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# Macroscopic and kinetic modelling of rarefied polyatomic gases

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A kinetic model and corresponding high-order macroscopic model for the accurate description of rarefied polyatomic gas flows are introduced. The different energy exchange processes are accounted for with a two term collision model. The proposed kinetic model, which is an extension of the S-model, predicts correct relaxation of higher moments and delivers the accurate Prandtl ($Pr$) number. Also, the model has a proven linear H-theorem. 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. At the first order, a modification of the Navier–Stokes–Fourier (NSF) equations is obtained. At third order of accuracy, a set of 19 regularized partial differential equations (R19) is obtained. Furthermore, the terms associated with the internal degrees of freedom yield various intermediate orders of accuracy, a total of 13 different orders. Thereafter, boundary conditions for the proposed macroscopic model are introduced. The unsteady heat conduction of a gas at rest is studied numerically and analytically as an example of a boundary value problem. The results for different gases are given and effects of Knudsen numbers, degrees of freedom, accommodation coefficients and temperature-dependent properties are investigated. For some cases, the higher-order effects are very dominant and the widely used first-order set of the NSF equations fails to accurately capture the gas behaviour and should be replaced by the proposed higher-order set of equations.

**Key words:** mathematical foundations, micro-/nano-fluid dynamics, rarefied gas flow

## 1. Introduction

The Knudsen number, $Kn$, is a measure illustrating the degree of rarefaction in a gas, therefore it is used to characterize processes in kinetic theory. It is defined as the ratio of molecular mean free path or time to the characteristic length or time of the system ($Kn = \lambda/L_0 = \tau/\tau_0$). At the low Knudsen range ($Kn < 0.01$), the flow is in the continuum regime and the classical Navier–Stokes–Fourier (NSF) equations are valid (Karniadakis, Beskok & Aluru 2006). However, in the transition flow regime, i.e. at intermediate Knudsen numbers, the equations of conventional hydrodynamics fail in the description of the gas behaviour. Flows in micro-electro-mechanical

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systems (MEMS) and high vacuum systems are in this regime (Gad-el Hak 2001; Rahimi & Niazmand 2014). Boltzmann (1872) proposed a transport equation which models the evolution of the velocity distribution function over time and space. This equation, known as the Boltzmann equation, was a breakthrough in the kinetic theory and offered accurate description of the gas flow for all $Kn$ numbers. However, solving the Boltzmann equation directly, deterministically or stochastically, is usually expensive and cumbersome. As an alternative to the Boltzmann equation, kinetic theory provides macroscopic models for not too large Knudsen numbers (Struchtrup 2005*b*). Macroscopic models are derived as approximations to the Boltzmann equation. These models offer high computational speed and explicit equations for macroscopic variables, which are helpful for understanding and analysing the flow behaviour (Rana, Torrilhon & Struchtrup 2013).

Macroscopic models are classically obtained by Chapman–Enskog (CE) method and Grad's moments method. Using the CE method, Nagnibeda & Kustova (2009) studied the strong vibrational non-equilibrium in diatomic gases (Kustova & Nagnibeda 1996) and reacting mixture of polyatomic gases for different cases with regards to the characteristic time of the microscopic processes (Chikhaoui *et al.* 1997; Kustova & Nagnibeda 1998; Kustova, Nagnibeda & Chauvin 1999; Chikhaoui *et al.* 2000), and derived the first-order distribution function and governing equations. Cai & Li (2014) extended the numerical regularized moment method of arbitrary order (NRxx) model to polyatomic gases using the ellipsoidal-statistical-Bhatnagar–Gross–Krook (ES-BGK) model of Andries *et al.* (2000) and Brull & Schneider (2009). Arima *et al.* (2012) developed a generalized macroscopic 14 field theory for the polyatomic gases, based on the methods of extended thermodynamics (Müller & Ruggeri 2013; Ruggeri & Sugiyama 2015). Tantos, Valougeorgis & Frezzotti (2015), Tantos *et al.* (2014) studied steady state heat transfer between parallel and coaxial cylinders using a BGK type model of Holway (1966) and DSMC simulations. The Burnett equations for monatomic gases in cylindrical coordinates obtained by the CE method are given by Singh & Agrawal (2014). Also, Sone (2012) developed systematic asymptotic solutions of the Boltzmann equation, and at small Knudsen numbers, an interesting phenomenon named the ghost effect was observed.

Recently, as a first attempt in the field, Rahimi & Struchtrup (2014*a*,*c*,*b*) developed a high-order macroscopic model for description of rarefied polyatomic gases using order of magnitude method. The proposed model consists of 18 regularized PDEs for third order of accuracy. This model is obtained using a simple BGK collision model, which is known to give incorrect Prandtl number and relaxation times for higher moments. Also, there was no boundary theory given for the polyatomic macroscopic model. In the present paper, we shall address these issues by introducing a generalized kinetic model and its boundary condition.

Our proposed kinetic model, which is an extension of the Rykov (1975) and Shakhov (1968) models, predicts correct relaxation of heat fluxes and delivers the accurate Prandtl number. In the model proposed here, the number of free relaxation parameters is increased to total of four to allow proper relaxation times for four higher moments compared to one and two parameters of the Shakhov and Rykov models, respectively.

We use the order of magnitude method (Struchtrup 2004, 2005*a*, 2012; Struchtrup & Torrilhon 2013) to derive a macroscopic model (the regularized set of equations) from the proposed kinetic equation. This method bridges between the CE and Grad moments method by using Knudsen number orders, and identifies the appropriate moment definitions and moment equations required for a given order.

The procedure of the order of magnitude method is as follows (Rahimi & Struchtrup 2014*a*):

(i) Construct large moments hierarchy: a system of moment equations using the Grad's method with arbitrary choice of definition and number of moments is constructed.

(ii) Reconstructing moments: apply the CE method on the moments and determine their leading-order terms. Define new moment definitions, using linear combination, based on the goal of having minimal number of moments in each order of magnitude.

(iii) Full set of equations: using the equations of old moments definitions, the set of new moments equations is constructed. Apply the CE method on the new moments to determine their leading order.

(iv) Model reduction: the full set of equations is rescaled considering the obtained order of the new moments. Then, the model can be reduced to any desired order of accuracy.

For the first time, the present paper establishes a theory of boundary conditions for the obtained regularized moment equations based on physical and mathematical requirements of the system. We use the recipe originally given by Grad (1949) based on the kinetic accommodation model of Maxwell (1879), which here is generalized for polyatomic gases. This gives a certain number of boundary conditions for the set of regularized equations, so that we can explore the confined fluid problems, e.g. flow in microchannels.

We lay out the foundation of the kinetic theory of polyatomic gases in the next chapter. The two term collision operator is discussed and the generalized Shakhov-BGK model is introduced. The general moments equation for polyatomic gases is introduced and the system of Grad's 36 moments equations is constructed in § 3, which is item 1 in the above list. The CE method is applied, leading-order terms are determined and the new set of moments is reconstructed in § 4, which is item 2 in the list. Model reduction, item 4 in the list, is done in the § 5 and the regularized equations for different orders of accuracy are presented. The theory of kinetic boundary condition is given in § 6 and corresponding macroscopic boundary conditions are introduced. Section 8 presents stationary heat conduction analysis. The unsteady heat conduction problem is solved numerically and the linear steady case is solved analytically. The obtained results from the proposed macroscopic model is compared with direct simulation Monte Carlo (DSMC) simulations and Holway and Andries kinetic results to show the good accuracy of the proposed model. Also, it is shown that the NSF equations could not produce accurate results and different effects on the gas, e.g. Knudsen numbers and degrees of freedom, are investigated. Final conclusions are given in § 10.

## 2. Kinetic model

A collection of numerous interacting particles is called a gas in kinetic theory. These particles are described by their position, $x_i$, velocity, $c_i$ and their internal energy,

$$e_{int} = I^{2/\delta}, \tag{2.1}$$

in a seven-dimensional space known as phase space at time, $t$. Here, $I$ is the internal energy parameter which is non-negative; $\delta$ is the measure of excitation of internal energy levels and non-translational degrees of freedom (DoF) of the gas. At a fully excited internal DoF, $\delta$ is an integer. However, internal energy levels are usually partially excited and $\delta$ is a fractional number. As temperature rises, that is increasing

the internal energy of the gas to higher levels, the value of $\delta$ continuously increases. Therefore, $\delta$ is a temperature-dependent continuous variable in our model, as given in (2.12).

By introducing the particle or velocity distribution function $f(\boldsymbol{x}, \boldsymbol{c}, I, t)$, the number of molecules in a phase space element $\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3\,\mathrm{d}c_1\,\mathrm{d}c_2\,\mathrm{d}c_3\,\mathrm{d}I$ is

$$\mathrm{d}N = f(\boldsymbol{x}, \boldsymbol{c}, I, t)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I. \tag{2.2}$$

The evolution of the particle distribution functions is determined by the Boltzmann equation, which is a nonlinear integro-differential equation written as (external forces are ignored)

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = S. \tag{2.3}$$

The left- and right-hand sides indicate free flight and particle collisions, respectively. The collision term, $S$, which is quadratic in distribution function, would take complex integral form (Nagnibeda & Kustova 2009; Kremer 2010) which is difficult to work with and costly in computing resources. Therefore, having simpler models to replace the Boltzmann collision term which could preserve the basic relaxation properties and give the correct transport coefficients is of more interest. We introduce a generalized S-model for polyatomic gases in § 2.2 to achieve this.

### 2.1. *Macroscopic quantities*

The macroscopic properties such as mass density, momentum, energy and pressure are moments of the distribution function. Other moments that have physical interpretations are the pressure tensor and heat flux vector. General moment definition based on the trace free part of the central moment is

$$u^{\varsigma,A}_{i_1\ldots i_n} = m \iint (I^{2/\delta})^A C^{2\varsigma} C_{<i_1} C_{i_2} \ldots C_{i_n>} f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I, \tag{2.4}$$

where

$$\left.\begin{array}{l} A = 0, 1, 2, 3, \ldots \\ \varsigma = 0, 1, 2, 3, \ldots. \end{array}\right\} \tag{2.5}$$

The basic and most important moments are:

$$\text{Density } \rho = m \iint f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = \int \rho_I\,\mathrm{d}I = u^{0,0}, \tag{2.6a}$$

$$\text{Velocity } \rho v_i = m \iint c_i f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I \quad \text{or} \quad 0 = m \iint C_i f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = u^{0,0}_i, \tag{2.6b}$$

$$\text{Stress } \boldsymbol{\sigma}_{ij} = m \iint C_{<i} C_{j>} f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = \boldsymbol{u}^{0,0}_{ij}, \tag{2.6c}$$

$$\text{Translational energy } \rho u_{tr} = \frac{3}{2} p = m \iint \frac{C^2}{2} f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = \frac{1}{2} u^{1,0}, \tag{2.6d}$$

$$\text{Internal energy } \rho u_{int} = m \iint I^{2/\delta} f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = \int I^{2/\delta} \rho_I\,\mathrm{d}I = u^{0,1}, \tag{2.6e}$$

$$\text{Translational heat flux } \boldsymbol{q}_{i,tr} = m \iint C_i \frac{C^2}{2} f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = \frac{1}{2} u^{1,0}_i, \tag{2.6f}$$

$$\text{Internal heat flux } \boldsymbol{q}_{i,int} = m \iint C_i I^{2/\delta} f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = u^{0,1}_i. \tag{2.6g}$$

Here, $C_i = c_i - v_i$, is the peculiar particle velocity and $\rho_I = m\int f\,\mathrm{d}\boldsymbol{c}$ is the density of molecules with the same internal energy. Moreover, $u_{tr}$ and $u_{int}$ are the translational energy and energy of the internal DoF, respectively, while $\boldsymbol{q}_{i,tr}$ and $\boldsymbol{q}_{i,int}$ are the translational and internal heat flux vectors.

Regarding the energies, $u_{tr}$ and $u_{int}$, the classical equipartition theorem (Reif 2009) states that in full thermal equilibrium, and with $\delta$ fully excited internal DoF, each DoF contributes an energy of $(1/2)\theta$ to the energy of a particle, where $\theta = (k_b/m)T$ is temperature in specific energy units. Therefore the energy in equilibrium, for fully excited internal DoF, can be written as

$$u = u_{tr|E} + u_{int|E} = \left(\frac{3}{2} + \frac{\delta}{2}\right)\theta, \tag{2.7}$$

where $u_{tr|E} = (3/2)\theta$ is the contribution from translational energy and $u_{int|E} = (\delta/2)\theta$ is the contribution from the internal DoF.

In non-equilibrium processes, translational energy and internal energies cannot be described by a single temperature, rather at least two distinct temperatures are required. Furthermore, the equipartition theorem as stated above is only valid when the internal DoF are either fully excited or frozen. Typically, for polyatomic gases, some internal DoF are only partially excited, with the degree of excitation determined by temperature. Therefore, $\delta$ is not an integer, but a continuous function of temperature, that has integer values only for fully excited internal DoF. For convenience we introduce the translational temperature $\theta_{tr}$ and the internal temperature $\theta_{int}$ which are defined through the energies as

$$u_{tr} = \frac{3}{2}\theta_{tr} \quad \text{and} \quad u_{int} = \frac{\delta(\theta_{int})}{2}\theta_{int}. \tag{2.8a,b}$$

We note that these temperatures are not measurable temperatures as in the equilibrium case, but rather convenient quantities to use instead of the energies $u_{tr}$ and $u_{int}$. In thermal equilibrium, both temperatures agree, and are equal to the thermodynamic temperature, $\theta_{tr} = \theta_{int} = \theta$. With these definitions, the ideal gas law in non-equilibrium reads $p = \rho\theta_{tr}$.

Just as we defined temperatures for the energies $u_{tr}$ and $u_{int}$, we can define an overall temperature $\theta$ for the total energy. Similar to $\theta_{tr}$ and $\theta_{int}$, the temperature $\theta$ is a measure for energy, and not a measurable temperature. By definition, in equilibrium $\theta$ is the thermodynamic temperature of the gas

$$u = \left(\frac{3}{2} + \frac{\delta(\theta)}{2}\right)\theta = \frac{3}{2}\theta_{tr} + \frac{\delta(\theta_{int})}{2}\theta_{int}. \tag{2.9}$$

The function $\delta$ can be found from measurements of specific heat in equilibrium as

$$C_v = \frac{\mathrm{d}u}{\mathrm{d}\theta} = \frac{3 + \delta(\theta) + \theta\dfrac{\mathrm{d}\delta(\theta)}{\mathrm{d}\theta}}{2}. \tag{2.10}$$

We will use third-order polynomial function for constant volume specific heat,

$$C_v = C_0 + C_1\theta + C_2\theta^2 + C_3\theta^3; \tag{2.11}$$

the coefficients $C_\alpha$ can be determined from tabulated data, and are available in databases (Borgnakke & Sonntag 2009). From (2.10) and (2.11) we find $\delta(\theta)$ as a polynomial of the same order,

$$\delta(\theta) = 2C_0 - 3 + C_1\theta + \frac{2}{3}C_2\theta^2 + \frac{C_3}{2}\theta^3. \tag{2.12}$$

From the definition of the overall temperature (2.9) we find a relation for $\delta$ evaluated at $\theta$ and $\theta_{int}$, $\delta(\theta) = \delta(\theta_{int})(\theta_{int}/\theta) - (3/2)((\theta - \theta_{tr})/\theta)$. From now on, we shall consider mainly states not far from equilibrium, so that $\theta_{int}/\theta \backsimeq 1 \gg (\theta - \theta_{tr})/\theta$ holds. For convenience, we shall ignore the small difference between $\delta(\theta_{int})$ and $\delta(\theta)$, and will have only the latter appear in our equations.

In equilibrium the three temperatures agree, $\theta_{tr|E} = \theta_{int|E} = \theta$, while in non-equilibrium they will differ. We define the non-equilibrium part of the temperature, named the dynamic temperature, as

$$\Delta\theta = \theta - \theta_{tr}. \tag{2.13}$$

The first 36 raw moments are listed as,

$$\Phi_{36} = \{\rho, v_i, \theta, \Delta\theta, \boldsymbol{\sigma}_{ij}, \boldsymbol{q}_{i,tr}, \boldsymbol{q}_{i,int}, \boldsymbol{u}_{ij}^{1,0}, u^{2,0}, \boldsymbol{u}_{ij}^{0,1}, u^{1,1}, \boldsymbol{u}_{ijk}^{0,0}\}. \tag{2.14}$$

### 2.2. *Generalized S-model*

The state of molecules and the distribution function will be changed by interaction between molecules (collisions). Different exchange processes occur on different characteristic time scales. In all collisions, the translational energy is exchanged between particles. However, only in some of the collisions is internal energy exchanged as well. These differences, and their relation to the macroscopic time scale, is a key feature for defining the state of a gas as being in non-equilibrium or equilibrium. The macroscopic time scale, which is the time needed for any changes to happen in the dynamics of the gas, is the reference time scale here. In cases when there are two different microscopic characteristic time scales, one smaller than and one comparable to, the macroscopic time scale, both rapid equilibrium and slow non-equilibrium processes exist in the gas. The case with a smaller time scale is associated with many collisions within the macroscopic time scale and results in a rapid equilibrium process. On the other hand, the case with a comparable time scale results in a slow non-equilibrium process. Also, all the processes with characteristics time much larger than macroscopic time scale appear to be frozen during the macroscopic time scale. While in every collision the translational energy is exchanged between molecules, internal energy is only exchanged in some of the collisions. Therefore, the translational microscopic time, $\tau_{tr}$, is smaller than the internal microscopic time, $\tau_{int}$.

To model the collision term, we use a two term BGK-type collision operator,

$$\frac{\partial f}{\partial t} + c_k\frac{\partial f}{\partial x_k} = S_{tr} + S_{int}, \tag{2.15a}$$

$$S_{tr} = -\frac{1}{\tau_{tr}}(f - f_{tr}), \tag{2.15b}$$

$$S_{int} = -\frac{1}{\tau_{int}}(f - f_{int}). \tag{2.15c}$$

The first term, $S_{tr}$, describes elastic collisions between particles, i.e. collisions in which the particles only exchange translational energy. The relaxation time $\tau_{tr}$ is the inverse

average collision frequency for this type of collision, which leads to a relaxation to the distribution function $f_{tr}$. The second term, $S_{int}$, describes inelastic collisions, i.e. collisions in which the particles exchange internal and translational energies at the same time. The relaxation time $\tau_{int}$ is the inverse average collision frequency for this type of collision, which leads to a relaxation to the distribution function $f_{int}$.

In the standard BGK model (Bourgat *et al.* 1994; Andries *et al.* 2000; Rahimi & Struchtrup 2014*a*), the targeted distributions, $f_{tr}$ and $f_{int}$ are chosen as the Maxwellian equilibrium distributions $f_{tr_0}$ and $f_{int_0}$, respectively, which are given by

$$f_{tr_0} = \frac{\rho_I}{m}\left(\frac{1}{2\pi\theta_{tr}}\right)^{3/2} \exp\left[-\frac{1}{2\theta_{tr}}C^2\right], \tag{2.16}$$

$$f_{int_0} = \frac{\rho}{m}\frac{1}{(2\pi)^{3/2}\theta^{(\delta+3)/2}}\frac{1}{\Gamma\left(1+\dfrac{\delta}{2}\right)} \exp\left[-\frac{1}{\theta}\left(\frac{C^2}{2}+I^{2/\delta}\right)\right]. \tag{2.17}$$

Here, $f_{tr_0}$ is the equilibrium distribution for particles with frozen internal DoF. Also, $f_{int_0}$ is the full equilibrium distribution for the gas, which experienced full exchange of the translational and internal energies.

However, the equations for moments $\boldsymbol{\sigma}_{ij}$, $\boldsymbol{q}_{i,tr}$, $\boldsymbol{q}_{i,int}$, $\boldsymbol{u}_{ij}^{1,0}$, $u^{2,0}$, $\boldsymbol{u}_{ij}^{0,1}$, $u^{1,1}$ and $\boldsymbol{u}_{ijk}^{0,0}$ corresponding to the original BGK model, have the form of (Rahimi & Struchtrup 2014*a*)

$$\frac{\partial u_{i_1\ldots i_n}^{\varsigma,A}}{\partial t} + \cdots = -\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right] u_{i_1\ldots i_n}^{\varsigma,A}, \tag{2.18}$$

with the same relaxation time for all of them. This could not predict the correct relaxation of the higher moments and the Prandtl number. Shakhov (1968) proposed a modified BGK model for a monatomic gases to obtain the correct $Pr$ number. Rykov (1975) introduced a model to diatomic molecules with rotational movements and Wu *et al.* (2015) extended this to polyatomic gases. Here, we introduce a generalized and modified S-model for polyatomic gases by obtaining $f_{tr}$ and $f_{int}$ which provide the correct $Pr$ number and distinct relaxation times for higher moments.

The relaxation times of the Boltzmann collision term for Maxwell molecules in the case of a monatomic gases for some higher moments are presented in table 1 (Truesdell & Muncaster 1980; Torrilhon, Au & Struchtrup 2003). The relaxation time of $\boldsymbol{u}_{ij}^{1,0}$ is close to the relaxation time of $\boldsymbol{\sigma}_{ij}$, but for other moments the differences are considerable and should not be ignored. Therefore, we obtained distribution functions, $f_{tr}$ and $f_{int}$, in order to predict distinct relaxation of these higher moments and their internal moment counterparts $\{\boldsymbol{q}_{i,tr}, \boldsymbol{q}_{i,int}, u^{2,0}, u^{1,1}\}$ by introducing four free relaxation parameters, $R_{q_{tr}}$, $R_{q_{int}}$, $R_{u^{2,0}}$ and $R_{u^{1,1}}$. The resulting relaxation time for these higher moments from our proposed model are shown in table 2 and compared with the relaxation of the BGK model. Values of these relaxation parameters will be obtained using fitting to experimental and DSMC simulation data. It should be pointed out here that two relaxation parameters, $R_{q_{tr}}$ and $R_{q_{int}}$, are analogies to the $Pr$ number (5.11). The microscopic relaxation in our model is independent of molecular velocity. In this sense the behaviour of our model is similar to the behaviour of Maxwell molecules. This basically influences the molecular velocity distribution function, but the physically meaningful moments are not influenced (Gallis & Torczynski 2011). The procedure and final form of the distribution functions are given in appendix A, along with some important features of the proposed model, e.g. recovering Maxwellian functions in equilibrium and the linear H-theorem.

| $\boldsymbol{\sigma}_{ij}$ | $q_i$ | $u^{2,0}$ | $\boldsymbol{u}^{1,0}_{ij}$ |
|---|---|---|---|
| $\tau$ | $Pr\,\tau$ | $\frac{2}{3}\tau$ | $\frac{7}{6}\tau$ |

TABLE 1. Maxwell molecule relaxation times.

| Moment | $q_{tr}$ | $q_{int}$ | $u^{2,0}$ | $u^{1,1}$ |
|---|---|---|---|---|
| Relaxation time GS model | $R_{q_{tr}}\nu$ | $R_{q_{int}}\nu$ | $R_{u^{2,0}}\nu$ | $R_{u^{1,1}}\nu$ |
| Relaxation time BGK model | $\nu$ | $\nu$ | $\nu$ | $\nu$ |

TABLE 2. Relaxation times for higher moments based on four new free parameters and comparison with the BGK model.

## 3. Moment equations

Moment methods replace the kinetic equation by a finite set of differential equations for the moments of the distribution function. Therefore, the moment equations can be used to approximately describe an ideal gas flow. Also, increasing the number of moments typically leads to a better approximation (Müller & Ruggeri 2013).

### 3.1. *General moment equation*

The moment equations are obtained by taking weighted averages of the kinetic equation. Multiplying the kinetic equation (2.15*a*) with $m(I^{2/\delta})^A C^{2\varsigma} C_{<i_1} C_{i_2} \ldots C_{i_n>}$ and subsequent integration over velocity space and the internal energy parameter gives the general moment equation as

$$\begin{aligned}
&\frac{\mathrm{D}u^{\varsigma,A}_{i_1\ldots i_n}}{\mathrm{D}t} + 2\varsigma u^{\varsigma-1,A}_{i_1\ldots i_n k}\frac{\mathrm{D}v_k}{\mathrm{D}t} + 2\varsigma u^{\varsigma-1,A}_{i_1\ldots i_n kj}\frac{\partial v_j}{\partial x_k} + \frac{n}{2n+1}2\varsigma u^{\varsigma,A}_{j<i_1\ldots i_{n-1}}\frac{\partial v_j}{\partial x_{i_n>}} \\
&\quad + \frac{\partial u^{\varsigma,A}_{i_1\ldots i_n k}}{\partial x_k} + 2\varsigma\frac{n+1}{2n+3}u^{\varsigma,A}_{<i_1\ldots i_n}\frac{\partial v_{k>}}{\partial x_k} + \frac{n}{2n+1}\frac{\partial u^{\varsigma+1,A}_{<i_1\ldots i_{n-1}}}{\partial x_{i_n>}} \\
&\quad + 2\varsigma\frac{n}{2n+1}u^{\varsigma,A}_{<i_1\ldots i_{n-1}}\frac{\mathrm{D}v_{i_n>}}{\mathrm{D}t} + \frac{n-1}{2n-1}nu^{\varsigma+1,A}_{<i_1\ldots i_{n-2}}\frac{\partial v_{i_{n-1}}}{\partial x_{i_n>}} + nu^{\varsigma,A}_{<i_1\ldots i_{n-1}}\frac{\mathrm{D}v_{i_n>}}{\mathrm{D}t} \\
&\quad + u^{\varsigma,A}_{i_1\ldots i_n}\frac{\partial v_k}{\partial x_k} + \frac{n}{2n+1}\frac{n-1}{2n-1}2\varsigma u^{\varsigma+1,A}_{<i_1\ldots i_{n-2}}\frac{\partial v_{i_{n-1}}}{\partial x_{i_n>}} + nu^{\varsigma,A}_{k<i_1\ldots i_{n-1}}\frac{\partial v_{i_n>}}{\partial x_k} \\
&= \frac{1}{\tau_{tr}}\left[u^{\varsigma,A}_{i_1\ldots i_n|E,tr} - u^{\varsigma,A}_{i_1\ldots i_n}\right] + \frac{1}{\tau_{int}}\left[u^{\varsigma,A}_{i_1\ldots i_n|E,int} - u^{\varsigma,A}_{i_1\ldots i_n}\right].
\end{aligned} \tag{3.1}$$

Here, the relation $u^{\varsigma,A}_{\langle i_1\ldots i_n\rangle k} = u^{\varsigma,A}_{i_1\ldots i_n k} + (n/(2n+1))u^{\varsigma+1,A}_{<i_1\ldots i_{n-1}}\delta_{i_n>k}$ is used (Struchtrup 2005*b*).

