. Hence, an additional equation for the dynamic temperature  $\Delta\theta$  is required, which at this order is simply the leading term. The heat flux and stress tensor are effectively zero. Accordingly, at  $\alpha$  order, the conservation laws (37) are closed with

$$\Delta\theta = \tau_{int} \frac{2\delta}{3(3+\delta)} \theta \frac{\partial v_i}{\partial x_i} \quad \text{and} \quad \sigma_{ij} = q_i = 0. \quad (38)$$

From the conservation laws, we recognize that in a moving gas the pressure is not just the equilibrium ideal gas pressure  $\rho\theta$ , but  $p = \rho\theta - \rho\Delta\theta$ . For this reason, one often denotes the second term as the *dynamic pressure*,<sup>15,60</sup>  $\Pi = -\rho\Delta\theta$ . In the classical Navier-Stokes equations, the dynamic pressure has the form  $\Pi = -v \frac{\partial v_i}{\partial x_i}$  where  $v$  is the bulk viscosity. Comparing with the above, we identify a relation between relaxation time  $\tau_{int}$  and the bulk viscosity,

$$v = \tau_{int} \frac{2\delta}{3(3+\delta)} \rho\theta. \quad (39)$$

The bulk viscosity is a function of the internal relaxation time, hence it will vanish in the monatomic gas where no internal energy exchange occurs ( $\delta = 0$ ).

### C. Order $\epsilon^{2\alpha}$ : Refined dynamic temperature

For all  $\alpha < 0.5$ , the next order appearing in (36) is  $\epsilon^{2\alpha}$ . Since  $\sigma_{ij}$  and  $q_i$  are of order  $\epsilon > \epsilon^{2\alpha}$ , they are still not relevant. The conservation laws do not contain terms of order  $2\alpha$ , hence they are unchanged from the previous case (order  $\epsilon^\alpha$ ). While the next higher order terms of  $\Delta\theta$ , which are of order  $\epsilon^\alpha$  and give overall contributions of order  $\epsilon^{2\alpha}$ , must be considered. This gives the closure

by a full balance equation for  $\Delta\theta$ , while stress and heat flux can still be ignored,

$$\rho \frac{D\Delta\theta}{Dt} + \frac{2\delta}{3(3+\delta)} \rho (\Delta\theta - \theta) \frac{\partial v_i}{\partial x_i} = -\frac{\rho}{\tau_{int}} \Delta\theta \quad \text{and} \quad \sigma_{ij} = q_i = 0. \quad (40)$$

This set of 6 field equations agrees with the set of equations used by Taniguchi *et al.*<sup>61</sup> to study shock waves in rarefied polyatomic gases.

#### D. Order $\epsilon^1$ : Refined Navier-Stokes-Fourier equations

For the first order, terms up to  $\epsilon^1$  order are considered in the conservation laws (37), for which now all terms are relevant. In addition to the balance law for  $\Delta\theta$  (40), the leading terms of the stress tensor and total heat flux are required as well,

$$\sigma_{ij} = -\tau_{tr} 2\rho\theta \frac{\partial v_{<i}}{\partial x_{j>}} \quad \text{and} \quad q_i = -\tau_{tr} \frac{5+\delta}{2} \rho\theta \frac{\partial \theta}{\partial x_i}. \quad (41)$$

These first order equations for  $\sigma_{ij}$  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. The factors between them are the shear viscosity  $\mu$  and the heat conductivity  $k$  which we identify as

$$\mu = \tau_{tr} \rho\theta \quad \text{and} \quad \kappa = \tau_{tr} \frac{5+\delta}{2} \rho\theta. \quad (42)$$

The obtained relation for the shear viscosity is identical to that of the monatomic gas. Internal degrees of freedom affect the heat conductivity, which differs from the monatomic gas as extra means of energy transport are present in the polyatomic gases.

However, what we have obtained here at first order are not the classical NSF equations, since we have to use the full balance law (40) for  $\Delta\theta$  (or dynamic pressure). The classical NSF equations are a five variables model for  $\{\rho, v_i, \theta\}$ . However, the refined Navier–Stokes–Fourier (RNSF) equations obtained have six independent field variables,  $\{\rho, v_i, \theta, \Delta\theta\}$ . This is a result of the scaling, where we assumed  $\alpha < 0.5$ . The classical Navier–Stokes–Fourier equations only arise for  $0.5 < \alpha < 1$ , this is shown in Sec. VII. The importance of the refined Navier–Stokes–Fourier equations with the extra balance law for dynamic pressure will be shown and discussed in the Sec. VII D.

#### E. Order $\epsilon^{1+\alpha}$ : RNSF equations with first internal DoF corrections

The next order of accuracy (for all  $\alpha < 0.5$ ) is obtained by considering the next higher terms in the equations for  $\Delta\theta$ ,  $\sigma_{ij}$ , and  $q_i$ , which are the contributions with factor  $\epsilon^1$  for the dynamic temperature (35d), and contributions with factor  $\epsilon^\alpha$  for stress (35e) and heat flux (35f), so that at order  $1 + \alpha$ , the conservation laws (37) must be closed by

$$\rho \frac{D\Delta\theta}{Dt} + \frac{2\delta}{3(3+\delta)} \rho (\Delta\theta - \theta) \frac{\partial v_i}{\partial x_i} - \frac{2\delta}{3(3+\delta)} \left( \frac{2}{5+\delta} \frac{\partial q_i}{\partial x_i} + \sigma_{ij} \frac{\partial v_j}{\partial x_i} \right) = -\frac{\rho}{\tau_{int}} \Delta\theta, \quad (43a)$$

$$\sigma_{ij} = -\tau_{tr} 2\rho [\theta - \Delta\theta] \frac{\partial v_{<i}}{\partial x_{j>}} \quad \text{and} \quad q_i = -\tau_{tr} \rho \left( \frac{5+\delta}{2} [\theta - \Delta\theta] \frac{\partial \theta}{\partial x_i} - \theta \frac{\partial \Delta\theta}{\partial x_i} \right). \quad (43b)$$

Additional corrections to the NSF equations occur due to the internal degrees of freedom.

#### F. Cases with $0 < \alpha < 0.25$

To proceed to the next order, we now have to distinguish further among the possible values of  $\alpha$ ; we begin with the window  $0 < \alpha < 0.25$ .

##### 1. Order $\epsilon^{1+2\alpha}$ : RNSF equations with second internal DoF corrections

Close inspection shows that the next higher terms in the balance for  $\Delta\theta$  add contributions to order  $1 + 2\alpha$ . Indeed, at this order the full balance law for dynamic temperature must be

considered,

$$\rho \frac{D\Delta\theta}{Dt} + \frac{2\delta}{3(3+\delta)}\rho(\Delta\theta - \theta) \frac{\partial v_i}{\partial x_i} - \frac{2\delta}{3(3+\delta)} \left( \frac{2}{5+\delta} \frac{\partial q_i}{\partial x_i} + \sigma_{ij} \frac{\partial v_j}{\partial x_i} \right) - \frac{2}{3} \frac{\delta}{5+\delta} \frac{\partial \Delta q_i}{\partial x_i} = -\frac{\rho}{\tau_{int}} \Delta\theta. \quad (44a)$$

This equation now has a contribution with the heat flux difference  $\Delta q_i$ , which here must be considered to leading order,

$$\Delta q_i = \tau_{tr} \frac{5(3+\delta)}{2\delta} \rho \theta \frac{\partial \Delta\theta}{\partial x_i}. \quad (44b)$$

At this order, the equation for stress remains unchanged, but the equation for heat flux now has also the terms with the factor  $\epsilon^{2\alpha}$  so that

$$\sigma_{ij} = -\tau_{tr} 2\rho [\theta - \Delta\theta] \frac{\partial v_{<i}}{\partial x_{>}}, \quad (44c)$$

$$q_i = -\tau_{tr} \left( \rho \left( \frac{5+\delta}{2} [\theta - \Delta\theta] \frac{\partial \theta}{\partial x_i} - \theta \frac{\partial \Delta\theta}{\partial x_i} - \Delta\theta \frac{\partial \Delta\theta}{\partial x_i} \right) - \Delta\theta^2 \frac{\partial \rho}{\partial x_i} - \frac{2}{39} \frac{\partial B^+}{\partial x_i} \right). \quad (44d)$$

For closing the set of equations, the leading order term of  $B^+$  is required,

$$B^+ = -\frac{39}{2} \rho \Delta\theta^2. \quad (44e)$$

Also at this order, all corrections to the NSF equations are due to the internal degrees of freedom.

## 2. Order $\epsilon^{1+3\alpha}$ : RNSF equations with third internal DoF corrections

The next order of accuracy is obtained by considering the conservation laws (37), the dynamic temperature equation (44a), the constitutive equations for the heat flux (44d) and stress (44c), and terms up to  $\alpha$  order in the heat flux difference as

$$\Delta q_i = \tau_{tr} \left[ \frac{5(3+\delta)}{\delta} \left\{ \frac{1}{2} \left( \rho (\theta + \Delta\theta) \frac{\partial \Delta\theta}{\partial x_i} + \Delta\theta^2 \frac{\partial \rho}{\partial x_i} \right) + \frac{1}{39} \frac{\partial B^+}{\partial x_i} \right\} \right]. \quad (45)$$

## 3. Order $\epsilon^{2-\alpha}$ : RNSF equations with full corrections

The equations at order  $2 - \alpha$  are the full conservation laws (37), the full dynamic temperature equation (44a), and the following constitutive equations for heat flux and stress (considering terms up to  $\epsilon^{1-\alpha}$  order),

$$\sigma_{ij} = -\frac{1}{\left[ \frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}} \right]} 2\rho [\theta - \Delta\theta] \frac{\partial v_{<i}}{\partial x_{>}}, \quad (46a)$$

$$q_i = -\frac{1}{\left[ \frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}} \right]} \left( \rho \left( \frac{5+\delta}{2} [\theta - \Delta\theta] \frac{\partial \theta}{\partial x_i} - \theta \frac{\partial \Delta\theta}{\partial x_i} - \Delta\theta \frac{\partial \Delta\theta}{\partial x_i} \right) - \Delta\theta^2 \frac{\partial \rho}{\partial x_i} - \frac{2}{39} \frac{\partial B^+}{\partial x_i} \right). \quad (46b)$$

The equations for the heat flux difference  $\Delta q_i$  and for  $B^+$  remain the same as for the previous case, i.e., (45) and (44e).

