A Macroscopic Approach to Model Rarefied Polyatomic Gas Behavior

by

Behnam Rahimi
B.Sc., Ferdowsi University of Mashhad, 2008
M.Sc., Ferdowsi University of Mashhad, 2011

A Dissertation Submitted in Partial Fulfillment of the
Requirements for the Degree of

DOCTOR OF PHILOSOPHY

in the Department of Mechanical Engineering

A Macroscopic Approach to Model Rarefied Polyatomic Gas Behavior

by

Behnam Rahimi
B.Sc., Ferdowsi University of Mashhad, 2008
M.Sc., Ferdowsi University of Mashhad, 2011

Supervisory Committee

Dr. H. Struchtrup, Supervisor
(Department of Mechanical Engineering)

Dr. B. Nadler, Departmental Member
(Department of Mechanical Engineering)

Dr. F. Herwig, Outside Member
(Department of Physics and Astronomy)

Supervisory Committee

Dr. H. Struchtrup, Supervisor
(Department of Mechanical Engineering)

Dr. B. Nadler, Departmental Member
(Department of Mechanical Engineering)

Dr. F. Herwig, Outside Member
(Department of Physics and Astronomy)

ABSTRACT

A high-order macroscopic model for the accurate description of rarefied polyatomic gas flows is introduced based on a simplified kinetic equation. The different energy exchange processes are accounted for with a two term collision model. The order of magnitude method is applied to the primary moment equations to acquire the optimized moment definitions and the final scaled set of Grad's 36 moment equations for polyatomic gases. The 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 H-theorem. At the first order, a modification of the Navier-Stokes-Fourier (NSF) equations is obtained, which shows considerable extended range of validity in comparison to the classical NSF equations in modeling sound waves. At third order of accuracy, a set of 19 regularized PDEs (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. Attenuation and speed of linear waves are studied as the first application of the many sets of equations. For frequencies were the internal degrees of freedom are effectively frozen, the equations reproduce the behavior of monatomic gases. Thereafter, boundary conditions for the proposed macroscopic model are introduced. The unsteady heat conduction of a gas at rest and steady Couette flow are studied numerically and analytically as examples of boundary value problems. 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 Navier Stokes Fourier equations fails to accurately capture the gas behavior and should be replaced by a higher order set of equations.

Contents

List of Tables

List of Figures

ACKNOWLEDGEMENTS

First I want to express my deepest appreciation to Prof. Henning Struchtrup, for his guidance and support, and the most important, his kindness when I needed it most. I acknowledge his inspirations, encouragements and limitless care.

My deepest gratitude goes to my parents for their love and blessings. I thank my brother, Behrouz, and my nephew, Hirbood, and all my family members, friends and relatives from the bottom of my heart. Without their love, support and help, this work wouldn't be completed.

I deeply acknowledge the support from my friends and colleagues Amin Cheraghi Shirazi, Alireza Akhgar, Mostafa Rahimpour, Fahimeh Moeindarbari, Dr. Amirreza Golestaneh, and Michael Fryer. I would like to thank my teachers at Ferdowsi University of Mashhad (Iran), Prof. Hamid Niazmand and Prof. Mohammad Pasandideh Fard.

I would also like to express my appreciation to various Professors of UVic as well as the technical and administrative staff at Department of Mechanical Engineering who helped me directly or indirectly during my research. I sincerely acknowledge the funding from Natural Sciences and Engineering Research Council (NSERC) of Canada.

DEDICATION

To my mother and father, Elaheh and Rahim. To my brother and nephew, Behrouz and Hirbood. And, to all who showed me kindness.

Chapter 1

Introduction

Find something that you love to do, and find a place that you really like to do it in. I found something I loved to do. I'm a mechanical engineer by training, and I loved it. I still do. My son is a nuclear engineer at MIT, a junior, and I get the same vibe from him. Your work has to be compelling. You spend a lot of time doing it.

Ursula Burns

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

The contemporary kinetic theory of gases starts to form when Maxwell proposed a general transport equation, which gives the changes of macroscopic quantities (density, temperature, velocity) over time as a function of microscopic quantities, and obtained the transport coefficients for a certain type of molecular interaction potential [1], known as Maxwellian potential. In 1872 Boltzmann [2] proposed a transport equation which models the evolution of velocity distribution function over time and space. This equation, known as Boltzmann equation, was a breakthrough in kinetic theory and created a big motivation in the field. Another great achievement in the kinetic theory was established by S. Chapman [3][4] and D. Enskog [5] independently as they studied closing the transport equations of hydrodynamics for the first time. They derived formulations for the stress tensor and energy flux as functions of gradients of hydrodynamic quantities and thus closed the system of hydrodynamic equations. First attempts into considering the effects of internal degrees of freedom on molecules behavior was made by Eucken [6] in 1913. Afterward, Wang Chang and Uhlenbeck [7][8] considered excitation of internal degrees of freedom and proposed a generalized Boltzmann equation, known as the Wang Chang and Uhlenbeck equation. Successful attempts for solving this equation using the Chapman-Enskog method in order to obtain the relations for shear and bulk viscosity and heat conductivity as functions of the relaxation times were made by Monchick et al. [9, 10, 11, 12, 13] and Morse et al. [14][15]. A modified quantum-mechanical Boltzmann equation for gases consisting of molecules with degenerate internal states was proposed by Snider [16] and solved using the Chapman-Enskog method to obtain an expression for the thermal conductivity [17]. Later, solving the Wang Chang and Uhlenbeck equation using the moment equations was considered [18][15]. A. M. Kogan [19] used the entropy maximization to obtain the generalized Grad's 13 moment equations for rough sphere polyatomic gases. The generalized 17-moment equations for polyatomic gases were derived by Zhdanov [20] and McCormack [21] to cover a wider range of physical problem. They also introduced expressions for slip velocity and temperature jump.