### 3.2. *Conservation laws*

Conservation laws for mass ($\varsigma = A = n = 0$), momentum ($\varsigma = A = 0$, $n = 1$) and the balance laws for translational ($\varsigma = 1$, $A = n = 0$) and internal ($\varsigma = 0$, $A = 1$, $n = 0$) energies are obtained from the general moment equation (3.1) as

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial v_i}{\partial x_i} = 0, \tag{3.2a}$$

$$\frac{\mathrm{D}v_i}{\mathrm{D}t}+\frac{1}{\rho}\frac{\partial \boldsymbol{\sigma}_{ij}}{\partial x_j}+\frac{\partial \theta_{tr}}{\partial x_i}+\frac{\theta_{tr}}{\rho}\frac{\partial \rho}{\partial x_i}=0, \tag{3.2b}$$

$$\frac{3}{2}\rho\frac{\mathrm{D}\theta_{tr}}{\mathrm{D}t}+\frac{\partial \boldsymbol{q}_{i,tr}}{\partial x_i}+\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}+\rho\theta_{tr}\frac{\partial v_i}{\partial x_i}=\frac{3\rho}{\tau_{int}}\frac{(\theta-\theta_{tr})}{2}, \tag{3.2c}$$

$$\rho\frac{\mathrm{D}\frac{\delta}{2}\theta_{int}}{\mathrm{D}t}+\frac{\partial \boldsymbol{q}_{i,int}}{\partial x_i}=-\frac{3\rho}{\tau_{int}}\frac{(\theta-\theta_{tr})}{2}. \tag{3.2d}$$

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

$$\rho\frac{3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\frac{\mathrm{D}\theta}{\mathrm{D}t}+\frac{\partial \boldsymbol{q}_{i,int}}{\partial x_i}+\frac{\partial \boldsymbol{q}_{i,tr}}{\partial x_i}+\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}+\rho(\theta-\Delta\theta)\frac{\partial v_i}{\partial x_i}=0. \tag{3.2e}$$

Therefore, the balance law for dynamic temperature (2.13) is obtained as

$$\rho\frac{\mathrm{D}\Delta\theta}{\mathrm{D}t}+\frac{2}{3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}\frac{\partial \boldsymbol{q}_{i,int}}{\partial x_i}-\frac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\frac{\partial \boldsymbol{q}_{i,tr}}{\partial x_i}-\frac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}$$
$$-\frac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\rho(\theta-\Delta\theta)\frac{\partial v_i}{\partial x_i}=-\frac{\rho}{\tau_{int}}\Delta\theta. \tag{3.2f}$$

### 3.3. *Balance laws*

Moment equations for stress tensor, $\boldsymbol{\sigma}_{ij}=\boldsymbol{u}^{0,0}_{ij}$, translational heat flux, $\boldsymbol{q}_{i,tr}=(1/2)u^{1,0}_i$ and internal heat flux, $u^{0,1}_i=\boldsymbol{q}_{i,int}$, which are present in the conservation laws, are obtained from the general moment equation (3.1) as

$$\frac{\mathrm{D}\boldsymbol{\sigma}_{ij}}{\mathrm{D}t}+\frac{\partial \boldsymbol{u}^{0,0}_{ijk}}{\partial x_k}+\frac{4}{5}\frac{\partial q_{<i,tr}}{\partial x_{j>}}+2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}$$
$$+2\rho[\theta-\Delta\theta]\frac{\partial v_{<i}}{\partial x_{j>}}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\sigma_{ij}, \tag{3.3a}$$

$$\frac{\mathrm{D}\boldsymbol{q}_{i,tr}}{\mathrm{D}t}-\frac{5}{2}[\theta-\Delta\theta]\left[\frac{\partial \boldsymbol{\sigma}_{ij}}{\partial x_j}+\rho\frac{\partial\theta}{\partial x_i}-\rho\frac{\partial\Delta\theta}{\partial x_i}\right]$$
$$+\sigma_{ik}\left[\frac{\partial\Delta\theta}{\partial x_k}-\frac{\partial\theta}{\partial x_k}-[\theta-\Delta\theta]\frac{\partial\ln\rho}{\partial x_k}-\frac{1}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right]$$
$$+\frac{1}{2}\frac{\partial u^{1,0}_{ik}}{\partial x_k}+\frac{1}{6}\frac{\partial u^{2,0}}{\partial x_i}+\boldsymbol{u}^{0,0}_{ijk}\frac{\partial v_j}{\partial x_k}+\frac{7}{5}\boldsymbol{q}_{i,tr}\frac{\partial v_k}{\partial x_k}+\frac{7}{5}q_{k,tr}\frac{\partial v_i}{\partial x_k}$$
$$+\frac{2}{5}q_{j,tr}\frac{\partial v_j}{\partial x_i}-\frac{5}{2}[\theta^2-2\theta\Delta\theta+\Delta\theta^2]\frac{\partial\rho}{\partial x_i}=-R_{q_{tr}}\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\boldsymbol{q}_{i,tr}, \tag{3.3b}$$

$$\frac{\mathrm{D}\boldsymbol{q}_{i,int}}{\mathrm{D}t}-\frac{\delta\theta+3\Delta\theta}{2}\left[\frac{\partial\boldsymbol{\sigma}_{ij}}{\partial x_j}+\rho\frac{\partial\theta}{\partial x_i}-\rho\frac{\partial\Delta\theta}{\partial x_i}+\rho[\theta-\Delta\theta]\frac{\partial\ln\rho}{\partial x_i}\right]+\frac{\partial u^{0,1}_{ik}}{\partial x_k}$$
$$+\frac{1}{3}\frac{\partial u^{1,1}}{\partial x_i}+q_{k,int}\frac{\partial v_i}{\partial x_k}+\boldsymbol{q}_{i,int}\frac{\partial v_k}{\partial x_k}=-R_{q_{int}}\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\boldsymbol{q}_{i,int}. \tag{3.3c}$$

These equations contain the higher moments $\boldsymbol{u}_{ij}^{1,0}$, $u^{2,0}$, $\boldsymbol{u}_{ijk}^{0,0}$, $\boldsymbol{u}_{ij}^{0,1}$ and $u^{1,1}$, for which full moment equations are obtained from (3.1) with the appropriate choices for $\varsigma$ and $A$. Choosing all moments mentioned so far as variables will construct a set of equations for 36 moments listed in (2.14).

Set of 36 moments equations contain higher moments, $\{\boldsymbol{u}_{ijk}^{1,0}, u_i^{2,0}, u_{ijkl}^{0,0}, \boldsymbol{u}_{ijk}^{0,1}, u_i^{1,1}\}$, under the space derivatives. We need constitutive equations for these higher moments to close the system of equations with only 36 variables. The generalized Grad's distribution function (B 1) for polyatomic gases (see appendix B) is used to obtain constitutive equations as

$$\left.\begin{aligned} \boldsymbol{u}_{ijk}^{1,0} &= 9\theta \boldsymbol{u}_{ijk}^{0,0}, \quad u_i^{2,0} = 28\theta \boldsymbol{q}_{i,tr}, \quad u_{ijkl}^{0,0} = 0, \\ \boldsymbol{u}_{ijk}^{0,1} &= \frac{\delta}{2}\theta \boldsymbol{u}_{ijk}^{0,0}, \quad u_i^{1,1} = (5\boldsymbol{q}_{i,int} + \delta \boldsymbol{q}_{i,tr})\theta. \end{aligned}\right\} \tag{3.4}$$

Substituting these equations into the balance laws for the moments $\boldsymbol{u}_{ij}^{1,0}$, $u^{2,0}$, $\boldsymbol{u}_{ijk}^{0,0}$, $\boldsymbol{u}_{ij}^{0,1}$ and $u^{1,1}$, results in

$$\begin{aligned} &\frac{\mathrm{D}\boldsymbol{u}_{ij}^{1,0}}{\mathrm{D}t} - \boldsymbol{u}_{ijk}^{0,0} 2\,[\theta - \Delta\theta]\,\frac{\partial \ln \rho}{\partial x_k} - \frac{28}{5}\,[\theta - \Delta\theta]\,q_{<i,tr}\frac{\partial \ln \rho}{\partial x_{j>}} \\ &\quad + 7\boldsymbol{u}_{ijk}^{0,0}\frac{\partial \theta}{\partial x_k} + 2\boldsymbol{u}_{ijk}^{0,0}\frac{\partial \Delta\theta}{\partial x_k} + \frac{28}{5}q_{<i,tr}\frac{\partial \theta}{\partial x_{j>}} \\ &\quad + \frac{28}{5}q_{<i,tr}\frac{\partial \Delta\theta}{\partial x_{j>}} + 9\theta\frac{\partial \boldsymbol{u}_{ijk}^{0,0}}{\partial x_k} + \frac{2}{5}28\theta\frac{\partial q_{<i,tr}}{\partial x_{j>}} + \frac{6}{7}u_{<ij}^{1,0}\frac{\partial v_{k>}}{\partial x_k} \\ &\quad + \frac{4}{5}u_{j<i}^{1,0}\frac{\partial v_j}{\partial x_{j>}} + 2u_{k<i}^{1,0}\frac{\partial v_{j>}}{\partial x_k} + \boldsymbol{u}_{ij}^{1,0}\frac{\partial v_k}{\partial x_k} + \frac{14}{15}u^{2,0}\frac{\partial v_{<i}}{\partial x_{j>}} \\ &\quad - 2\frac{1}{\rho}\boldsymbol{u}_{ijk}^{0,0}\frac{\partial \sigma_{kl}}{\partial x_l} - \frac{28}{5}\frac{1}{\rho}q_{<i,tr}\frac{\partial \sigma_{j>l}}{\partial x_l} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\boldsymbol{u}_{ij}^{1,0}, \end{aligned} \tag{3.5a}$$

$$\begin{aligned} &\frac{\mathrm{D}u^{2,0}}{\mathrm{D}t} - 8q_{k,tr}[\theta - \Delta\theta]\frac{\partial \ln \rho}{\partial x_k} + 28\theta\frac{\partial q_{k,tr}}{\partial x_k} - 8\frac{q_{k,tr}}{\rho}\frac{\partial \sigma_{kj}}{\partial x_j} \\ &\quad + 20q_{k,tr}\frac{\partial \theta}{\partial x_k} + 8q_{k,tr}\frac{\partial \Delta\theta}{\partial x_k} + 4u_{kj}^{1,0}\frac{\partial v_j}{\partial x_k} + \frac{7}{3}u^{2,0}\frac{\partial v_k}{\partial x_k} \\ &= \frac{R_{u^{2,0}}}{\tau_{tr}}[(15\rho[\theta^2 - 2\theta\Delta\theta + \Delta\theta^2]) - u^{2,0}] + \frac{R_{u^{2,0}}}{\tau_{int}}[(15\rho\theta^2) - u^{2,0}], \end{aligned} \tag{3.5b}$$

$$\begin{aligned} &\frac{\mathrm{D}\boldsymbol{u}_{ijk}^{0,0}}{\mathrm{D}t} - 3\frac{\sigma_{<ij}}{\rho}\frac{\partial \sigma_{k>l}}{\partial x_l} + \frac{3}{7}\frac{\partial u_{<ij}^{1,0}}{\partial x_{k>}} - 3\sigma_{<ij}\frac{\partial \theta}{\partial x_{k>}} \\ &\quad - 3[\theta - \Delta\theta]\sigma_{<ij}\frac{\partial \ln \rho}{\partial x_{k>}} + 3\sigma_{<ij}\frac{\partial \Delta\theta}{\partial x_{k>}} + 3u_{l<ij}^{0,0}\frac{\partial v_{k>}}{\partial x_l} \\ &\quad + \boldsymbol{u}_{ijk}^{0,0}\frac{\partial v_l}{\partial x_l} + \frac{12}{5}q_{<i,tr}\frac{\partial v_j}{\partial x_{k>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\boldsymbol{u}_{ijk}^{0,0}, \end{aligned} \tag{3.5c}$$

$$\frac{\mathrm{D}\boldsymbol{u}_{ij}^{0,1}}{\mathrm{D}t} - 2q_{<i,int}\frac{1}{\rho}\frac{\partial \sigma_{j>k}}{\partial x_k} - 2\frac{[\theta - \Delta\theta]}{\rho}q_{<i,int}\frac{\partial \rho}{\partial x_{ij>}} + \frac{\delta}{2}\theta\frac{\partial \boldsymbol{u}_{ijk}^{0,0}}{\partial x_k}$$

$$+\boldsymbol{u}_{ijk}^{0,0}\frac{\theta}{2}\frac{\partial\delta}{\partial x_k}+\frac{\delta}{2}\boldsymbol{u}_{ijk}^{0,0}\frac{\partial\theta}{\partial x_k}+\frac{2\delta}{5}q_{<i,tr}\frac{\partial\theta}{\partial x_{j>}}+2q_{<i,int}\frac{\partial\Delta\theta}{\partial x_{j>}}$$
$$+2\theta\frac{\partial q_{<i,int}}{\partial x_{j>}}+\frac{2\delta}{5}\theta\frac{\partial q_{<i,tr}}{\partial x_{j>}}+\frac{2}{5}\theta q_{<i,tr}\frac{\partial\delta}{\partial x_{j>}}+2u_{k<i}^{0,1}\frac{\partial v_{j>}}{\partial x_k}$$
$$+\boldsymbol{u}_{ij}^{0,1}\frac{\partial v_k}{\partial x_k}+\frac{2}{3}u^{1,1}\frac{\partial v_{<i}}{\partial x_{j>}}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\boldsymbol{u}_{ij}^{0,1},\tag{3.5d}$$

$$\frac{\mathrm{D}u^{1,1}}{\mathrm{D}t}-2\frac{q_{k,int}}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}-2q_{k,int}[\theta-\Delta\theta]\frac{\partial\ln\rho}{\partial x_k}+2q_{k,int}\frac{\partial\Delta\theta}{\partial x_k}$$
$$+(3q_{k,int}+\delta q_{k,tr})\frac{\partial\theta}{\partial x_k}+5\theta\frac{\partial q_{k,int}}{\partial x_k}+\delta\theta\frac{\partial q_{k,tr}}{\partial x_k}$$
$$+\theta q_{k,tr}\frac{\partial\delta}{\partial x_k}+2u_{kj}^{0,1}\frac{\partial v_j}{\partial x_k}+\frac{5}{3}u^{1,1}\frac{\partial v_k}{\partial x_k}$$
$$=\frac{R_{u^{1,1}}}{\tau_{tr}}\left[3\rho\left[\frac{\delta}{2}\theta+\frac{3}{2}\Delta\theta\right][\theta-\Delta\theta]-u^{1,1}\right]+\frac{R_{u^{1,1}}}{\tau_{int}}\left[\left(3\frac{\delta}{2}\rho\theta^2\right)-u^{1,1}\right].\tag{3.5e}$$

These balance laws, along with the conservation laws (3.2*f*), form a closed set of 36 equations associated with the variables listed in (2.14).

Applying the order of magnitude method to this set of 36 moment equations will ensure that the minimum number of moments with optimized definitions are used for any wanted order of accuracy in terms of the powers of the Knudsen numbers. This method, in the first step, applies the CE expansion on the moment equations to find their leading-order terms. Then, new moment definitions 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 CE expansion is carried out and new optimized moment definitions are obtained in the next section.

## 4. Optimizing moment definitions

For the proposed polyatomic kinetic model (2.15*a*), we have two different relaxation times corresponding to two different mean free paths and two distinct Knudsen numbers, $Kn_{tr}=\tau_{tr}/\tau_0$ and $Kn_{int}=\tau_{int}/\tau_0$. The expansion parameter in the CE method is the Knudsen number, of which we have two, $Kn_{tr}$ and $Kn_{int}$, to account for translational and internal energy exchange. $Kn_{tr}$ should be less than $Kn_{int}$, 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 $\varepsilon$ as

$$Kn_{tr}=\epsilon\quad\text{and}\quad Kn_{int}=\epsilon^{\alpha}.\tag{4.1a,b}$$

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 given by $\alpha=1$ and the upper limit is reached when $\alpha=0$. While the ratio of relaxation times $\tau_{tr}/\tau_{int}$ depends on the state of the gas, the ratio $\tau_{tr}/\tau_0=\epsilon=Kn_{tr}$ depends on the relevant macroscopic time scale $\tau_0$. Accordingly, the values of both $\alpha$ and $\epsilon=Kn_{tr}$ depend on the chosen scale. We (Rahimi & Struchtrup 2014*a*) show that usually small values of $\alpha$ are relevant and here we only consider $\alpha<0.25$.

The CE 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 $Kn_{int}^2 \simeq Kn_{tr}$, proper accounting to first order in $Kn_{tr}$ might require consideration of different orders in the CE expansion: expansion to first order in $Kn_{tr}$, but to second order in $Kn_{int}$. The conserved variables, density, velocity and total temperature, have equilibrium values and hence are at zero order. The remaining variables in the list of (2.14) are expanded in the smallness parameter $\epsilon$, where we account series in $\epsilon$ and $\epsilon^\alpha$ as

$$\begin{aligned}\psi \;=\; & \epsilon^{0\alpha}[\epsilon^0\psi^{(0,0)} + \epsilon^1\psi^{(0,1)} + \epsilon^2\psi^{(0,2)} + \epsilon^3\psi^{(0,3)} + \cdots] \\ & + \epsilon^{1\alpha}[\epsilon^0\psi^{(1,0)} + \epsilon^1\psi^{(1,1)} + \epsilon^2\psi^{(1,2)} + \cdots] + \epsilon^{2\alpha}[\epsilon^0\psi^{(2,0)} + \epsilon^1\psi^{(2,1)} + \cdots] + \cdots,\end{aligned} \tag{4.2}$$

where, $\psi^{(a,b)}$ is the moment expansion coefficient at order $\epsilon^{a\alpha+b}$.

The leading-order terms of the moments are found as the first non-vanishing term in their expansion; we find

$$O(\epsilon^0): \quad u^{2,0(0,0)} = 15\rho\theta^2, \tag{4.3a}$$

$$O(\epsilon^0): \quad u^{1,1(0,0)} = \frac{3\delta}{2}\rho\theta^2, \tag{4.3b}$$

$$O(\epsilon^\alpha): \quad \Delta\theta^{(1,0)} = \tau_{int}\frac{2\left(\delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3 + \delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\theta\frac{\partial v_i}{\partial x_i}, \tag{4.3c}$$

$$O(\epsilon^1): \quad \boldsymbol{q}_{i,tr}^{(0,1)} = -\frac{\tau_{tr}}{R_{q_{tr}}}\frac{5}{2}\rho\theta\frac{\partial\theta}{\partial x_i}, \tag{4.3d}$$

$$O(\epsilon^1): \quad \boldsymbol{u}_{ij}^{1,0(0,1)} = -\tau_{tr}14\rho\theta^2\frac{\partial v_{<i}}{\partial x_{j>}}, \tag{4.3e}$$

$$O(\epsilon^1): \quad \boldsymbol{u}_{ij}^{0,1(0,1)} = -\tau_{tr}\delta\rho\theta^2\frac{\partial v_{<i}}{\partial x_{j>}}, \tag{4.3f}$$

$$O(\epsilon^1): \quad \boldsymbol{\sigma}_{ij}^{(0,1)} = -\tau_{tr}2\rho\theta\frac{\partial v_{<i}}{\partial x_{j>}}, \tag{4.3g}$$

$$O(\epsilon^1): \quad \boldsymbol{q}_{i,int}^{(0,1)} = -\frac{\tau_{tr}}{R_{q_{int}}}\frac{\left(\delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{2}\rho\theta\frac{\partial\theta}{\partial x_i}, \tag{4.3h}$$

$$O(\epsilon^2): \quad \boldsymbol{u}_{ijk}^{0,0(0,2)} = -\tau_{tr}\left(\frac{3}{7}\frac{\partial u_{<ij}^{1,0}}{\partial x_{k>}} - 3\sigma_{<ij}\frac{\partial\theta}{\partial x_{k>}} - 3\theta\sigma_{<ij}\frac{\partial\ln\rho}{\partial x_{k>}} + \frac{12}{5}q_{<i,tr}\frac{\partial v_j}{\partial x_{k>}}\right). \tag{4.3i}$$

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, $\boldsymbol{q}_{i,tr}^{(0,1)}$ and $\boldsymbol{q}_{i,int}^{(0,1)}$, are proportional to each other, and also the three tensorial moments, $\boldsymbol{\sigma}_{ij}^{(0,1)}$, $\boldsymbol{u}_{ij}^{0,1(0,1)}$ and $\boldsymbol{u}_{ij}^{1,0(0,1)}$, 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 (4.3) to define new variables at higher orders as

$$w^{2,0} \;=\; u^{2,0} - 15\rho\theta^2, \tag{4.4a}$$

$$w^{1,1} = u^{1,1} - \tfrac{3}{2}\delta\rho\theta^2. \tag{4.4b}$$

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

The linear dependent vectors $\boldsymbol{q}_{i,tr}$ and $\boldsymbol{q}_{i,int}$, which are of first order, can be combined into one first-order vector, the total heat flux,

$$q_i = \boldsymbol{q}_{i,tr} + \boldsymbol{q}_{i,int}, \tag{4.5a}$$

and one unique higher-order variable, the heat flux difference, which is defined by subtracting leading-order terms (4.3) to cancel them in the new variable as

$$\Delta q_i = \boldsymbol{q}_{i,tr} - \frac{5R_{q_{int}}}{\left(\delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\boldsymbol{q}_{i,int}. \tag{4.5b}$$

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

$$\boldsymbol{u}_{ij}^{-} = \boldsymbol{u}_{ij}^{1,0} - \frac{14}{\delta}\boldsymbol{u}_{ij}^{0,1}, \tag{4.6a}$$

$$\boldsymbol{u}_{ij}^{+} = \boldsymbol{u}_{ij}^{1,0} + \boldsymbol{u}_{ij}^{0,1} - \frac{(14+\delta)}{2}\theta\boldsymbol{\sigma}_{ij}. \tag{4.6b}$$

The second-order moment $\boldsymbol{u}_{ijk}^{0,0}$ is the only three-tensor in the equations and thus remains unchanged.

Equations for the new moments are obtained based on their definitions and a linear combination of the primary moment equations. The above procedure:

(i) applying CE expansion on the moment equations;
(ii) obtaining leading-order term of moments;
(iii) defining new optimized linearly independent moments from linearly dependent moments;

is repeated until full linearly independent moments are achieved. At the end, we have defined four new moments as,

$$B_{ij}^{-} = \boldsymbol{u}_{ij}^{+} - \frac{11}{14}\frac{\delta}{\delta+3}\boldsymbol{u}_{ij}^{-}, \tag{4.7a}$$

$$B_{ij}^{+} = \boldsymbol{u}_{ij}^{+} + \boldsymbol{u}_{ij}^{-}, \tag{4.7b}$$

$$B^{+} = w^{1,1} - w^{2,0} - \left(\tfrac{3}{2}[3-\delta] + 30\right)\rho\theta\Delta\theta, \tag{4.7c}$$

$$B^{-} = w^{1,1} + \tfrac{3}{10}w^{2,0} + \left(9 - \tfrac{3}{2}[3-\delta]\right)\rho\theta\Delta\theta. \tag{4.7d}$$

Therefore, we have the final set of 36 optimized moments at different orders as

$$O(\epsilon^0): \quad \rho,\, v_i,\, \theta, \tag{4.8a}$$

$$O(\epsilon^{\alpha}): \quad \Delta\theta, \tag{4.8b}$$

$$O(\epsilon^{2\alpha}): \quad B^{+}, \tag{4.8c}$$

$$O(\epsilon^{1}): \quad \boldsymbol{\sigma}_{ij},\, q_i,\, B^{-}, \tag{4.8d}$$

$$O(\epsilon^{1+\alpha}): \quad \Delta q_i,\, B_{ij}^{+}, \tag{4.8e}$$

$$O(\epsilon^{2}): \quad B_{ij}^{-},\, \boldsymbol{u}_{ijk}^{0,0}. \tag{4.8f}$$

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

## 5. Model reduction

The explicit orders will now be used for model reduction such that in each order under consideration, only terms up to the corresponding power of $\epsilon$ are kept while all other terms can be ignored. We require the explicit order of all terms to be clearly visible in the equations, hence the orders are made explicit with power of $\epsilon$ and $\epsilon^\alpha$. In the next section, $\epsilon$ will be substituted by 1 so that the original form of equations is recovered. The introduced notation allows us to arrange all terms by their explicit $\epsilon$ orders.

The scaled conservation laws for mass, momentum and energy read

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial v_i}{\partial x_i} = 0, \tag{5.1a}$$

$$\frac{\mathrm{D}v_i}{\mathrm{D}t} + \theta\frac{\partial \ln\rho}{\partial x_i} + \frac{\partial\theta}{\partial x_i} - \epsilon^\alpha\left[\frac{\partial\Delta\theta}{\partial x_i} + \Delta\theta\frac{\partial\ln\rho}{\partial x_i}\right] + \epsilon^1\left[\frac{1}{\rho}\frac{\partial\boldsymbol{\sigma}_{ij}}{\partial x_j}\right] = 0, \tag{5.1b}$$

$$\frac{3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\rho\frac{\mathrm{D}\theta}{\mathrm{D}t} + \rho\theta\frac{\partial v_i}{\partial x_i} - \epsilon^\alpha\left[\rho\Delta\theta\frac{\partial v_i}{\partial x_i}\right] + \epsilon^1\left[\frac{\partial q_i}{\partial x_i} + \boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}\right] = 0. \tag{5.1c}$$

The remaining scaled equations are presented in appendix C. While the expansion series (4.2) contains all mixed powers of $\epsilon$ and $\epsilon^\alpha$, the final equations only contain some terms. We are interested in terms up to $\epsilon^3$, and find only sets of equations at the following powers:

$$\{\epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \epsilon^{1+2\alpha}, \epsilon^{1+3\alpha}, \epsilon^{2-\alpha}, \epsilon^2, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^{2+3\alpha}, \epsilon^{2+4\alpha}, \epsilon^3\}. \tag{5.2}$$

### 5.1. *A recipe for choosing the set of equations*

The relaxation of the internal DoF 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. In order to decide which set of equations we need to consider for a particular problem, the relaxation times, their ratios and characteristic time or length scale 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 $Kn_{tr}$ is rather small while $Kn_{int}$ is relatively large, one will choose a model with high power in $\epsilon^\alpha$ and low power in $\epsilon$; these are models with internal corrections to the NSF equations. On the other hand, if both Knudsen numbers are small, one can use a lower accuracy model, like the refined NSF equations. In problems when both Knudsen numbers are large, particularly for order-unity values of $Kn_{tr}$, a higher order of accuracy is an essential choice, e.g. one would choose the third-order R19 equations.

The following sections will discuss different sets of equations based on the desired order of accuracy in the powers of $\epsilon$. For this, we will consider the increasing orders as laid out in (5.2) up to third order, but only present four main cases, $\epsilon^0$, $\epsilon^1$, $\epsilon^2$ and $\epsilon^3$.

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

We begin the reduction process with considering only the zeroth-order terms in the conservation laws,

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial v_i}{\partial x_i} = 0, \tag{5.3a}$$

$$\frac{\mathrm{D}v_i}{\mathrm{D}t} + \theta \frac{\partial \ln \rho}{\partial x_i} + \frac{\partial \theta}{\partial x_i} = 0, \tag{5.3b}$$

$$\frac{3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\rho\frac{\mathrm{D}\theta}{\mathrm{D}t} + \rho\theta\frac{\partial v_i}{\partial x_i} = 0. \tag{5.3c}$$

These equations form a closed set of equations for the variables $\{\rho, v_i, \theta\}$, the Euler equations for polyatomic gases, with specific heat given in (2.10).

### 5.3. *Order $\epsilon^1$: Refined Navier–Stokes–Fourier equations*

For the first order, terms up to $\epsilon^1$ order must be considered in the conservation laws. Hence, now all terms are relevant in the conservation laws,

$$\left.\begin{aligned} \frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial v_i}{\partial x_i} = 0, \\ \rho\frac{\mathrm{D}v_i}{\mathrm{D}t} + \frac{\partial \rho(\theta-\Delta\theta)}{\partial x_i} + \frac{\partial \boldsymbol{\sigma}_{ij}}{\partial x_j} = 0, \\ \frac{3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\rho\frac{\mathrm{D}\theta}{\mathrm{D}t} + \frac{\partial q_i}{\partial x_i} + \rho(\theta-\Delta\theta)\frac{\partial v_i}{\partial x_i} + \boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i} = 0. \end{aligned}\right\} \tag{5.4}$$

These equations must be furnished with equations for $\Delta\theta$, $\boldsymbol{\sigma}_{ij}$, $q_i$ at the required order. To first order, the balance law for $\Delta\theta$, which is at order $\epsilon^\alpha$, with terms up to order $\epsilon^{1-\alpha}$ must be considered as

$$\rho\frac{\mathrm{D}\Delta\theta}{\mathrm{D}t} + \frac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\rho\,(\Delta\theta-\theta)\,\frac{\partial v_i}{\partial x_i} = -\frac{\rho}{\tau_{int}}\Delta\theta, \tag{5.5}$$

while the leading terms for stress tensor and total heat flux are obtained from (C 1*b*) and (C 1*c*) as

$$\left.\begin{aligned} \boldsymbol{\sigma}_{ij} &= -\tau_{tr} 2\rho\theta\frac{\partial v_{<i}}{\partial x_{j>}}, \\ q_i &= -\tau_{tr}\frac{5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}\rho\theta\frac{\partial\theta}{\partial x_i}. \end{aligned}\right\} \tag{5.6}$$

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, (Kremer 2010; Arima *et al.* 2012), $\Pi = -\rho\Delta\theta$.

These first-order equations for $\boldsymbol{\sigma}_{ij}$ and $q_i$ are the classical 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 $\kappa$ which we identify as

$$\mu = \tau_{tr}\rho\theta \quad \text{and} \quad \kappa = \tau_{tr}\frac{5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}\rho\theta. \tag{5.7a,b}$$

We have internal DoF corrections to the (5.6) by considering order-$\epsilon^{\alpha}$ terms from (C 1*b*) and (C 1*c*), which results in corrected shear viscosity and heat conductivity as,

$$\mu = \tau_{tr}\rho(\theta - \Delta\theta) \quad \text{and} \quad \kappa = \tau_{tr}\frac{5R_{q_{int}} + \left(\delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}\rho(\theta - \Delta\theta). \tag{5.8a,b}$$

The obtained relation between relaxation time and the shear viscosity is identical to that for a monatomic gas. Internal DoF affect the heat conductivity, which differs from the monatomic gas as extra means of energy transport (internal DoF) are present in polyatomic gases. Therefore, the heat conductivity (5.8) consists of two parts based on (4.3*d*) and (4.3*h*) as,

$$\kappa_{tr} = \tau_{tr}\frac{5}{2R_{q_{tr}}}\rho(\theta - \Delta\theta), \tag{5.9a}$$

$$\kappa_{int} = \tau_{tr}\frac{\left(\delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{2R_{q_{int}}}\rho(\theta - \Delta\theta). \tag{5.9b}$$

In the classical Navier–Stokes equations, the dynamic pressure has the form $\Pi = -\nu(\partial v_i/\partial x_i)$ where $\nu$ is the bulk viscosity. Comparing with the above, we identify a relation between relaxation time $\tau_{int}$ and the bulk viscosity,

$$\upsilon = \tau_{int}\frac{2\left(\delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3 + \delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\rho(\theta - \Delta\theta). \tag{5.10}$$

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

Experimental data of viscosities and specific heat (Poling *et al.* 2001; Borgnakke & Sonntag 2009; Cramer 2012) will be used to obtain the temperature-dependent relaxation times, $\tau_{tr}$ and $\tau_{int}$, using (5.10) and (5.8).