## 4. Order $\epsilon^2$ : Refined Grad's 14 moment equations

Starting with the second order of accuracy, balance laws for stress  $\sigma_{ij}$  and heat flux  $q_i$  must be considered. To reduce the number of equations shown, we again adopt a notation with brackets and



write (35e) and (35f) as

$$\frac{D\sigma_{ij}}{Dt} + \frac{4}{5+\delta} \frac{\partial q_{<i}}{\partial x_{j>}} + 2\sigma_{k<i} \frac{\partial v_{j>}}{\partial x_k} + \sigma_{ij} \frac{\partial v_k}{\partial x_k} - 2\rho\Delta\theta \frac{\partial v_{<i}}{\partial x_{j>}} + \left[ \frac{4}{5} \frac{\delta}{5+\delta} \frac{\partial \Delta q_{<i}}{\partial x_{j>}} \right] + \left[ \left[ \left[ \frac{\partial u_{ijk}^{0,0}}{\partial x_k} \right] \right] \right] = -2\rho\theta \frac{\partial v_{<i}}{\partial x_{j>}} - \left( \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right) \sigma_{ij}, \quad (47a)$$

$$\begin{aligned} \frac{Dq_i}{Dt} + \frac{1}{5+\delta} \left\{ (7+\delta) \left( q_k \frac{\partial v_i}{\partial x_k} + q_i \frac{\partial v_k}{\partial x_k} \right) + 2q_j \frac{\partial v_j}{\partial x_i} \right\} + \sigma_{ij} \left( \frac{5+\delta}{2} \frac{\partial \theta}{\partial x_j} - \theta \frac{\partial \ln \rho}{\partial x_j} \right) + \theta \frac{\partial \sigma_{ij}}{\partial x_j} \\ - \rho\theta \frac{\partial \Delta\theta}{\partial x_i} - \frac{(\delta+5)}{2} \rho \Delta\theta \frac{\partial \theta}{\partial x_i} - \rho \Delta\theta \frac{\partial \Delta\theta}{\partial x_i} - \Delta\theta^2 \frac{\partial \rho}{\partial x_i} - \frac{2}{39} \frac{\partial B^+}{\partial x_i} \\ + \left[ \frac{4\delta}{25\delta+42} \frac{\partial B_{ik}^+}{\partial x_k} + \frac{\delta}{5+\delta} \left( \Delta q_k \frac{\partial v_i}{\partial x_k} + \Delta q_i \frac{\partial v_k}{\partial x_k} + \frac{2}{5} \Delta q_j \frac{\partial v_j}{\partial x_i} \right) + \sigma_{ij} \Delta\theta \frac{\partial \ln \rho}{\partial x_j} + \frac{\partial \Delta\theta \sigma_{ij}}{\partial x_j} \right] \\ + \left[ \left[ \frac{3}{26} \frac{\partial B^-}{\partial x_i} \right] \right] + \left[ \left[ \left[ \frac{7(\delta+3)(14+3\delta)}{(25\delta+42)(14+\delta)} \frac{\partial B_{ik}^-}{\partial x_k} - \frac{\sigma_{ik}}{\rho} \frac{\partial \sigma_{kj}}{\partial x_j} + u_{ijk}^{0,0} \frac{\partial v_j}{\partial x_k} \right] \right] \right] \\ = -\frac{(\delta+5)}{2} \rho\theta \frac{\partial \theta}{\partial x_i} - \left( \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right) q_i. \quad (47b) \end{aligned}$$

For the second order accuracy discussed presently, all terms of the above equations *except* the bracketed terms must be included; these are the terms with factors up to  $\epsilon^1$  in (35e) and (35f). The other relevant equations are the conservation laws (37), the dynamic temperature equation (44a), and the previous constitutive equations for  $\Delta q_i$  and  $B^+$ , (45) and (44e).

With balance laws for stress and heat flux, the second order equations form a set of partial differential equations (PDEs) for the 14 variables  $\{\rho, v_i, \theta, \Delta\theta, \sigma_{ij}, q_i\}$ . Other authors discuss a 14 moment set for polyatomic gases,<sup>14,15,42</sup> where the equations differ from what we find. Indeed, our refined Grad's 14 moment (RG14) equations contain additional terms of order  $\epsilon^{1+2\alpha}$ , which are the single underlined terms in the equations for overall heat flux (47b) and the dynamic temperature (44a), along with the constitutive equation for  $B^+$  (44e) and  $\Delta q_i$  (45). These terms would not appear for  $\alpha > 0.5$ , where they would give contributions of higher than second order in  $\epsilon$ . Hence we can say that the equations in Refs. 14, 15, and 42 are only relevant for the case that  $\alpha > 0.5$ , and second order accuracy.

The mentioned 14 field theory<sup>14,15,42</sup> contains the three double underlined nonlinear terms in (47b), which according to our analysis are of orders  $\epsilon^{2+\alpha}$  and  $\epsilon^3$ , respectively. As will be seen below, if one wishes to have a theory at these orders, there will be additional terms that must be included (those that stand in the same bracket, as well as contributions in other equations).

### 5. Order $\epsilon^{2+\alpha}$ : RG14 equations with internal DoF corrections

In the next order of accuracy, the terms in single brackets in the equations for heat flux (47b) and stress (47a) must be added, which are those with factors up to  $\epsilon^{1+\alpha}$  in (35f)–(35e). Together with the conservation laws (37) and the full balance law for dynamic temperature (44a), we still have a set of PDEs for 14 variables, which is closed by the constitutive equations for  $\Delta q_i$  and  $B^+$  up to  $1 - \alpha$  order,

$$\Delta q_i = \frac{1}{\left[ \frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}} \right]} \left[ \frac{5(3+\delta)}{\delta} \left\{ \frac{1}{2} \left( \rho(\theta + \Delta\theta) \frac{\partial \Delta\theta}{\partial x_i} + \Delta\theta^2 \frac{\partial \rho}{\partial x_i} \right) + \frac{1}{39} \frac{\partial B^+}{\partial x_i} \right\} - \frac{2}{5+\delta} \left( q_i \frac{\partial v_k}{\partial x_k} + q_k \frac{\partial v_i}{\partial x_k} + q_j \frac{\partial v_j}{\partial x_i} \right) - \theta \left( \frac{\partial \sigma_{ij}}{\partial x_j} - \sigma_{ik} \frac{\partial \ln \rho}{\partial x_k} \right) \right], \quad (48a)$$

$$B^+ = -\frac{1}{\left[\frac{1}{\tau_{rr}} + \frac{1}{\tau_{int}}\right]} \left( \frac{39}{2} \frac{\rho \Delta \theta^2}{\tau_{rr}} + \frac{26\delta}{3+\delta} \rho \theta \Delta \theta \frac{\partial v_k}{\partial x_k} \right), \quad (48b)$$

and the leading order contribution to  $B_{ij}^+$ ,

$$B_{ij}^+ = \tau_{rr} \frac{42 + 25\delta}{\delta} \rho \theta \Delta \theta \frac{\partial v_{<i}}{\partial x_{j>}}. \quad (48c)$$

## 6. Order $\epsilon^{2+2\alpha}$ : Refined Grad's 18 moment equations

Increasing the accuracy to  $2 + 2\alpha$ , require the following equations: the conservation laws (37), the full equation for dynamic temperature (44a), the equations for stress and heat flux (47a) and (47b) without the terms in triple brackets, and balance laws for  $\Delta q_i$  and  $B^+$ ,

$$\begin{aligned} \frac{D\Delta q_i}{Dt} + \frac{25 + 7\delta}{5(5 + \delta)} \Delta q_k \frac{\partial v_i}{\partial x_k} + \frac{5}{2} \frac{3 + \delta}{\delta} \Delta \theta \frac{\partial \sigma_{ij}}{\partial x_j} + \sigma_{ik} \Delta \theta \frac{\partial \ln \rho}{\partial x_k} + \sigma_{ik} \frac{\partial \Delta \theta}{\partial x_k} \\ + \frac{1}{5(5 + \delta)} \left( (25 + 7\delta) \Delta q_i \frac{\partial v_k}{\partial x_k} + 2\delta \Delta q_k \frac{\partial v_i}{\partial x_k} \right) + \frac{15 + 7\delta}{42 + 25\delta} \frac{\partial B_{ik}^+}{\partial x_k} \\ - \left( \frac{5(3 + \delta)}{2\delta} \rho \Delta \theta \frac{\partial \Delta \theta}{\partial x_i} + \frac{5}{2} \frac{3 + \delta}{\delta} \Delta \theta^2 \frac{\partial \rho}{\partial x_i} + \frac{5(\delta + 3)}{39\delta} \frac{\partial B^+}{\partial x_i} \right) \\ + \frac{2}{5 + \delta} \left( q_i \frac{\partial v_k}{\partial x_k} + q_k \frac{\partial v_i}{\partial x_k} + q_j \frac{\partial v_j}{\partial x_i} \right) + \theta \left( \frac{\partial \sigma_{ij}}{\partial x_j} - \sigma_{ik} \frac{\partial \ln \rho}{\partial x_k} \right) \\ + \left[ \frac{5(\delta - 10)}{39\delta} \frac{\partial B^-}{\partial x_i} \right] = \frac{5(3 + \delta)}{2\delta} \rho \theta \frac{\partial \Delta \theta}{\partial x_i} - \left( \frac{1}{\tau_{rr}} + \frac{1}{\tau_{int}} \right) \Delta q_i, \quad (49a) \end{aligned}$$

$$\begin{aligned} \frac{DB^+}{Dt} + \frac{85}{39} B^+ \frac{\partial v_k}{\partial x_k} + \frac{(23 - \delta)}{3 + \delta} 3\rho \Delta \theta^2 \frac{\partial v_k}{\partial x_k} + \frac{26\delta}{3 + \delta} \rho \theta \Delta \theta \frac{\partial v_k}{\partial x_k} \\ - \left[ \left[ \frac{240 - \delta(47 - \delta)}{2(3 + \delta)(5 + \delta)} \theta \frac{\partial q_i}{\partial x_i} + \frac{2}{5 + \delta} q_k \left( \frac{100 - 8\delta}{2} \frac{\partial \theta}{\partial x_k} - (20 - \delta) \theta \frac{\partial \ln \rho}{\partial x_k} \right) + 8\theta \sigma_{kj} \frac{\partial v_j}{\partial x_k} \right] \right] \\ = -\frac{39}{2} \frac{\rho \Delta \theta^2}{\tau_{rr}} - \left( \frac{1}{\tau_{rr}} + \frac{1}{\tau_{int}} \right) B^+. \quad (49b) \end{aligned}$$