More recently, Bourgat et al. [22] introduced a model which uses just one additional continuous internal parameter to represent the internal degrees of freedom of the polyatomic gas and derived the corresponding equilibrium distribution function. Mallinger [23] generalized the Grad's method and derived the 14 moments equations based on Bourgat's model. Desvillettes et al. [24] developed a model for a mixture of reactive polyatomic gases based on Bourgat's model. Kustova, Nagnibeda and co-workers studied the strong vibrational nonequilibrium in diatomic gases [25] and reacting mixture of polyatomic gases for different cases with regards to the characteristic time of the microscopic processes [26, 27, 28, 29] using the Chapman-Enskog method, and derived the first order distribution function and the corresponding governing equations [30]. Andries et al. [31] introduced the ellipsoidal Gaussian BGK model for polyatomic gases considering the additional internal parameter and proved the H-theorem. Brull et al. [32] used the maximization of entropy and obtained the same BGK type model as Andries et al. [31]. Cai and Li [33] extended the NRxx model, introduced in [34][35], to polyatomic gases using the ES-BGK model of Andries et al. [31] and Brull et al. [32].

In the past four years, Ruggeri, Sugiyama and co-workers developed a generalized

14 field theory for polyatomic gases in the context of rational extended thermodynamics [36]. They adopted 14 field variables to construct the theory for the dense gases [37] and showed that the rarefied gas limit of their theory is inconsistent with Mallinger's model [23] of kinetic theory. They studied [38] the dispersion relation for sound and showed that their results have a good consistency with experimental data up to the non-dimensional frequency of 0.1. Also, the equivalency between extended thermodynamics and maximization of entropy was shown in [39] for polyatomic gases. Furthermore, recovering the monatomic gas model as a singular limit of the extended thermodynamics model of the polyatomic gases was studied in [40]. We will show that this 14 field theory is not fully at second order of accuracy. Our proposed third order accurate model is valid at higher Knudsen numbers, where the second order models loose accuracy.

The macroscopic models at higher order in Knudsen number were shown to work well for monatomic gases in the transition regime [41]. One of the newly developed macroscopic models which was shown to work well without being unstable is called the regularized 13 moment (R13) [42][43][44]. This model has third order accuracy in the Kn number, and unlike the super-Burnett equations which are unstable, gives physically meaningful results [45]. The damping and phase speed of ultra sound waves obtained by this method proofed to be accurate [44]. This model gives, even at high Mach numbers, smooth shocks [46] and is linearly stable [42][44]. After the set of R13 equations was completed by boundary conditions [47], several engineering problems were solved successfully both analytically and numerically. Couette and Poiseuille flow were solved for flat [48], cylindrical [49][50] and annular channels [51] geometries. Also, the transpiration flow was solved for both linear and non-linear cases [52]. Furthermore, this model captures Knudsen boundary layers [53]. The set of R26 were derived by Gu and Emerson [54] and solved for similar problems [55][56]. The numerical results of the R13 equations are obtained for heat transfer in partial vacuum in a micro cavity and the lid driven cavity [57][58]. Recently, the R13 equations for monatomic gases consists of hard sphere molecules are studied in [59]. All these good results are obtained for monatomic gases. However, realistic gases are polyatomic, and having the same results for polyatomic gases is a perfect tool to incorporate in design processes.

The present thesis aims at introducing a rigorous macroscopic models for rarefied polyatomic gases which is obtained from our introduced kinetic model. In order to obtain such a model we developed a model based on meeting the following requirements:

1. be stable,
2. ability to capture Knudsen boundary layers and predict correct relaxation of higher moments,
3. clearly obtained definition of moments which could construct the model's field of variables at it's minimized number,
4. explicitly shown number of the field variables need to be considered for different levels of accuracy based on power of the Knudsen number,
5. have high order of accuracy. Specifically, higher than existing first, NSF, and second order, G14, theories,
6. model the different exchange processes between particles based on their characteristics microscopic time scale and at the same time, have a nice, firm and simple mathematical structure.

The Chapman-Enskog method at higher order expansions, second or higher, usually yields unstable equations [60][61]. Therefore, the first item in the list eliminates the use of Chapman-Enskog method and bring the stable Grad's moment method [62][63] into attention. However, the items 2 and 3 imply the need of a more genuine model which satisfies all the requirements. This means that the regularization method [42][43][44] should be applied and generalized to cover the polyatomic gasses. The regularization method have another advantage over the Grad's moment method, the Knudsen number is related to the model and the moment set needs to be considered for a given order is clear which is the item 4 in the list. In the procedure of regularization, as shortly will be described, the minimal number of the moments is assured and item 3 is satisfied. Regarding item 6 in the list, our introduced kinetic equation models the exchange processes under two different time scales, using a two term collision operator. Furthermore, we use a continuous internal energy parameter to model the internal degrees of freedom, instead of having discrete internal energy levels. This is also used by other researchers too [22, 24, 31, 32]. Also, a generalized BGK type collision model [64] [65] is introduced in the kinetic model for having a nice and simple structure of the Boltzmann collision term to enable us to investigate the model reduction at high orders. These considerations would satisfy the requirements in item 6.