The Prandtl number is defined as the dimensionless ratio of specific heat and shear viscosity over heat conductivity (Struchtrup 2005*b*),

$$Pr = \frac{5 + \delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\frac{\mu}{k}. \tag{5.11}$$

This is a measure of the importance of momentum over thermal diffusivity. Based on the obtained shear viscosity and heat conductivity definitions (5.8), the Prandtl number is

$$Pr = \frac{\left(5 + \delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{int}}R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}. \tag{5.12}$$

The values of the modelling parameters $R_{q_{int}}$ and $R_{q_{tr}}$ are restricted by the Prandtl number and one of them depends on the other one through the $Pr$ number. Viscosity and heat conductivity values could be used to determine the heat fluxes relaxation parameters. Therefore, the model provides the freedom to fit two parameters ($R_{u^{2,0}}$ and $R_{u^{1,1}}$). These values can be found from fitting to experimental or DSMC simulation

data for rarefied flows, such as heat conduction, damping of ultrasound, light scattering experiments or shockwave structure.

What we have obtained here at first order are not the classical NSF equations, since we have to use the full balance law (5.5) for $\Delta\theta$ (or dynamic pressure). The classical NSF equations constitute a five variables model for $\{\rho, v_i, \theta\}$, while, the refined NSF (RNSF) equations obtained have six independent field variables, $\{\rho, v_i, \theta, \Delta\theta\}$.

### 5.4. *Order $\epsilon^2$: refined Grad's 14 moment equations*

The relevant equations at the second order of accuracy are the conservation laws (5.4) and the dynamic temperature equation with additional terms up to order $\epsilon^{2-\alpha}$,

$$\rho\frac{\mathrm{D}\Delta\theta}{\mathrm{D}t}+\frac{2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\rho\Delta\theta\frac{\partial v_i}{\partial x_i}+\frac{2}{3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}}\frac{\partial q_i}{\partial x_i}-\frac{2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\rho\theta\frac{\partial v_i}{\partial x_i}$$
$$-\frac{2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}-\frac{10R_{q_{int}}}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}$$
$$\times\left[\frac{\partial q_i}{\partial x_i}+\frac{R_{q_{tr}}\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\left(\Delta q_i\frac{\partial\theta}{\partial x_i}-q_i\frac{\partial\theta}{\partial x_i}\right)\right]$$
$$-\frac{2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_i}{\partial x_i}=-\frac{\rho}{\tau_{int}}\Delta\theta. \tag{5.13}$$

For the second order of accuracy, the balance laws for stress and heat flux must be considered up to first order, because the variables, $\boldsymbol{\sigma}_{ij}$ and $q_i$, are at first order, see (4.8). From (C 1*b*) and (C 1*c*) with terms up to order $\epsilon^1$, we have second-order equations as

$$\frac{\mathrm{D}\boldsymbol{\sigma}_{ij}}{\mathrm{D}t}+\frac{4R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\frac{\partial q_{<i}}{\partial x_{j>}}-\frac{4R_{q_{int}}R_{q_{tr}}\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}q_{<i}\frac{\partial\theta}{\partial x_{j>}}$$
$$+2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}+2\rho(\theta-\Delta\theta)\frac{\partial v_{<i}}{\partial x_{j>}}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\boldsymbol{\sigma}_{ij}, \tag{5.14}$$

$$\frac{\mathrm{D}q_i}{\mathrm{D}t}+\sigma_{ik}\left[\frac{5+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\frac{\partial\theta}{\partial x_k}-\theta\frac{\partial\ln\rho}{\partial x_k}\right]-\frac{2}{39}\frac{\partial B^+}{\partial x_i}+\frac{5}{13}\frac{\partial B^-}{\partial x_i}$$
$$+\left(1+\frac{2R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\left[q_k\frac{\partial v_i}{\partial x_k}+q_i\frac{\partial v_k}{\partial x_k}\right]$$

$$+\frac{2R_{q_{int}}q_k}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\frac{\partial v_k}{\partial x_i}-\Delta\theta^2\frac{\partial\rho}{\partial x_i}+\theta\frac{\partial\sigma_{ik}}{\partial x_k}$$

$$-\rho(\theta+\Delta\theta)\frac{\partial\Delta\theta}{\partial x_i}+\frac{5+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\rho(\theta-\Delta\theta)\frac{\partial\theta}{\partial x_i}$$

$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}q_i+\frac{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\Delta q_i\right). \tag{5.15}$$

For closing the set of equations we need constitutive equations for $B^+$ and $\Delta q_i$ up to order $\epsilon^{1-2\alpha}$ from (C 2*b*) and (C 1*d*), as

$$B^+=-\frac{39}{2}\rho\Delta\theta^2+\frac{3\tau_{tr}}{\tau_{int}}\left[\frac{10}{R_{u^{2,0}}}+\frac{3-\delta}{2R_{u^{1,1}}}-\frac{23-\delta}{2}\right]\rho\theta\Delta\theta, \tag{5.16}$$

$$\begin{aligned}\Delta q_i=&\frac{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5R_{q_{int}}^2+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}^2}\frac{5}{2}\tau_{tr}\left[\left(1+\frac{3R_{q_{int}}}{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\right.\\&\times\left(\rho\left(\theta+\Delta\theta\right)\frac{\partial\Delta\theta}{\partial x_i}+\Delta\theta^2\frac{\partial\rho}{\partial x_i}+\frac{2}{39}\frac{\partial B^+}{\partial x_i}\right)\\&\left.+\frac{\left(R_{q_{int}}-R_{q_{tr}}\right)}{R_{q_{tr}}}\rho\left(\theta+\Delta\theta\right)\frac{\partial\theta}{\partial x_i}\right]-\frac{\left[1+\frac{\tau_{tr}}{\tau_{int}}\right]5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}^2+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}^2}q_i,\end{aligned} \tag{5.17}$$

and for $B^-$ at leading order from (C 2*a*) as,

$$B^-=-\frac{3\tau_{tr}}{\tau_{int}}\left[\frac{3}{R_{u^{2,0}}}-\frac{3-\delta}{2R_{u^{1,1}}}-\frac{3+\delta}{2}\right]\rho\theta\Delta\theta. \tag{5.18}$$

With balance laws for stress and heat flux, the second-order equations form a set of PDEs for the 14 variables $\{\rho, v_i, \theta, \Delta\theta, \boldsymbol{\sigma}_{ij}, q_i\}$. Other authors discuss a 14 moment set for polyatomic gases, (Ruggeri & Sugiyama 2015) 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 terms in the equations for overall heat flux (C 1*c*) and the dynamic temperature (5.13) containing $B^+$, $\Delta q_i$ and $B^-$ along with their constitutive equations, (5.16)–(5.18). Therefore, the proposed model is not a second-order accurate model. Also, the mentioned 14 field theory (Ruggeri & Sugiyama 2015) contains three nonlinear terms from (C 1*c*), 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.

The leading-order term of $\Delta q_i$ at order $\epsilon^{1+\alpha}$ from (C 1*d*) and (C 1*c*) is obtained as

$$\Delta q_i = \tau_{tr} \frac{5\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}} \rho\theta \frac{\partial \Delta\theta}{\partial x_i}. \tag{5.19}$$

We name the factor relating the heat flux difference and the gradient of dynamic temperature the dynamic heat conductivity,

$$\kappa_\Delta = \tau_{tr} \frac{5\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}} \rho\theta. \tag{5.20}$$

### 5.5. *Order $\epsilon^3$: regularized 19 (R19) equations*

Finally, we present the equations at third order of accuracy, which are: the conservation laws (5.4); the full equation for the dynamic temperature (5.13); the equation for heat flux difference with terms up to order $\epsilon^{2-2\alpha}$, due to the fact that $\Delta q_i$ is at order $\epsilon^{1+\alpha}$ and first appears in the $\Delta\theta$ equation (5.13) which itself is at order $\epsilon^{\alpha}$,

$$\begin{aligned}
&\frac{\mathrm{D}\Delta q_i}{\mathrm{D}t} + \sigma_{ik}\left[\frac{\partial\Delta\theta}{\partial x_k} + \Delta\theta\frac{\partial \ln\rho}{\partial x_k}\right] \\
&\quad + \frac{10R_{q_{int}}\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)(\Delta\theta-\theta)(\Delta q_i - q_i)}{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{\partial v_k}{\partial x_k} \\
&\quad + \frac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\Delta q_j}{5\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{\partial v_j}{\partial x_i} + \frac{\delta}{(42+25\delta)}\left(7+\frac{15R_{q_{int}}}{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\frac{\partial B_{ij}^{+}}{\partial x_j} \\
&\quad + \left(\frac{25R_{q_{int}}+7\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\right)\left(\Delta q_i\frac{\partial v_k}{\partial x_k}+\Delta q_k\frac{\partial v_i}{\partial x_k}\right) \\
&\quad + \frac{42}{(42+25\delta)^2}\left(7+\frac{15R_{q_{int}}}{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\frac{\mathrm{d}\delta}{\mathrm{d}\theta}B_{ij}^{+}\frac{\partial\theta}{\partial x_j} + \theta\frac{\partial\sigma_{ik}}{\partial x_k} \\
&\quad + \frac{5}{39}\left(1-\frac{10R_{q_{int}}}{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{-}}{\partial x_i} - \frac{5}{39}\left(1+\frac{3R_{q_{int}}}{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{+}}{\partial x_i}
\end{aligned}$$

$$+\frac{5}{2}\left[1-\frac{R_{q_{int}}}{R_{q_{tr}}}\right]\rho\left(\theta+\Delta\theta\right)\frac{\partial\theta}{\partial x_i}+\sigma_{ik}\left(\frac{5}{2}\left[1-\frac{R_{q_{int}}}{R_{q_{tr}}}\right]\frac{\partial\theta}{\partial x_k}-\theta\frac{\partial\ln\rho}{\partial x_k}\right)$$
$$+\frac{2R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\left[q_j\frac{\partial v_j}{\partial x_i}+q_i\frac{\partial v_k}{\partial x_k}+q_k\frac{\partial v_i}{\partial x_k}\right]$$
$$+\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{R_{q_{tr}}\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\right)\left[\Delta\theta\frac{\partial\boldsymbol{\sigma}_{ij}}{\partial x_j}-\Delta\theta\frac{\partial\rho\Delta\theta}{\partial x_i}-\rho\theta\frac{\partial\Delta\theta}{\partial x_i}\right]$$
$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}q_i+\frac{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}^2+5R_{q_{int}}^2}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\Delta q_i\right), \tag{5.21}$$

the equations for stress tensor and total heat flux with terms up to order $\epsilon^2$, because the variables, $\boldsymbol{\sigma}_{ij}$ and $q_i$, are at first order,

$$\frac{\mathrm{D}\boldsymbol{\sigma}_{ij}}{\mathrm{D}t}+\frac{4R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\frac{\partial q_{<i}}{\partial x_{j>}}-\frac{4R_{q_{int}}R_{q_{tr}}\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}q_{<i}\frac{\partial\theta}{\partial x_{j>}}$$
$$+\frac{4\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_{<i}}{\partial x_{j>}}+2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}$$
$$+\frac{4R_{q_{int}}R_{q_{tr}}}{\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}}+\frac{\partial\boldsymbol{u}_{ijk}^{0,0}}{\partial x_k}$$
$$+2\rho\left(\theta-\Delta\theta\right)\frac{\partial v_{<i}}{\partial x_{j>}}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\sigma_{ij}, \tag{5.22}$$

$$\frac{\mathrm{D}q_i}{\mathrm{D}t}+\sigma_{ik}\left[\frac{5+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\frac{\partial\theta}{\partial x_k}-\theta\frac{\partial\ln\rho}{\partial x_k}\right]-\frac{\sigma_{ik}}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}$$
$$+\left(1+\frac{2R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\left[q_k\frac{\partial v_i}{\partial x_k}+q_i\frac{\partial v_k}{\partial x_k}\right]-\frac{2}{39}\frac{\partial B^+}{\partial x_i}$$
$$+\frac{5}{13}\frac{\partial B^-}{\partial x_i}+\frac{2R_{q_{int}}q_k}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\frac{\partial v_k}{\partial x_i}-\Delta\theta^2\frac{\partial\rho}{\partial x_i}$$
$$+\theta\frac{\partial\sigma_{ik}}{\partial x_k}-\rho\left(\theta+\Delta\theta\right)\frac{\partial\Delta\theta}{\partial x_i}+\frac{5+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\rho\left(\theta-\Delta\theta\right)\frac{\partial\theta}{\partial x_i}$$

$$+\frac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\left[\Delta q_k\frac{\partial v_i}{\partial x_k}+\Delta q_i\frac{\partial v_k}{\partial x_k}+\Delta q_k\frac{\partial v_k}{\partial x_i}\right]$$
$$+\frac{168}{(42+25\delta)^2}B^+_{ij}\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\frac{\partial\theta}{\partial x_j}+\frac{4\delta}{(42+25\delta)}\frac{\partial B^+_{ij}}{\partial x_j}+\Delta\theta\frac{\partial\boldsymbol{\sigma}_{ij}}{\partial x_j}+\sigma_{ik}\left(\frac{\partial\Delta\theta}{\partial x_k}+\Delta\theta\frac{\partial\ln\rho}{\partial x_k}\right)$$
$$+7\left(\frac{1}{(14+\delta)^2}-\frac{24}{(42+25\delta)^2}\right)\frac{\mathrm{d}\delta}{\mathrm{d}\theta}B^-_{ij}\frac{\partial\theta}{\partial x_j}+\frac{7\,(3+\delta)\,(14+3\delta)}{(14+\delta)(42+25\delta)}\frac{\partial B^-_{ij}}{\partial x_j}+\boldsymbol{u}^{0,0}_{ijk}\frac{\partial v_j}{\partial x_k}$$
$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}q_i+\frac{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\Delta q_i\right), \tag{5.23}$$

equation for $B^+$ with terms up to order $\epsilon^{2-2\alpha}$, due to the fact that $B^+$ is at order $\epsilon^{2\alpha}$ and first appears in the $\boldsymbol{\sigma}_{ij}$ and $q_i$ equations, which themselves are at order $\epsilon^1$,

$$\frac{\mathrm{D}B^+}{\mathrm{D}t}-8\theta\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}+\frac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}-40R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_k}{\partial x_k}$$
$$+\left(\frac{50R_{q_{int}}R_{q_{tr}}\theta\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}+\frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)-100R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)$$
$$\times q_k\frac{\partial\theta}{\partial x_k}-\left(2-\frac{50R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\theta q_k\frac{\partial\ln\rho}{\partial x_k}-\frac{20}{39}B^-\frac{\partial v_k}{\partial x_k}$$
$$+\frac{85}{39}B^+\frac{\partial v_k}{\partial x_k}+\frac{3\left(23-\delta-\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i}+\left(26-\frac{78}{3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}\right)\rho\theta\Delta\theta\frac{\partial v_i}{\partial x_i}$$
$$=-\frac{1}{\tau_{tr}}\left(\frac{9}{2}R_{u^{1,1}}+15R_{u^{2,0}}\right)\rho\Delta\theta^2-\frac{1}{\tau_{int}}\left[\frac{3}{2}\left(\left(3-\delta\right)R_{u^{1,1}}+20R_{u^{2,0}}-\left(23-\delta\right)\right)\rho\theta\Delta\theta\right]$$
$$-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{3R_{u^{1,1}}+10R_{u^{2,0}}}{13}B^+\frac{10}{13}\left(R_{u^{1,1}}-R_{u^{2,0}}\right)B^-\right), \tag{5.24}$$

and the balance law for $B^-$ with terms up to order $\epsilon^1$, because $B^+$ is at order $\epsilon^1$ and first appears in the $\boldsymbol{\sigma}_{ij}$ and $q_i$ equations, which themselves are at order $\epsilon^1$,

$$\frac{\mathrm{D}B^{-}}{\mathrm{D}t}+\frac{12}{5}\theta\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}+\frac{12R_{q_{int}}+2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_k}{\partial x_k}-\frac{2}{13}B^{+}\frac{\partial v_k}{\partial x_k}$$
$$+\left(\frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)+30R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}-\frac{2R_{q_{tr}}R_{q_{int}}\theta\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\right)q_k\frac{\partial\theta}{\partial x_k}$$
$$-2\left(1+\frac{R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\theta q_k\frac{\partial\ln\rho}{\partial x_k}-3\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i}+\frac{71}{39}B^{-}\frac{\partial v_k}{\partial x_k}$$
$$=-\frac{1}{\tau_{tr}}\frac{9\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{2}\rho\Delta\theta^2-\frac{1}{\tau_{int}}\left(\frac{3}{2}\left(3+\delta+\left[3-\delta\right]R_{u^{1,1}}-6R_{u^{2,0}}\right)\rho\theta\Delta\theta\right)$$
$$-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{10R_{u^{1,1}}+3R_{u^{2,0}}}{13}B^{-}+\left[\frac{3\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{13}B^{+}\right]\right). \tag{5.25}$$

These 19 PDEs are closed with the constitutive equations for $B_{ij}^{+}$ up to $1-\alpha$ order, because $B_{ij}^{+}$ is at order $\epsilon^{1+\alpha}$ and first appears in the $\boldsymbol{\sigma}_{ij}$ and $q_i$ equations, which themselves are at order $\epsilon^1$,

$$B_{ij}^{+}=-\frac{1}{\left[\dfrac{1}{\tau_{tr}}+\dfrac{1}{\tau_{int}}\right]}\left[2\left(\frac{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}-\frac{14-\delta}{\delta}\right)\theta\frac{\partial q_{<i}}{\partial x_{j>}}\right.$$
$$-\frac{4\left(70-19\delta\right)}{39\delta}B^{-}\frac{\partial v_{<i}}{\partial x_{j>}}+\frac{(14-\delta)\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}-\delta(14+\delta)}{\delta\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\theta\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}$$
$$-2\left(\frac{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}-\frac{14-\delta}{\delta}\right)\theta q_{<i}\frac{\partial\ln\rho}{\partial x_{j>}}$$
$$-\frac{2(42+25\delta)}{39\delta}B^{+}\frac{\partial v_{<i}}{\partial x_{j>}}+2R_{q_{int}}\left(\frac{14+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right.$$
$$\left.-\theta\frac{10\left(7R_{q_{int}}+2\left(7+3\delta\right)R_{q_{tr}}\right)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+14R_{q_{tr}}\theta\left(\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)^2+\left(70+23\delta\right)R_{q_{tr}}\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\right)$$
$$\left.\times\ q_{<i}\frac{\partial\theta}{\partial x_{j>}}+4\theta\left(2\sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}}+2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}\right)-\frac{(42+25\delta)}{\delta}\rho\theta\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}\right], \tag{5.26}$$

and for $\boldsymbol{u}_{ijk}^{0,0}$ and $B_{ij}^{-}$ at their leading orders, due to the fact that they are at order $\epsilon^2$ and first appear in the $\boldsymbol{\sigma}_{ij}$ and $q_i$ equations, which themselves are at order $\epsilon^1$,

$$\boldsymbol{u}_{ijk}^{0,0} = -\tau_{tr}\left[3\theta\frac{\partial\sigma_{<ij}}{\partial x_{k>}} - 3\theta\sigma_{<ij}\frac{\partial \ln\rho}{\partial x_{k>}} + \frac{12R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}} q_{<i}\frac{\partial v_j}{\partial x_{k>}}\right], \tag{5.27}$$

$$\begin{aligned} B_{ij}^{-} \;=\; -\tau_{tr}\Bigg[ & \frac{6(14+\delta)}{7\,(3+\delta)}\theta\left(\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k} + \sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}} - \frac{2}{3}\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}\right) \\ & + \frac{2(14+\delta)R_{q_{int}}}{(3+\delta)\left(5R_{q_{int}} + \left(\delta + \theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\left(5R_{q_{int}}\left[3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right]\right. \\ & \left. + R_{q_{tr}}\left[(3+\delta)\,\delta + (7+2\delta)\,\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta} + \left(\left(\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)^2 + 2\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)\theta^2\right]\right) q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\ & + \frac{2(14+\delta)}{3\,(3+\delta)}B^{-}\frac{\partial v_{<i}}{\partial x_{j>}} - \frac{2(14+\delta)\left(3R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}{(3+\delta)\left(5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\theta q_{<i}\frac{\partial \ln\rho}{\partial x_{j>}} \\ & + 2\frac{(14+\delta)\left(3R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}{(3+\delta)\left(5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial q_{<i}}{\partial x_{j>}}\Bigg]. \end{aligned} \tag{5.28}$$

This is the set of original regularized 19 (R19) equations corresponding to the third order of accuracy.

Next, we will introduce new forms of the balance and constitutive equations to replace (5.24)–(5.28) in the set of R19 equations. New forms eliminate some derivatives by substitution with stress tensor, heat flux and dynamic temperature while keeping the current order of accuracy. The new form requires the same number of boundary conditions for both linear and nonlinear cases, while this is not the case for the original R19 equations. Also, the boundary conditions needed for the new form of R19 equations are clear; and they are derived and presented in the next section. However, the exact type of boundary conditions needed for the original nonlinear R19 equations are not clear. The boundary conditions will be discussed further in the coming section.

### 5.5.1. *Transformation of equations*

The balance laws for $B^{+}$ and $B^{-}$ and the constitutive equations in the set of R19 equations can be rewritten using the leading-order heat flux difference, NSF stress and viscosities as

$$\boldsymbol{\sigma}_{ij}^{NSF} \;=\; -2\mu\frac{\partial v_{<i}}{\partial x_{j>}} = \boldsymbol{\sigma}_{ij} + O(\epsilon^{1+\alpha}) + \cdots, \tag{5.29a}$$

$$q_i^{NSF} \;=\; -\kappa\frac{\partial\theta}{\partial x_i} = q_i + O(\epsilon^{1+\alpha}) + \cdots, \tag{5.29b}$$

$$\kappa_\Delta \frac{\partial \Delta\theta}{\partial x_i} = \Delta q_i + O(\epsilon^{1+2\alpha}) + \cdots , \tag{5.29c}$$

$$\Delta\theta^{NSF} = \frac{\upsilon}{\rho}\frac{\partial v_i}{\partial x_i} = \Delta\theta + O(\epsilon^{2\alpha}) + \cdots , \tag{5.29d}$$

in a way that we still keep the proper order of accuracy. The balance laws take the form of

$$\begin{aligned}
&\frac{\mathrm{D}B^+}{\mathrm{D}t} - 2\frac{20R_{q_{int}} - \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\theta\left[\frac{\partial q_k}{\partial x_k} - q_k\frac{\partial \ln\rho\,(\theta-\Delta\theta)}{\partial x_k}\right] \\
&\quad + \left[\left(26 - \frac{78}{3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}}\right)\rho\theta\Delta\theta + \frac{3\left(23-\delta-\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}}\rho\Delta\theta^2 + \frac{85}{39}B^+ - \frac{20}{39}B^-\right] \\
&\quad \times \frac{\partial v_k}{\partial x_k} - \left(\frac{50R_{q_{int}}R_{q_{tr}}\theta\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta} + \theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2} + \frac{(5R_{q_{int}}+3R_{q_{tr}})\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) - 100R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right) \\
&\quad \times \frac{q_k q_k}{\kappa} + 2\frac{20R_{q_{int}} - \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\frac{\theta}{\theta-\Delta\theta}\left[\frac{q_k q_k}{\kappa} + \frac{q_k\Delta q_k}{\kappa_\Delta}\right] + 4\theta\frac{\sigma_{ij}\boldsymbol{\sigma}_{ij}}{\mu} \\
&= -\frac{1}{\tau_{tr}}\left(\frac{9}{2}R_{u^{1,1}} + 15R_{u^{2,0}}\right)\rho\Delta\theta^2 - \frac{1}{\tau_{int}}\left[\frac{3}{2}((3-\delta)R_{u^{1,1}} + 20R_{u^{2,0}} - (23-\delta))\rho\theta\Delta\theta\right] \\
&\quad - \left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\left(\frac{3R_{u^{1,1}} + 10R_{u^{2,0}}}{13}B^+ + \frac{10}{13}\left(R_{u^{1,1}} - R_{u^{2,0}}\right)B^-\right),
\end{aligned} \tag{5.30}$$

$$\begin{aligned}
&\frac{\mathrm{D}B^-}{\mathrm{D}t} - 2\frac{6R_{q_{int}} + \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\frac{\theta}{(\theta-\Delta\theta)}\left[\frac{q_k q_k}{\kappa} + \frac{q_k\Delta q_k}{\kappa_\Delta}\right] \\
&\quad - \left(\frac{(5R_{q_{int}}+3R_{q_{tr}})\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) + 30R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}} - \frac{2R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta} + \theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\right)\frac{q_k q_k}{\kappa} \\
&\quad - \frac{6}{5}\theta\frac{\boldsymbol{\sigma}_{ij}\boldsymbol{\sigma}_{ij}}{\mu} - \left(3\rho\Delta\theta^2 - \frac{71}{39}B^- + \frac{2}{13}B^+\right)\frac{\partial v_k}{\partial x_k} \\
&\quad + 2\frac{6R_{q_{int}} + \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\theta\left[\frac{\partial q_k}{\partial x_k} - q_k\frac{\partial \ln\rho\,(\theta-\Delta\theta)}{\partial x_k}\right]
\end{aligned}$$

$$= -\frac{1}{\tau_{tr}}\frac{9\left(R_{u^{1,1}} - R_{u^{2,0}}\right)}{2}\rho\Delta\theta^2 - \frac{1}{\tau_{int}}\left(\frac{3}{2}\left(3+\delta+\left[3-\delta\right]R_{u^{1,1}} - 6R_{u^{2,0}}\right)\rho\theta\Delta\theta\right)$$
$$- \left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\left(\frac{10R_{u^{1,1}} + 3R_{u^{2,0}}}{13}B^- + \left[\frac{3\left(R_{u^{1,1}} - R_{u^{2,0}}\right)}{13}B^+\right]\right). \tag{5.31}$$

The new constitutive equations for $B_{ij}^+$, $B_{ij}^-$ and $\boldsymbol{u}_{ijk}^{0,0}$ in the set of R19 equations after some manipulation become

$$B_{ij}^+ = -\frac{1}{\left[1 + \dfrac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\mu}{3\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\upsilon}\right]\rho\theta}\left(\frac{2\left(70-19\delta\right)B^- + \left(42+25\delta\right)B^+}{39\delta}\boldsymbol{\sigma}_{ij}\right.$$
$$+ \frac{\left(42+25\delta\right)}{2\delta}\rho\theta\Delta\theta\sigma_{ij} - 2R_{q_{int}}\left[\frac{14+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right.$$
$$\left.\left. - \theta\frac{10\left(7R_{q_{int}} + 2\left(7+3\delta\right)R_{q_{tr}}\right)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta} + 14R_{q_{tr}}\theta\left(\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)^2 + \left(70+23\delta\right)R_{q_{tr}}\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\right]\right.$$
$$\left.\times\ \frac{\mu}{\kappa}q_{<i}q_{j>} + \left[\frac{\left(14-\delta\right)\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta} - \delta\left(14+\delta\right)}{\delta\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)} + \frac{28}{3}\right]\frac{\mu}{\upsilon}\rho\theta\Delta\theta\boldsymbol{\sigma}_{ij} - 8\theta\sigma_{k<i}\sigma_{j>k}\right)$$
$$+ \frac{2\mu}{1 + \dfrac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\mu}{3\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\upsilon}}\left(\frac{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)} - \frac{14-\delta}{\delta}\right)\frac{q_{<i}}{\rho\left(\theta-\Delta\theta\right)}$$
$$\times\left[\frac{q_{j>}}{\kappa} + \frac{\Delta q_{j>}}{\kappa_\Delta}\right] - \frac{2}{\dfrac{1}{\mu} + \dfrac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\upsilon}}\left(\frac{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\right.$$
$$\left. - \frac{14-\delta}{\delta}\right)\frac{1}{\rho}\left[\frac{\partial q_{<i}}{\partial x_{j>}} - q_{<i}\frac{\partial\ln\rho\left(\theta-\Delta\theta\right)}{\partial x_{j>}}\right], \tag{5.32}$$

$$
\begin{aligned}
B_{ij}^{-} = & -\frac{1}{\rho\theta}\left[-\frac{6(14+\delta)}{7\,(3+\delta)}\theta\sigma_{k<i}\sigma_{j>k}-\frac{(14+\delta)}{3\,(3+\delta)}B^{-}\boldsymbol{\sigma}_{ij}\right.\\
& -\frac{2(14+\delta)R_{q_{int}}}{(3+\delta)\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^{2}}\left(5R_{q_{int}}\left[3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right]\right.\\
& \left.\left.+R_{q_{tr}}\left[(3+\delta)\,\delta+(7+2\delta)\,\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\left(\left(\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)^{2}+2\frac{\mathrm{d}^{2}\delta}{\mathrm{d}\theta^{2}}\right)\theta^{2}\right]\right)\frac{\mu}{\kappa}q_{<i}q_{j>}\right]\\
& +\mu\frac{2(14+\delta)\left(3R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}{(3+\delta)\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{q_{<i}}{\rho\,(\theta-\Delta\theta)}\left[\frac{q_{j>}}{\kappa}+\frac{\Delta q_{j>}}{\kappa_{\Delta}}\right]\\
& -\mu\frac{2(14+\delta)\left(3R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}{(3+\delta)\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{1}{\rho}\left(\frac{\partial q_{<i}}{\partial x_{j>}}-q_{<i}\frac{\partial\ln\rho\,(\theta-\Delta\theta)}{\partial x_{j>}}\right),
\end{aligned}
\tag{5.33}
$$

$$
\begin{aligned}
\boldsymbol{u}_{ijk}^{0,0} = & \frac{6R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\frac{q_{<i}\sigma_{jk>}}{\rho\theta}+3\mu\frac{\sigma_{<ij}}{\rho\,(\theta-\Delta\theta)}\left[\frac{q_{k>}}{\kappa}+\frac{\Delta q_{k>}}{\kappa_{\Delta}}\right]\\
& -3\frac{\mu}{\rho}\left(\frac{\partial\sigma_{<ij}}{\partial x_{k>}}-\sigma_{<ij}\frac{\partial\ln\rho\,(\theta-\Delta\theta)}{\partial x_{k>}}\right),
\end{aligned}
\tag{5.34}
$$

where the microscopic time scales are substituted by viscosities and specific heat using (5.8).