Once more we use square brackets to distinguish between terms at different orders. At the order  $(2 + 2\alpha)$ , presently discussed, only the terms outside the brackets in Eqs. (49a) and (49b) must be included. Closure of this set of equations requires constitutive equations for  $B_{ij}^+$  (up to  $\alpha$  order) and  $B^-$  (at leading order), which read,

$$B_{ij}^+ = \tau_{rr} \left[ \frac{42 + 25\delta}{\delta} \left( \rho \theta \Delta \theta + \frac{2}{39} B^+ \right) \frac{\partial v_{<i}}{\partial x_{j>}} \right], \quad (49c)$$

$$B^- = \tau_{rr} \left[ \frac{2}{13} B^+ + 3\rho \Delta \theta^2 \right] \frac{\partial v_i}{\partial x_i}. \quad (49d)$$

At this order, we have PDEs for the 18 variables  $\{\rho, v_i, \theta, \Delta \theta, \sigma_{ij}, q_i, \Delta q_i, B^+\}$ , which are the refined Grad's 18 moment (RG18) equations based on the proper ordering.

## 7. Order $\epsilon^{2+3\alpha}$ : RG18 equations with internal DoF corrections

At the next order,  $2 + 3\alpha$ , the equations are the same as for  $2 + 2\alpha$ , only that now one additional term, which is the single-bracket term in (49a), must be included.

### 8. Order $\epsilon^3$ : Regularized 18 (R18) equations

Finally, we present the equations at third order of accuracy, which are: the conservation laws (37); the full equation for the dynamic temperature (44a); Eqs. (47a), (47b), (49a), and (49b)—with all terms—for stress, heat flux, heat flux difference, and  $B^+$ . These 18 PDEs are closed with the constitutive equations for  $B_{ij}^+$  up to  $1 - \alpha$  order,

$$B_{ij}^+ = \frac{1}{\left[\frac{1}{\tau_{rr}} + \frac{1}{\tau_{im}}\right]} \left[ -\theta \left( 12\sigma_{<ij} \frac{\partial v_{k>}}{\partial x_k} + \frac{56}{5} \sigma_{k<i} \frac{\partial v_k}{\partial x_{j>}} - \frac{14 + \delta}{3 + \delta} \sigma_{ij} \frac{\partial v_k}{\partial x_k} \right) + \frac{42 + 25\delta}{\delta} \left( \rho\theta\Delta\theta + \frac{2}{39} B^+ \right) \frac{\partial v_{<i}}{\partial x_{j>}} - \frac{2(14 + \delta)}{5 + \delta} \left( \theta \frac{\partial q_{<i}}{\partial x_{j>}} + q_{<i} \frac{\partial \theta}{\partial x_{j>}} - \theta q_{<i} \frac{\partial \ln \rho}{\partial x_{j>}} \right) \right], \quad (50a)$$

for  $B^-$  up to  $1 - 2\alpha$  order,

$$B^- = \tau_{rr} \left[ \left( \frac{2}{13} B^+ + 3\rho\Delta\theta^2 \right) \frac{\partial v_i}{\partial x_i} - \frac{12}{5} \theta \sigma_{kj} \frac{\partial v_j}{\partial x_k} - \frac{1}{2(5 + \delta)} \left( (24 - \delta) \theta \frac{\partial q_i}{\partial x_i} + 4q_k \left[ (15 + 4\delta) \frac{\partial \theta}{\partial x_k} - (6 + \delta) \theta \frac{\partial \ln \rho}{\partial x_k} \right] \right) \right], \quad (50b)$$

and for  $u_{ijk}^{0,0}$  and  $B_{ij}^-$  at their leading orders,

$$u_{ijk}^{0,0} = -\tau_{rr} \left[ 3\theta \frac{\partial \sigma_{<ij}}{\partial x_{k>}} - 3\sigma_{<ij} \theta \frac{\partial \ln \rho}{\partial x_{k>}} + \frac{12}{5 + \delta} q_{<i} \frac{\partial v_j}{\partial x_{k>}} \right], \quad (50c)$$

$$B_{ij}^- = \tau_{rr} \left[ -2 \frac{14 + \delta}{5 + \delta} \theta \frac{\partial q_{<i}}{\partial x_{j>}} - 2 \frac{14 + \delta}{5 + \delta} q_{<i} \frac{\partial \theta}{\partial x_{j>}} + 2 \frac{14 + \delta}{5 + \delta} \theta q_{<i} \frac{\partial \ln \rho}{\partial x_{j>}} - \frac{\delta + 14}{\delta + 3} \frac{6}{7} \theta \left( \sigma_{k<i} \frac{\partial v_{j>}}{\partial x_k} + \sigma_{k<j} \frac{\partial v_k}{\partial x_{i>}} - \frac{2}{3} \sigma_{ij} \frac{\partial v_k}{\partial x_k} \right) \right]. \quad (50d)$$

This is the set of regularized 18 (R18) equations corresponding to the third order of accuracy.

### G. Cases with $0.25 < \alpha < 0.33$

The ordering of terms depends on the value of  $\alpha$ , as outlined in Eq. (36). Above, we considered the model reduction for  $\alpha < 0.25$ , which gave a hierarchical sequence of equations. When we consider slightly larger values of  $\alpha$ , those in the interval  $0.25 < \alpha < 0.33$ , the ordering of contributions changes. Specifically, only two orders change position in the ordering sequence (36), namely,  $\epsilon^{2-\alpha}$  and  $\epsilon^{1+3\alpha}$ . The difference is relatively small: all set of equations corresponding to orders  $\{\epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \epsilon^{1+2\alpha}, \epsilon^2, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^{2+3\alpha}, \epsilon^3\}$  are the same as those in Subsection VI F. The two changed sets of equations are discussed below.

#### 1. Order $\epsilon^{2-\alpha}$

The  $2 - \alpha$  order of accuracy requires the full conservation laws (37), the dynamic temperature equation (44a), the constitutive equations for the heat flux and stress (46), the heat flux difference (44b), and the leading term of  $B^+$  (44e). To save space, we will not show the equations in detail.

#### 2. Order $\epsilon^{1+3\alpha}$

At order  $1 + 3\alpha$  one must consider the full conservation laws (37), the dynamic temperature equation (44a), the constitutive equations for the heat flux and stress (46), the leading order of  $B^+$  (44e), and the equation for heat flux difference (45).

## H. Cases with $0.33 < \alpha < 0.5$

At even larger values of  $\alpha$ , in the range of  $0.33 < \alpha < 0.5$ , four orders change position in the ordering sequence (36), viz.  $\epsilon^{2-\alpha}$ ,  $\epsilon^{1+2\alpha}$ ,  $\epsilon^2$ , and  $\epsilon^{1+3\alpha}$ . Moreover, the  $2 + 3\alpha$  order is greater than third order and is not further considered. The changed sets of equations are presented below, the equations at all other orders remain same as those of Sec. VI G.

### 1. Order $\epsilon^{2-\alpha}$

The  $2 - \alpha$  order of accuracy is gained by considering the full conservation laws (37), the dynamic temperature equation (44a) without terms in double brackets (i.e., terms up to  $2 - 2\alpha$  order), and terms up to  $1 - \alpha$  order in the heat flux and stress tensor,

$$\sigma_{ij} = -\frac{1}{\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]} 2\rho [\theta - \Delta\theta] \frac{\partial v_{<i}}{\partial x_{j>}}, \quad (51a)$$

$$q_i = -\frac{1}{\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]} \rho \left( \frac{5 + \delta}{2} [\theta - \Delta\theta] \frac{\partial \theta}{\partial x_i} - \theta \frac{\partial \Delta\theta}{\partial x_i} \right). \quad (51b)$$

### 2. Order $\epsilon^{1+2\alpha}$

At order  $1 + 2\alpha$  the polyatomic gas must be described by the conservation laws (37), the dynamic temperature equation (44a), the constitutive equations for the heat flux difference (44b), and the following equations for stress and heat flux:

$$\sigma_{ij} = -\frac{1}{\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]} 2\rho [\theta - \Delta\theta] \frac{\partial v_{<i}}{\partial x_{j>}}, \quad (52a)$$

$$q_i = -\frac{1}{\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]} \left( \rho \left( \frac{5 + \delta}{2} [\theta - \Delta\theta] \frac{\partial \theta}{\partial x_i} - \theta \frac{\partial \Delta\theta}{\partial x_i} - \Delta\theta \frac{\partial \Delta\theta}{\partial x_i} \right) - \Delta\theta^2 \frac{\partial \rho}{\partial x_i} - \frac{2}{39} \frac{\partial B^+}{\partial x_i} \right). \quad (52b)$$

For closing the set of equations, the leading order term of  $B^+$  (44e) is required.