Our proposed kinetic model, which is an extension of the Rykov and Shakov models [65, 66], predicts correct relaxation of heat fluxes and delivers the accurate Prandtl number. Compared to the BGK, Shakov and Rykov model, in the model proposed here the number of free relaxation parameters is increased to 4 to allow proper higher moment relaxation times. The proposed model has a proven H-theorem. Also, we incorporated the temperature variation of internal degrees of freedom into the model. Furthermore, based on experimental data of shear and bulk viscosities, the relaxation times in the proposed model are temperature dependent too.

Our proposed macroscopic models are derived from this kinetic model. The order of magnitude method [43][67][68][59] is used to obtain macroscopic models and derive the regularized set of equations. The procedure of this method is as follows,

1. Construct infinite moments hierarchy: A system of moment equations using the Grad's method with arbitrary choice of definition and number of moments is constructed.

2. Reconstructing moments: Apply the Chapman-Enskog 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.

3. Full set of equations: Using the equations of old moments definition, the set of new moments equations is constructed. Apply the Chapman-Enskog on the new moments and determine their leading order.

4. Model reduction: The full set of equations is rescaled considering the obtained order of the new moments. Then, the model could be reduce to any wanted order of accuracy.

The proposed kinetic model and macroscopic models, and results obtained from the models are all original contributions. Our proposed macroscopic model, extends the level of accuracy of common macroscopic models, e.g. first order and second order models mentioned above, for polyatomic gases. We will show that results obtained from our models are valid in transition regime, where the first order models, e.g. Navier Stokes Fourier equations, and second order equations loose validity.

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 S-BGK type model is introduced along with derivation of equilibrium distribution functions and H-theorem. From introduced general moments equation for polyatomic gases, the system of Grad's 36 moments equations is constructed in chapter 3, which is item 1 in the above list. The Chapman-Enskog procedure is applied, leading order terms are determined and the new set of moments is reconstructed in chapter 4, which is item 2 in the list. The full set of new moments equation, item 3 in the list, is obtained in chapter 5. Model reduction, item 4 in the list, performed in the chapter 5 leads to the regularized equations for different order of accuracy. The linear wave analysis for different sets of regularized equations is discussed in chapter 6. The dispersion and damping coefficients of high frequency sound waves for different sets of equations are compared. The theory of microscopic boundary condition is given in Chapter 7 and the corresponding macroscopic boundary conditions are given in subsequent chapters. Chapters 8 and 9 are dedicated to solving boundary value problems and analyzing different effects on the flow field, e.g. Knudsen numbers and degrees of freedom. Chapter 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 model are compared with DSMC simulations to show the good accuracy of the proposed model. Also, it is shown that Navier–Stokes–Fourier equations could not produce accurate results. Analysis of Couette flow is done in Chapter 9. The linear system of equations is solved analytically and the effect of Kn numbers, internal degrees of freedom, Pr number, and accommodation coefficients on the behavior of the Couette flow is investigated. Final conclusions and recommendations are given in Chapter 10.

Chapter 2

Kinetic model

There are those who work all day. Those who dream all day. And those who spend an hour dreaming before setting to work to fulfill those dreams. Go into the third category because theres virtually no competition.

Steven J Ross

In this chapter, we present the kinetic theory of polyatomic gases and will introduce our kinetic model for modeling polyatomic gases and explore some of its properties.

2.1 Kinetic theory of polyatomic gases

The number of independent variables which are required to specify the full state of a system is called the degree of freedom of that system. A particle in space can move independently in three directions. Therefore, there are three translational degrees of freedom associated with any gas molecule in free flight. Besides the translational degrees of freedom, there are other degrees of freedom due to internal energy of molecules. These degrees of freedom may be divided into two categories based on rotational and vibrational movements of the molecules. For example, a diatomic gas could have rotational movements around two axes, the ones perpendicular to the connecting line between two atoms [69] and a vibrational degree of freedom in the direction of the connecting line. Therefore, a diatomic gas has six degrees of freedom. However, one should keep in mind that based on quantum mechanic analysis, spaces between the energy levels of vibration and other kinds of molecular energy are big and usually at room temperature the vibrational levels of internal energy are frozen

[69].

State of molecules changes due to interaction between molecules (collisions). Energy and momentum are conserved, but exchange between different energy forms and particles. 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 the internal energy is exchanged as well. These differences and their relation to the reference or macroscopic time scale is a key feature for defining the state of a gas as being in non-equilibrium or equilibrium. In cases when there are two different characteristic time scales, one smaller than and the other one comparable to the macroscopic time scale, both rapid equilibrium and slow non-equilibrium processes would be present in the gas. The rapid processes are in equilibrium state at the macroscopic time scale, due to the fact that lots of collisions with rapid processes occur in the time needed for any changes in the dynamics of the gas. Also, all the processes with characteristics time much larger than macroscopic time scale would be assumed to be frozen during the macroscopic time scale.