## 6. Kinetic boundary condition

In this section, we introduce a kinetic boundary condition using the idea of two distinguished exchanged processes, internal and translational. Then we incorporate this condition to obtain the corresponding macroscopic boundary conditions. Having the macroscopic boundary conditions will enable us to solve boundary value problems, e.g. stationary heat transfer, using the macroscopic models introduced above.

The microscopic wall boundary condition prescribes the distribution function of the particles reflected from the wall when the distribution function of the incoming particles towards the wall is known. The most common used model is the Maxwell (1879) accommodation model. Maxwell proposed that the gas particles are reflected from the wall specularly or diffusivity. A portion $\chi$, where $\chi$ is the wall accommodation coefficient, of the particles hit the wall and accommodate at the wall so that they are reflected with the equilibrium distribution of the wall. The other portion, $1-\chi$, is reflected specularly. In this case, the normal component of the velocity changes sign and the distribution function describing the reflected particles is akin to the incoming particles distribution function with corresponding transformed velocities, i.e. $f^{*}(\boldsymbol{c})=f(\boldsymbol{c}-\mathbf{2}(\boldsymbol{n}\cdot\boldsymbol{c})\boldsymbol{n})$.

For polyatomic particles that are diffusively reflected, we have two Maxwellian-type equilibrium distribution functions (2.16) and (2.17) corresponding to only translational

energy equilibrium and total energy equilibrium. We adopt the generalized Grad's 36 distribution function (B 1) and its corresponding form as the phase density ($f^*$), for incoming and specularly reflected particles. We introduce the wall boundary condition as the velocity distribution function in the infinitesimal precinct of the wall,

$$\tilde{f}(c) = \begin{cases} \chi[(1-\zeta)f_{tr,w}(\boldsymbol{c},\boldsymbol{I}) + \zeta f_{int,w}(\boldsymbol{c},\boldsymbol{I})] + (1-\chi)f^*_{|36}(\boldsymbol{c},\boldsymbol{I}) & \boldsymbol{n}\cdot(\boldsymbol{c}-\boldsymbol{v}_w) \succ 0, \\ f_{|36}(\boldsymbol{c},\boldsymbol{I}) & \boldsymbol{n}\cdot(\boldsymbol{c}-\boldsymbol{v}_w) \prec 0, \end{cases} \tag{6.1}$$

where the two wall accommodation coefficients, $\zeta$ and $\chi$, are specifying the level of accommodation of the particle on the wall. Full accommodation is specified by $\zeta = 1$ and $\chi = 1$, partial accommodation for particles only accommodated translationally identified by $\zeta = 0$ and $\chi = 1$ and the pure specularly reflected particles are described by $\chi = 0$. Moreover, $\boldsymbol{n}$ is the wall-normal pointing towards the gas.

Wall boundary conditions for gases must obey a number of requirements, most importantly proper normalization and reciprocity (Sharipov 2003). The above is a variant of the Maxwell boundary conditions and obeys these requirements. Normalization implies that the number of particles is conserved, and this is ensured here by adjusting the densities for the wall Maxwellians, $f_{tr,w}$ and $f_{int,w}$, accordingly, see (7.6). The distribution used on the wall are Maxwellian distributions which are normalized and the Grad's distribution is an expansion on the Maxwellian distribution, which are designed to ensure conservation of the particle number, as will be seen in (7.6). This means the kernel is normalized and the number of particles hitting the wall is the same as that of reflecting particles and the normalization condition is satisfied (Sharipov 2003).

## 7. Macroscopic boundary condition

For obtaining boundary conditions for our field of macroscopic equations, we do the similar procedure as we did to obtain the balance law for moments: we multiply the wall distribution function ($\tilde{f}$) by corresponding velocity and internal parameter functions and take the integral over velocity and internal parameter space. This will give us the relations between the macroscopic properties at the wall and the wall properties given in the wall equilibrium distribution functions, $f_{tr,w}$ and $f_{int,w}$. We define peculiar velocity based on average velocity, $\boldsymbol{C} = \boldsymbol{c} - \boldsymbol{V}_{gas}$, and slip velocity as $V_s = \boldsymbol{V}_{gas} - \boldsymbol{V}_w$. This will give us the integral of the weighted wall distribution function as,

$$\begin{aligned} &\int \Psi(\boldsymbol{C},\boldsymbol{I})\tilde{f}(\boldsymbol{C})\,\mathrm{d}\boldsymbol{C}\,\mathrm{d}\boldsymbol{I} \\ &\quad = \iint_{\boldsymbol{C}\cdot\boldsymbol{n}\prec 0} [\Psi(\boldsymbol{C},\boldsymbol{I}) + (1-\chi)\Psi(\boldsymbol{C}-\boldsymbol{2}(\boldsymbol{n}\cdot\boldsymbol{C})\boldsymbol{n},\boldsymbol{I})]f_{|36}(\boldsymbol{C},\boldsymbol{I})\,\mathrm{d}\boldsymbol{C}\,\mathrm{d}I \\ &\qquad + \chi\left[\iint_{\boldsymbol{C}\cdot\boldsymbol{n}\succ 0} \Psi(\boldsymbol{C}_w - V_s, I)[(1-\zeta)f_{tr,w}(\boldsymbol{C}_w, I) + \zeta f_{int,w}(\boldsymbol{C}_w, I)]\,\mathrm{d}\boldsymbol{C}_w\,\mathrm{d}I\right], \end{aligned} \tag{7.1}$$

where, $\boldsymbol{C}_w = \boldsymbol{C} + V_s$. We consider that $\boldsymbol{n} = (0, 1, 0)$ and $\boldsymbol{V}_w = (V_w, 0, 0)$.

For any velocity and internal parameter function, $\Psi(\boldsymbol{C},\boldsymbol{I})$, a relation between the corresponding moment and the wall properties could be obtained from (7.1). In order

to have meaningful boundary conditions, Grad (1949) discussed the argument of specular reflection such that the velocity function should be odd in the normal component of the particle velocity. This is due to the fact that the even polynomials at the wall boundary condition will produce identities and are uncontrollable. Also, the theory of balance laws states that, at the boundary, we need to prescribe fluxes not variables (Torrilhon & Struchtrup 2008). Considering a two-dimensional process in the $x$–$y$ plane, the flux moments corresponding to odd powers in the $y$ component, $\boldsymbol{n} = (0, 1, 0)$, of the particle velocity are

$$u_\Psi = \left\{ v_y, \boldsymbol{\sigma}_{xy}, q_y, \Delta q_y, B^-_{xy}, u^{0,0}_{xxy}, u^{0,0}_{yyy} \right\}. \tag{7.2}$$

Therefore, the corresponding velocity and internal parameter function, $\Psi$, for two-dimensional R19 equations occurring in the $y$-direction is obtained as,

$$\begin{aligned}\Psi \;=\; \Bigg\{ & C_y,\, C_xC_y,\, C_y\left(\frac{C^2}{2}+I^{2/\delta}\right),\\ & C_xC_y\left(\left[1-\frac{11}{14}\frac{\delta}{\delta+3}\right]C^2+\left[1+\frac{11}{\delta+3}\right]I^{2/\delta}-\frac{14+\delta}{2}\theta\right),\\ & C_y\left(\frac{C^2}{2}-\frac{5R_{q_{int}}}{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}I^{2/\delta}\right),\, C_y\left(C_yC_y-\frac{3}{5}C^2\right),\, C_y\left(C_xC_x-\frac{1}{5}C^2\right)\Bigg\}. \end{aligned} \tag{7.3}$$

The general boundary condition (7.1) is used here to obtain macroscopic boundary conditions for different functions in $\Psi$.

The first condition is obtained by considering $\Psi = C_y$. For this we rewrite the part representing incoming particles as

$$f_{|36}(\boldsymbol{c}) = \chi[(1-\zeta)f_{|36}(\boldsymbol{c}) + \zeta f_{|36}(\boldsymbol{c})] + (1-\chi)f_{|36}(\boldsymbol{c}). \tag{7.4}$$

So, we have three identity relations,

$$-(1-\chi)\iint_{\boldsymbol{C}\cdot\boldsymbol{n}<0} C_y f_{|36}\,\mathrm{d}\boldsymbol{C}\,\mathrm{d}\boldsymbol{I} \;=\; (1-\chi)\iint_{\boldsymbol{C}\cdot\boldsymbol{n}>0} C_y f^*_{|36}\,\mathrm{d}\boldsymbol{C}\,\mathrm{d}\boldsymbol{I}, \tag{7.5a}$$

$$-\chi(1-\zeta)\int_{\boldsymbol{C}\cdot\boldsymbol{n}<0} C_y f_{|36}\,\mathrm{d}\boldsymbol{C} \;=\; \chi(1-\zeta)\int_{\boldsymbol{C}\cdot\boldsymbol{n}>0} C_y f_{tr,w}\,\mathrm{d}\boldsymbol{C}, \tag{7.5b}$$

$$-\chi\zeta\iint_{\boldsymbol{C}\cdot\boldsymbol{n}<0} C_y f_{|36}\,\mathrm{d}\boldsymbol{C}\,\mathrm{d}\boldsymbol{I} \;=\; \chi\zeta\iint_{\boldsymbol{C}\cdot\boldsymbol{n}>0} C_y f_{int,w}\,\mathrm{d}\boldsymbol{C}\,\mathrm{d}\boldsymbol{I}, \tag{7.5c}$$

which state that the flux of molecules towards the wall is the same as that leaving for all three reflection types, pure specular, partial accommodation and full accommodation. The first identity is always true based on the definition of $f^*_{|36}$ and $f_{|36}$, (B 1). The second identity gives us a relation for $\rho_{I,w}$ as,

$$\rho_{I,w}\sqrt{\theta_w} = -\frac{\exp\left[-\dfrac{I^{2/\delta}}{\theta_w}\right]}{\Gamma\left(1+\dfrac{\delta}{2}\right)840\delta\sqrt{2}\theta^{(\delta+5)/2}}\left[\frac{70\sqrt{2}\delta}{13}\theta\left(21B^- + 5B^+ \right.\right.$$
$$+ 78\left[\frac{(3+\delta)\,(14+27\delta)}{(14+\delta)(42+25\delta)}B^-_{yy} - \frac{2\delta}{42+25\delta}B^+_{yy}\right.$$
$$\left.\left.\left.+ \frac{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\sqrt{2\pi\theta}R_{q_{tr}}}{\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\left(\Delta q_y - q_y\right) + \theta\left(2\rho\left[2\Delta\theta-\theta\right]-\sigma_{yy}\right)\right]\right)\right.$$
$$- 140I^{2/\delta}\left(\frac{12\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\sqrt{\pi}R_{q_{tr}}}{\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\sqrt{\theta}(\Delta q_y - q_y) + \frac{168\sqrt{2}\delta\,(3+\delta)}{(14+\delta)(42+25\delta)}\right.$$
$$\left.\left.\times B^-_{yy} + \frac{20\sqrt{2}}{13}B^- + \frac{6\sqrt{2}}{13}B^+ - \frac{18\sqrt{2}\delta}{(42+25\delta)}B^+_{yy} + \frac{18\sqrt{2}}{(42+25\delta)}\rho\theta\Delta\theta\right)\right], \tag{7.6}$$

and the third one gives us,

$$\Upsilon = \rho_w\sqrt{\theta_w} = -\frac{(14-\delta)(3+\delta)}{2(14+\delta)(42+25\delta)\theta^{3/2}}B^-_{yy} + \frac{1}{156}\frac{B^+ - B^-}{\theta^{3/2}}$$
$$- \frac{\delta}{2(42+25\delta)\theta^{3/2}}B^+_{yy} + \frac{1}{2}\frac{\sigma_{yy}}{\sqrt{\theta}} + \frac{1}{2\sqrt{\theta}}\rho(2\theta-\Delta\theta). \tag{7.7}$$

Choosing different $\Psi$ functions from (7.3) we obtain boundary condition for the stress tensor,

$$\boldsymbol{\sigma}_{xy} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi}}\left[\Upsilon V_s + \frac{5R_{q_{int}}q_x + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\Delta q_x}{5\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)\sqrt{\theta}} + \frac{u^{0,0}_{xyy}}{2\sqrt{\theta}}\right], \tag{7.8}$$

the boundary condition for the total heat flux,

$$q_y = -\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{\Upsilon}{2}\sqrt{\theta}\left[(4+\delta\zeta)\,(\theta-\theta_w) - (1-\zeta)\,(\delta\theta+3\Delta\theta) - V_s^2\right]\right.$$
$$+ (3+\delta)\,\frac{(140+\delta\,(32+\delta)+(14-\delta)\delta\zeta)}{4(14+\delta)(42+25\delta)}B^-_{yy} + \frac{[(1-\zeta)\,\delta-4]}{312}B^+$$
$$+ \frac{\delta\,(4-\delta\,(1-\zeta))}{4\,(42+25\delta)}B^+_{yy} - \frac{(2+\delta\,(1-\zeta))}{4}\theta\left(\rho\Delta\theta-\sigma_{yy}\right)$$
$$\left.+ \frac{(56-\delta\,(1-\zeta))}{312}B^- + \frac{\delta\,(1-\zeta)}{2}\rho\theta^2\right], \tag{7.9}$$

the boundary condition for heat flux difference $\Delta q_y$,

$$\begin{aligned}\Delta q_y \;=\; & \frac{\chi}{(2-\chi)R_{q_{tr}}\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{5\,(40-\delta)\,R_{q_{int}}-12\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{312}B^{-}\right.\\
&+\frac{5\,(12+\delta)\,R_{q_{int}}+12\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{312}B^{+}\\
&+\frac{5\delta R_{q_{int}}-6\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4}\theta\sigma_{yy}-\delta\frac{5\,(6+\delta)\,R_{q_{int}}+6\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4(42+25\delta)}B^{+}_{yy}\\
&+\frac{10\delta R_{q_{int}}-8\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4}\rho\theta^2+\frac{5\,(6-\delta)\,R_{q_{int}}+12\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4}\rho\theta\,\Delta\theta\\
&+[3+\delta]\,\frac{5\delta\,(42+\delta)\,R_{q_{int}}-6(14-\delta)\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4(14+\delta)(42+25\delta)}B^{-}_{yy}\\
&+\frac{\Upsilon}{2}\sqrt{\theta}\left[\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}V_s^2-15R_{q_{int}}\,(1-\zeta)\,\Delta\theta\right.\\
&\left.\left.-\left(5\delta R_{q_{int}}-4\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)\theta+\left(5\delta\zeta R_{q_{int}}-4\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)(\theta-\theta_W)\right]\right],\end{aligned}\tag{7.10}$$

the boundary condition for $B^{-}_{xy}$,

$$\begin{aligned}B^{-}_{xy} \;=\; & \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi}}\frac{3(14+\delta)}{14\,(3+\delta)}\left(\frac{37\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{15\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\sqrt{\theta}\Delta q_x\right.\\
&-\frac{14\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}+33R_{q_{int}}}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\sqrt{\theta}q_x-\frac{1}{2}\sqrt{\theta}u^{0,0}_{xyy}\\
&\left.-\Upsilon V_s\left(V_s^2-\theta+7\,(1-\zeta)\,\Delta\theta-\frac{(18+7\zeta\delta)}{3}\,[\theta-\theta_W]\right)\right),\end{aligned}\tag{7.11}$$

the boundary condition for $u^{0,0}_{yyy}$,

$$\begin{aligned}5u^{0,0}_{yyy} \;=\; & \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{(-14+\delta)\,(3+\delta)}{(14+\delta)\,(42+25\delta)}B^{-}_{yy}-\frac{\delta B^{+}_{yy}}{42+25\delta}-\frac{2\left(B^{+}-B^{-}\right)}{195}\right.\\
&\left.-\frac{7\sigma_{yy}+2\rho\Delta\theta}{5}\theta-\Upsilon\frac{\sqrt{\theta}}{5}\left(3V_s^2-2\,[\theta-\theta_W]\right)\right],\end{aligned}\tag{7.12}$$

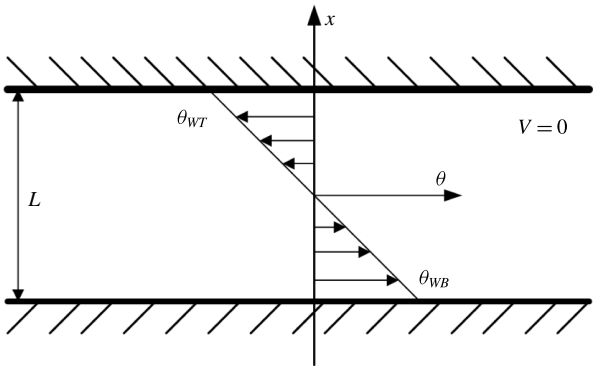


FIGURE 1. General stationary heat conduction schematic. Top and bottom walls are at different temperatures, $\theta_{WT}$, $\theta_{WB}$.

and the boundary condition for $u^{0,0}_{xxy}$,

$$u^{0,0}_{xxy} = \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{(-14+\delta)\,(3+\delta)}{(14+\delta)\,(42+25\delta)}B^{-}_{xx} - \frac{\delta B^{+}_{xx}}{42+25\delta} + \frac{\left(B^{+}-B^{-}\right)}{195} + \frac{\theta}{5}\left(\rho\Delta\theta+\sigma_{yy}-5\sigma_{xx}\right) + \Upsilon\frac{\sqrt{\theta}}{5}\left(4V_s^2-[\theta-\theta_W]\right)\right]. \tag{7.13}$$

## 8. One-dimensional stationary heat conduction

Next, one-dimensional heat transfer within a stationary polyatomic gas is studied using numerical and analytical methods to solve nonlinear and linear systems. Specifically, for the set of R19 and the RNSF equations. We consider unsteady heat conduction which is homogeneous in $y$ and $z$ directions. The gas is confined between two infinite plates and is stationary, i.e. $v = 0$, as shown in figure 1. The walls are at different temperatures and the flow properties and variables depend only on the $x$-direction. We study different gases and different test case scenarios.

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

$$\left.\begin{gathered}\bar{x}_i = \frac{x_i}{\tau_0\sqrt{\theta_0}} = \frac{x_i}{L},\quad \bar{t} = \frac{t}{\tau_0},\quad \bar{\tau}_{int} = \frac{\tau_{int}}{\tau_0},\quad \bar{\tau}_{tr} = \frac{\tau_{tr}}{\tau_0},\quad \bar{\rho} = \frac{\rho}{\rho_0} - 1,\\ \bar{\theta} = \frac{\theta}{\theta_0} - 1,\quad \Delta\bar{\theta} = \frac{\Delta\theta}{\theta_0},\quad \bar{\sigma}_{ij} = \frac{\boldsymbol{\sigma}_{ij}}{\rho_0\theta_0},\quad \bar{q}_i = \frac{q_i}{\rho_0\sqrt{\theta_0}^3},\quad \Delta\bar{q}_i = \frac{\Delta q_i}{\rho_0\sqrt{\theta_0}^3},\\ \bar{u}^{0,0}_{ijk} = \frac{\boldsymbol{u}^{0,0}_{ijk}}{\rho_0\sqrt{\theta_0}^3},\quad \bar{B}^{+}_{ij} = \frac{B^{+}_{ij}}{\rho_0\theta_0^2},\quad \bar{B}^{-}_{ij} = \frac{B^{-}_{ij}}{\rho_0\theta_0^2},\quad \bar{B}^{+} = \frac{B^{+}}{\rho_0\theta_0^2},\quad \bar{B}^{-} = \frac{B^{-}}{\rho_0\theta_0^2}.\end{gathered}\right\} \tag{8.1}$$

Note that the dimensionless relaxation times, $\bar{\tau}_{int}$ and $\bar{\tau}_{tr}$, are the Knudsen numbers. From now on, the overbars are dropped to avoid any unnecessary complexity in stating equations. The dimensionless set of R19 equations describing the considered problem consists of energy and momentum conservation,

$$\frac{\partial\rho}{\partial x} + \frac{\partial\,(\theta-\Delta\theta)}{\partial x} + \frac{\partial\sigma_{11}}{\partial x} = 0, \tag{8.2}$$

$$\frac{3+\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}(1+\rho)\,\frac{\partial\theta}{\partial t}+\frac{\partial q}{\partial x}=0, \tag{8.3}$$

and 11 equations for $\{\Delta\theta,\ \sigma_{11},\ q,\ \Delta q,\ B^{+},\ B^{-},\ B^{+}_{ij},\ B^{-}_{ij},\ \boldsymbol{u}^{0,0}_{ijk}\}$ which are presented in appendix D.

### 8.1. *Refined NSF equations*

For this case, the RNSF equations (5.4)–(5.6), reduce to

$$\frac{\partial\rho}{\partial x}+\frac{\partial\theta}{\partial x}=0, \tag{8.4a}$$

$$\frac{3+\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}(1+\rho)\,\frac{\partial\theta}{\partial t}+\frac{\partial q}{\partial x}=0, \tag{8.4b}$$

$$\Delta\theta=0, \tag{8.4c}$$

$$\sigma_{11}=0, \tag{8.4d}$$

$$q=-\tau_{tr}\frac{5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}(1+\rho)\,(1+\theta)\,\frac{\partial\theta}{\partial x}. \tag{8.4e}$$

### 8.2. *Boundary conditions*

For obtaining the boundary conditions, we consider the steady state condition with 11 variables,

$$\Phi=\left\{\theta,\ \Delta\theta,\ q,\ \Delta q,\ B^{+},\ B^{-},\ B^{+}_{11},\ B^{-}_{11},\ \rho,\ \sigma_{11},\ u^{0,0}_{111}\right\}, \tag{8.5}$$

and write the system of equations as

$$B(\Phi)\frac{\partial\Phi}{\partial y}=P(\Phi)\Phi. \tag{8.6}$$

The number of boundary conditions which must be described is the number of variables of the system (11) minus the number of multiplicity of the zero eigenvalues of the matrix $\boldsymbol{A}(\Phi)$ (Torrilhon & Struchtrup 2008). Calculation of the eigenvalues shows that the matrix $\boldsymbol{A}(\Phi)$ possesses a zero eigenvalue with a multiplicity of 4. Therefore, we need to prescribe a total number of 7 boundary conditions for regularized 19 equations. Four associated null spaces of the matrix $\boldsymbol{A}(\Phi)$ give relations which describe $B^{+}$, $B^{-}$, $B^{+}_{11}$ and $B^{-}_{11}$ as functions of the rest of the variables of (8.5). Therefore, only 7 independent variables remain. Based on this reduced 7 field of variables of $\Phi$, we have the velocity and internal energy parameter functions corresponding to the fluxes with odd powers in the normal velocity component ($q$, $\Delta q$ and $u^{0,0}_{111}$) as

$$\Psi=\left\{C_1\left(\frac{C^2}{2}+I^{2/\delta}\right),\ C_1\left(\frac{C^2}{2}-\frac{5R_{q_{int}}}{\left(\delta+\theta\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}I^{2/\delta}\right),\ C_1\left(C_1C_1-\frac{3}{5}C^2\right)\right\}. \tag{8.7}$$

The microscopic boundary condition along with the $\Psi$ function (7.1) are used to obtain 6 macroscopic boundary conditions which correspond to the boundary conditions for $q$, $\Delta q$ and $u^{0,0}_{111}$ (7.9), (7.10) and (7.12), on each wall, and are given in appendix D.

Here, the fluid is considered to be stationary and the flow which exists due to the density changes in the unsteady state is ignored. We apply the prescribed mass condition as the seventh boundary condition to update the density during the unsteady processes as

$$\int_{-L/2}^{L/2} \rho \, \mathrm{d}x = \rho_0 L. \tag{8.8}$$

If we were to allow gas movements and convection to be a part of the problem, the conservation of mass and normal velocity of gas on the wall would replace the prescribed mass condition. Here we are interested in only stationary heat conduction, therefore all the velocities are set to zero; and the prescribed mass condition (8.2) is solved by the trapezoidal rule along with conservation of momentum to gain the distribution of density at each time step in the unsteady processes.

Also, the boundary condition for the RNSF equations along with the prescribed mass condition is the temperature jump condition obtained from (D 10) at order $\varepsilon^1$ as,

$$\theta - \theta_w = n_y \tau_{tr} \frac{(2-\chi)}{\chi} \sqrt{\frac{\pi\theta}{2}} \frac{5R_{q_{int}} + \left(\delta + \theta \dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}}{(4+\delta\zeta) R_{q_{int}} R_{q_{tr}}} \frac{\partial\theta}{\partial x}. \tag{8.9}$$

### 8.3. *Numerical scheme*

The finite difference method is used to discretize our system of equations with central difference scheme in spatial discretization and first-order explicit discretization in time. The steady state condition is

$$\frac{|\theta^{n+1}_{m/2} - \theta^{n}_{m/2}|}{|\theta^{n}_{m/2}|} \leqslant 10^{-6}. \tag{8.10}$$

For RNSFs temperature jump boundary condition (8.9), second-order backward and forward finite difference discretizations are used.

### 8.4. *Linear and steady case*

First, we study the steady linearized set of equations with small disturbances from an equilibrium ground state $\{\rho_0, v^0_i = 0, \theta_0\}$. The set of linear steady equations are reduced to 5 coupled equations for $\Phi = \{\Delta q, q, u^{0,0}_{111}, \sigma_{11}, \Delta\theta\}$. Equations for the rest of the variables $\{\rho, \theta, B^+, B^-\}$ are functions of coupled variables. The solution of the set of coupled equations, $A_{5\times5}(\partial\Phi/\partial x) = B_{5\times5}\Phi$, is obtained using the eigenvalue method as

$$\Phi(x) = \sum_{n=1}^{5} C_n \boldsymbol{\vartheta}_n \mathrm{e}^{\lambda_n x}, \tag{8.11}$$

where, $\lambda$ and $\boldsymbol{\vartheta}$ are eigenvalues and eigenvectors of the coefficient matrix, $\boldsymbol{A}^{-1}\boldsymbol{B}$. The solution for the remaining variables are obtained by integrating of their equations.

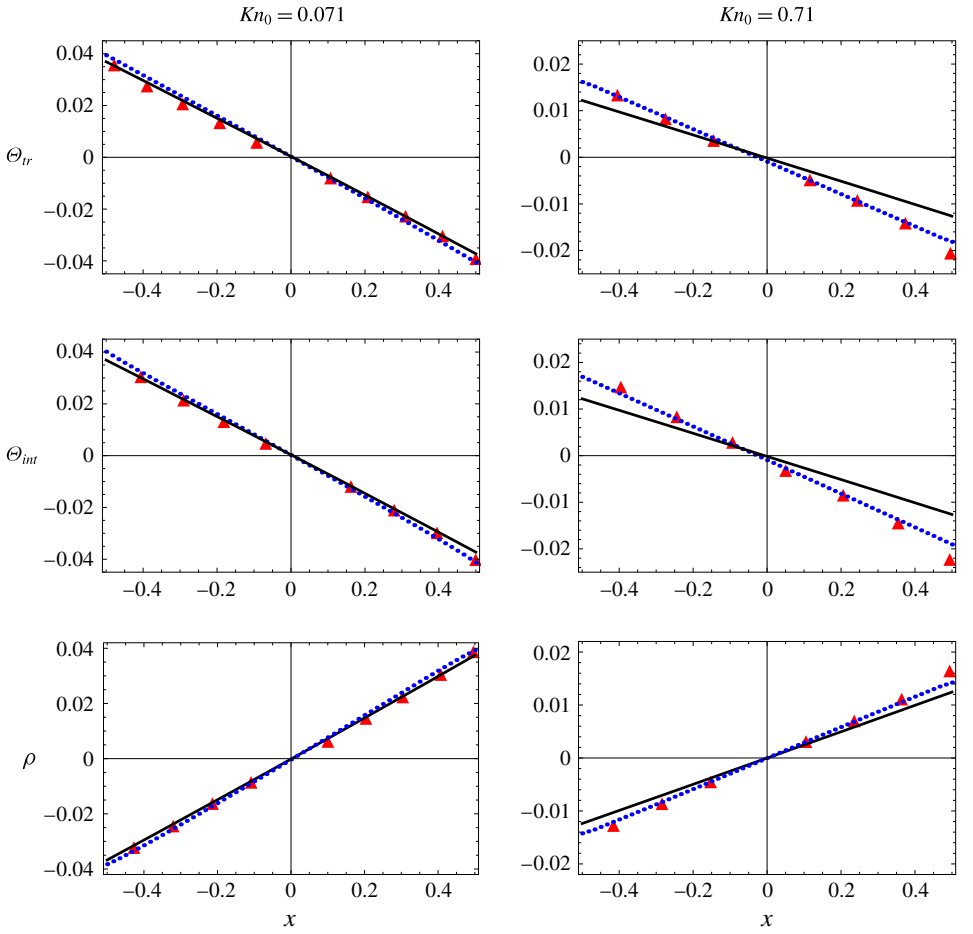


FIGURE 2. (Colour online) Comparison of temperature and density profiles for $Kn$ numbers equal to 0.071 and 0.71 with $t_{int}/t_{tr} = 1$. Results shown are obtained from: R19 equations (blue dashed line); RNSF equations (black line); DSMC method (red triangles).