### 3. Order $\epsilon^2$

The second order of accuracy requires all terms in the stress and heat flux balance up to factors  $\epsilon^1$ , which are Eqs. (47a) and (47b) without all terms in brackets, as well as the conservation laws (37), the dynamic temperature equation (44a), and the constitutive equations for  $B^+$  (44e) and the heat flux difference (44b). The second order equations form a set of PDEs for the 14 variables  $\{\rho, v_i, \theta, \Delta\theta, \sigma_{ij}, q_i\}$ .

### 4. Order $\epsilon^{1+3\alpha}$

In  $1 + 3\alpha$  order of accuracy, almost all equations are the same as at second order, only that, in order to include the proper higher order terms, the constitutive equation for heat flux difference must be replaced by (45).

### 5. Order $\epsilon^3$

The third order of accuracy corresponds to the  $0.33 < \alpha < 0.5$ , the only change from the set of R18 equations at lower  $\alpha$  ( $0 < \alpha < 0.33$ ) is the balance law for the heat flux difference, which now only terms outside brackets in the Eq. (49a) are needed.

## I. Classical Navier-Stokes-Fourier equations, $0.5 < \alpha < 1$

The classical Navier-Stokes-Fourier equations arise only for cases with  $0.5 < \alpha < 1$ , where they are the appropriate system at order  $\varepsilon$ . Here, the powers  $\varepsilon^0$ ,  $\varepsilon^\alpha$ , and  $\varepsilon^1$  are required, while the corrections to dynamic temperature of order  $\varepsilon^{2\alpha}$  and higher must be discarded. Accordingly, the proper first order set is the conservation laws (37), together with the stress and heat flux as given in (41), while the equation for dynamic temperature is (38),

$$\Delta\theta = \frac{2}{3} \frac{\delta}{3 + \delta} \tau_{int} \theta \frac{\partial v_i}{\partial x_i}. \quad (53)$$

The classical NSF equations give a five variables model for  $\{\rho, v_i, \theta\}$ . As discussed in Sec. IV,  $\alpha$  will assume values *below* 0.5 for rarefied flows. Thus, the classical Navier-Stokes-Fourier equations have rather limited applicability in the rarefied regime. As was shown earlier, for  $0 < \alpha < 0.5$ , the refined NSF equations are the appropriate model at first order in  $\varepsilon$ . These use the full balance law for dynamic temperature (40) instead of (38), and have the six independent field variables,  $\{\rho, v_i, \theta, \Delta\theta\}$ .

## J. Intermediate summary

The relaxation of the internal degrees of freedom leads to various ordering sequences for different values of  $\alpha$ , which differ in particular in the terms associated with the dynamic temperature  $\Delta\theta$ . The accounting of these terms, which depends on the value of  $\alpha$  and the accuracy under consideration, needs great care.

At the first order of accuracy, a refined version of the classical Navier-Stokes-Fourier equations is obtained, which includes *the balance law* for the dynamic temperature (Sec. VI D).

At the second order, a refined variant of Grad's 14 moment equations is obtained, which includes some corrections and two extra constitutive equations for  $\Delta q_i$  and  $B^+$ . We note that the higher order terms in the dynamic temperature introduce higher space derivatives into these equations, which are not present in the typical Grad 14 moment system.<sup>14,15</sup>

At order  $2 + 2\alpha$ , a refined variant of Grad's 18 moment equations is obtained which consists of 18 PDEs and two constitutive equations.

Finally at the third order, the regularized 18 moment equations (R18) are obtained which consist of 18 PDEs and four constitutive equations, and contribute regularizing terms similar to what appears in the R13 equations for monatomic gases.<sup>20</sup>

In order to decide which set of equations we need to consider for a particular problem, the relaxation times and their ratios must be known. Therefore, the particular problem under consideration determines which set of equations should be used. This choice depends on the values of both Knudsen numbers: If the value of  $\text{Kn}_{tr}$  is rather small while  $\text{Kn}_{int}$  is relatively large, one will choose a model with high power in  $\varepsilon^\alpha$  and low power in  $\varepsilon$ ; these are models with corrections to the NSF equations, i.e., the set of  $1 + 3\alpha$  order equations (Sec. VI F 2). On the other hand, if both Knudsen numbers are small, one can use a lower accuracy model, like the refined NSF equations (Sec. VI D). In problems when both Knudsen numbers are large, particularly order unity values of  $\text{Kn}_{tr}$ , a higher order of accuracy is an essential choice, e.g., one would choose the third order R18 equations (Sec. VI F 8).

## VII. LINEAR WAVE ANALYSIS

As a first application of the introduced model, we study the behavior of one-dimensional linear waves as forecasted in the obtained different orders of equations. We compare the predictions of the various equations in the hierarchies among each other as well as to those of the classical Navier-Stokes-Fourier equations, and its modification containing the balance law for the dynamic temperature. Moreover, we study the influence of excitations of the internal degrees of freedom by comparing with results for monatomic gases, where we will highlight the influence of the ratio of collision times,  $\tau_{tr}/\tau_{int}$ .

### A. Linearized equations

Sound waves are small disturbances of an equilibrium ground state  $\{\rho_0, v_i^0 = 0, \theta_0\}$ , and hence it suffices to study the linearized equations. For this, we write all variables in terms of their ground state values plus a small deviation, denoted by a hat, as

$$\rho = \rho_0 + \hat{\rho}, \theta = \theta_0 + \hat{\theta}, v_i = \hat{v}_i, \Delta\theta = \Delta\hat{\theta}, \sigma_{ij} = \hat{\sigma}_{ij}, q_i = \hat{q}_i, \Delta q_i = \Delta\hat{q}_i, B_{ij}^+ = \hat{B}_{ij}^+, B^- = \hat{B}^-, B_{ij}^- = \hat{B}_{ij}^-, B^- = \hat{B}^-, u_{ijk}^{0,0} = \hat{u}_{ijk}^{0,0}. \quad (54)$$

All deviations are considered to be very small, and the systems of equations are being linearized by keeping only linear terms in the deviations.

The equilibrium rest state  $\{\rho_0, \theta_0\}$  is used to non-dimensionalize all quantities and equations. Specifically, we set

$$\begin{aligned} \bar{x}_i &= \frac{x_i}{\tau_0 \sqrt{\theta_0}}, \bar{t} = \frac{t}{\tau_0}, \bar{\tau}_{int} = \frac{\tau_{int}}{\tau_0}, \bar{\tau}_{tr} = \frac{\tau_{tr}}{\tau_0}, \bar{\rho} = \frac{\rho}{\rho_0} - 1, \\ \bar{\theta} &= \frac{\theta}{\theta_0} - 1, \Delta\bar{\theta} = \frac{\Delta\theta}{\theta_0}, \bar{v}_i = \frac{v_i}{\sqrt{\theta_0}}, \bar{\sigma}_{ij} = \frac{\sigma_{ij}}{\rho_0 \theta_0}, \bar{q}_i = \frac{q_i}{\rho_0 \sqrt{\theta_0}^3}, \Delta\bar{q}_i = \frac{\Delta q_i}{\rho_0 \sqrt{\theta_0}^3}, \\ \bar{u}_{ijk}^{0,0} &= \frac{u_{ijk}^{0,0}}{\rho_0 \sqrt{\theta_0}^3}, \bar{B}_{ij}^+ = \frac{B_{ij}^+}{\rho_0 \theta_0^2}, \bar{B}_{ij}^- = \frac{B_{ij}^-}{\rho_0 \theta_0^2}, \bar{B}^+ = \frac{B^+}{\rho_0 \theta_0^2}, \bar{B}^- = \frac{B^-}{\rho_0 \theta_0^2}. \end{aligned} \quad (55)$$

Note that the dimensionless relaxation times,  $\bar{\tau}_{int}$  and  $\bar{\tau}_{tr}$ , are the Knudsen numbers. In order to do the one-dimensional wave analysis, all variables should depend only on time and x-direction. For simplicity we use the following notation for the relevant elements of vectors and tensors:

$$v_1 = v, \sigma_{11} = \sigma, q_1 = q, \Delta q_1 = \Delta q, u_{111}^{0,0} = u^{0,0}. \quad (56)$$

To avoid complexity, the over bars and hats are dropped from now on, wherever applicable. For deriving the trace free tensors in the 1D equations, care must be taken. For instance, the trace free parts of derivatives of stress and velocity are  $\frac{\partial \sigma_{<11}}{\partial x_{1>}} = \frac{3}{5} \frac{\partial \sigma}{\partial x}$  and  $\frac{\partial v_{<1}}{\partial x_{1>}} = \frac{2}{3} \frac{\partial v}{\partial x}$ . The final set of one-dimensional linear dimensionless equations are presented next.