A collection of numerous interacting particles is called gas in kinetic theory. One mole of gas at reference temperature and pressure of 273.15 K and 1 atmosphere will have numer of molecules equal to Avogadro number ($N_A = 6.022 \times 10^{23}$) and occupies a volume of $2.2 \times 10^{-2}\ m^3$. These particles are described by their position, x_i, velocity, c_i, and their internal energy, e_{int}, at any given time. Each molecule could be described by this 7-dimensional space known as phase space at time, t. Using continuos spectrum internal energy, which is a simplified model where all degrees are fully developed or frozen, the internal energy is defined as

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

I is internal energy parameter which is non-negative; δ is the number of non-translational degrees of freedom of the gas. By introducing the particle or velocity distribution function $f(\mathbf{x}, \mathbf{c}, e_{int}, t)$, the number of molecules in a phase space element $dx_1dx_2dx_3dc_1dc_2dc_3de_{int}$ is computed as

$$dN = f(\mathbf{x}, \mathbf{c}, e_{int}, t)d\mathbf{x}d\mathbf{c}de_{int}\ . \tag{2.2}$$

The evolution of particle distribution functions is determined by the Boltzmann equation, which is a nonlinear integro-differential equation written in the absence of external forces, as

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

The left and right-hand sides take into account the effects of the particles free flight and particles collisions, respectively. The quadratic collision term,

$$S = \sum_{\alpha_1,\alpha',\alpha'_1} \int \left(f_{\alpha'} f_{\alpha'_1} - f_\alpha f_{\alpha_1} \right) \ \sigma_{\alpha\alpha_1}^{\alpha'\alpha'_1} g \ d\mathbf{\Omega} \ dc_1 \ ,$$

would take different complex forms which is difficult to work with and costly in computing resources [70, 30]. Here, α and α_1 denotes the incoming particles before collision, α' and α'_1 are denotes particles after collision, σ is the differential cross section, g is relative velocity of the incoming particles, and $d\mathbf{\Omega}$ is the element of solid angle. Therefore, having simpler models to replace the Boltzmann collision term which could preserve the basic relaxation properties and give the correct transport coefficients is more of our interest.

2.2 Kn number

Processes in kinetic theory are characterized by a dimensionless parameter called the Knudsen number,

$$Kn = \frac{\lambda}{L} = \frac{\tau}{\tau_0} \ , \tag{2.4}$$

L is the characteristic length scale of the process and λ is the mean-free path of gas particles. τ is the relaxation time of the microscopic exchange processes. In dimensionless form of the Boltzmann equation, relaxation time (microscopic time scale) is non-dimensionalized by dividing by a typical reference or macroscopic time of the process τ_0. This dimensionless time presents the Knudsen number. When Kn number is small, we are at hydrodynamic regime and continuum assumption is valid. As the mean-free path becomes comparable with the characteristic length, which means less collisions, we are in the transition regime and the continuum assumption starts to break down and particle-based methods need to be employed. In this situation, the flow is in rarefied state and one has either to solve the Boltzmann equation, or develop advanced macroscopic models that include rarefaction effects. When the mean-free path becomes longer than the characteristic length, we are in the free molecular flow, which means very rare or none collisions.

There are several applications that illustrate comparable mean-free path and the characteristic length [71, 72, 73, 74]. At the small scale devices, e.g. MEMS, the characteristics length becomes comparable to the mean free length, which for air at standard condition is around 0.1 μm. Vacuum devices have large mean free path due to low density, e.g. mean free path is around 1 mm at pressure of 10^{-4} Pa. Also, at high altitude applications we have large mean free path as the air becomes dilute. Decrease of density and increase of mean free path with increasing altitude is a exponential function, the mean free path gain the values around 0.1 and 100 m at 100 and 200 km elevations.

2.3 Macroscopic quantities

The macroscopic properties such as mass density, momentum, energy, and pressure are moments of phase density. Other than that, there are other moments that have physical interpretations, e.g., pressure tensor and heat flux vector. Based on the definition of the trace free part of the central moments,

$$\begin{aligned} u^{\varsigma,A}_{i_1...i_n} &= m\int\int (e_{int})^A C^{2\varsigma} C_{<i_1}C_{i_2}...C_{i_n>} f_e d\mathbf{c} de_{int} \\ &= m\int\int (I^{\frac{2}{\delta}})^A C^{2\varsigma} C_{<i_1}C_{i_2}...C_{i_n>} f d\mathbf{c} dI \ , \end{aligned} \quad (2.5)$$

where

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

and due to substitution $e_{int} \rightarrow I$,

$$f = \frac{2}{\delta} I^{\frac{2}{\delta}-1} f_e \ .$$

The basic and most important moments are:

$$\text{Density} \quad \rho = m\int\int f d\mathbf{c} dI = \int \rho_I dI = u^{0,0} \ , \tag{2.6a}$$

$$\text{Velocity} \quad \rho v_i = m\int\int c_i f d\mathbf{c} dI \quad \text{or } 0 = m\int\int C_i f d\mathbf{c} dI = u_i^{0,0} \ , \tag{2.6b}$$

$$\text{Stress} \quad \sigma_{ij} = m\int\int C_{<i}C_{j>} f d\mathbf{c} dI = u_{ij}^{0,0} \ , \tag{2.6c}$$

$$\text{Translational energy} \quad \rho u_{tr} = \frac{3}{2}p = m\int\int \frac{C^2}{2} f d\mathbf{c} dI = \frac{1}{2}u^{1,0} \ , \tag{2.6d}$$

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

$$\text{Translational heat flux} \quad q_{i,tr} = m\int\int C_i \frac{C^2}{2} f d\mathbf{c} dI = \frac{1}{2}u_i^{1,0} \ , \tag{2.6f}$$

$$\text{Internal heat flux} \quad q_{i,int} = m\int\int C_i I^{2/\delta} f d\mathbf{c} dI = u_i^{0,1} \ . \tag{2.6g}$$