## 9. Results

We first compare the results of our proposed models with the direct simulation Monte Carlo method data of Tantos *et al.* (2015). Comparison between numerical solution of the R19, the RNSF equations and DSMC results are shown in figure 2. Dimensionless wall temperatures are deviations of $\pm 0.0476$ from the reference temperature at 350 K. We investigate two different reference $Kn$ numbers, 0.071 and 0.71, which represent slip and transition flow regimes, respectively. Relaxation parameters are set to $R_{q_{tr}} = R_{u^{2,0}} = 0.72$ and $R_{u^{1,1}} = R_{q_{int}} = 0.7537$ in order to have Prandtl number equal to 0.73, the same as the DSMC simulation, based on (5.12). Changing the values of $R_{q_{tr}}$ so that they remain close to 3/2 will fine tune the results. However, if we lift this restriction and let $R_{q_{tr}}$ be lower and $R_{q_{int}}$ higher than the 3/2 value, the influence on the results will be considerable, especially on moments corresponding to internal-translational interactions. Also, the number of excited internal DoF is set to 2, the same as the DSMC simulation. The DSMC simulation is performed by considering identical translational-rotational relaxation

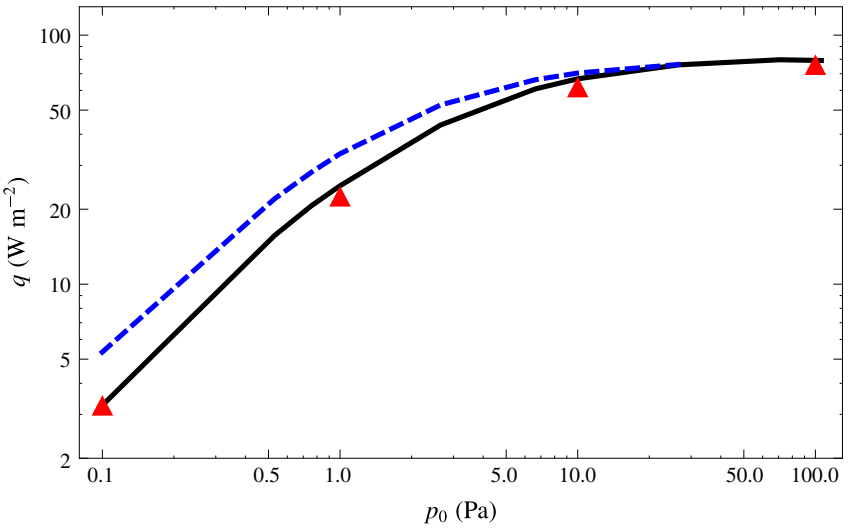


FIGURE 3. (Colour online) Comparison of total heat flux as a function of reference pressure, ranging from continuum to transition regime. Results shown are obtained from: R19 equations (black line); RNSF equations (blue dashed line); DSMC (red triangles).

rates, therefore we used $t_{int}/t_{tr} = 1$. It is evident from figure 2 that there is a good agreement between the DSMC and the R19 results. In contrast, in transition regime, there is a considerable deviation of RNSF equations results from the DSMC results and the first-order set of equations fails to accurately model the problem.

We compare the values of dimensional total heat flux from R19 equations with those from the DSMC simulation of Gallis, Torczynski & Rader (2007) at various reference pressures, ranging from continuum to transition regime in figure 3. The simulation case is a channel with 1 μm width filled with $N_2$ gas and wall temperatures at 285 and 315 K. The Prandtl number is set to 0.71, and the reference temperature and reference shear viscosity are 300 K and 1.775 Pa s$^{-1}$, respectively. Also, full accommodation coefficients are considered. Reference pressures of $10^2$, 1 and 0.1 Pa correspond to reference $Kn_{tr}$ equal to 0.005, 0.5 and 5. As it is depicted in figure 3, there is good agreement between our data and the DSMC data. However in transition regime, there is a considerable deviation of RNSF equations results from R19 and DSMC results and the first-order set of equations fails to accurately model the problem. It is seen that the total heat flux is independent of pressure at very low Knudsen numbers. However, at high Knudsen numbers, heat flux changes abruptly with changing pressure. Here, we use the values for Maxwell molecules of relaxation parameters for pure translational moments, $R_{u^{2,0}} = R_{q_{tr}} = 3/2$, from table 1. Prandtl number is equal to 0.71 and based on (5.12) we obtain $R_{q_{int}} = 0.847$. Also, we use the obtained value of $R_{q_{int}}$ for $R_{u^{1,1}} = 0.847$, and as is clear from figure 3, this value produces a good fit to the DSMC results. Therefore, the relaxation time of internal heat flux equals to 0.79 of the translational heat flux relaxation time.

Next, we compare results from our macroscopic R19 model and results obtained deterministically from the Holway (1966) and Andries *et al.* (2000) kinetic models. Values of total heat flux obtained from R19 equations are compared with the values obtained using the Holway (1966) model (Tantos *et al.* 2015) in figure 4. The simulation case is a diatomic gas with excited internal DoF equal to 2, the

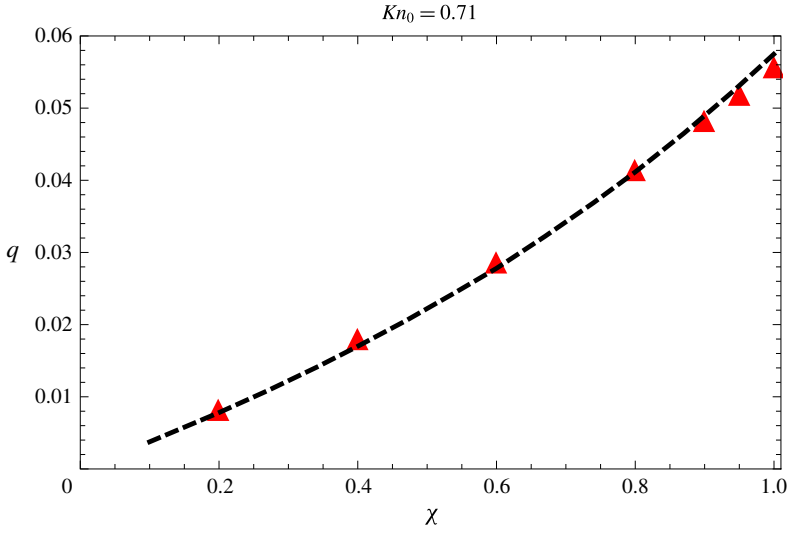


FIGURE 4. (Colour online) Comparison of total heat flux as a function of wall accommodation coefficient, ranging from specular reflection to full accommodation at wall. Results shown are obtained from: R19 equations (black dashed line); Holway model (red triangles).

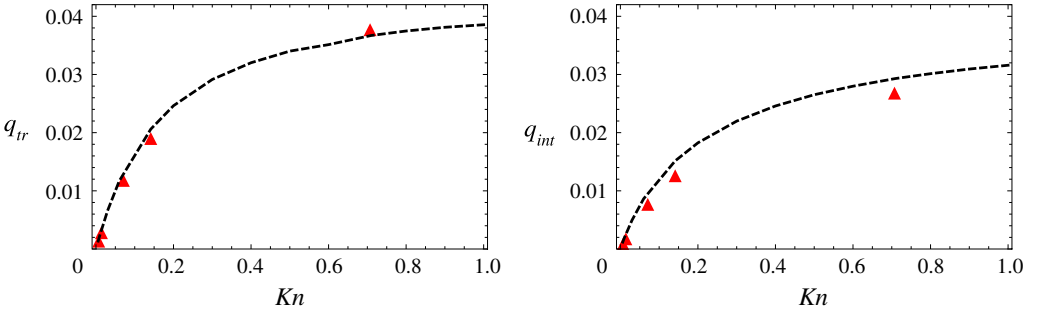


FIGURE 5. (Colour online) Comparison of translational and internal heat fluxes as a function of reference Knudsen number, ranging from continuum to transition regime. Results shown are obtained from: R19 equations (black dashed line); Andries model (red triangles).

Prandtl number and reference Knudsen number are equal to 0.71. At different wall accommodation coefficients, $\chi$, total heat fluxes from our macroscopic model and deterministically solved kinetic model are in a good agreement. As the wall accommodation coefficient decreases, the value of total heat flux decreases too.

Translational and internal heat fluxes of a polyatomic gas with excited internal DoF equal to 3, obtained by the deterministic method from the Andries *et al.* (2000) model (Tantos *et al.* 2015) and our R19 equations are compared in figure 5. The Prandtl number is set to 0.72. The heat fluxes at different reference Knudsen numbers are depicted and a good agreement between our macroscopic model and Andries kinetic model is observed, especially for translational heat flux.

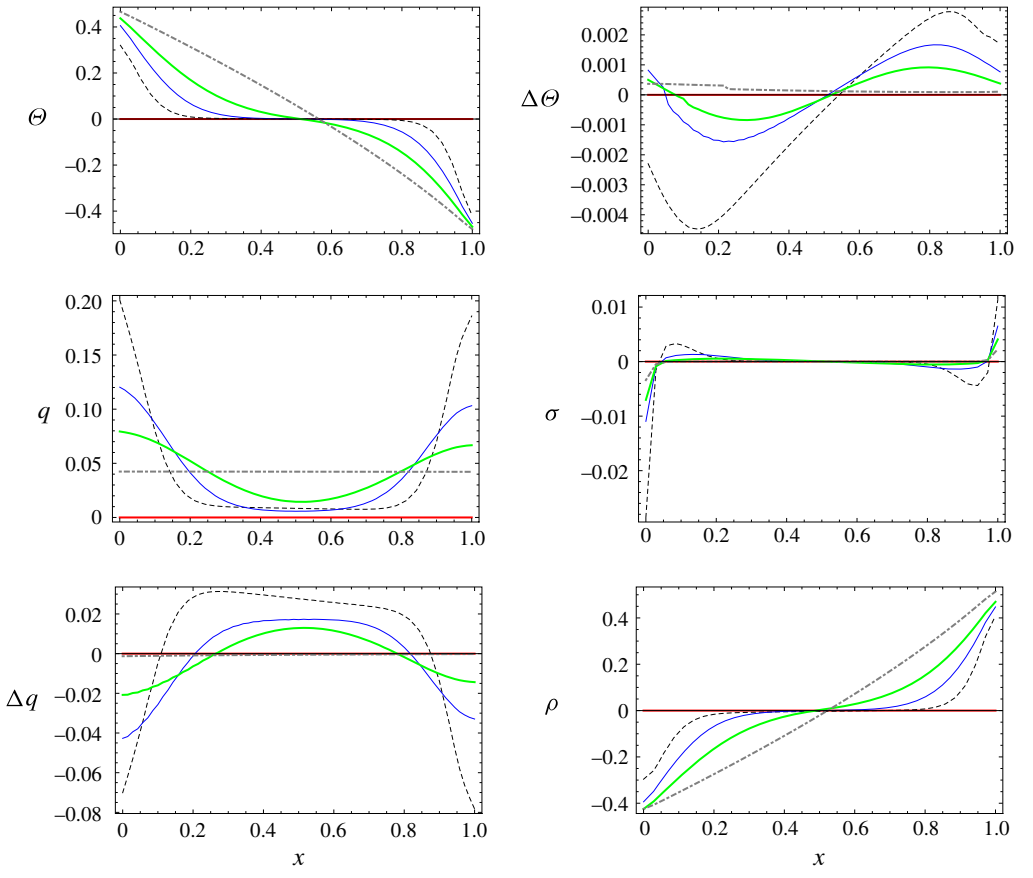


FIGURE 6. (Colour online) Numerical results of stationary heat conduction from set of R19 equations. Red line is at $t = 0$ s; black dashed line is at $t = 0.2$ s; blue thin line is at $t = 0.6$ s; green thick line is at $t = 1.5$ s; grey dot-dashed line is at $t = 29$ s.

In all the comparisons with other methods we have good agreement between results at various Knudsen number values. However, in the cases with fluid flow present, we expect that at high Knudsen numbers, the agreements might not be as good as for the heat transfer case.

### 9.1. *Unsteady state analysis*

The developing profiles from the equilibrium ground state initial condition $\{\rho_0, \theta_0\}$ to the steady state condition are presented for $H_2$ gas in figure 6. Prandtl number is set to 0.69, reference temperature is at 300 K and dimensionless wall temperatures are $\pm 0.5$. The shear viscosity temperature exponent is set to 0.5. Reference time scale is set to be equal to reference internal time scale, $\tau_0 = \tau_{int}$. Therefore, based on (5.8) we have

$$\left.\begin{array}{c} Kn_{tr} = 0.0091 \\ Kn_{int} = 1. \end{array}\right\} \tag{9.1}$$

The results presented in figure 6 are obtained from numerical solution of the R19 equations with the initial conditions of the reference equilibrium state $\{\rho_0, \theta_0\}$. It is

depicted that deviations of total temperature and density rise from zero starting from regions near the walls and gradually, in time, move towards the central region. Other variables start from zero at the initial state and jump to their maximum value first of all as the boundary feels the temperature jump and then start to decay over time to reach their steady state profiles as the boundary effects reach the middle section. As shown in figure 6, the speed of these decays are not constant and their values keep reducing in time as the temperature differences in the fluid decay. The values of non-equilibrium variables at the beginning of the process are an order of magnitude higher than their values in steady state.

### 9.2. *Steady state analysis of various gases*

Next, we analyse an $N_2$ gas. The reference time scale is chosen so that, based on (5.8), we have

$$\left.\begin{aligned} Kn_{tr} &= 0.207 \\ Kn_{int} &= 0.444. \end{aligned}\right\} \tag{9.2}$$

This implies the need for a set of equations with high-order accuracy in both $Kn_{tr}$ and $Kn_{int}$, that is the set of R19 equations. The reference temperature is 400 K and the dimensionless temperature at the walls is $\pm 0.3$. For a $N_2$ gas, the shear viscosity temperature exponent is set to 0.74 and the Prandtl number to 0.69. Figure 7 illustrates the steady state profiles obtained numerically from the R19 and RNSF equations, and analytically from the linear R19 equations. Results from RNSF equations are not in agreement with the R19 profiles, which reflects the fact that at these $Kn$ numbers they are not expected to be accurate. Temperature gradient on the walls and normal heat flux are lower for R19 equations. Here, effects of the gradients of dynamic temperature and stress tensor are in opposition to the gradient of the temperature and reduce the total heat flux. Also, it is evident that the effects of the nonlinear and temperature-dependent properties are more dominant in profiles associated with variables corresponding to internal and translational interactions ($\Delta\theta$ and $\Delta q$), and differ in the analytical and numerical results. The linear and temperature-independent cases produce lower total heat flux and and symmetry profiles in comparison to the unsymmetrical profiles of the full R19 equations.

The effects of a different range of temperatures is studied on a $N_2$ gas in figure 8. We investigate two cases with upper dimensionless wall temperatures at 0.5 and 2.5. The lower wall temperature and reference temperature are kept fixed at 300 K and referenced $Kn$ numbers are fixed at $Kn_{tr} = 0.077$ and $Kn_{int} = 0.2$. As can be seen, the main effect here is the promotion of the non-symmetry effects by the temperature-dependent properties and relaxation times in the case with higher upper wall temperature. This emphasizes the importance of a model with the capability to model temperature-dependent properties in problems with relatively high temperature variations.

Now, we compare three different gases with distinguished characteristics, $H_2$, $N_2$ and $CH_4$, in figure 9. Reference and wall temperatures are fixed at 700 K, 0 and 0.5, respectively. Translational Knudsen number is also kept fixed at 0.032. The corresponding reference $Kn_{int}$ are obtained from (5.8) to be

$$Kn_{int} = \begin{cases} N_2\text{: } 0.158 \\ H_2\text{: } 3.78 \\ CH_4\text{: } 10. \end{cases} \tag{9.3}$$

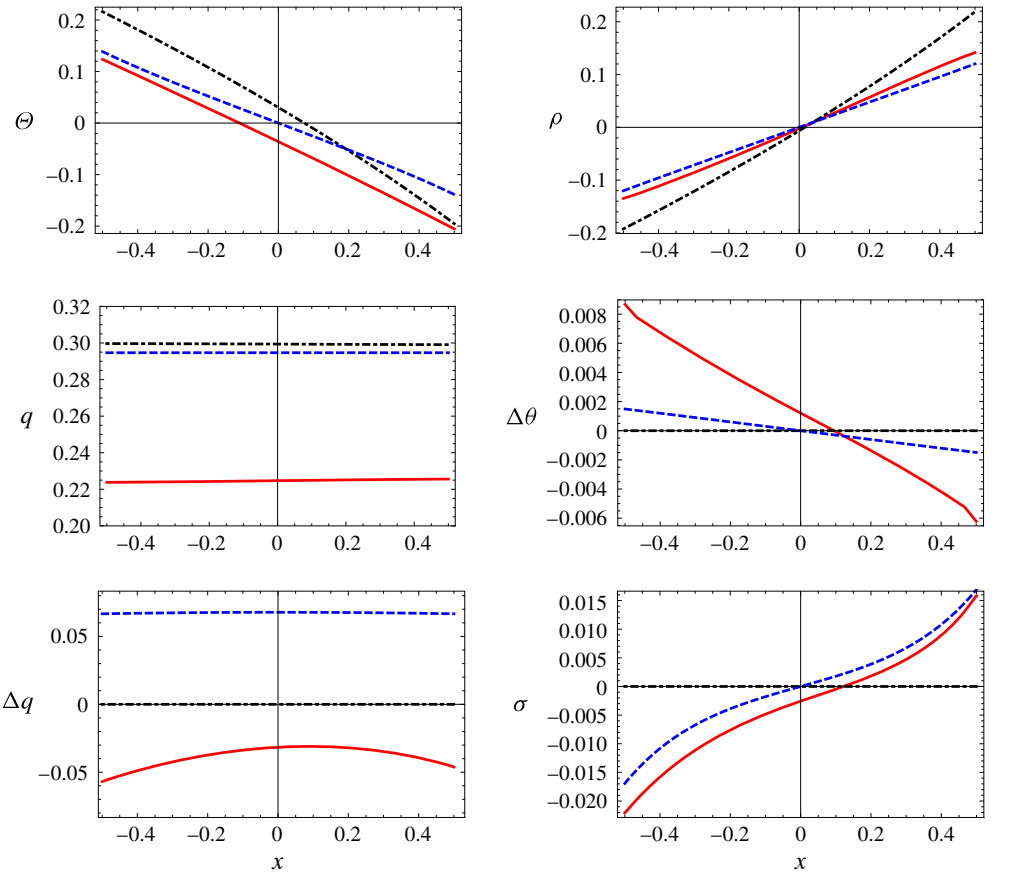


FIGURE 7. (Colour online) Steady state profiles of $N_2$ gas obtained from numerical and analytical methods. Red line: R19-numerical; black dot-dashed line: RNSF-numerical; blue dotted line: R19-analytical.

Number of excited internal DoF at reference temperature of these gases are

$$\delta + \theta \frac{\mathrm{d}\delta}{\mathrm{d}\theta} = \begin{cases} N_2\text{: } 2.41 \\ H_2\text{: } 2.09 \\ CH_4\text{: } 8.89. \end{cases} \tag{9.4}$$

$H_2$ and $CH_4$ gases both have large differences between internal and translational relaxation times. However, internal and translational relaxation times of the $N_2$ gas have comparable values. On the other hand, $H_2$ and $N_2$ gases both have similar excited internal DoF. Nonetheless, excited internal DoF of the $CH_4$ gas is higher than the other two gases. The effects of having internal and translational relaxation times of the same order are seen in profiles of moments corresponding to deviations from total values, $\Delta\theta$ and $\Delta q$, which are derived by translational-internal interactions. These effects promote the temperature dependency of the profiles, which now cover a larger range of values between the two walls. The cases with higher internal *Kn* number have a higher temperature jump. Due to the lower internal relaxation times and more active internal exchange processes in the $N_2$ case, the value of dynamic

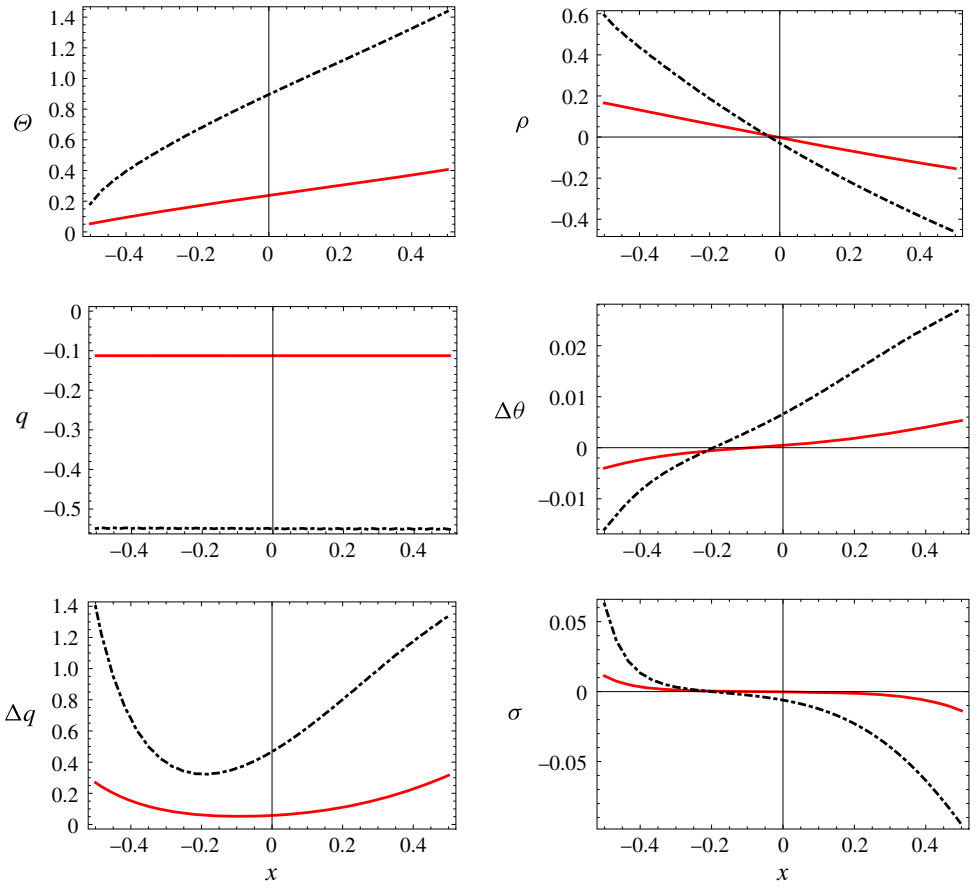


FIGURE 8. (Colour online) Steady state profiles of $N_2$ gas obtained from numerical method with $\theta_{WB} = 0$ and red line: $\theta_{WT} = 0.5$; black dot-dashed line: $\theta_{WT} = 2.5$.

temperature is slightly higher compared to the $H_2$ case. Also, less active internal exchange processes produced higher heat fluxes. The strong effects of different ratios of *Kn* numbers are diminished at low translational Knudsen number. The effects of different internal DoF are most seen in the total heat flux and stress tensor. A $CH_4$ gas with higher DoF gains a higher total heat flux and stress tensor in comparison with other two gases. Also, increasing the internal DoF slightly increases the temperature jump.

Effects of the reference temperature on the variables are studied in figure 10. A $N_2$ gas with fixed reference translational Knudsen number at 0.077 and dimensionless wall temperatures at 0 and 0.5 is used with different reference temperatures of 300 and 700 K. The corresponding reference internal Knudsen numbers are 0.2 and 0.38, respectively. As is depicted in figure 10, the case with a higher reference temperature, which means more excited internal DoF, has a higher heat flux value and flatter deviation moments, $\Delta\theta$ and $\Delta q$, in comparison with the lower reference temperature. Also, there is a slightly higher temperature jump, especially on the bottom wall in the case of the higher reference temperature in comparison with the lower one.

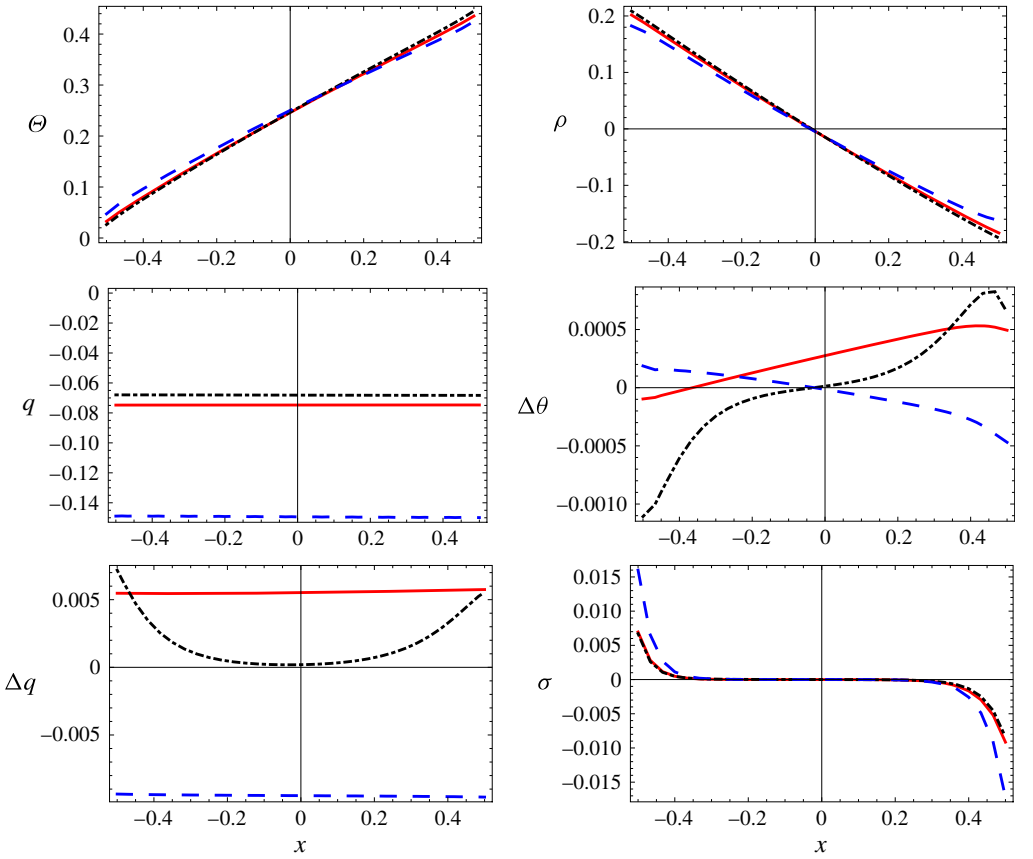


FIGURE 9. (Colour online) Steady state profiles of different gases obtained from numerical solution of the R19 equations. Red line: $H_2$; black dot-dashed line: $N_2$; blue dashed line: $CH_4$.

### 9.3. *Accommodation coefficients analysis*

Effects of the accommodation coefficients are investigated in figure 11. Three cases are shown with different accommodation coefficients,

$$\left.\begin{array}{l}\text{case no. 1: } \chi = 1 \text{ and } \zeta = 1\\ \text{case no. 2: } \chi = 0.5 \text{ and } \zeta = 1\\ \text{case no. 3: } \chi = 1 \text{ and } \zeta = 0.5.\end{array}\right\} \tag{9.5}$$

Case no. 1 is the case with full accommodation. Case nos. 2 and 3 are partial accommodations with full internal and half internal-translational accommodations, respectively. Partial accommodation with full internal accommodation, case no. 2, shows lower temperature and density gradients and heat flux but higher stress tensor in comparison with the fully accommodated case (no. 1). Comparing case nos. 1 and 3 shows that the effects of half internal-translational accommodation are dominant on the dynamic temperature and heat flux difference, which correspond to internal-translational interactions. Its effects are towards a lower temperature gradient and heat flux. The drastic changes in dynamic temperature between case nos. 1 or 2 and 3 are due to differences in the gradient of heat flux difference.