### B. One-dimensional linear dimensionless equations

For having the Grad's 36 moment equations, the conservation laws,

$$\frac{\partial \rho}{\partial t} + \frac{\partial v}{\partial x} = 0, \quad (57a)$$

$$\frac{\partial v}{\partial t} + \frac{\partial \rho}{\partial x} + \frac{\partial \theta}{\partial x} + \frac{\partial \sigma}{\partial x} - \frac{\partial \Delta \theta}{\partial x} = 0, \quad (57b)$$

$$\frac{\partial \theta}{\partial t} + \frac{2}{3 + \delta} \frac{\partial v}{\partial x} + \frac{2}{3 + \delta} \frac{\partial q}{\partial x} = 0, \quad (57c)$$

full balance laws for the dynamic temperature, heat flux and stress,

$$\frac{\partial \Delta \theta}{\partial t} - \frac{2\delta}{3(3 + \delta)} \frac{\partial v}{\partial x} - \frac{4\delta}{3(3 + \delta)(5 + \delta)} \frac{\partial q}{\partial x} - \frac{2\delta}{3(5 + \delta)} \frac{\partial \Delta q}{\partial x} = -\frac{\Delta \theta}{\tau_{int}}, \quad (57d)$$

$$\frac{\partial \sigma}{\partial t} + \frac{4}{3} \frac{\partial v}{\partial x} + \frac{8}{3(5 + \delta)} \frac{\partial q}{\partial x} + \frac{8\delta}{15(5 + \delta)} \frac{\partial \Delta q}{\partial x} + \frac{\partial u^{0,0}}{\partial x_k} = -\left[ \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right] \sigma, \quad (57e)$$

$$\begin{aligned} \frac{\partial q}{\partial t} + \frac{5 + \delta}{2} \frac{\partial \theta}{\partial x} + \frac{\partial \sigma}{\partial x} - \frac{\partial \Delta \theta}{\partial x} + \frac{4\delta}{25\delta + 42} \frac{\partial B_{11}^+}{\partial x} - \frac{2}{39} \frac{\partial B^+}{\partial x} \\ + \frac{7(14 + 3\delta)(3 + \delta)}{(14 + \delta)(42 + 25\delta)} \frac{\partial B_{11}^-}{\partial x} + \frac{5}{13} \frac{\partial B^-}{\partial x} = -\left[ \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right] q, \end{aligned} \quad (57f)$$

should be considered along with balance laws,

$$\frac{\partial \Delta q}{\partial t} - \frac{5(3+\delta)}{2\delta} \frac{\partial \Delta \theta}{\partial x} + \frac{\partial \sigma}{\partial x} + \frac{15+7\delta}{42+25\delta} \frac{\partial B_{11}^+}{\partial x} - \frac{5(3+\delta)}{39\delta} \frac{\partial B^+}{\partial x_i} + \frac{5(\delta-10)}{39\delta} \frac{\partial B^-}{\partial x} - 7 \frac{3+\delta}{14+\delta} \frac{\delta+6}{42+25\delta} \frac{\partial B_{11}^-}{\partial x} = - \left[ \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right] \Delta q, \quad (57g)$$

$$\frac{\partial B^+}{\partial t} - \frac{240-\delta(47-\delta)}{2(3+\delta)(5+\delta)} \frac{\partial q}{\partial x} - \frac{10\delta}{5+\delta} \frac{\partial \Delta q}{\partial x} = - \left[ \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right] B^+, \quad (57h)$$

$$\frac{\partial B_{11}^+}{\partial t} + \frac{4(14+\delta)}{3(5+\delta)} \frac{\partial q}{\partial x} + 4 \frac{\partial u^{0,0}}{\partial x} + \frac{4(70+23\delta)}{15(5+\delta)} \frac{\partial \Delta q}{\partial x} = - \left[ \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right] B_{11}^+, \quad (57i)$$

$$\frac{\partial u^{0,0}}{\partial t} + \frac{9}{5} \frac{\partial \sigma}{\partial x} + \frac{18\delta}{5(25\delta+42)} \frac{\partial B_{11}^+}{\partial x} + \frac{18(14-\delta)(3+\delta)}{5(14+\delta)(42+25\delta)} \frac{\partial B_{11}^-}{\partial x} = - \left[ \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right] u^{0,0}, \quad (57j)$$

$$\frac{\partial B^-}{\partial t} + \frac{(24-\delta)}{2(5+\delta)} \frac{\partial q}{\partial x} + \frac{2\delta}{5(5+\delta)} \frac{\partial \Delta q}{\partial x} = - \left[ \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right] B^-, \quad (57k)$$

$$\frac{\partial B_{11}^-}{\partial t} + \frac{4(14+\delta)}{3(5+\delta)} \frac{\partial q}{\partial x} + \frac{3(14+\delta)}{7(3+\delta)} \frac{\partial u^{0,0}}{\partial x} - \frac{8\delta(14+\delta)}{15(3+\delta)(5+\delta)} \frac{\partial \Delta q}{\partial x} = - \left[ \frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}} \right] B_{11}^-. \quad (57l)$$

The set of equations for first, second, and third order could be obtained by zeroing the corresponding underlined terms, e.g., zeroing the second and third underlined terms reproduce the second order set of equations.

### C. Plane harmonic waves

All sets of linearized one-dimensional equations can be written in the general form

$$A_{AB} \frac{\partial u_B}{\partial t} + C_{AB} \frac{\partial u_B}{\partial x} = L_{AB} u_B, \quad (58)$$

with the coefficients matrices  $A_{AB}$ ,  $C_{AB}$ , and  $L_{AB}$  corresponding to the equations and variables vector defined as

$$u^{[14]} = \{\rho, v_i, \theta, \sigma_{ij}, \Delta\theta, q_i\} \quad \text{first and second order,} \quad (59a)$$

$$u^{[36]} = \{\rho, v_i, \theta, \sigma_{ij}, \Delta\theta, q_i, \Delta q_i, B^+, B^-, u_{ijk}^{0,0}, B_{ij}^+, B_{ij}^-\} \quad \text{third order and G36.} \quad (59b)$$

Making the harmonic wave ansatz,

$$u_A(x, t) = \check{u}_A \exp[i(\omega t - kx)], \quad (60)$$

with the complex amplitude  $\check{u}_A$ , frequency  $\omega$ , and wave number  $k$ , and inserting the harmonic wave into the general form of the equations results in an algebraic equation,

$$[i\omega A_{AB} - ikC_{AB} - L_{AB}] \check{u}_B = 0. \quad (61)$$

The only non-trivial solution for this equation is obtained when the determinant of the complex matrix inside the bracket becomes zero, which gives the dispersion relation. For different set of equations, the dispersion relation has different numbers of branches.

#### D. Phase velocity and damping factor

The phase velocity and damping factor are defined as

$$v_{ph} = \frac{\omega}{k_r} \text{ and } \phi = -k_i. \quad (62)$$

We found 2, 3, 4, and 4 pairs of branches for first, second, and third order set of equations, and G36, respectively. Each of these pairs consist of two waves with the same damping and velocity magnitude moving in opposite direction.

The frequency is made dimensionless such that it can be considered as a Knudsen number,<sup>62</sup>

$$\bar{\omega} = \omega\tau_0 = \text{Kn}. \quad (63)$$

For convenience, the internal Knudsen number is set to unity,  $\text{Kn}_{int} = 1$ , so that the reference time scale is the internal mean free time,  $\tau_0 = \tau_{int}$ . This means frequency is a measure of the internal Knudsen number.

Figure 2 shows the branches associated with the lowest damping, this is the sound wave,<sup>62</sup> for the different sets of equations, where only one branch is plotted. The dimensionless inverse phase velocity and the reduced damping factor  $\phi/\omega$  for a wide range of dimensionless frequency and two different ratios of Knudsen numbers,  $10^{-2}$  and  $10^{-3}$ , are shown as functions of inverse frequency.

All sets of equations agree for low frequency (i.e., small Knudsen number). However, as the Knudsen number rises (i.e., for smaller inverse frequency), first the refined NSF equations start to deviate, followed by the second order set of equations. The third order equations, R18, have agreement with the full set of 36 equations up to higher Knudsen numbers. Therefore, the range of validity for the set of R18 equations is near  $1/\omega\tau_{int} = \text{Kn}_{tr}/\text{Kn}_{int}$ ; this value of dimensionless frequency corresponds to the case of  $\text{Kn}_{tr} = 1$ . Based on Fig. 2, the expected validity of the R18 is up to  $\text{Kn}_{tr} = 0.6$ .

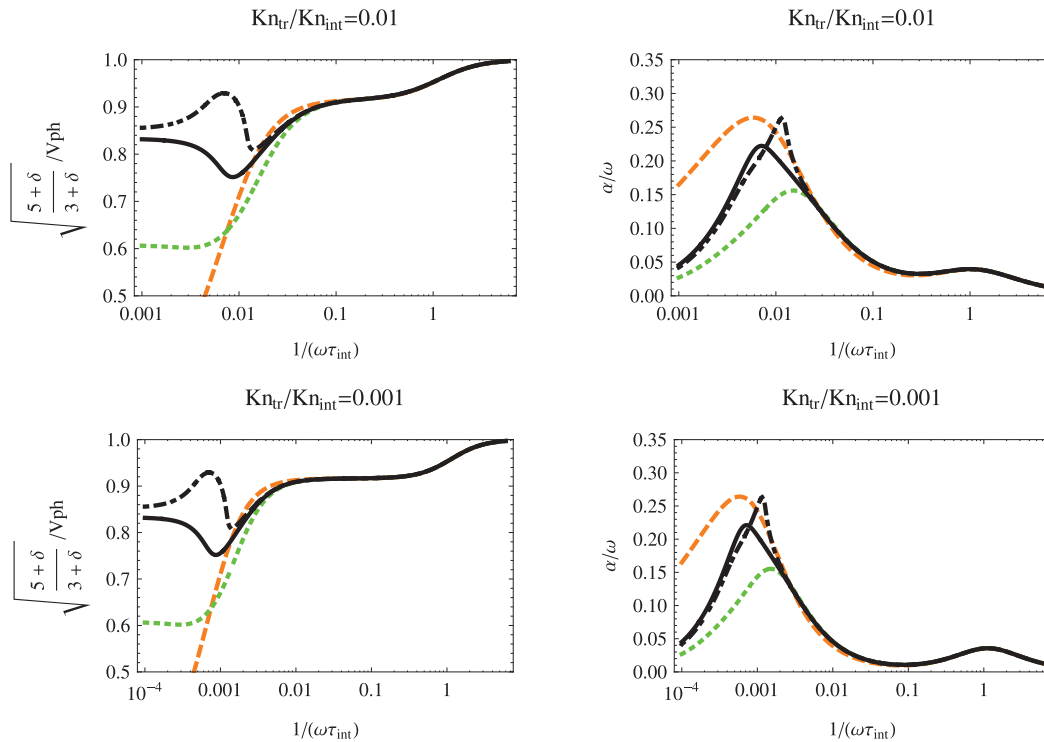


FIG. 2. Inverse dimensionless phase velocity  $\sqrt{(5+\delta)/(3+\delta)}/v_{ph}$  (left) and reduced damping  $\phi/\omega$  (right) as functions of inverse frequency  $1/\omega$  for various Knudsen number ratios and different sets of equations: refined NSF (orange dashed), second order (green dotted), R18 (black continuous), G36 (black dashed-dotted).