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

The classical equipartition theorem states that in thermal equilibrium, each degree of freedom contributes an energy of $\frac{1}{2}\theta$ to the energy of particle, where $\theta = \frac{k_b}{m}T$ is temperature in specific energy units [44]. Thus in equilibrium, the translational and internal energies are

$$u_{tr|E} = \frac{3}{2}\theta \quad \text{and} \quad u_{int|E} = \frac{\delta}{2}\theta \ . \tag{2.7}$$

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

$$u_{tr} = \frac{3}{2}\theta_{tr} \quad \text{and} \quad u_{int} = \frac{\delta}{2}\theta_{int} \ . \tag{2.8}$$

With these definitions, the ideal gas law in non-equilibrium reads $p = \rho\theta_{tr}$. The total thermal energy, $u = u_{int} + u_{tr}$, is defined as the sum of the internal and translational energies, and we use the equipartition theorem to define the overall temperature θ as

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

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

2.4 BGK model

One of the models to replace Boltzmann equation's quadratic collision term is the BGK model [64] which was introduced by Bhatnagar, Gross and Krook for monatomic gases. This model is based on relaxation towards Maxwellian distribution and is written as

$$S = \frac{1}{\tau}\left(\mathcal{M} - f\right) \ . \tag{2.10}$$

Here, the Maxwellian $\mathcal{M}$ is the distribution function at equilibrium state and τ is the characteristic time (mean free time).

As discussed earlier, there are many different processes with distinct time scales for polyatomic gases [30]. While translational energy is exchanged in all collisions, internal energy is exchanged only in some collisions, due to details of molecular interaction, and leads to different time scales. Our model considers continuous internal states, and all the internal exchange processes are modeled to relax by only a single characteristic relaxation time, τ_{int}. This implies restriction on our model, specially at higher temperatures where distance of the energy levels between internal states are considerable and the assumption of one continuous internal state is not feasible. For description of these exchanges we use a two term BGK-type collision operator following [75]. The first term, indicated by subscript tr, represents the translational energy exchange during the collisions. The second one, indicated by subscript int, models the exchange of the internal energy between colliding molecules. Therefore,

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

Table 2.1: Maxwell molecules's relaxation times.

Gas	H_2	N_2	CO_2	CO	CH_4
Pr	0.69	0.72	0.76	0.74	0.72

Table 2.2: Prandtl number of different gases at temperature of 300 K.

the Boltzmann equation can be written as,

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = S_{tr} + S_{int} \ , \tag{2.11a}$$

$$S_{tr} = -\frac{1}{\tau_{tr}}(f - f_{tr}) \ , \tag{2.11b}$$

$$S_{int} = -\frac{1}{\tau_{int}}(f - f_{int}) \ . \tag{2.11c}$$

Here, τ_{tr} and τ_{int} are the corresponding mean free times that we assume to depend only on the macroscopic equilibrium variables (ρ, θ). Also, f_{tr} and f_{int} are equilibrium distribution functions that describe the different equilibria to which the distribution function will relax due to the collisions; they depend on the collisional invariants. The maximum entropy principle will be used to obtain these equilibrium distribution functions in section 2.7.

2.5 General moment equation

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

$$\frac{Du^{\varsigma,A}_{i_1\ldots i_n}}{Dt} + 2\varsigma u^{\varsigma-1,A}_{i_1\ldots i_n k}\frac{Dv_k}{Dt} + 2\varsigma u^{\varsigma-1,A}_{i_1\ldots i_n kj}\frac{\partial v_j}{\partial x_k} + \frac{n}{2n+1}2\varsigma u^{\varsigma,A}_{j<i_1\ldots i_{n-1}}\frac{\partial v_j}{\partial x_{i_n>}}$$
$$+\frac{\partial u^{\varsigma,A}_{i_1\ldots i_n k}}{\partial x_k} + 2\varsigma\frac{n+1}{2n+3}u^{\varsigma,A}_{<i_1\ldots i_n}\frac{\partial v_{k>}}{\partial x_k} + \frac{n}{2n+1}\frac{\partial u^{\varsigma+1,A}_{<i_1\ldots i_{n-1}}}{\partial x_{i_n>}}$$
$$+2\varsigma\frac{n}{2n+1}u^{\varsigma,A}_{<i_1\ldots i_{n-1}}\frac{Dv_{i_n>}}{Dt} + \frac{n-1}{2n-1}nu^{\varsigma+1,A}_{<i_1\ldots i_{n-2}}\frac{\partial v_{i_{n-1}}}{\partial x_{i_n>}} + nu^{\varsigma,A}_{<i_1\ldots i_{n-1}}\frac{Dv_{i_n>}}{Dt}$$
$$+u^{\varsigma,A}_{i_1\ldots i_n}\frac{\partial v_k}{\partial x_k} + \frac{n}{2n+1}\frac{n-1}{2n-1}2\varsigma u^{\varsigma+1,A}_{<i_1\ldots i_{n-2}}\frac{\partial v_{i_{n-1}}}{\partial x_{i_n>}} + nu^{\varsigma,A}_{k<i_1\ldots i_{n-1}}\frac{\partial v_{i_n>}}{\partial x_k}$$
$$= \frac{1}{\tau_{tr}}\left[u^{\varsigma,A}_{i_1\ldots i_n|E,tr} - u^{\varsigma,A}_{i_1\ldots i_n}\right] + \frac{1}{\tau_{int}}\left[u^{\varsigma,A}_{i_1\ldots i_n|E,int} - u^{\varsigma,A}_{i_1\ldots i_n}\right] \quad (2.12)$$

Here, the relation $u^{\varsigma,A}_{<i_1\ldots i_n>k} = u^{\varsigma,A}_{i_1\ldots i_n k} + \frac{n}{2n+1}u^{\varsigma+1,A}_{<i_1\ldots i_{n-1}}\delta_{i_n>k}$ is used [44], and $\frac{D}{Dt} = \frac{\partial}{\partial t} + v_i\frac{\partial}{\partial x_i}$.