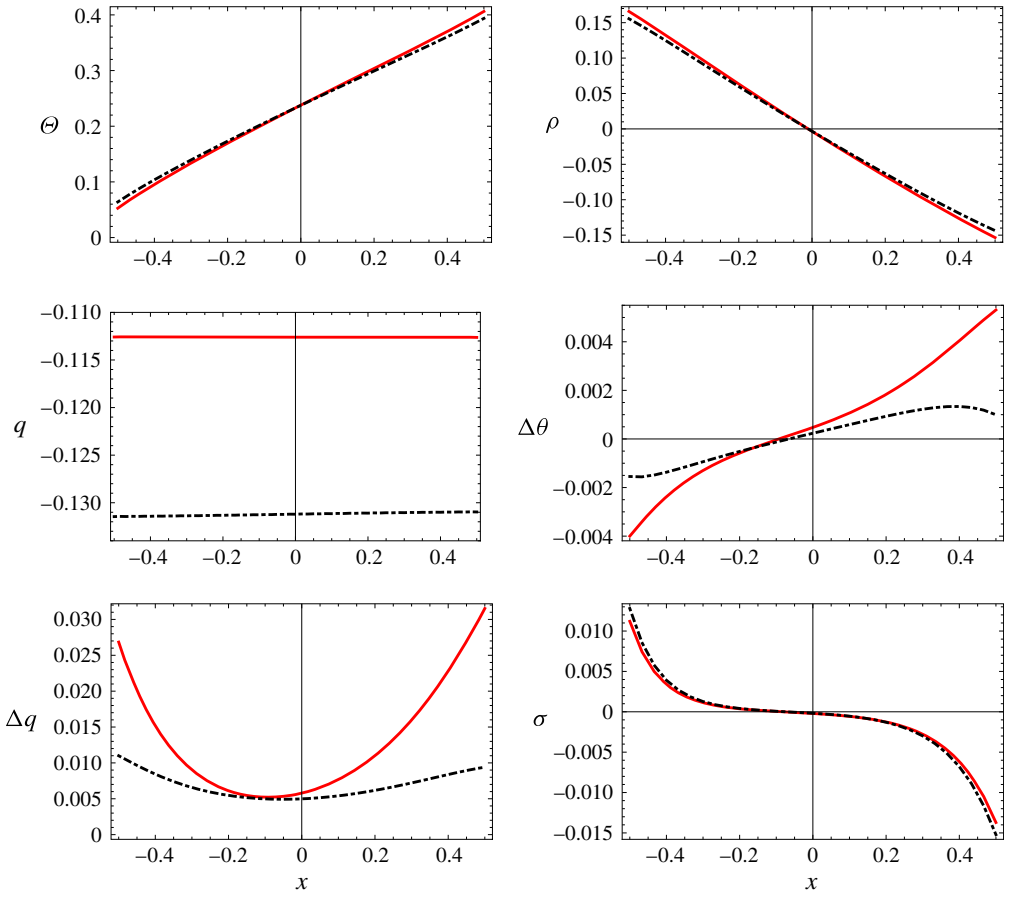


FIGURE 10. (Colour online) Steady state profiles of $N_2$ gas obtained from numerical method of the R19 equations with $\theta_{WB} = 0$ and $\theta_{WT} = 0.5$. Red line: $T_0 = 300$; black dot-dashed line: $T_0 = 700$.

## 10. Conclusions

The present study introduced a new kinetic model and macroscopic model for the accurate description of polyatomic gas flows in the transition regime. Such flows are presents in many applications, e.g. MEMS and partial vacuumed devices. It was depicted that the proposed model offers accurate results and the ability to interpret results in terms of macroscopic quantities. This is achieved with much less computational cost compared to that required for the DSMC simulations. As the first applications of the introduced model, we studied stationary heat conduction.

Polyatomic gases are governed by at least two distinct time scales, the mean free times for processes that exchange only translational energy, or translational and internal energies. We introduced a generalized S-model with the following features:

(i) The model predicts correct relaxation times of higher moments and $Pr$ number.
(ii) The correct relaxation of the model towards equilibrium phase densities for different exchange processes.
(iii) The model conserves the collision invariants.
(iv) The linear H-theorem for the proposed model was proven.

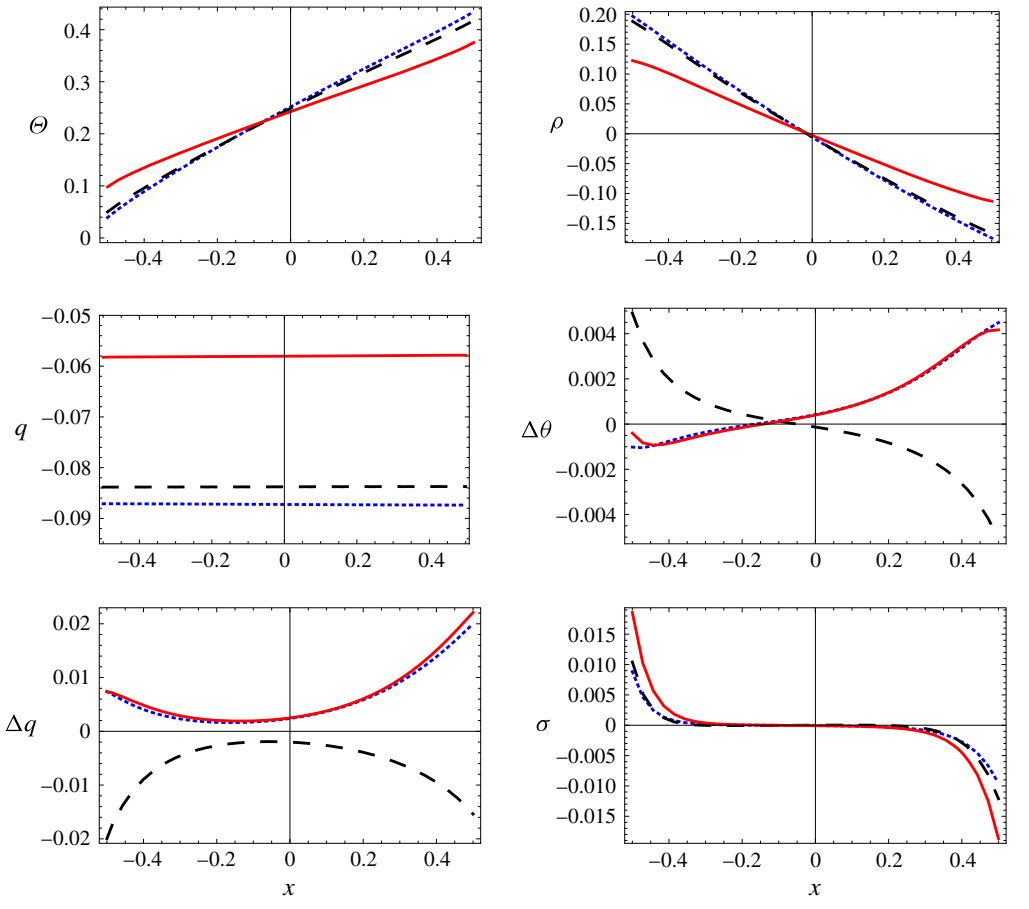


FIGURE 11. (Colour online) Steady state profiles of $N_2$ gases obtained from numerical solution of the R19 equations with $Kn_{tr} = 0.04$ and $Kn_{int} = 0.2$. Blue dotted line: $\chi = 1$ and $\zeta = 1$; red line: $\chi = 1$ and $\zeta = 0.5$; black dashed line: $\chi = 0.5$ and $\zeta = 1$.

Moment equations for the raw 36 moments were obtained from the proposed kinetic equation. We introduced the generalized Grad's distribution function to cover polyatomic gases based on these 36 variables. The proposed distribution function was used to obtain constitutive equations to close the set of 36 moments equations.

Closed system of 36 raw moments was used to optimize the moment definitions. The relations between *Kn* numbers were explored. We obtained orders of all 36 moments in two *Kn* numbers by applying CE expansion on the system of raw moment equations. New optimized moment definitions for polyatomic gases were defined in a way that all the optimized moments are linearly independent at the first order. This ensures that at each order of accuracy, we have the least moment numbers possible. Also, introduced optimized moment definitions are used to obtain the set of optimized 36 moment equations for polyatomic gases.

Model reduction was applied on the set of 36 moment equations and the obtained orders of different optimized moments were used to eliminate higher-order terms and equations at different levels of accuracy. Sets of equations corresponding to $\epsilon^0$, $\epsilon^1$, $\epsilon^2$ and $\epsilon^3$ orders of accuracy were obtained. At the first order of accuracy, a refined

version of the classical NSF equations was obtained, which includes the balance law for the dynamic temperature. At the second order, a refined variant of Grad's 14 moment equations was obtained, which includes some corrections and three extra constitutive equations for $\Delta q_i$, $B^-$ and $B^+$. Finally at the third order, the regularized 19 moment equations (R19) were obtained which consists of 19 PDEs and three constitutive equations. Also, temperature-dependent internal DoF and relaxation times were calculated based on specific heat and shear viscosities, and incorporated into the proposed model. Also, we discussed the changes in the equations due to the ratio of the Knudsen numbers.

We introduced a microscopic boundary condition using same idea that we used to model the two distinguished exchanged processes, internal and translational. In the proposed boundary condition, a portion of the particles hit the wall and accommodate at the wall so that they are reflected with the equilibrium distribution of the wall. The other portion is reflected specularly. For polyatomic particles that are diffusively reflected, we had two Maxwellian-type equilibrium distribution functions, (2.16) and (2.17), corresponding to the translational only energy equilibrium and the total energy equilibrium. Corresponding macroscopic boundary conditions are obtained using the proposed kinetic boundary condition.

We solved unsteady one-dimensional stationary heat conduction numerically and analytically with the set of R19 and RNSF equations and compared the results with DSMC simulations. It was shown that the NSF equations were not accurate in the transition regime. The results from set of R19 equations was in a good agreement with the DSMC simulations and deterministically solved kinetic models. The values of non-equilibrium variables at the beginning of the unsteady process found to be an order of magnitude higher than their values in steady state. Effects of nonlinearity and temperature-dependent properties were more dominant in profiles associated with translational-internal variables ($\Delta\theta$ and $\Delta q$). The importance of our proposed model, with the capability to model temperature-dependent properties, was shown in problems with relatively high temperature variations. The effects of having internal and translational relaxation times of the same order were found to be acting on moments corresponding to deviations from total values, $\Delta\theta$ and $\Delta q$, which were derived by translational-internal interactions. These effects were towards promoting the temperature-dependency effects and the obtained profiles covered a larger range of values. The effects of different internal DoF were most seen in the total heat flux and stress tensor, where gases with higher DoF gain a higher total heat flux and stress tensor in comparison with gases with lower DoF. Higher reference temperature, which means more excited internal DoF, produced higher heat flux values and flatter deviation moment profiles, $\Delta\theta$ and $\Delta q$, in comparison to the lower reference temperature case. Also, different accommodation coefficients are investigated and the drastic effects of $\zeta$ on dynamic temperature and heat flux difference were seen.

## Acknowledgement

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## Appendix A

In the first part of this appendix, we present the formulization of our proposed generalized S-model. Based on the definition of $\{\boldsymbol{q}_{i,tr}, \boldsymbol{q}_{i,int}, u^{2,0}, u^{1,1}\}$ moments, we introduce translational and internal distribution functions by expansion about the

equilibrium Maxwellian functions (2.16) and (2.17) in corresponding polynomials in specular velocity and the particle's internal energy as,

$$f_{tr} = f_{tr_0}\,[1 + (\,a^{0,0} + a_i^{0,0}C_i + a^{1,0}C^2 + a_{ij}^{0,0}C_{<i}C_{j>} + a_i^{1,0}C_iC^2 + a_i^{0,1}C_ie_{int} + a^{1,1}C^2e_{int} + a^{2,0}C^2C^2\,)], \tag{A 1}$$

$$f_{int} = f_{int_0}\,[1 + (b^{0,0} + b_i^{0,0}C_i + b^{1+1}(C^2 + e_{int}) + b_{ij}^{0,0}C_{<i}C_{j>} + b_i^{1,0}C_iC^2 + b_i^{0,1}C_ie_{int} + b^{1,1}C^2e_{int} + b^{2,0}C^2C^2)]\,. \tag{A 2}$$

The unknown coefficients in $f_{tr}$ and $f_{int}$ are obtained based on the conditions that the proposed two term collision model predicts correct relaxation for higher moments by introducing four free relaxation parameters $R_{q_{tr}}$, $R_{q_{int}}$, $R_{u^{2,0}}$, $R_{u^{1,1}}$ as shown in table 2. A similar idea was used by Marques (1999) to introduce a simple polyatomic kinetic model with a single relaxation term. These conditions along with the collision invariants result in coefficients for the translational distribution function as,

$$a_{ij}^{0,0} = 0, \quad a^{0,0} = \frac{(1 - R_{u^{2,0}})(u^{2,0} - 15\rho\theta_{tr}^2)}{8\rho\theta_{tr}^2}, \tag{A 3a}$$

$$a_i^{0,0} = -\left[\frac{(1 - R_{q_{tr}})\boldsymbol{q}_{i,tr} + 2\delta\left(1 - R_{q_{int}}\right)\boldsymbol{q}_{i,int}\dfrac{\rho\theta_{tr}\theta_{int}}{4u^{0,2} - \delta^2\rho\theta_{int}^2}}{\rho\theta_{tr}^2}\right], \tag{A 3b}$$

$$a^{1,0} = \frac{-5(1 - R_{u^{2,0}})\left(u^{2,0} - 15\rho\theta_{tr}^2\right) - 8\delta\rho\theta_{tr}\theta_{int}\,(1 - R_{u^{1,1}})\,\dfrac{u^{1,1} - \frac{3}{2}\delta\rho\theta_{tr}\theta_{int}}{4u^{0,2} - \delta^2\rho\theta_{int}^2}}{60\rho\theta_{tr}^3}, \tag{A 3c}$$

$$a_i^{1,0} = \frac{(1 - R_{q_{tr}})\boldsymbol{q}_{i,tr}}{5\rho\theta_{tr}^3}, \quad a_i^{0,1} = \frac{4\left(1 - R_{q_{int}}\right)\boldsymbol{q}_{i,int}}{4u^{0,2}\theta_{tr} - \delta^2\rho\theta_{int}^2\theta_{tr}}, \tag{A 3d}$$

$$a^{1,1} = \frac{4\,(1 - R_{u^{1,1}})\left(u^{1,1} - \frac{3}{2}\delta\rho\theta_{tr}\theta_{int}\right)}{15\theta_{tr}^2\left[4u^{0,2} - \delta^2\rho\theta_{int}^2\right]}, \tag{A 3e}$$

$$a^{2,0} = \frac{(1 - R_{u^{2,0}})\left(u^{2,0} - 15\rho\theta_{tr}^2\right)}{120\rho\theta_{tr}^4}, \tag{A 3f}$$

and internal distribution function as,

$$b^{0,0} = (6 + \delta)\,\frac{28\,(1 - R_{u^{1,1}})\left[u^{1,1} - \frac{3}{2}\delta\rho\theta^2\right] + (5 - \delta)\,(1 - R_{u^{2,0}})\left[u^{2,0} - 15\rho\theta^2\right]}{8\rho\theta^2\,(30 + \delta\,(3 + \delta))}, \tag{A 4a}$$

$$b_i^{0,0} = -\left[\frac{(1 - R_{q_{tr}})\boldsymbol{q}_{i,tr} + \left(1 - R_{q_{int}}\right)\boldsymbol{q}_{i,int}}{\rho\theta^2}\right], \tag{A 4b}$$

$$b^{1+1} = \frac{-28\,(1 - R_{u^{1,1}})\left[u^{1,1} - \frac{3}{2}\delta\rho\theta^2\right] - (5 - \delta)\,(1 - R_{u^{2,0}})\left[u^{2,0} - 15\rho\theta^2\right]}{2\rho\theta^3\,(30 + \delta\,(3 + \delta))}, \tag{A 4c}$$

$$b_{ij}^{0,0} = 0, \quad b_i^{1,0} = \frac{(1 - R_{q_{tr}})\boldsymbol{q}_{i,tr}}{5\rho\theta^3}, \quad b_i^{0,1} = \frac{2\left(1 - R_{q_{int}}\right)\boldsymbol{q}_{i,int}}{\delta\rho\theta^3}, \tag{A 4d}$$

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

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

In the rest of this appendix we examine some important properties of our proposed model. First, we consider equilibrium. Using the Maxwellian distribution functions, we get

$$\left.\begin{aligned} u^{1,1}_{|E,tr} &= m\iint C^2 e_{int} f_{tr_0} t\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}e_{int} = \frac{3}{2}\delta\rho\theta_{int}\theta_{tr},\\ u^{2,0}_{|E,tr} &= m\iint C^4 f_{tr_0}\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}e_{int} = 15\rho\theta_{tr}^2, \quad \text{and}\\ u^{1,1}_{|E,int} &= m\iint C^2 e_{int} f_{int_0}\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}e_{int} = \frac{3}{2}\delta\rho\theta^2,\\ u^{2,0}_{|E,int} &= m\iint C^4 f_{int_0}\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}e_{int} = 15\rho\theta^2. \end{aligned}\right\} \tag{A 5}$$

In equilibrium we have zero collision term and all moments of the collision term must vanish, e.g. $\boldsymbol{q}_{i,tr} = \boldsymbol{q}_{i,int} = 0$. Therefore, based on (A 1) and (A 2), all the expanding coefficients become zero and we will get $f = f_{tr} = f_{tr_0}$ when we have equilibrium in translational processes only, and $f = f_{int} = f_{int_0}$ when we have equilibrium in both internal and translational processes.

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

$$\left.\begin{aligned} \rho_I &= m\int f_{tr}\,\mathrm{d}\boldsymbol{c} = m\int f\,\mathrm{d}\boldsymbol{c},\\ 0 &= m\iint C_i f_{tr}\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = m\iint C_i f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I,\\ \frac{3}{2}\rho\theta_{tr} &= \frac{m}{2}\iint C^2 f_{tr}\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = \frac{m}{2}\iint C^2 f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I. \end{aligned}\right\} \tag{A 6a}$$

$$\left.\begin{aligned} \rho &= m\iint f_{int}\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = m\iint f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I,\\ 0 &= m\iint C_i f_{int}\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = m\iint C_i f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I,\\ \left(\frac{3}{2}+\frac{\delta}{2}\right)\rho\theta &= m\iint\left(\frac{C^2}{2}+e_{int}\right) f_{int}\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I = m\iint\left(\frac{C^2}{2}+e_{int}\right) f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}I. \end{aligned}\right\} \tag{A 6b}$$

These equalities are satisfied, and the conservation of mass, momentum and energy is guaranteed by using the proposed model.

In the rest of this appendix we prove the linear H-theorem for the proposed kinetic model. It should be pointed out that the nonlinear H-theorem is not proven here. Multiplication of the kinetic equation (2.15*a*) with $-k\ln f$ and subsequent integration over velocities and internal energy give the transport equation for the entropy density. Consequently, the entropy generation is obtained as

$$\begin{aligned}\sum &= -k\int \ln f\, S\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I \\ &= \frac{k}{\tau_{int}}\iint \ln f(f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I + \frac{k}{\tau_{tr}}\iint \ln f(f-f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I \geqslant \boldsymbol{0},\end{aligned} \tag{A 7}$$

non-equality shows that the entropy generation ought to be non-negative. The right-hand side of (A 7) has two terms, first we consider the first term.

We write the first term associated with the internal exchange processes as

$$\begin{aligned}\frac{k}{\tau_{int}}\iint \ln f(f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I \;=\; &\frac{k}{\tau_{int}}\iint \frac{\ln f}{\ln f_{int}}(f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I \\ &+ \frac{k}{\tau_{int}}\iint \ln f_{int}(f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I.\end{aligned} \tag{A 8}$$

Here, the first term on the right-hand side is always positive by structure. Now, we focus on the second term. Considering a near equilibrium situation with small non-equilibrium variables $\boldsymbol{q}_{i,tr}$, $\boldsymbol{q}_{i,int}$, $[u^{1,1}-(3/2)\delta\rho\theta^2]$, $[u^{2,0}-15\rho\theta^2]$, we write $\ln f_{int}$ as,

$$\begin{aligned}\ln f_{int} \;=\; &\ln f_{int_0} + (b^{0,0} + b_i^{0,0}C_i + b^{1+1}(C^2+e_{int}) + b_{ij}^{0,0}C_{<i}C_{j>} \\ &+ b_i^{1,0}C_iC^2 + b_i^{0,1}C_ie_{int} + b^{1,1}C^2e_{int} + b^{2,0}C^2C^2);\end{aligned} \tag{A 9}$$

here, we used the relation $\ln[1+x]=x$ with $x$ being small. Due to the conservation of energy, momentum and mass, we have

$$\left.\begin{aligned}&\iint \ln f_{int_0}(f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I \\ &= \iint \left[\ln\left[\frac{\rho}{m}\frac{1}{(2\pi)^{3/2}\theta^{3/2}}\frac{1}{\Gamma\left(1+\frac{\delta}{2}\right)}\right] - \frac{1}{\theta}\left(\frac{C^2}{2}+e_{int}\right)\right](f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = 0, \\ &\int b^{0,0}(f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = 0, \quad \int b_i^{0,0}C_i(f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = 0, \\ &\text{and} \quad \int b^{1+1}(C^2+e_{int})(f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = 0.\end{aligned}\right\} \tag{A 10}$$

Therefore, remaining terms of the first term of (A 7) are

$$\iint b_i^{1,0}C_iC^2(f-f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}e_{int} \;=\; b_i^{1,0}2R_{q_{tr}}\boldsymbol{q}_{i,tr} = \frac{2R_{q_{tr}}(1-R_{q_{tr}})}{5\rho\theta^3}\boldsymbol{q}_{i,tr}^2, \tag{A 11$a$}$$

$$\iint b_i^{0,1} C_i I^{2/\delta} (f - f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}e_{int} = b_i^{0,1} R_{q_{int}} \boldsymbol{q}_{i,int} = \frac{2R_{q_{int}}(1 - R_{q_{int}})}{\delta\rho\theta^3} \boldsymbol{q}_{i,int}^2, \quad \text{(A 11}b\text{)}$$

which are always positive for $\{R_{q_{tr}}, R_{q_{int}}\} \leqslant 1$ and

$$\begin{aligned} A_1 &= \iint b^{2,0} C^2 C^2 (f - f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}e_{int} = b^{2,0} \left[ R_{u^{2,0}} \left( u^{2,0} - 15\rho\theta^2 \right) \right] \\ &= \frac{20\delta\,(6-\delta)\, R_{u^{2,0}}\,(1 - R_{u^{1,1}}) \left[ u^{1,1} - \frac{3}{2}\delta\rho\theta^2 \right]}{120\delta\rho\theta^4\,(30 + \delta\,(3+\delta))} \left[ u^{2,0} - 15\rho\theta^2 \right] \\ &\quad + \frac{\delta\,(30 - \delta\,(7-\delta))\, R_{u^{2,0}} (1 - R_{u^{2,0}})}{120\delta\rho\theta^4\,(30 + \delta\,(3+\delta))} \left[ u^{2,0} - 15\rho\theta^2 \right]^2, \end{aligned} \quad \text{(A 12)}$$

$$\begin{aligned} A_2 &= \iint b^{1,1} C^2 I^{2/\delta} (f - f_{int})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}e_{int} = b^{1,1} \left[ R_{u^{1,1}} \left( u^{1,1} - \frac{3}{2}\delta\rho\theta^2 \right) \right] \\ &= \frac{480\,(1+\delta)\, R_{u^{1,1}}\,(1 - R_{u^{1,1}})}{120\delta\rho\theta^4\,(30 + \delta\,(3+\delta))} \left[ u^{1,1} - \frac{3}{2}\delta\rho\theta^2 \right]^2 \\ &\quad + \frac{20\delta\,(3-\delta)\, R_{u^{1,1}}\,(1 - R_{u^{2,0}})}{120\delta\rho\theta^4\,(30 + \delta\,(3+\delta))} \left[ u^{2,0} - 15\rho\theta^2 \right] \left( u^{1,1} - \frac{3}{2}\delta\rho\theta^2 \right). \end{aligned} \quad \text{(A 13)}$$

It should be pointed out here that the two relaxation parameters, $R_{q_{tr}}$ and $R_{q_{int}}$, are analogies to the $Pr$ number and their typical values are around 0.6–0.9. We use the Onsager relation due to the coupling between these last two equations as

$$A_1 + A_2 = L_{AB} X_B \cdot X_A, \quad \text{(A 14}a\text{)}$$

with Onsager phenomenological matrix,

$$L_{AB} = \begin{pmatrix} \dfrac{\delta\,(30 - \delta\,(7-\delta))\, R_{u^{2,0}}(1 - R_{u^{2,0}})}{120\delta\rho\theta^4\,(30 + \delta\,(3+\delta))} & \dfrac{20\delta\,(6-\delta)\, R_{u^{2,0}}\,(1 - R_{u^{1,1}})}{120\delta\rho\theta^4\,(30 + \delta\,(3+\delta))} \\ \dfrac{20\delta\,(3-\delta)\, R_{u^{1,1}}\,(1 - R_{u^{2,0}})}{120\delta\rho\theta^4\,(30 + \delta\,(3+\delta))} & \dfrac{480\,(1+\delta)\, R_{u^{1,1}}\,(1 - R_{u^{1,1}})}{120\delta\rho\theta^4\,(30 + \delta\,(3+\delta))} \end{pmatrix}, \quad \text{(A 14}b\text{)}$$

and forces,

$$X_1 = u^{2,0} - 15\rho\theta^2 \quad \text{and} \quad X_2 = u^{1,1} - \tfrac{3}{2}\delta\rho\theta^2. \quad \text{(A 14}c\text{)}$$

The coefficient matrix has proportional non-diagonal terms, non-negative diagonal terms and determinant for $\{R_{u^{1,1}}, R_{u^{2,0}}\} \leqslant 1$. Therefore, we conclude that

$$b^{2,0}[R_{u^{2,0}}(u^{2,0} - 15\rho\theta^2)] + b^{1,1} \left[ R_{u^{1,1}} \left( u^{1,1} - \tfrac{3}{2}\delta\rho\theta^2 \right) \right] \geqslant 0. \quad \text{(A 14}d\text{)}$$

The relaxation parameter, $R_{u^{2,0}}$, has a value of approximately 0.7 for a monatomic gas, as mentioned in table 1. Now that we have proved that the first term on the right-hand side of the entropy production equation (A 7) is non-negative, the second term is now analysed.

We re-write the second term in the entropy production equation (A 7) which is related to translational exchange processes as,

$$\int \ln f (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = \int \frac{\ln f}{\ln f_{tr}} (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I + \int \ln f_{tr} (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I. \quad \text{(A 15)}$$

The first term is always positive by structure. Therefore, we now focus on the second term here. Applying the same technique as we did for $\ln f_{int}$, we will have the $\ln f_{tr}$ as,

$$\ln f_{tr} = \ln f_{tr_0} + (a^{0,0} + a_i^{0,0} C_i + a^{1,0} C^2 + a_i^{1,0} C_i C^2 + a_i^{0,1} C_i e_{int} + a^{2,0} C^2 C^2 + a^{1,1} C^2 e_{int}) \tag{A 16a}$$

$$\ln f_{tr_0} = \ln \left[ \frac{\rho_I}{m} \left( \frac{1}{2\pi\theta_{tr}} \right)^{3/2} \right] - \frac{1}{2\theta_{tr}} C^2. \tag{A 16b}$$

Due to the conservation of the translational energy, momentum and mass, we have

$$\left.\begin{aligned} &\iint \ln f_{tr_0}(f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = \iint \left[ \ln \left[ \frac{\rho_I}{m} \left( \frac{1}{2\pi\theta_{tr}} \right)^{3/2} \right] - \frac{1}{2\theta_{tr}} C^2 \right] (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = 0, \\ &\int a^{0,0}(f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = 0, \quad \int a_i^{0,0} C_i (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = 0 \\ &\text{and} \quad \int a^{1,0} C^2 (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = 0. \end{aligned}\right\} \tag{A 17}$$

Therefore the remaining parts are,

$$\int a_i^{1,0} C_i C^2 (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = \frac{2R_{q_{tr}}(1 - R_{q_{tr}})}{5\rho\theta_{tr}^3} \boldsymbol{q}_{i,tr}^2, \tag{A 18a}$$

$$\int a_i^{0,1} C_i I^{2/\delta} (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = \frac{4R_{q_{int}}(1 - R_{q_{int}})}{\theta_{tr} \left[ 4u^{0,2} - \delta^2 \rho \theta_{int}^2 \right]} \boldsymbol{q}_{i,int}^2, \tag{A 18b}$$

$$\int a^{2,0} C^2 C^2 (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = \frac{R_{u^{2,0}}\,(1 - R_{u^{2,0}})}{120\rho\theta_{tr}^4} \left( u^{2,0} - 15\rho\theta_{tr}^2 \right)^2, \tag{A 18c}$$

$$\int a^{1,1} C^2 I^{2/\delta} (f - f_{tr})\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I = \frac{4R_{u^{1,1}}\,(1 - R_{u^{1,1}})}{15\theta_{tr}^2 \left[ 4u^{0,2} - \delta^2 \rho \theta_{int}^2 \right]} \left( u^{1,1} - \frac{3}{2} \delta \rho \theta_{tr} \theta_{int} \right)^2, \tag{A 18d}$$

which are always non-negative for $\{R_{q_{tr}}, R_{q_{int}}, R_{u^{2,0}}, R_{u^{1,1}}\} \leqslant 1$. Here, based on the obtained Grad 36 (G36) distribution function (B 1) we calculate the moment $u^{0,2}$ to be

$$u_{|G36}^{0,2} = \tfrac{1}{4}(2 + \delta)\rho\theta[(6 + \delta)\theta - 6\theta_{tr}], \tag{A 19a}$$

$$[4u_{|G36}^{0,2} - \delta^2 \rho \theta_{int}^2] = \rho[2\delta\theta^2 + 3\Delta\theta(4\theta - 3\Delta\theta)]. \tag{A 19b}$$

Therefore, both terms in the entropy production inequality are non-negative. It follows from (A 7) that the linear H-theorem is fulfilled as,

$$\sum = -k \int \ln f\, S\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I \geqslant 0 \quad \text{for } \{R_{q_{tr}}, R_{q_{int}}, R_{u^{2,0}}, R_{u^{1,1}}\} \leqslant 1. \tag{A 20}$$

Therefore, the H-theorem demands that the values of relaxation parameters be less than or equal to 1. Also, this agrees with our obtained values of relaxation parameters from fitting to DSMC simulation data, as is shown in § 8.