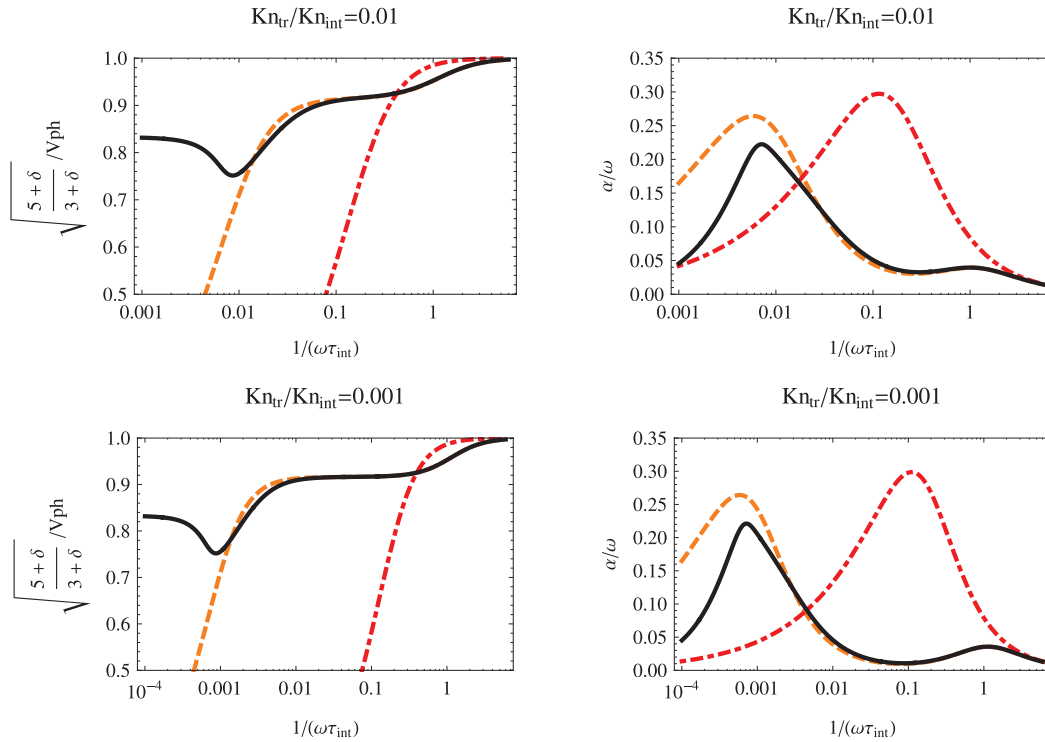


FIG. 3. Inverse dimensionless phase velocity  $\sqrt{(5+\delta)/(3+\delta)}/v_{ph}$  (left) and reduced damping  $\alpha/\omega$  (right) as functions of inverse frequency  $1/\omega$  for two Knudsen number ratios and different sets of equations: R18 (black continuous), classical NSF (red dashed-dotted), refined NSF (orange dashed).

A comparison between the refined and classical NSF equations is made in Fig. 3. The difference between the two sets is simply the time derivative  $\frac{\partial \Delta \theta}{\partial t}$  in Eq. (57d), which is there for the refined case, but not for the classical NSF equations. Original NSF deviates from R18 for almost all frequencies plotted, while refined NSF agrees to R18 for dimensionless inverse frequencies  $1/(\omega\tau_{int})$  down to the values of  $Kn_{tr}/Kn_{int}$ . Considering the proposed refined version of the NSF equations, instead of the classical one, will extend the range of validity of the NSF equations considerably.

### E. Monatomic limit

The cases with very low relaxation time ratio, so that  $\tau_{tr} < \tau_0 \ll \tau_{int}$ , correspond to frozen internal exchange processes. Therefore, if the internal mean free time becomes much larger than the macroscopic time and translational mean free time, the internal degrees of freedom are frozen and the polyatomic gas acts like a monatomic gas.

For convenience, now the translational Knudsen number is set to unity,  $Kn_{tr} = 1$ , so that the reference time scale is the translational mean free time,  $\tau_0 = \tau_{tr}$ . This means frequency is a measure of the translational Knudsen number. In Fig. 4 results from the R18 equations for three different relaxation times ratios are compared with the result from monatomic counterpart, which are the R13 equations.<sup>20</sup> The three relaxation times considered here correspond to two extreme cases, excited ( $\tau_{tr} \approx \tau_{int}$ ) and frozen ( $\tau_{tr} \ll \tau_{int}$ ) internal degrees of freedom, and one case in between  $\tau_{tr}/\tau_{int} = 0.5$ ,  $0.05$ ,  $10^{-5}$ . The case with  $\tau_{tr}/\tau_{int} = 10^{-5}$  corresponds to the frozen internal state and exhibits a good agreement with the monatomic results from the R13 equations. A polyatomic gas with  $\delta = 2$  behaves like a monatomic gas with  $\delta = 0$ , if the internal degrees of freedom are frozen. For intermediate values of  $\tau_{tr}/\tau_{int}$ , the speed of sound is strongly dependent on frequency. If the frequency is small (large  $1/\omega\tau$ ), the internal degrees of freedom have time to relax, and the speed of sound is that for  $\delta$

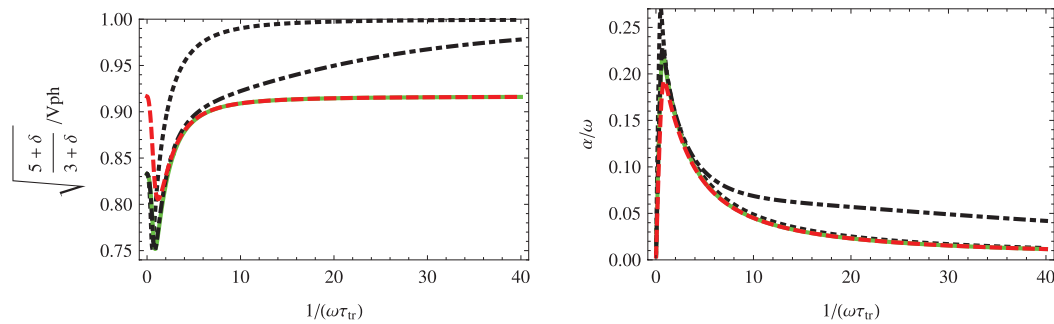


FIG. 4. Inverse dimensionless phase velocity  $\sqrt{(5 + \delta)/(3 + \delta)}/v_{ph}$  (left) and reduced damping  $\phi/\omega$  (right) as functions of inverse frequency  $1/\omega$  for set of R18 equations for Knudsen number ratios, 0.5 (black dotted), 0.05 (black dashed-dotted),  $10^{-5}$  (red dashed), and for the set of R13 equations corresponds to the monatomic gas (green continuous).

$= 2$ , but for larger frequency, the internal degree of freedom does not have sufficient time to relax, which results in an increased speed of sound.

Here, we reproduce the monatomic gas behavior as an asymptotic solution of the equations, without setting the internal degrees of freedom to zero, as was done in Ref. 43.

### VIII. CONCLUSIONS AND OUTLOOK

The present paper introduced new macroscopic models for the accurate description of polyatomic gas flows in the transition regime by employing the order of magnitude method. Different energy exchange processes have been described using the two term BGK collision model. We defined optimized moment definitions such that only linearly independent variables at each order exists. The final closed form of the Grad's 36 moments equations for polyatomic gasses has been presented. We applied the model reduction and obtained 13 different set of equations associated with various order of accuracy. Also, we discussed the changes in the equations due to the ratio of the Knudsen numbers. A brief discussion on the appropriate set of equations which should be used to model different physical problems and some examples on the determining parameters have been given.

The emphasis of the present paper is on the derivation of the equations and introducing a comprehensive model for polyatomic gases in the transition regime. As the first application of the introduced model, we studied the linear wave analysis.

A modification of the classical Navier-Stokes-Fourier equations, which we denoted as refined Navier-Stokes-Fourier (RNSF) equations, was obtained at the first order of accuracy. This modification, which includes the full balance law for the dynamic temperature, extends the range of validity of the classical NSF equations considerably. At the second order of accuracy, a corrected version, RG14, of the existing 14 field theory of moments has been obtained by considering two additional constitutive equations. At order  $2 + 2\alpha$ , a refined variant of Grad's 18 moment (RG18) equations is obtained which consists of 18 PDEs and two constitutive equations. The regularized 18 (R18) equations, consisting of 18 PDEs and 4 constitutive equations, have been acquired at the third order of accuracy as the final reduced set of stable equations which describes the polyatomic gas flows in the transition regime with high order of accuracy. Based on the results for sound waves, the expected validity of the R18 equations is up to  $Kn_{tr} = 0.6$ . Several sets of equations for in-between orders of accuracy have been presented as well.

Finally, as an asymptotic solution to our model, we reproduced the monatomic gas behavior by considering frozen internal exchange processes, and not the zero internal DoF as in Ref. 43.

The next important steps in this research program are: (a) development of suitable boundary conditions for the equations, including boundary conditions for the refined NSF model and (b) 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, fully developed, or frozen, internal energy states. Rederivation 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, and temperature dependent specific heat).