2.6 S-model

In the original BGK model f_{tr_0} and f_{int_0} are the Maxwellian equilibrium distribution functions corresponding to different collision types which could not predict correct relaxation of the higher moments, Eq. 2.12, and the Prandtl number [76, 77]. Shakhov [65] proposed a modified BGK model for monatomic gases to obtain the correct Pr number and Rykov [66] extended this model to molecules with rotational movements. In order to overcome these defects we introduce a generalized and modified S-model for polyatomic gases.

The relaxation times of the Boltzmann collision term for Maxwell molecules in the case of monatomic gases for some higher moments are presented in table 2.1 [44] [78]. The relaxation time for all higher moments in the original BGK model are the same as stress tensor. The relaxation time of $u^{1,0}_{ij}$ is close to the relaxation time of σ_{ij}, but for other moments the differences are considerable and should not be ignored. Therefore, we introduce a model which correctly predicts the relaxation of these higher moments and their internal moment counterparts $\{q_{i,tr},\, q_{i,int},\, \sigma_{ij},\, u^{2,0},\, u^{1,1}\}$. Prandtl numbers of some polyatomic and diatomic gases are given in table 2.2 [79, 80]. Based on the definition of these higher moments, we introduce translational and internal distribution functions by expansion about the equilibrium Maxwellian functions, f_{tr_0} and f_{int_0}, in corresponding polynomials in specular velocity and particle's internal

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

Table 2.3: Correct relaxation times for higher moments based on four new free parameters.

energy as

$$\begin{aligned} f_{tr} = f_{tr_0}\Big[1+\big(&a^{0,0}+a_i^{0,0}C_i+a^{1,0}C^2+a_{ij}^{0,0}C_{<i}C_{j>} \\ &+a_i^{1,0}C_iC^2+a_i^{0,1}C_ie_{int}+a^{1,1}C^2e_{int}+a^{2,0}C^2C^2\big)\Big] \ , \end{aligned} \tag{2.13}$$

$$\begin{aligned} f_{int} = f_{int_0}\Big[1+\big(&b^{0,0}+b_i^{0,0}C_i+b^{1+1}\left(C^2+e_{int}\right) \\ &+b_{ij}^{0,0}C_{<i}C_{j>}+b_i^{1,0}C_iC^2+b_i^{0,1}C_ie_{int}+b^{1,1}C^2e_{int}+b^{2,0}C^2C^2\big)\Big] \ . \end{aligned} \tag{2.14}$$

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 2.3. The relaxation parameters will be obtained using fitting to experimental and simulation data. These conditions along with the collision invariants result in coefficients for the translational distribution function as,

$$a_{ij}^{0,0}=0 \quad , \quad a^{0,0}=\frac{\left(1-R_{u^{2,0}}\right)\left(u^{2,0}-15\rho\theta_{tr}^2\right)}{8\rho\theta_{tr}^2} \ , \tag{2.15a}$$

$$a_i^{0,0}=-\left[\frac{\left(1-R_{q_{tr}}\right)q_{i,tr}+2\delta\left(1-R_{q_{int}}\right)q_{i,int}\frac{\rho\theta_{tr}\theta_{int}}{4u^{0,2}-\delta^2\rho\theta_{int}^2}}{\rho\theta_{tr}^2}\right] , \tag{2.15b}$$

$$a^{1,0}=\frac{-5\left(1-R_{u^{2,0}}\right)\left(u^{2,0}-15\rho\theta_{tr}^2\right)-8\delta\rho\theta_{tr}\theta_{int}\left(1-R_{u^{1,1}}\right)\frac{u^{1,1}-\frac{3}{2}\delta\rho\theta_{tr}\theta_{int}}{4u^{0,2}-\delta^2\rho\theta_{int}^2}}{60\rho\theta_{tr}^3} , \tag{2.15c}$$

$$a_i^{1,0}=\frac{\left(1-R_{q_{tr}}\right)q_{i,tr}}{5\rho\theta_{tr}^3} \quad , \quad a_i^{0,1}=\frac{4\left(1-R_{q_{int}}\right)q_{i,int}}{4u^{0,2}\theta_{tr}-\delta^2\rho\theta_{int}^2\theta_{tr}} , \tag{2.15d}$$

$$a^{1,1}=\frac{4\left(1-R_{u^{1,1}}\right)\left(u^{1,1}-\frac{3}{2}\delta\rho\theta_{tr}\theta_{int}\right)}{15\theta_{tr}^2\left[4u^{0,2}-\delta^2\rho\theta_{int}^2\right]} , \tag{2.15e}$$

$$a^{2,0}=\frac{\left(1-R_{u^{2,0}}\right)\left(u^{2,0}-15\rho\theta_{tr}^2\right)}{120\rho\theta_{tr}^4} \ , \tag{2.15f}$$

and internal distribution function as,

$$b^{0,0} = (6+\delta)\,\frac{28\left(1-R_{u^{1,1}}\right)\left[u^{1,1}-\frac{3}{2}\delta\rho\theta^2\right]+(5-\delta)\left(1-R_{u^{2,0}}\right)\left[u^{2,0}-15\rho\theta^2\right]}{8\rho\theta^2\left(30+\delta\left(3+\delta\right)\right)}\ , \tag{2.16a}$$