## Appendix B

Generalized Grad closure for 36 moments is presented in this appendix. Grad (1949, 1958) 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

$$\begin{aligned} f_{|36} = f_{int_0}\,(&\lambda^{0,0} + \lambda_i^{0,0} C_i + \lambda^{1,0} C^2 + \lambda_{\langle ij\rangle}^{0,0} C_{<i} C_{j>} + \lambda^{0,1} e_{int} \\ &+ \lambda_i^{1,0} C_i C^2 + \lambda_i^{0,1} C_i e_{int} + \lambda_{\langle ij\rangle}^{1,0} C^2 C_{<i} C_{j>} + \lambda^{2,0} C^4 \\ &+ \lambda_{\langle ijk\rangle}^{0,0} C_{<i} C_j C_{k>} + \lambda_{\langle ij\rangle}^{0,1} C_{<i} C_{j>} e_{int} + \lambda^{1,1} C^2 e_{int}), \end{aligned} \tag{B 1}$$

where $\lambda_{\langle i_1 i_2 \ldots i_n\rangle}^{S,A}$ are expansion coefficients, which are chosen such that Grad's 36 distribution function reproduces the set of 36 moments, i.e.

$$u_A = m \iint \Psi_A f_{|36}\, \mathrm{d}\boldsymbol{c}\, \mathrm{d}I, \tag{B 2a}$$

with

$$u_A = \{\rho,\ \rho\theta_{tr},\ \rho\theta_{int},\ \boldsymbol{\sigma}_{ij},\ \boldsymbol{q}_{i,tr},\ \boldsymbol{q}_{i,int},\ \boldsymbol{u}_{ij}^{1,0},\ u^{2,0},\ \boldsymbol{u}_{ijk}^{0,0},\ \boldsymbol{u}_{ij}^{0,1},\ u^{1,1}\}, \tag{B 2b}$$

and

$$\begin{aligned} \Psi_A = \Big\{&1,\ C_i,\ \frac{C^2}{3},\ \frac{2}{\delta} e_{int},\ C_{<i} C_{j>},\ \frac{C_i C^2}{2},\ C_i e_{int}, \\ &C_{<i} C_{j>} C^2,\ C^4,\ C_{<i} C_j C_{k>},\ C_{<i} C_{j>} e_{int},\ C^2 e_{int}\Big\}. \end{aligned} \tag{B 2c}$$

The obtained coefficients are

$$\lambda^{0,0} = \frac{4u^{1,1} + u^{2,0}}{8\rho\theta^2} + \frac{5}{8} - \frac{3\,(2+\delta)\,\theta_{tr}}{4\theta}, \tag{B 3a}$$

$$\lambda^{0,1} = -\frac{u^{1,1}}{\delta\rho\theta^3} + \frac{15}{2\delta\theta} - \frac{3\,(5-\delta)\,\theta_{tr}}{2\delta\theta^2}, \tag{B 3b}$$

$$\lambda^{1,0} = -\frac{2u^{1,1} + u^{2,0}}{12\rho\theta^3} - \frac{1}{\theta} + \frac{(9+\delta)\,\theta_{tr}}{4\theta^2}, \tag{B 3c}$$

$$\lambda^{2,0} = \frac{u^{2,0}}{120\rho\theta^4} + \frac{1}{8\theta^2} - \frac{\theta_{tr}}{4\theta^3}, \tag{B 3d}$$

$$\lambda^{1,1} = \frac{u^{1,1}}{3\delta\rho\theta^4} - \frac{3}{2\delta\theta^2} + \frac{(9-\delta)\,\theta_{tr}}{6\delta\theta^3}, \tag{B 3e}$$

$$\lambda_i^{0,0} = -\frac{\boldsymbol{q}_{i,tr} + \boldsymbol{q}_{i,int}}{\rho\theta^2}, \quad \lambda_{\langle ij\rangle}^{1,0} = \frac{\boldsymbol{u}_{ij}^{1,0}}{28\rho\theta^4} - \frac{\boldsymbol{\sigma}_{ij}}{4\rho\theta^3}, \tag{B 3f}$$

$$\lambda_i^{1,0} = \frac{\boldsymbol{q}_{i,tr}}{5\rho\theta^3}, \quad \lambda_i^{0,1} = \frac{2\boldsymbol{q}_{i,int}}{\delta\rho\theta^3}, \tag{B 3g}$$

$$\lambda_{\langle ij\rangle}^{0,0} = -\frac{2\boldsymbol{u}_{ij}^{0,1} + \boldsymbol{u}_{ij}^{1,0}}{4\rho\theta^3} + \frac{(9+\delta)\,\boldsymbol{\sigma}_{ij}}{4\rho\theta^2}, \tag{B 3h}$$

$$\lambda_{\langle ijk\rangle}^{0,0} = \frac{\boldsymbol{u}_{ijk}^{0,0}}{6\rho\theta^3}, \quad \lambda_{\langle ij\rangle}^{0,1} = \frac{\boldsymbol{u}_{ij}^{0,1}}{\delta\rho\theta^4} - \frac{\boldsymbol{\sigma}_{ij}}{2\rho\theta^3}. \tag{B 3i}$$

Grad's distribution function implies a relation between the internal state density, $\rho_I$, total density, $\rho$, and the temperatures, $\theta$ and $\Delta\theta = \theta - \theta_{tr}$ based on (2.6*a*), *viz.*

$$\rho_I = \frac{\rho}{\theta^{1+\delta/2}\Gamma\left(1+\frac{\delta}{2}\right)}\left[\frac{I^{2/\delta}}{\delta}\frac{\delta\theta-(\delta-3)\,\Delta\theta}{\theta}+\frac{2\theta-3\Delta\theta}{2}\right]\exp\left(-\frac{1}{\theta}I^{2/\delta}\right). \quad \text{(B 4)}$$

## Appendix C

Scaled moments equations used in the model reduction procedure are given here as the balance laws for dynamic temperature $\Delta\theta$, stress tensor $\boldsymbol{\sigma}_{ij}$, overall heat flux $q_i$, heat flux difference $\Delta q_i$:

$$\begin{aligned}
&\epsilon^{\alpha}\left[\rho\frac{\mathrm{D}\Delta\theta}{\mathrm{D}t}+\frac{2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\rho\Delta\theta\frac{\partial v_i}{\partial x_i}\right]\\
&+\epsilon^{1}\left[\left(\frac{2}{3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}}-\frac{10R_{q_{int}}}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\right)\frac{\partial q_i}{\partial x_i}\right]\\
&+\epsilon^{1}\left[\frac{10R_{q_{int}}R_{q_{tr}}\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}q_i\frac{\partial\theta}{\partial x_i}-\frac{2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}\right]\\
&-\epsilon^{1+\alpha}\left[\frac{10R_{q_{int}}R_{q_{tr}}\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\Delta q_i\frac{\partial\theta}{\partial x_i}+\frac{2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_i}{\partial x_i}\right]\\
&-\frac{2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3\left(3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\rho\theta\frac{\partial v_i}{\partial x_i}=-\frac{\rho}{\tau_{int}}\Delta\theta, \qquad \text{(C 1}a\text{)}
\end{aligned}$$

$$\begin{aligned}
&\epsilon^{1}\left[\frac{\mathrm{D}\boldsymbol{\sigma}_{ij}}{\mathrm{D}t}-\frac{4R_{q_{int}}R_{q_{tr}}\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}q_{<i}\frac{\partial\theta}{\partial x_{j>}}\right]\\
&+\epsilon^{1}\left[\frac{4R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\frac{\partial q_{<i}}{\partial x_{j>}}+2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}\right]
\end{aligned}$$

$$
\begin{aligned}
&-\epsilon^{\alpha}\left[2\rho\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}\right]+\epsilon^{1+\alpha}\left[\frac{4\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_{<i}}{\partial x_{j>}}\right]\\
&+\epsilon^{1+\alpha}\left[\frac{4R_{q_{int}}R_{q_{tr}}}{\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^{2}}\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\frac{\mathrm{d}^{2}\delta}{\mathrm{d}\theta^{2}}\right)\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}}\right]\\
&+\epsilon^{2}\left[\frac{\partial \boldsymbol{u}^{0,0}_{ijk}}{\partial x_k}\right]+2\rho\theta\frac{\partial v_{<i}}{\partial x_{j>}}=-\left[\frac{1}{\tau_{tr}}+\frac{\epsilon^{1-\alpha}}{\tau_{int}}\right]\boldsymbol{\sigma}_{ij},
\end{aligned}
\tag{C 1b}
$$

$$
\begin{aligned}
&\epsilon^{1}\left[\frac{\mathrm{D}q_i}{\mathrm{D}t}+\theta\frac{\partial\sigma_{ik}}{\partial x_k}+\sigma_{ik}\left(\frac{5+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\frac{\partial\theta}{\partial x_k}-\theta\frac{\partial\ln\rho}{\partial x_k}\right)\right]\\
&+\epsilon^{1}\left[\left(1+\frac{2R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\left[q_k\frac{\partial v_i}{\partial x_k}+q_i\frac{\partial v_k}{\partial x_k}\right]\right]\\
&+\epsilon^{1}\left[\frac{2R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}q_k\frac{\partial v_k}{\partial x_i}+\frac{5}{13}\frac{\partial B^{-}}{\partial x_i}\right]\\
&-\epsilon^{\alpha}\left[\rho\theta\frac{\partial\Delta\theta}{\partial x_i}+\frac{5+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\rho\Delta\theta\frac{\partial\theta}{\partial x_i}\right]\\
&-\epsilon^{2\alpha}\left[\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}\right]\\
&+\epsilon^{1+\alpha}\left[\frac{2\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\left(\Delta q_k\frac{\partial v_i}{\partial x_k}+\Delta q_i\frac{\partial v_k}{\partial x_k}+\Delta q_k\frac{\partial v_k}{\partial x_i}\right)\right]\\
&+\epsilon^{1+\alpha}\left[\frac{168}{(42+25\delta)^{2}}B^{+}_{ij}\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\frac{\partial\theta}{\partial x_j}+\frac{4\delta}{(42+25\delta)}\frac{\partial B^{+}_{ij}}{\partial x_j}+\Delta\theta\frac{\partial\boldsymbol{\sigma}_{ij}}{\partial x_j}\right]\\
&+\epsilon^{1+\alpha}\left[\sigma_{ik}\left(\frac{\partial\Delta\theta}{\partial x_k}+\Delta\theta\frac{\partial\ln\rho}{\partial x_k}\right)\right]+\frac{5+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}\rho\theta\frac{\partial\theta}{\partial x_i}\\
&+\epsilon^{2}\left[7\left(\frac{1}{(14+\delta)^{2}}-\frac{24}{(42+25\delta)^{2}}\right)B^{-}_{ij}\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\frac{\partial\theta}{\partial x_j}-\frac{1}{\rho}\sigma_{ik}\frac{\partial\sigma_{kj}}{\partial x_j}\right]
\end{aligned}
$$

$$+\epsilon^2\left[\frac{7\,(3+\delta)\,(14+3\delta)}{(14+\delta)(42+25\delta)}\frac{\partial B_{ij}^{-}}{\partial x_j}+\boldsymbol{u}_{ijk}^{0,0}\frac{\partial v_j}{\partial x_k}\right]=-\left[\frac{1}{\tau_{tr}}+\frac{\epsilon^{1-\alpha}}{\tau_{int}}\right]$$
$$\times\left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}q_i+\epsilon^{\alpha}\left[\frac{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\Delta q_i\right]\right),\tag{C 1c}$$

$$\epsilon^1\left[\frac{\mathrm{D}\Delta q_i}{\mathrm{D}t}+\sigma_{ik}\left[\frac{\partial\Delta\theta}{\partial x_k}+\Delta\theta\frac{\partial\ln\rho}{\partial x_k}\right]-\varsigma_2\Delta\theta q_i\frac{\partial v_k}{\partial x_k}\right.$$
$$+\frac{\delta}{(42+25\delta)}\varsigma_4\frac{\partial B_{ij}^{+}}{\partial x_j}+\frac{42}{(42+25\delta)^2}\varsigma_4\frac{\mathrm{d}\delta}{\mathrm{d}\theta}B_{ij}^{+}\frac{\partial\theta}{\partial x_j}$$
$$-\varsigma_2\theta\Delta q_i\frac{\partial v_k}{\partial x_k}+\frac{2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\Delta q_j\frac{\partial v_j}{\partial x_i}+\frac{5}{2}\varsigma_3\Delta\theta\frac{\partial\boldsymbol{\sigma}_{ij}}{\partial x_j}$$
$$\left.+\left(\frac{25R_{q_{int}}+7\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\right)\left(\Delta q_i\frac{\partial v_k}{\partial x_k}+\Delta q_k\frac{\partial v_i}{\partial x_k}\right)\right]$$
$$-\epsilon^{\alpha}\left[\frac{5}{2}\varsigma_3\Delta\theta^2\frac{\partial\rho}{\partial x_i}+\frac{5}{2}\varsigma_3\rho\Delta\theta\frac{\partial\Delta\theta}{\partial x_i}+\frac{5}{39}\varsigma_3\frac{\partial B^{+}}{\partial x_i}\right]$$
$$+\epsilon^{1-\alpha}\left[\frac{5}{39}\left(1-\frac{10R_{q_{int}}}{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{-}}{\partial x_i}+\varsigma_2\theta q_i\frac{\partial v_k}{\partial x_k}+\theta\frac{\partial\sigma_{ik}}{\partial x_k}\right.$$
$$+\frac{2R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\left[q_j\frac{\partial v_j}{\partial x_i}+q_i\frac{\partial v_k}{\partial x_k}+q_k\frac{\partial v_i}{\partial x_k}\right]$$
$$\left.+\ \sigma_{ik}\left(\frac{5}{2}\left[1-\frac{R_{q_{int}}}{R_{q_{tr}}}\right]\frac{\partial\theta}{\partial x_k}-\theta\frac{\partial\ln\rho}{\partial x_k}\right)+\varsigma_2\Delta\theta\Delta q_i\frac{\partial v_k}{\partial x_k}\right]$$
$$-\epsilon^2\left[\varsigma_2\left(\frac{\Delta q_i}{\rho}\frac{\partial q_k}{\partial x_k}+\Delta q_i\frac{\sigma_{kl}}{\rho}\frac{\partial v_l}{\partial x_k}\right)\right]+\epsilon^{2-\alpha}\left[\varsigma_2\frac{q_i}{\rho}\frac{\partial q_k}{\partial x_k}+\boldsymbol{u}_{ijk}^{0,0}\frac{\partial v_j}{\partial x_k}-\frac{\sigma_{ik}}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right.$$
$$\left.+\frac{7\,(3+\delta)}{(14+\delta)\,(42+25\delta)}\left(14-\delta-\frac{20\delta R_{q_{int}}}{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\frac{\partial B_{ij}^{-}}{\partial x_j}+\varsigma_2\frac{q_i\sigma_{kl}}{\rho}\frac{\partial v_l}{\partial x_k}\right.$$

$$-\varsigma_1\frac{\mathrm{d}\delta}{\mathrm{d}\theta}B_{ij}^{-}\frac{\partial\theta}{\partial x_j}\Bigg]-\frac{5}{2}\rho\left(\varsigma_3\theta\frac{\partial\Delta\theta}{\partial x_i}-\frac{\left[R_{q_{int}}-R_{q_{tr}}\right]}{R_{q_{tr}}}\Delta\theta\frac{\partial\theta}{\partial x_i}\right)$$
$$-\epsilon^{-\alpha}\left[\frac{5\left[R_{q_{int}}-R_{q_{tr}}\right]}{2R_{q_{tr}}}\rho\theta\frac{\partial\theta}{\partial x_i}\right]=-\left[\frac{1}{\tau_{tr}}+\frac{\epsilon^{1-\alpha}}{\tau_{int}}\right]$$
$$\times\left(\epsilon^{-\alpha}\left[\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}q_i\right]+\frac{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}^2+5R_{q_{int}}^2}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\Delta q_i\right),\quad(\mathrm{C}\,1d)$$

where,

$$\varsigma_1=7\left(\frac{1}{(14+\delta)^2}+\frac{42}{(42+25\delta)^2}+\frac{10R_{q_{int}}}{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\left[\frac{1}{(14+\delta)^2}+\frac{9}{(42+25\delta)^2}\right]\right),\quad(\mathrm{C}\,1e)$$

$$\varsigma_2=\frac{10R_{q_{int}}\left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\left(3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)},\quad(\mathrm{C}\,1f)$$

$$\varsigma_3=\left(1+\frac{3R_{q_{int}}}{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right),\quad(\mathrm{C}\,1g)$$

$$\varsigma_4=\left(7+\frac{15R_{q_{int}}}{\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right).\quad(\mathrm{C}\,1h)$$

Balance laws for higher moments $B^-$ and $B^+$,

$$\epsilon^1\left[\frac{\mathrm{D}B^-}{\mathrm{D}t}+\frac{71}{39}B^-\frac{\partial v_k}{\partial x_k}+\frac{12}{5}\theta\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}\right]$$
$$+\epsilon^1\left[\varsigma_5 q_k\frac{\partial\theta}{\partial x_k}+\frac{12R_{q_{int}}+2\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_k}{\partial x_k}-2\varsigma_6\theta q_k\frac{\partial\ln\rho}{\partial x_k}\right]$$
$$-\epsilon^{2\alpha}\left[\frac{2}{13}B^+\frac{\partial v_k}{\partial x_k}+3\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i}\right]+\epsilon^{1+\alpha}\left[\frac{54\delta}{5(42+25\delta)}B_{ij}^{+}\frac{\partial v_j}{\partial x_i}\right]$$

$$
\begin{aligned}
&+\epsilon^{1+\alpha}\left[2\varsigma_6 q_k\left(\frac{\partial\Delta\theta}{\partial x_k}+\Delta\theta\frac{\partial\ln\rho}{\partial x_k}\right)+\varsigma_7\Delta q_k\frac{\partial\theta}{\partial x_k}\right]\\
&+\epsilon^{1+\alpha}\left[3\Delta\theta\left(\frac{\partial q_k}{\partial x_k}+\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}\right)+\frac{2}{5}\frac{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\theta\frac{\partial\Delta q_k}{\partial x_k}\right]\\
&-\epsilon^{1+\alpha}\left[\varsigma_8\theta\Delta q_k\frac{\partial\ln\rho}{\partial x_k}\right]+\epsilon^{1+2\alpha}\left[\varsigma_8\Delta q_k\left(\frac{\partial\Delta\theta}{\partial x_k}+\Delta\theta\frac{\partial\ln\rho}{\partial x_k}\right)\right]\\
&+\epsilon^{2}\left[\frac{196\,(6+\delta)\,(3+\delta)}{5(14+\delta)(42+25\delta)}B^{-}_{ij}\frac{\partial v_j}{\partial x_i}-2\varsigma_6\frac{q_k}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right]-\epsilon^{2+\alpha}\left[\varsigma_8\frac{\Delta q_k}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right]\\
=&-\left[\frac{1}{\tau_{tr}}+\frac{\epsilon^{1-\alpha}}{\tau_{int}}\right]\left(\frac{10R_{u^{1,1}}+3R_{u^{2,0}}}{13}B^{-}+\epsilon^{2\alpha-1}\left[\frac{3\,(R_{u^{1,1}}-R_{u^{2,0}})}{13}B^{+}\right]\right)\\
&-\epsilon^{2\alpha-1}\left[\frac{1}{\tau_{tr}}\frac{9\,(R_{u^{1,1}}-R_{u^{2,0}})}{2}\rho\Delta\theta^2\right]\\
&-\frac{1}{\tau_{int}}\left(\frac{3}{2}\left(3+\delta+[3-\delta]\,R_{u^{1,1}}-6R_{u^{2,0}}\right)\rho\theta\Delta\theta\right).
\end{aligned}
\tag{C 2a}
$$

$$
\begin{aligned}
&\epsilon^{1}\left[\frac{\mathrm{D}B^{+}}{\mathrm{D}t}+\frac{85}{39}B^{+}\frac{\partial v_k}{\partial x_k}+\varsigma_{13}\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i}\right]+\epsilon^{1-\alpha}\left[\left(26-\frac{78}{3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}\right)\rho\theta\Delta\theta\frac{\partial v_i}{\partial x_i}\right]\\
&+\epsilon^{2-2\alpha}\left[\varsigma_9 q_k\frac{\partial\theta}{\partial x_k}-8\theta\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}+\varsigma_{14}\theta\frac{\partial q_k}{\partial x_k}-\varsigma_{10}\theta q_k\frac{\partial\ln\rho}{\partial x_k}-\frac{20}{39}B^{-}\frac{\partial v_k}{\partial x_k}\right]\\
&+\epsilon^{2-\alpha}\left[\varsigma_{10}q_k\left[\frac{\partial\Delta\theta}{\partial x_k}+\Delta\theta\frac{\partial\ln\rho}{\partial x_k}\right]-\frac{62\delta}{(42+25\delta)}B^{+}_{ij}\frac{\partial v_j}{\partial x_i}+\varsigma_{12}\Delta q_k\frac{\partial\theta}{\partial x_k}\right]\\
&+\epsilon^{2-\alpha}\left[\varsigma_{11}\theta\left(\Delta q_k\frac{\partial\ln\rho}{\partial x_k}-\frac{\partial\Delta q_k}{\partial x_k}\right)-\varsigma_{13}\Delta\theta\left(\frac{\partial q_k}{\partial x_k}+\boldsymbol{\sigma}_{ij}\frac{\partial v_j}{\partial x_i}\right)\right]\\
&-\epsilon^{2}\left[\varsigma_{11}\Delta q_k\left(\frac{\partial\Delta\theta}{\partial x_k}+\Delta\theta\frac{\partial\ln\rho}{\partial x_k}\right)\right]+\epsilon^{3-\alpha}\left[\varsigma_{11}\frac{\Delta q_k}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right]\\
&-\epsilon^{3-2\alpha}\left[\frac{112\,(7-\delta)\,(3+\delta)}{(14+\delta)(42+25\delta)}B^{-}_{ij}\frac{\partial v_j}{\partial x_i}+\varsigma_{10}\frac{q_k}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right]\\
=&-\left[\frac{1}{\tau_{tr}}+\frac{\epsilon^{1-\alpha}}{\tau_{int}}\right]\left(\frac{3R_{u^{1,1}}+10R_{u^{2,0}}}{13}B^{+}+\epsilon^{1-2\alpha}\left[\frac{10}{13}\,(R_{u^{1,1}}-R_{u^{2,0}})\,B^{-}\right]\right)\\
&-\frac{1}{\tau_{tr}}\left(\frac{9}{2}R_{u^{1,1}}+15R_{u^{2,0}}\right)\rho\Delta\theta^2\\
&-\epsilon^{1-2\alpha}\left[\frac{1}{\tau_{int}}\frac{3}{2}\left((3-\delta)\,R_{u^{1,1}}+20R_{u^{2,0}}-(23-\delta)\right)\rho\theta\Delta\theta\right],
\end{aligned}
\tag{C 2b}
$$

where,

$$
\varsigma_5=\left(\frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)+30R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}-\frac{2R_{q_{tr}}R_{q_{int}}\theta\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\right),
\tag{C 2c}
$$

$$\varsigma_6 = 1 + \frac{R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}}, \tag{C 2d}$$

$$\varsigma_7 = \frac{\left(3 + \delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}} \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}} + \frac{2R_{q_{tr}}R_{q_{int}}\theta \left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta} + \theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}\right)^2}, \tag{C 2e}$$

$$\varsigma_8 = \frac{2}{5}\left(1 - \frac{5R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}}\right), \tag{C 2f}$$

$$\varsigma_9 = \left(\frac{50R_{q_{int}}R_{q_{tr}}\theta \left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta} + \theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}\right)^2} + \frac{\left(5R_{q_{int}} + 3R_{q_{tr}}\right)\left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) - 100R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}}\right), \tag{C 2g}$$

$$\varsigma_{10} = \left(2 - \frac{50R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}}\right), \tag{C 2h}$$

$$\varsigma_{11} = \frac{10\left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}}, \tag{C 2i}$$

$$\varsigma_{12} = \left(\frac{\left(-23 + \delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}} \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}} - \frac{50R_{q_{tr}}R_{q_{int}}\theta \left(2\frac{\mathrm{d}\delta}{\mathrm{d}\theta} + \theta\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}\right)^2}\right), \tag{C 2j}$$

$$\varsigma_{13} = \frac{3\left(23 - \delta - \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{3 + \delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}} \tag{C 2k}$$

$$\varsigma_{14} = \frac{2\left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}} - 40R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right) R_{q_{tr}}}. \tag{C 2l}$$