## ACKNOWLEDGMENTS

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## APPENDIX: GRAD'S DISTRIBUTION FUNCTION AND MOMENT EQUATIONS

### 1. Coefficients of Grad's distribution function

The generalized Grad phase density for polyatomic molecules is

$$f_{|Grad} = f_{int} \sum_{n=0} \sum_{\zeta=0} \sum_{A=0} \lambda_{\langle i_1 i_2 \dots i_n \rangle}^{\zeta, A} I^{A(2/\delta)} C^{2\zeta} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle}. \quad (A1)$$

This distribution function for 36 moments (17) must reproduce the set of 36 moments as

$$u_A = m \int \int \Psi_A f_{|36} d\mathbf{c} dI, \quad (A2)$$

with

$$u_A = \{\rho, \rho\theta_{tr}, \rho\theta_{int}, \sigma_{ij}, q_{i,tr}, q_{i,int}, u_{ij}^{1,0}, u^{2,0}, u_{ijk}^{0,0}, u_{ij}^{0,1}, u^{1,1}\},$$

$$\Psi_A = \{1, C_i, \frac{C^2}{3}, \frac{2}{\delta} I^{2/\delta}, C_{\langle i} C_{j \rangle}, \frac{C_i C^2}{2}, C_i I^{2/\delta}, C_{\langle i} C_{j \rangle} C^2, C^4, C_{\langle i} C_j C_{k \rangle}, C_{\langle i} C_{j \rangle} I^{2/\delta}, C^2 I^{2/\delta}\}.$$

The coefficients of the distribution function, Eq. (17), are obtained using the above equations as

$$\begin{aligned} \lambda^{0,0} &= \frac{4u^{1,1} + u^{2,0}}{8\rho\theta^2} + \frac{5}{8} - \frac{3(2+\delta)\theta_{tr}}{4\theta}, & \lambda^{0,1} &= -\frac{u^{1,1}}{\delta\rho\theta^3} + \frac{15}{2\delta\theta} - \frac{3(5-\delta)\theta_{tr}}{2\delta\theta^2}, \\ \lambda^{1,0} &= -\frac{2u^{1,1} + u^{2,0}}{12\rho\theta^3} - \frac{1}{\theta} + \frac{(9+\delta)\theta_{tr}}{4\theta^2}, & \lambda^{2,0} &= \frac{u^{2,0}}{120\rho\theta^4} + \frac{1}{8\theta^2} - \frac{\theta_{tr}}{4\theta^3}, \\ \lambda^{1,1} &= \frac{u^{1,1}}{3\delta\rho\theta^4} - \frac{3}{2\delta\theta^2} + \frac{(9-\delta)\theta_{tr}}{6\delta\theta^3}, & \lambda_i^{0,0} &= -\frac{q_{i,tr} + q_{i,int}}{\rho\theta^2}, \\ \lambda_i^{1,0} &= \frac{q_{i,tr}}{5\rho\theta^3}, & \lambda_i^{0,1} &= \frac{2q_{i,int}}{\delta\rho\theta^3}, \\ \lambda_{\langle ij \rangle}^{0,0} &= -\frac{2u_{ij}^{0,1} + u_{ij}^{1,0}}{4\rho\theta^3} + \frac{(9+\delta)\sigma_{ij}}{4\rho\theta^2}, & \lambda_{\langle ij \rangle}^{1,0} &= -\frac{u_{ij}^{1,0}}{28\rho\theta^4} - \frac{\sigma_{ij}}{4\rho\theta^3}, \\ \lambda_{\langle ijk \rangle}^{0,0} &= \frac{u_{ijk}^{0,0}}{6\rho\theta^3}, & \lambda_{\langle ij \rangle}^{0,1} &= \frac{u_{ij}^{0,1}}{\delta\rho\theta^4} - \frac{\sigma_{ij}}{2\rho\theta^3}. \end{aligned}$$

### 2. Moment equations

The moment equations for higher 18 moments,  $B^-$ ,  $B_{ij}^+$ ,  $u_{ijk}^{0,0}$ , and  $B_{ij}^-$ , are presented here. The moment equations for lower 18 moments,  $\rho$ ,  $v_i$ ,  $\theta$ ,  $\Delta\theta$ ,  $\sigma_{ij}$ ,  $q_i$ ,  $B^+$ , and  $\Delta q_i$  were presented in

Eqs. (35a)–(35h).

$$\begin{aligned}
& \epsilon^1 \left[ \frac{D\tilde{B}^-}{Dt} + \frac{71}{39}\tilde{B}^- \frac{\partial v_k}{\partial x_k} \right] + \left\{ \begin{array}{l} \epsilon^1 \\ \epsilon^{2\alpha} \end{array} \right\} \left[ \frac{2\delta}{5(5+\delta)} \Delta \tilde{q}_k \left( \frac{\partial \Delta \tilde{\theta}}{\partial x_k} + \Delta \tilde{\theta} \frac{\partial \ln \rho}{\partial x_k} \right) \right] \\
& + \left\{ \begin{array}{l} \epsilon^{1-2\alpha} \\ \epsilon^0 \end{array} \right\} \left[ \frac{1}{2(5+\delta)} \left( (24-\delta)\theta \frac{\partial \tilde{q}_i}{\partial x_i} + 4\tilde{q}_k \left[ (15+4\delta) \frac{\partial \theta}{\partial x_k} - (6+\delta)\theta \frac{\partial \ln \rho}{\partial x_k} \right] \right) + \frac{12}{5}\theta \tilde{\sigma}_{kj} \frac{\partial v_j}{\partial x_k} \right] \\
& + \left\{ \begin{array}{l} \epsilon^{1-\alpha} \\ \epsilon^\alpha \end{array} \right\} \left[ \frac{2(6+\delta)}{5+\delta} \tilde{q}_k \left( \frac{\partial \Delta \tilde{\theta}}{\partial x_k} + \Delta \tilde{\theta} \frac{\partial \ln \rho}{\partial x_k} \right) + 3\Delta \tilde{\theta} \left( \frac{\partial \tilde{q}_i}{\partial x_i} + \tilde{\sigma}_{kj} \frac{\partial v_j}{\partial x_k} \right) \right] \\
& + \left\{ \begin{array}{l} \epsilon^{1-\alpha} \\ \epsilon^\alpha \end{array} \right\} \left[ \frac{2\delta}{5(5+\delta)} \theta \left( \frac{\partial \Delta \tilde{q}_k}{\partial x_k} - \Delta \tilde{q}_k \frac{\partial \ln \rho}{\partial x_k} \right) + \frac{36\delta}{42+25\delta} \tilde{B}_{kj}^+ \frac{\partial v_j}{\partial x_k} + \frac{\delta(3+\delta)}{(5+\delta)} \Delta \tilde{q}_k \frac{\partial \theta}{\partial x_k} \right] \\
& + \left\{ \begin{array}{l} \epsilon^{2-2\alpha} \\ \epsilon^1 \end{array} \right\} \left[ \frac{196(\delta+6)(\delta+3)\tilde{B}_{kj}^-}{5(\delta+14)(25\delta+42)} \frac{\partial v_j}{\partial x_k} - \frac{2(6+\delta)\tilde{q}_k}{(5+\delta)\rho} \frac{\partial \tilde{\sigma}_{kj}}{\partial x_j} \right] - \left\{ \begin{array}{l} \epsilon^{2-\alpha} \\ \epsilon^{1+\alpha} \end{array} \right\} \left[ \frac{2\delta \Delta \tilde{q}_k}{5(5+\delta)\rho} \frac{\partial \tilde{\sigma}_{kj}}{\partial x_j} \right] \\
& = \left\{ \begin{array}{l} \epsilon^0 \\ \epsilon^{1-2\alpha} \end{array} \right\} \left[ 3\rho \Delta \theta^2 \frac{\partial v_i}{\partial x_i} + \frac{2}{13} \tilde{B}^+ \frac{\partial v_k}{\partial x_k} \right] - \left( \frac{1}{\tilde{\tau}_{tr}} + \frac{\epsilon^{1-\alpha}}{\tilde{\tau}_{int}} \right) \tilde{B}^-, \quad (\text{A3a})
\end{aligned}$$