$$b_i^{0,0} = -\left[\frac{\left(1-R_{q_{tr}}\right)q_{i,tr}+\left(1-R_{q_{int}}\right)q_{i,int}}{\rho\theta^2}\right]\ , \tag{2.16b}$$

$$b^{1+1} = \frac{-28\left(1-R_{u^{1,1}}\right)\left[u^{1,1}-\frac{3}{2}\delta\rho\theta^2\right]-(5-\delta)\left(1-R_{u^{2,0}}\right)\left[u^{2,0}-15\rho\theta^2\right]}{2\rho\theta^3\left(30+\delta\left(3+\delta\right)\right)}\ , \tag{2.16c}$$

$$b_{ij}^{0,0} = 0 \quad , \quad b_i^{1,0} = \frac{\left(1-R_{q_{tr}}\right)q_{i,tr}}{5\rho\theta^3} \quad , \quad b_i^{0,1} = \frac{2\left(1-R_{q_{int}}\right)q_{i,int}}{\delta\rho\theta^3}\ , \tag{2.16d}$$

$$b^{2,0} = \frac{20\,(6-\delta)\left(1-R_{u^{1,1}}\right)\left[u^{1,1}-\frac{3}{2}\delta\rho\theta^2\right]+\left(30-\delta\left(7-\delta\right)\right)\left(1-R_{u^{2,0}}\right)\left[u^{2,0}-15\rho\theta^2\right]}{120\rho\theta^4\left(30+\delta\left(3+\delta\right)\right)}\ , \tag{2.16e}$$

$$b^{1,1} = \frac{24\,(1+\delta)\left(1-R_{u^{1,1}}\right)\left[u^{1,1}-\frac{3}{2}\delta\rho\theta^2\right]+\delta\,(3-\delta)\left(1-R_{u^{2,0}}\right)\left[u^{2,0}-15\rho\theta^2\right]}{6\delta\rho\theta^4\left(30+\delta\left(3+\delta\right)\right)}\ . \tag{2.16f}$$

2.7 Equilibrium distributions

A gas which is isolated and there is no disturbance or force acting on it, will have an entropy elevation until its entropy reaches its maximum value. This maximum value is limited by the conserved quantities during the collisions. In 1987, Dreyer [81] proposed the maximum entropy principle in non-equilibrium state motivated by the work of Kogan [82]. We obtain the equilibrium distributions using the maximum entropy principle here.

The energy of internal states of molecules does not change during translational collisions. So, the number of molecules with the same internal energy level is an invariant for this type of collisions. However, in internal processes due to exchange of the internal energy, the total number of the molecules is an invariant. Also, momentum is conserved in all the collisions. Conservation of the energy for the translational processes results in conserved translational and internal energies, separately. Total energy is conserved for the internal processes.

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

$$\rho s = -k_b \int\!\!\int f \ln\frac{f}{y}\, d\mathbf{c}\, dI\ , \tag{2.17}$$

under the collision invariants constraints is solved using the method of Lagrange multipliers [44]. Here, k_b is the Boltzmann's constant and y is volume of inverse of phase space element. This method is based on the fact that finding the extremum of a function, L, under constraints $G_i = 0$, is the same as finding the extremum of $L - \sum_i \lambda_i G_i$, where λ_i is the vector of Lagrange multipliers. The unknown multipliers are obtained using the constraints. Therefore, the function that should be maximized for the translational processes is

$$\begin{aligned}\Phi = -k_b \int\int f \ln \frac{f}{y} d\mathbf{c} dI + \int \mathbf{\Lambda}_{\rho_I} \left(\rho_I - m \int f d\mathbf{c}\right) dI \\ + \mathbf{\Lambda}_{\rho_{v_k}} \left(0 - m \int\int C_i f d\mathbf{c} dI\right) + \mathbf{\Lambda}_{\rho u_{tr}} \left(\frac{3}{2}\rho\theta_{tr} - m \int\int \frac{C^2}{2} f d\mathbf{c} dI\right) \ . \end{aligned} \tag{2.18}$$

This is a variational calculus problem with the solution

$$f = y \exp[-1 - \frac{m}{k_b}(\mathbf{\Lambda}_{\rho_I} + \mathbf{\Lambda}_{\rho_{v_k}} C_k + \mathbf{\Lambda}_{\rho u_{tr}} \frac{C^2}{2})] \ . \tag{2.19}$$

The unknown multipliers are obtained using the constraints (prescribed values of number of molecules, translational energy and momentum balance) to be

$$\begin{aligned} \mathbf{\Lambda}_{\rho u_{tr}} &= \frac{k_b}{m\theta_{tr}} \ , \\ \mathbf{\Lambda}_{\rho_{v_k}} &= 0 \ , \\ \exp[-1 - \frac{m}{k_b}(\mathbf{\Lambda}_{\rho_I})] &= \frac{\rho_I}{my}(\frac{1}{2\pi\theta_{tr}})^{\frac{3}{2}} \ . \end{aligned} \tag{2.20}$$

Substituting the multipliers back into the distribution function, the equilibrium distribution function of the translational processes is obtained to be a Maxwellian distribution function,

$$f_{tr_0} = \frac{\rho_I}{m} \left(\frac{1}{2\pi\theta_{tr}}\right)^{\frac{3}{2}} \exp\left[-\frac{1}{2\theta_{tr}} C^2\right] \ . \tag{2.21}$$