The equations for higher moments $B^{+}_{ij}$, $B^{-}_{ij}$ and $\boldsymbol{u}^{0,0}_{ijk}$,

$$
\begin{aligned}
&\epsilon^1\left[\frac{\mathrm{D}B^{+}_{ij}}{\mathrm{D}t}+\frac{2\,(70+23\delta)\,R_{q_{tr}}\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial\Delta q_{<i}}{\partial x_{j>}}+\Gamma_3\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}}+2B^{+}_{k<i}\frac{\partial v_{j>}}{\partial x_k}\right]\\
&+\epsilon^1\left[\frac{8\delta}{(42+25\delta)}\left(\frac{14}{5}B^{+}_{k<i}\frac{\partial v_k}{\partial x_{j>}}+3B^{+}_{<ij}\frac{\partial v_{k>}}{\partial x_k}\right)\right.\\
&\left.-\frac{(14-\delta)\,\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}-\delta\,(14+\delta)}{\delta\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\Delta\theta\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}\right]\\
&-\epsilon^1\left[(\Gamma_1-1)\,B^{+}_{ij}\frac{\partial v_k}{\partial x_k}+\frac{2\,(70+23\delta)\,R_{q_{tr}}\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\theta\Delta q_{<i}\frac{\partial\ln\rho}{\partial x_{j>}}\right]\\
&+\epsilon^1\left[2\left(\frac{(70+23\delta)\,R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}-\frac{(14-\delta)}{\delta}\right)q_{<i}\left(\frac{\partial\Delta\theta}{\partial x_{j>}}+\Delta\theta\frac{\partial\ln\rho}{\partial x_{j>}}\right)\right]\\
&+\epsilon^{1+\alpha}\left[\frac{2\,(70+23\delta)\,R_{q_{tr}}\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\Delta q_{<i}\left(\frac{\partial\Delta\theta}{\partial x_{j>}}+\Delta\theta\frac{\partial\ln\rho}{\partial x_{j>}}\right)+\Gamma_1B^{+}_{ij}\Delta\theta\frac{\partial v_k}{\partial x_k}\right]\\
&+\epsilon^{1-\alpha}\left[2\left(\frac{(70+23\delta)\,R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}-\frac{(14-\delta)}{\delta}\right)\theta\frac{\partial q_{<i}}{\partial x_{j>}}+\Gamma_2q_{<i}\frac{\partial\theta}{\partial x_{j>}}\right]\\
&+\epsilon^{1-\alpha}\left[4\theta\left(2\sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}}+2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}\right)\right.\\
&\left.+\frac{(14-\delta)\,\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}-\delta\,(14+\delta)}{\delta\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\theta\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}\right]\\
&-\epsilon^{1-\alpha}\left[2\left(\frac{(70+23\delta)\,R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}-\frac{(14-\delta)}{\delta}\right)\theta q_{<i}\frac{\partial\ln\rho}{\partial x_{j>}}\right.
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{4\,(70-19\delta)}{39\delta} B^{-} \frac{\partial v_{<i}}{\partial x_{j>}} \Bigg] \\
&+ \epsilon^{2-\alpha} \left[ \boldsymbol{u}^{0,0}_{ijk} \left( \frac{14+\delta+\dfrac{\delta-14}{\delta}\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2} \frac{\partial\theta}{\partial x_k} - 4\theta \frac{\partial \ln\rho}{\partial x_k} \right) \right. \\
&\left. + \frac{(14-\delta)\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta} - \delta\,(14+\delta)}{\delta\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)} \frac{\boldsymbol{\sigma}_{ij}}{\rho} \frac{\partial q_k}{\partial x_k} \right] \\
&+ \epsilon^{2-\alpha} \left[ \frac{(14-\delta)\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta} - \delta(14+\delta)}{\delta\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)} \frac{\boldsymbol{\sigma}_{ij}\sigma_{kl}}{\rho} \frac{\partial v_l}{\partial x_k} + \frac{784\,(3+\delta)\,\Gamma_1}{84(14+\delta)} B^{-}_{ij} \frac{\partial v_k}{\partial x_k} \right] \\
&- \epsilon^{2-\alpha} \left[ 2 \left( \frac{(70+23\delta)\,R_{q_{int}}}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)} - \frac{(14-\delta)}{\delta} \right) \frac{q_{<i}}{\rho} \frac{\partial \sigma_{j>k}}{\partial x_k} \right] \\
&+ \epsilon^{2-\alpha} \left[ \frac{8(14-\delta)\,(3+\delta)}{(14+\delta)(42+25\delta)} \left( \frac{14}{5} B^{-}_{k<i} \frac{\partial v_k}{\partial x_{j>}} + 3B^{-}_{<ij} \frac{\partial v_{k>}}{\partial x_k} \right) \right] \\
&- \epsilon^{2} \left[ \frac{\Gamma_1}{3(14+\delta)\theta} \left( 3(14+\delta) \frac{B^{+}_{ij}}{\rho} \left[ \frac{\partial q_k}{\partial x_k} - \sigma_{kl} \frac{\partial v_l}{\partial x_k} \right] + 28\,(3+\delta)\, B^{-}_{ij} \Delta\theta \frac{\partial v_k}{\partial x_k} \right) \right] \\
&+ \epsilon^{2} \left[ 4\boldsymbol{u}^{0,0}_{ijk} \left[ \Delta\theta \frac{\partial \ln\rho}{\partial x_k} + \frac{\partial \Delta\theta}{\partial x_k} \right] - \frac{2\,(70+23\delta)\,R_{q_{tr}} \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5\delta\left(5R_{q_{int}} + \left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)} \frac{\Delta q_{<i}}{\rho} \frac{\partial \sigma_{j>k}}{\partial x_k} \right] \\
&+ \epsilon^{3-\alpha} \left[ \frac{784\,(3+\delta)\,\Gamma_1}{84(14+\delta)} \frac{B^{-}_{ij}}{\rho\theta} \left( \sigma_{kl} \frac{\partial v_l}{\partial x_k} + \frac{\partial q_k}{\partial x_k} \right) - 4 \frac{\boldsymbol{u}^{0,0}_{ijk}}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l} \right] \\
&- \epsilon^{\alpha} \left[ \frac{2(42+25\delta)}{39\delta} B^{+} \frac{\partial v_{<i}}{\partial x_{j>}} \right] - \frac{(42+25\delta)}{\delta} \rho\theta\Delta\theta \frac{\partial v_{<i}}{\partial x_{j>}} = - \left[ \frac{1}{\tau_{tr}} + \frac{\epsilon^{1-\alpha}}{\tau_{int}} \right] B^{+}_{ij}, \quad \text{(C 3}a\text{)}
\end{aligned}
$$

$$
\begin{aligned}
&\epsilon^{1} \left[ \frac{\mathrm{D}B^{-}_{ij}}{\mathrm{D}t} - \frac{14+\delta}{3+\delta} \frac{\boldsymbol{\sigma}_{ij}}{\rho} \left[ \frac{\partial q_k}{\partial x_k} + \sigma_{kl} \frac{\partial v_l}{\partial x_k} \right] \right] \\
&- \epsilon^{1} \left[ \frac{22\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{(3+\delta)\,(14+\delta)\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)} B^{-}_{ij} \frac{\partial v_k}{\partial x_k} - \frac{14+\delta+\dfrac{14+\delta}{3+\delta}\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2} + 2B^{-}_{k<i} \frac{\partial v_{j>}}{\partial x_k} \right] \\
&+ \epsilon^{1} \left[ \frac{6(14-\delta)}{(42+25\delta)} \left[ \frac{3}{7} B^{-}_{<ij} \frac{\partial v_{k>}}{\partial x_k} + \frac{2}{5} B^{-}_{k<i} \frac{\partial v_k}{\partial x_{j>}} \right] \boldsymbol{u}^{0,0}_{ijk} \frac{\partial\theta}{\partial x_k} \right]
\end{aligned}
$$

$$
\begin{aligned}
&+\epsilon^1\left[B_{ij}^{-}\frac{\partial v_k}{\partial x_k}+\frac{3(14+\delta)}{7\,(3+\delta)}\theta\frac{\partial \boldsymbol{u}_{ijk}^{0,0}}{\partial x_k}-\frac{3(14+\delta)}{7\,(3+\delta)}\theta\boldsymbol{u}_{ijk}^{0,0}\frac{\partial\,\ln\rho}{\partial x_k}-\Gamma_5\frac{q_{<i}}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_k}\right]\\
&+\epsilon^{\alpha}\left[\frac{14+\delta}{3+\delta}\Delta\theta\sigma_{ij}\frac{\partial v_k}{\partial x_k}+\frac{2\,(70+23\delta)\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial\Delta q_{<i}}{\partial x_{j>}}\right.\\
&\left.+4\Gamma_4\theta\Delta q_{<i}\frac{\partial\,\ln\rho}{\partial x_{j>}}\right]\\
&+\epsilon^{\alpha}\left[\frac{10}{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\Gamma_4\left(\frac{\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5}\left(3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\right.\right.\\
&\left.\left.-\frac{2\theta\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}}\right]\\
&+\epsilon^{\alpha}\left[\frac{6\delta(14+\delta)}{(3+\delta)\,(42+25\delta)}\left(\frac{3}{7}B_{<ij}^{+}\frac{\partial v_{k>}}{\partial x_k}+\frac{2}{5}B_{k<i}^{+}\frac{\partial v_k}{\partial x_{j>}}\right)\right]\\
&+\epsilon^{\alpha}\left[\Gamma_5 q_{<i}\left(\frac{\partial\Delta\theta}{\partial x_{j>}}+\Delta\theta\frac{\partial\,\ln\rho}{\partial x_{j>}}\right)\right]-\epsilon^{2\alpha}\left[4\Gamma_4\Delta q_{<i}\left(\frac{\partial\Delta\theta}{\partial x_{j>}}+\Delta\theta\frac{\partial\,\ln\rho}{\partial x_{j>}}\right)\right]\\
&+\epsilon^{1+\alpha}\left[\frac{3(14+\delta)}{7\,(3+\delta)}\boldsymbol{u}_{ijk}^{0,0}\left(\Delta\theta\frac{\partial\,\ln\rho}{\partial x_k}+\frac{\partial\Delta\theta}{\partial x_k}\right)+4\Gamma_4\frac{\Delta q_{<i}}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_k}\right]\\
&+\epsilon^{1+\alpha}\left[\frac{22\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{(3+\delta)\,(14+\delta)\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\Delta\theta B_{ij}^{-}\frac{\partial v_k}{\partial x_k}\right]-\epsilon^2\left[\frac{3\,(14+\delta)}{7\,(3+\delta)}\frac{\boldsymbol{u}_{ijk}^{0,0}}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l}\right]\\
&-\epsilon^2\left[\frac{22\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{(3+\delta)\,(14+\delta)\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\frac{B_{ij}^{-}}{\rho}\left(\frac{\partial q_k}{\partial x_k}+\sigma_{lk}\frac{\partial v_k}{\partial x_l}\right)\right]\\
&+\frac{2(14+\delta)R_{q_{int}}}{(3+\delta)\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\left(5R_{q_{int}}\left[3+\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right]\right.\\
&\left.+R_{q_{tr}}\left[(3+\delta)\,\delta+(7+2\delta)\,\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}+\left(\left(\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)^2+2\frac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)\theta^2\right]\right)q_{<i}\frac{\partial\theta}{\partial x_{j>}}\\
&+\frac{6(14+\delta)}{7\,(3+\delta)}\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}\boldsymbol{\sigma}_{ij}\frac{\partial v_k}{\partial x_k}\right)\\
&+\Gamma_5\theta\left(\frac{\partial q_{<i}}{\partial x_{j>}}-q_{<i}\frac{\partial\,\ln\rho}{\partial x_{j>}}\right)+\frac{2\,(14+\delta)}{3\,(3+\delta)}B^{-}\frac{\partial v_{<i}}{\partial x_{j>}}=-\left[\frac{1}{\tau_{tr}}+\frac{\epsilon^{1-\alpha}}{\tau_{int}}\right]B_{ij}^{-},
\end{aligned}
\tag{C 3b}
$$

$$\epsilon^1\left[\frac{\mathrm{D}\boldsymbol{u}^{0,0}_{ijk}}{\mathrm{D}t}-3\frac{\sigma_{<ij}}{\rho}\frac{\partial\sigma_{k>l}}{\partial x_l}+\frac{6\,(14-\delta)\,(3+\delta)}{(14+\delta)\,(42+25\delta)}\frac{\partial B^{-}_{<ij}}{\partial x_{k>}}\right]$$
$$-\epsilon^1\left[\left(\frac{6}{(14+\delta)^2}+\frac{252}{(42+25\delta)^2}\right)\frac{\mathrm{d}\delta}{\mathrm{d}\theta}B^{-}_{<ij}\frac{\partial\theta}{\partial x_{k>}}\right]$$
$$+\epsilon^1\left[\boldsymbol{u}^{0,0}_{ijk}\frac{\partial v_l}{\partial x_l}+3u^{0,0}_{l<ij}\frac{\partial v_{k>}}{\partial x_l}\right]+\epsilon^\alpha\left[\frac{6\delta}{42+25\delta}\frac{\partial B^{+}_{,<ij}}{\partial x_{k>}}\right]$$
$$+\epsilon^\alpha\left[\frac{252\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{(42+25\delta)^2}B^{+}_{,<ij}\frac{\partial\theta}{\partial x_{k>}}+3\sigma_{<ij}\left(\frac{\partial\Delta\theta}{\partial x_{k>}}+\Delta\theta\frac{\partial\ln\rho}{\partial x_{k>}}\right)\right]$$
$$+\epsilon^\alpha\left[\frac{12\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\Delta q_{<i}\frac{\partial v_j}{\partial x_{k>}}\right]+3\theta\left(\frac{\partial\sigma_{<ij}}{\partial x_{k>}}-\sigma_{<ij}\frac{\partial\ln\rho}{\partial x_{k>}}\right)$$
$$+\frac{12R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}q_{<i}\frac{\partial v_j}{\partial x_{k>}}=-\left[\frac{1}{\tau_{tr}}+\frac{\epsilon^{1-\alpha}}{\tau_{int}}\right]\boldsymbol{u}^{0,0}_{ijk}. \tag{C 3c}$$

where,

$$\Gamma_1=\frac{84(14+\delta)\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{\delta(14+\delta)\left(3+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)(42+25\delta)}, \tag{C 3d}$$

$$\Gamma_2=2R_{q_{int}}\left(\frac{\left[14+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right]}{5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right.$$
$$\left.-\theta\frac{10\left(7R_{q_{int}}+2\,(7+3\delta)\,R_{q_{tr}}\right)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+14R_{q_{tr}}\theta\left(\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)^2+(70+23\delta)\,R_{q_{tr}}\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\right), \tag{C 3e}$$

$$\Gamma_3=2R_{q_{tr}}\left(\frac{\left(\delta\left[14+\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right]-14\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\right.$$
$$\left.+\frac{2R_{q_{tr}}R_{q_{int}}\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+\theta\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)(70+\delta\,[14+9\theta])}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\right), \tag{C 3f}$$

$$\Gamma_4 = \frac{(14+\delta)\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\,(3+\delta)\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}, \tag{C 3g}$$

$$\Gamma_5 = \frac{2(14+\delta)\left(3R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}{(3+\delta)\left(5R_{q_{int}}+\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}. \tag{C 3h}$$

## Appendix D

The corresponding equations and boundary conditions for the stationary heat conduction are presented here. To avoid complexity, the overbars and hats are dropped in the following dimensionless set of R19 equations describing the considered problem: the balance laws for dynamic temperature $\Delta\theta$, stress tensor $\boldsymbol{\sigma}_{ij}$,

$$(1+\rho)\frac{\partial\Delta\theta}{\partial t}+\left(\frac{2}{3+\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}-\frac{10R_{q_{int}}}{3\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\right)\frac{\partial q}{\partial x}$$
$$-\frac{2\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{3\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q}{\partial x}$$
$$+\frac{10R_{q_{int}}R_{q_{tr}}\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+(1+\theta)\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{3\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}(q-\Delta q)\frac{\partial\theta}{\partial x}=-\frac{(1+\rho)}{\tau_{int}}\Delta\theta, \tag{D 1}$$

$$\frac{\partial\sigma_{11}}{\partial t}+\frac{2}{3}\frac{4R_{q_{int}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\frac{\partial q}{\partial x}+\frac{2}{3}\frac{4\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}$$
$$\times\frac{\partial\Delta q}{\partial x}+\frac{2}{3}\frac{4R_{q_{int}}R_{q_{tr}}\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+(1+\theta)\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}(\Delta q-q)\frac{\partial\theta}{\partial x}+\frac{\partial u^{0,0}_{111}}{\partial x}$$
$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\sigma_{11}, \tag{D 2}$$

overall heat flux $q$, heat flux difference $\Delta q$,

$$\frac{\partial q}{\partial t}+\left(1+\theta+\Delta\theta-\frac{1}{\rho}\sigma_{11}\right)\frac{\partial\sigma_{11}}{\partial x}+\frac{5+\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{2}$$
$$\times\left[(1+\rho)\left[1+\theta-\Delta\theta\right]+\sigma_{11}\right]\frac{\partial\theta}{\partial x}$$

$$+\frac{168}{(42+25\delta)^2}B_{11}^{+}\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\frac{\partial\theta}{\partial x}+\frac{4\delta}{(42+25\delta)}\frac{\partial B_{11}^{+}}{\partial x}-\frac{2}{39}\frac{\partial B^{+}}{\partial x}+\frac{5}{13}\frac{\partial B^{-}}{\partial x}$$
$$+\frac{7\,(3+\delta)\,(14+3\delta)}{(14+\delta)\,(42+25\delta)}\frac{\partial B_{11}^{-}}{\partial x}+\left[\sigma_{11}-(1+\rho)\,[1+\theta+\Delta\theta]\right]\frac{\partial\Delta\theta}{\partial x}$$
$$-\left[\frac{(1+\theta-\Delta\theta)\,\sigma_{11}}{(1+\rho)}+\Delta\theta^2\right]\frac{\partial\rho}{\partial x}+7\left(\frac{1}{(14+\delta)^2}-\frac{24}{(42+25\delta)^2}\right)B_{11}^{-}\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\frac{\partial\theta}{\partial x}$$
$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}q\right.$$
$$\left.+\frac{\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\Delta q\right), \tag{D 3}$$

$$\frac{\partial\Delta q}{\partial t}+\left[\sigma_{11}-\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)(1+\rho)\,(1+\theta+\Delta\theta)\right]\frac{\partial\Delta\theta}{\partial x}$$
$$+\left[\frac{(\Delta\theta-1-\theta)}{1+\rho}\sigma_{11}-\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\Delta\theta^2\right]\frac{\partial\rho}{\partial x}$$
$$+\left[1+\theta+\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{R_{q_{tr}}\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\right)\Delta\theta\right]\frac{\partial\sigma_{11}}{\partial x}$$
$$-\frac{5}{39}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{+}}{\partial x}$$
$$+\frac{5}{39}\left(1-\frac{10R_{q_{int}}}{\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{-}}{\partial x}$$
$$+\frac{\delta}{(42+25\delta)}\left(7+\frac{15R_{q_{int}}}{\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)\frac{\partial B_{11}^{+}}{\partial x}$$

$$+\left(\frac{5}{2}\left[1-\frac{R_{q_{int}}}{R_{q_{tr}}}\right]\left[\sigma_{11}+(1+\rho)\,(1+\theta+\Delta\theta)\right]\right.$$
$$\left.+\frac{42\left(7+\dfrac{15R_{q_{int}}}{\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right)}{(42+25\delta)^2}\frac{\mathrm{d}\delta}{\mathrm{d}\theta}B_{11}^{+}\right)\frac{\partial\theta}{\partial x}$$
$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}q\right.$$
$$\left.+\frac{\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}^2+5R_{q_{int}}^2}{5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\Delta q\right), \tag{D 4}$$

and higher moments $B^+$ and $B^-$,

$$\frac{\partial B^+}{\partial t}-2\,(1+\theta)\left[\frac{\partial q}{\partial x}-\frac{q}{(1+\rho)\,(1+\theta-\Delta\theta)}\frac{\partial\rho\,(\theta-\Delta\theta)}{\partial x}\right]$$
$$=\frac{5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{20R_{q_{int}}-\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\left[-\frac{1}{\tau_{tr}}\left(\frac{9}{2}R_{u^{1,1}}+15R_{u^{2,0}}\right)(1+\rho)\,\Delta\theta^2-\frac{1}{\tau_{int}}\right.$$
$$\left.\times\left(\frac{3}{2}\left((3-\delta)\,R_{u^{1,1}}+20R_{u^{2,0}}-(23-\delta)\right)(1+\rho)\,(1+\theta)\,\Delta\theta\right)-6\,(1+\theta)\,\frac{\sigma_{11}\sigma_{11}}{\mu}\right.$$
$$\left.+\left(\frac{50R_{q_{int}}R_{q_{tr}}\,(1+\theta)\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+(1+\theta)\,\dfrac{\mathrm{d}^2\delta}{\mathrm{d}\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^2}\right.\right.$$

$$+\frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)-100R_{q_{int}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\Bigg)\frac{qq}{\kappa}$$

$$-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{3R_{u^{1,1}}+10R_{u^{2,0}}}{13}B^{+}+\frac{10}{13}\left(R_{u^{1,1}}-R_{u^{2,0}}\right)B^{-}\right)\Bigg]$$

$$-\frac{2\,(1+\theta)}{1+\theta-\Delta\theta}\left[\frac{qq}{\kappa}+\frac{q\Delta q}{\kappa_{\Delta}}\right], \tag{D 5}$$

$$\frac{\partial B^{-}}{\partial t}+2\,(1+\theta)\left[\frac{\partial q}{\partial x}-\frac{q}{(1+\rho)\,(1+\theta-\Delta\theta)}\frac{\partial\rho\,(\theta-\Delta\theta)}{\partial x}\right]$$

$$=\frac{5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{6R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\Bigg[-\frac{1}{\tau_{tr}}\frac{9\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{2}(1+\rho)\,\Delta\theta^{2}$$

$$-\frac{1}{\tau_{int}}\left(\frac{3}{2}\left(3+\delta+[3-\delta]\,R_{u^{1,1}}-6R_{u^{2,0}}\right)(1+\rho)\,(1+\theta)\,\Delta\theta\right)+\frac{9}{5}\,(1+\theta)\,\frac{\sigma_{11}\sigma_{11}}{\mu}$$

$$+\Bigg(\frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)+30R_{q_{int}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}$$

$$-\frac{2R_{q_{tr}}R_{q_{int}}\,(1+\theta)\left(2\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+(1+\theta)\,\dfrac{\mathrm{d}^{2}\delta}{\mathrm{d}\theta^{2}}\right)}{\left(5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^{2}}\Bigg)\frac{qq}{\kappa}$$

$$-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{10R_{u^{1,1}}+3R_{u^{2,0}}}{13}B^{-}+\frac{3\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{13}B^{+}\right)\Bigg]$$

$$+2\frac{(1+\theta)}{(1+\theta-\Delta\theta)}\left[\frac{qq}{\kappa}+\frac{q\Delta q}{\kappa_{\Delta}}\right], \tag{D 6}$$

the constitutive equations for the higher moments $B^{+}_{ij}$, $B^{-}_{ij}$ and $\boldsymbol{u}^{0,0}_{ijk}$,

$$\frac{\dfrac{(1+\rho)\,(1+\theta)}{(70+23\delta)\,R_{q_{int}}}}{\delta\left(5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}-\frac{14-\delta}{\delta}\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]B^{+}_{11}$$

$$=\frac{4}{3}\frac{(1+\theta)\,q}{(1+\theta-\Delta\theta)}\left[\frac{q}{\kappa}+\frac{\Delta q}{\kappa_{\Delta}}\right]$$

$$
\begin{aligned}
&-\frac{4}{3}(1+\theta)\left[\frac{\partial q}{\partial x}-\frac{q}{(1+\rho)(1+\theta-\Delta\theta)}\frac{\partial\rho(\theta-\Delta\theta)}{\partial x}\right]\\
&-\frac{1}{\left(\dfrac{(70+23\delta)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}-\dfrac{14-\delta}{\delta}\right)}\left(\frac{2(70-19\delta)B^{-}+(42+25\delta)B^{+}}{\mu 39\delta}\sigma_{11}\right.\\
&+\frac{(42+25\delta)}{\mu 2\delta}(1+\rho)(1+\theta)\Delta\theta\sigma_{11}-\frac{4\sigma_{11}\sigma_{11}}{(1+\rho)\tau_{tr}}-\frac{4}{3}R_{q_{int}}\frac{qq}{\kappa}\\
&\left[\frac{14+\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}}{5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}\right.\\
&\left.\left.-\frac{10\left(7R_{q_{int}}+2(7+3\delta)R_{q_{tr}}\right)(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+14R_{q_{tr}}\left((1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)^{2}+(70+23\delta)R_{q_{tr}}^{2}(1+\theta)\dfrac{\mathrm{d}^{2}\delta}{\mathrm{d}\theta^{2}}}{\delta\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^{2}}\right]\right.\\
&\left.+\left[\frac{(14-\delta)(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}-\delta(14+\delta)}{\delta\left(3+\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}+\frac{28}{3}\right]\frac{3\left(3+\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}{2\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)\tau_{int}}\Delta\theta\sigma_{11}\right),
\end{aligned}
\tag{D 7}
$$

$$
\begin{aligned}
&\frac{(3+\delta)\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}{(14+\delta)\left(3R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{B_{11}^{-}}{\tau_{tr}}=\frac{4}{3}\frac{(1+\theta)q}{(1+\theta-\Delta\theta)}\left[\frac{q}{\kappa}+\frac{\Delta q}{\kappa_{\Delta}}\right]\\
&-\frac{4}{3}(1+\theta)\left(\frac{\partial q}{\partial x}-\frac{q}{(1+\rho)(1+\theta-\Delta\theta)}\frac{\partial\rho(\theta-\Delta\theta)}{\partial x}\right)\\
&-\frac{(3+\delta)\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}{(14+\delta)\left(3R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{1}{(1+\rho)(1+\theta)\tau_{tr}}\\
&\left[-\frac{3(14+\delta)}{7(3+\delta)}(1+\theta)\sigma_{11}\sigma_{11}-\frac{(14+\delta)}{3(3+\delta)}B^{-}\sigma_{11}-4(14+\delta)R_{q_{int}}\right.\\
&\times\frac{5R_{q_{int}}\left[3+\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right]+R_{q_{tr}}\left[(3+\delta)\delta+(7+2\delta)(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}+\left(\left(\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)^{2}+2\dfrac{\mathrm{d}^{2}\delta}{\mathrm{d}\theta^{2}}\right)(1+\theta)^{2}\right]}{3(3+\delta)\left(5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)^{2}}\\
&\left.\times\frac{2R_{q_{int}}R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}qq\right],
\end{aligned}
\tag{D 8}
$$

$$\frac{u_{111}^{0,0}}{\tau_{tr}} = \frac{9}{5}\frac{(1+\theta)\,\sigma_{11}}{(1+\theta-\Delta\theta)}\left[\frac{q}{\kappa}+\frac{\Delta q}{\kappa_{\Delta}}\right] + \frac{18R_{q_{int}}}{5\left(5R_{q_{int}}+\left(\delta+(1+\theta)\,\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)}\frac{q\sigma_{11}}{(1+\rho)\,(1+\theta)\,\tau_{tr}} - \frac{9}{5}(1+\theta)\left(\frac{\partial\sigma_{11}}{\partial x}-\frac{\sigma_{11}}{(1+\rho)\,(1+\theta-\Delta\theta)}\frac{\partial\rho\,(\theta-\Delta\theta)}{\partial x}\right). \tag{D 9}$$

### D.1. *Boundary conditions*

The corresponding boundary conditions for the stationary heat conduction are as follows: boundary condition for total heat flux,

$$\begin{aligned} q = {} & -n_y\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{(56-\delta\,(1-\zeta))}{312}B^{-}\right. \\ & + (3+\delta)\,\frac{(140+\delta\,(32+\delta)+(14-\delta)\,\delta\zeta)}{4(14+\delta)\,(42+25\delta)}B_{11}^{-} \\ & + \frac{[(1-\zeta)\,\delta-4]}{312}B^{+}+\frac{\delta\,(4-\delta\,(1-\zeta))}{4\,(42+25\delta)}B_{11}^{+}-\frac{(2+\delta\,(1-\zeta))}{4}\theta\,(\rho\Delta\theta-\sigma_{11}) \\ & \left.+\frac{\delta\,(1-\zeta)}{2}\rho\theta^{2}+\frac{\Upsilon}{2}\sqrt{\theta}\,[(4+\delta\zeta)\,(\theta-\theta_{w})-(1-\zeta)\,(\delta\theta+3\Delta\theta)]\right], \end{aligned} \tag{D 10}$$

boundary condition for heat flux difference,

$$\begin{aligned} \Delta q = {} & n_y\frac{\chi}{(2-\chi)R_{q_{tr}}\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{5\,(40-\delta)\,R_{q_{int}}-12\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{312}B^{-}\right. \\ & + \frac{5\,(12+\delta)\,R_{q_{int}}+12\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{312}B^{+}+\frac{10\delta R_{q_{int}}-8\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4}\rho\theta^{2} \\ & + [3+\delta]\,\frac{5\delta\,(42+\delta)\,R_{q_{int}}-6(14-\delta)\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4(14+\delta)(42+25\delta)}B_{11}^{-} \\ & + \frac{5\delta R_{q_{int}}-6\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4}\theta\sigma_{yy}+\frac{5\,(6-\delta)\,R_{q_{int}}+12\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4}\rho\theta\Delta\theta \\ & - \delta\frac{5\,(6+\delta)\,R_{q_{int}}+6\left(\delta+\theta\dfrac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}}{4(42+25\delta)}B_{11}^{+} \\ & \left.+\frac{\Upsilon}{2}\sqrt{\theta}\left[\left(\delta+\theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}V_{s}^{2}-15R_{q_{int}}\,(1-\zeta)\,\Delta\theta\right.\right. \end{aligned}$$

$$- \left(5\delta R_{q_{int}} - 4\left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)\theta$$

$$+ \left(5\delta\zeta R_{q_{int}} - 4\left(\delta + \theta\frac{\mathrm{d}\delta}{\mathrm{d}\theta}\right)R_{q_{tr}}\right)(\theta - \theta_W)\Bigg]\Bigg], \tag{D 11}$$

and, boundary condition for $u^{0,0}_{yyy}$,

$$u^{0,0}_{111} = n_y\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{(-14+\delta)(3+\delta)}{(14+\delta)(42+25\delta)}B^-_{11} - \frac{\delta B^+_{11}}{42+25\delta} - \frac{2(B^+ - B^-)}{195}\right.$$
$$\left. - \frac{7\sigma_{11} + 2\rho\Delta\theta}{5}\theta + \Upsilon\frac{2}{5}\sqrt{\theta}\,[\theta - \theta_W]\right], \tag{D 12}$$

where,

$$\Upsilon = \rho_w\sqrt{\theta_w} = -\frac{(14-\delta)(3+\delta)}{2(14+\delta)(42+25\delta)\theta^{3/2}}B^-_{11} + \frac{1}{156}\frac{B^+ - B^-}{\theta^{3/2}} - \frac{\delta}{2(42+25\delta)\theta^{3/2}}B^+_{11}$$
$$+ \frac{1}{2}\frac{\sigma_{11}}{\sqrt{\theta}} + \frac{1}{2\sqrt{\theta}}\rho(2\theta - \Delta\theta). \tag{D 13}$$

These boundary conditions have to hold on both walls with $n_y = \pm 1$ for the lower and upper wall, respectively.

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