$$\begin{aligned}
& \epsilon^1 \left[ \frac{D\tilde{B}_{ij}^+}{Dt} + \frac{2(14+\delta)}{5+\delta} \left( \Delta \tilde{\theta} \tilde{q}_{<i} \frac{\partial \ln \rho}{\partial x_{j>}} + \tilde{q}_{<i} \frac{\partial \Delta \tilde{\theta}}{\partial x_{j>}} + \frac{\delta}{5} \Delta \tilde{q}_{<i} \frac{\partial \theta}{\partial x_{j>}} \right) \right] \\
& + \epsilon^1 \left[ \frac{2(23\delta+70)}{5(5+\delta)} \theta \left( \frac{\partial \Delta \tilde{q}_{<i}}{\partial x_{j>}} - \Delta \tilde{q}_{<i} \frac{\partial \ln \rho}{\partial x_{j>}} \right) + \frac{12(2\delta+3)}{25\delta+42} \left( \frac{14}{15} \tilde{B}_{k<i}^+ \frac{\partial v_k}{\partial x_{j>}} + \tilde{B}_{<ij}^+ \frac{\partial v_{k>}}{\partial x_k} \right) \right] \\
& + \epsilon^1 \left[ 2\tilde{B}_{k<i}^+ \frac{\partial v_{j>}}{\partial x_k} + \tilde{B}_{ij}^+ \frac{\partial v_k}{\partial x_k} + \frac{14+\delta}{3+\delta} \tilde{\sigma}_{ij} \Delta \tilde{\theta} \frac{\partial v_k}{\partial x_k} \right] - \epsilon^\alpha \left[ \frac{84+50\delta}{39\delta} \tilde{B}^+ \frac{\partial v_{<i}}{\partial x_{j>}} \right] \\
& + \epsilon^{1-\alpha} \left[ \theta \left( 12\tilde{\sigma}_{<ij} \frac{\partial v_{k>}}{\partial x_k} + \frac{56}{5} \tilde{\sigma}_{k<i} \frac{\partial v_k}{\partial x_{j>}} - \frac{14+\delta}{3+\delta} \tilde{\sigma}_{ij} \frac{\partial v_k}{\partial x_k} \right) + 2 \frac{14+\delta}{5+\delta} \left( \theta \frac{\partial \tilde{q}_{<i}}{\partial x_{j>}} + \tilde{q}_{<i} \frac{\partial \theta}{\partial x_{j>}} - \theta \tilde{q}_{<i} \frac{\partial \ln \rho}{\partial x_{j>}} \right) \right] \\
& + \epsilon^{1+\alpha} \left[ \frac{70+23\delta}{5+\delta} \frac{2}{5} \Delta \tilde{q}_{<i} \left( \frac{\partial \Delta \tilde{\theta}}{\partial x_{j>}} + \Delta \tilde{\theta} \frac{\partial \ln \rho}{\partial x_{j>}} \right) \right] - \left\{ \begin{array}{l} \epsilon^{1+\alpha} \\ \epsilon^{2-\alpha} \end{array} \right\} \left[ \frac{4(70-19\delta)}{39\delta} \tilde{B}^- \frac{\partial v_{<i}}{\partial x_{j>}} \right] \\
& + \epsilon^{2-\alpha} \left[ 4\theta \left( \frac{\partial \tilde{u}_{ijk}^{0,0}}{\partial x_k} - \tilde{u}_{ijk}^{0,0} \frac{\partial \ln \rho}{\partial x_k} \right) - \frac{14+\delta}{3+\delta} \frac{\tilde{\sigma}_{ij}}{\rho} \left( \frac{\partial \tilde{q}_k}{\partial x_k} + \tilde{\sigma}_{kl} \frac{\partial v_l}{\partial x_k} \right) \right] \\
& - \epsilon^{2-\alpha} \left[ \frac{8\delta(3+\delta)}{(14+\delta)(42+25\delta)} \left( 3\tilde{B}_{<ij}^- \frac{\partial v_{k>}}{\partial x_k} + \frac{14}{5} \tilde{B}_{k<i}^- \frac{\partial v_k}{\partial x_{j>}} \right) \right] \\
& + \epsilon^{2-\alpha} \left[ \frac{\delta+14}{2} \tilde{u}_{ijk}^{0,0} \frac{\partial \theta}{\partial x_k} - \frac{14+\delta}{5+\delta} \frac{2}{\rho} \tilde{q}_{<i} \frac{\partial \tilde{\sigma}_{j>k}}{\partial x_k} \right] - \epsilon^{3-\alpha} \left[ \frac{4}{\rho} \tilde{u}_{ijk}^{0,0} \frac{\partial \tilde{\sigma}_{kl}}{\partial x_l} \right] \\
& + \epsilon^2 \left[ 4\tilde{u}_{ijk}^{0,0} \left( \Delta \tilde{\theta} \frac{\partial \ln \rho}{\partial x_k} + \frac{\partial \Delta \tilde{\theta}}{\partial x_k} \right) - \frac{2(70+23\delta)}{5(5+\delta)} \frac{\Delta \tilde{q}_{<i}}{\rho} \frac{\partial \tilde{\sigma}_{j>k}}{\partial x_k} \right] \\
& = \left[ \frac{42+25\delta}{\delta} \rho \theta \Delta \tilde{\theta} \frac{\partial v_{<i}}{\partial x_{j>}} - \left( \frac{1}{\tilde{\tau}_{tr}} + \frac{\epsilon^{1-\alpha}}{\tilde{\tau}_{int}} \right) \tilde{B}_{ij}^+ \right], \quad (\text{A3b})
\end{aligned}$$

$$\begin{aligned} \epsilon^1 & \left[ \frac{D\tilde{u}_{ijk}^{0,0}}{Dt} - \frac{3\tilde{\sigma}_{<ij}}{\rho} \frac{\partial \tilde{\sigma}_{k>l}}{\partial x_l} + \frac{6(14-\delta)(3+\delta)}{(14+\delta)(42+25\delta)} \frac{\partial \tilde{B}_{<ij}^-}{\partial x_k} + 3\tilde{u}_{l<ij}^{0,0} \frac{\partial v_{k>}}{\partial x_l} + \tilde{u}_{ijk}^{0,0} \frac{\partial v_l}{\partial x_l} \right] \\ & + \epsilon^\alpha \left[ \frac{6\delta}{25\delta+42} \frac{\partial \tilde{B}_{<ij}^+}{\partial x_k} + 3\tilde{\sigma}_{<ij} \left( \frac{\partial \Delta\tilde{\theta}}{\partial x_k} + \Delta\tilde{\theta} \frac{\partial \ln \rho}{\partial x_k} \right) + \frac{12\delta}{5(5+\delta)} \Delta\tilde{q}_{<i} \frac{\partial v_j}{\partial x_k} \right] \\ & = - \left[ 3\theta \left( \frac{\partial \tilde{\sigma}_{<ij}}{\partial x_k} - \tilde{\sigma}_{<ij} \frac{\partial \ln \rho}{\partial x_k} \right) + \frac{12}{5+\delta} \tilde{q}_{<i} \frac{\partial v_j}{\partial x_k} + \tilde{u}_{ijk}^{0,0} \left( \frac{1}{\tilde{\tau}_{ir}} + \frac{\epsilon^{1-\alpha}}{\tilde{\tau}_{int}} \right) \right], \quad (\text{A3c}) \end{aligned}$$

$$\begin{aligned} \epsilon^1 & \left[ \frac{D\tilde{B}_{ij}^-}{Dt} + \frac{14+\delta}{3+\delta} \left( \frac{3}{7}\theta \left( \frac{\partial \tilde{u}_{ijk}^{0,0}}{\partial x_k} - \tilde{u}_{ijk}^{0,0} \frac{\partial \ln \rho}{\partial x_k} \right) - \frac{\tilde{\sigma}_{ij}}{\rho} \left[ \frac{\partial \tilde{q}_k}{\partial x_k} + \tilde{\sigma}_{kl} \frac{\partial v_l}{\partial x_k} \right] \right) \right] \\ & + \epsilon^1 \left[ 2\tilde{B}_{k<i}^- \frac{\partial v_{j>}}{\partial x_k} + \left( \frac{14-\delta}{14+\delta} \frac{14(\delta+3)}{25\delta+42} + \frac{11\delta}{25\delta+42} \right) \left( \frac{6}{7}\tilde{B}_{<ij}^- \frac{\partial v_{k>}}{\partial x_k} + \frac{4}{5}\tilde{B}_{k<i}^- \frac{\partial v_k}{\partial x_{j>}} \right) \right] \\ & + \epsilon^1 \left[ (\delta+14) \left( \frac{\tilde{u}_{ijk}^{0,0}}{2} \frac{\partial \theta}{\partial x_k} - \frac{2}{(5+\delta)\rho} \tilde{q}_{<i} \frac{\partial \tilde{\sigma}_{j>k}}{\partial x_k} \right) + \tilde{B}_{ij}^- \frac{\partial v_k}{\partial x_k} \right] \\ & + \epsilon^\alpha \left[ (14+\delta) \left( \frac{2}{5+\delta} \left[ \frac{\delta}{5} \Delta\tilde{q}_{<i} \frac{\partial \theta}{\partial x_{j>}} + \Delta\tilde{\theta} \tilde{q}_{<i} \frac{\partial \ln \rho}{\partial x_{j>}} + \tilde{q}_{<i} \frac{\partial \Delta\tilde{\theta}}{\partial x_{j>}} \right] + \frac{\Delta\tilde{\theta} \tilde{\sigma}_{ij}}{3+\delta} \frac{\partial v_k}{\partial x_k} \right) \right] \\ & + \epsilon^\alpha \left[ \frac{4\delta(14+\delta)}{5(\delta+3)(\delta+5)} \theta \left( \Delta\tilde{q}_{<i} \frac{\partial \ln \rho}{\partial x_{j>}} - \frac{\partial \Delta\tilde{q}_{<i}}{\partial x_{j>}} \right) + \frac{3\delta}{25\delta+42} \left( \frac{6}{7}\tilde{B}_{<ij}^+ \frac{\partial v_{k>}}{\partial x_k} + \frac{4}{5}\tilde{B}_{k<i}^+ \frac{\partial v_k}{\partial x_{j>}} \right) \right] \\ & + \left\{ \frac{\epsilon^{2\alpha}}{\epsilon^1} \right\} \frac{2(14+\delta)}{3(3+\delta)} \tilde{B}_{ij}^- \frac{\partial v_{<i}}{\partial x_{j>}} - \epsilon^{2\alpha} \left[ \frac{4\delta(14+\delta)}{5(\delta+3)(\delta+5)} \Delta\tilde{q}_{<i} \left( \Delta\tilde{\theta} \frac{\partial \ln \rho}{\partial x_{j>}} + \frac{\partial \Delta\tilde{\theta}}{\partial x_{j>}} \right) \right] \\ & + \epsilon^{1+\alpha} \left[ \frac{14+\delta}{3+\delta} \left( \frac{3}{7}\tilde{u}_{ijk}^{0,0} \left[ \Delta\tilde{\theta} \frac{\partial \ln \rho}{\partial x_k} + \frac{\partial \Delta\tilde{\theta}}{\partial x_k} \right] - \frac{4\delta}{5(5+\delta)} \frac{\Delta\tilde{q}_{<i}}{\rho} \frac{\partial \tilde{\sigma}_{j>k}}{\partial x_k} \right) \right] \\ & - \epsilon^2 \left[ \frac{3(\delta+14)}{7(\delta+3)} \frac{\tilde{u}_{ijk}^{0,0}}{\rho} \frac{\partial \tilde{\sigma}_{kl}}{\partial x_l} \right] = - \frac{6(\delta+14)}{7(\delta+3)} \theta \left( \sigma_{k<i} \frac{\partial v_{j>}}{\partial x_k} + \sigma_{k<i} \frac{\partial v_k}{\partial x_{j>}} - \frac{2}{3} \sigma_{ij} \frac{\partial v_k}{\partial x_k} \right) \\ & - \frac{2(14+\delta)}{5+\delta} \left( \theta \frac{\partial \tilde{q}_{<i}}{\partial x_{j>}} + \tilde{q}_{<i} \frac{\partial \theta}{\partial x_{j>}} - \theta \tilde{q}_{<i} \frac{\partial \ln \rho}{\partial x_{j>}} \right) - \tilde{B}_{ij}^- \left( \frac{1}{\tilde{\tau}_{ir}} + \frac{\epsilon^{1-\alpha}}{\tilde{\tau}_{int}} \right). \quad (\text{A3d}) \end{aligned}$$

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