Also, the function that is maximized for the internal processes is

$$\begin{aligned}\Phi = -k_b \int\int f \ln \frac{f}{y} d\mathbf{c} dI + \mathbf{\Lambda}_{\rho} \left(\rho - m \int\int f d\mathbf{c} dI\right) + \mathbf{\Lambda}_{\rho_{v_k 2}} \left(0 - m \int\int C_i f d\mathbf{c} dI\right) \\ + \mathbf{\Lambda}_{\rho u} \left(\frac{3+\delta}{2}\rho\theta_{tr} - m \int\int \left(\frac{C^2}{2} + e_{int}\right) f d\mathbf{c} dI\right) \ , \end{aligned} \tag{2.22}$$

Similarly, this is a variational calculus problem with the solution

$$f = y \exp\left[-1 - \frac{m}{k_b}\left(\mathbf{\Lambda}_{\rho} + \mathbf{\Lambda}_{\rho_{v_k}2} C_k + \mathbf{\Lambda}_{\rho u}\left[\frac{C^2}{2} + e_{int}\right]\right)\right] \ , \tag{2.23}$$

using the collision invariants of the internal processes (prescribed values of total number of molecules, total energy and momentum balance), we have,

$$\begin{aligned} \mathbf{\Lambda}_{\rho u} &= \frac{k_b}{m\theta} \ , \\ \mathbf{\Lambda}_{\rho_{v_k}2} &= 0 \ , \\ \exp[-1 - \frac{m}{k}(\mathbf{\Lambda}_{\rho_I})] &= \frac{\rho}{m}\frac{1}{(2\pi)^{\frac{3}{2}}\,\theta^{(\delta+3)/2}}\frac{1}{\Gamma\left(1+\frac{\delta}{2}\right)} \ . \end{aligned} \tag{2.24}$$

Accordingly, the equilibrium distribution function of the internal processes is

$$f_{int_0} = \frac{\rho}{m}\frac{1}{(2\pi)^{\frac{3}{2}}\,\theta^{(\delta+3)/2}}\frac{1}{\Gamma\left(1+\frac{\delta}{2}\right)} \exp\left[-\frac{1}{\theta}\left(\frac{C^2}{2} + I^{2/\delta}\right)\right] \ . \tag{2.25}$$

These obtained equilibrium distribution functions are first derived as Maxwellian distribution function by Bourgat et al. [22] and Andries et al. [31].

Moments of the two equilibrium distributions are

$$u^{\varsigma,A}_{|E,int} = \frac{(2\varsigma+1)!!}{\Gamma\left(\frac{\delta}{2}\right)}\rho\theta^{\varsigma+A}\Gamma\left(A + \frac{\delta}{2}\right) \ , \tag{2.26a}$$

$$u^{\varsigma,A}_{|E,tr} = (2\varsigma+1)!!\theta^{\varsigma}_{tr}\int (I^{2/\delta})^A \rho_I dI \ , \tag{2.26b}$$

$$u^{\varsigma,A}_{i_1\ldots i_n|E} = 0 \qquad\qquad n \neq 0 \ , \tag{2.26c}$$

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

2.8 Important properties of the proposed model

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

$$
\begin{aligned}
u^{1,1}_{|E,tr} &= m\int\int C^2 e_{int} f_{tr_0} t d\mathbf{c} de_{int} = \frac{3}{2}\delta\rho\theta_{int}\theta_{tr} \ , \\
u^{2,0}_{|E,tr} &= m\int\int C^4 f_{tr_0} d\mathbf{c} de_{int} = 15\rho\theta^2_{tr} \ , \quad \text{and} \\
u^{1,1}_{|E,int} &= m\int\int C^2 e_{int} f_{int_0} d\mathbf{c} de_{int} = \frac{3}{2}\delta\rho\theta^2 \ , \\
u^{2,0}_{|E,int} &= m\int\int C^4 f_{int_0} d\mathbf{c} de_{int} = 15\rho\theta^2 \ .
\end{aligned}
\tag{2.27}
$$

In equilibrium we have zero collision term and all moments of the collision term must vanish, e.g., $q_{i,tr} = q_{i,int} = 0$. Therefore based on Eqs. (2.13,2.14), 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 number of particles with the same internal energy level should be conserved. Internal exchange processes conserves the total mass and number of particles. Both internal and translational exchange processes conserve the momentum. The total energy is conserved in the internal exchange processes, where the translational processes conserves the translational and internal energies separately. The above conditions imply that the two phase densities , f_{tr} and f_{int}, should have the moments related to mass, momentum and energy in common with f as,

$$
\begin{aligned}
\rho_I &= m\int f_{tr} d\mathbf{c} = m\int f d\mathbf{c} \ , \\
0 &= m\int\int C_i f_{tr} d\mathbf{c} dI = m\int\int C_i f d\mathbf{c} dI \ , \\
\frac{3}{2}\rho\theta_{tr} &= \frac{m}{2}\int\int C^2 f_{tr} d\mathbf{c} dI = \frac{m}{2}\int\int C^2 f d\mathbf{c} dI \ .
\end{aligned}
\tag{2.28a}
$$

$$\begin{aligned}\rho = m\int\int f_{int} d\mathbf{c}dI = m\int\int f d\mathbf{c}dI \quad , \\ 0 = m\int\int C_i f_{int} d\mathbf{c}dI = m\int\int C_i f d\mathbf{c}dI \ , \\ \left(\frac{3}{2}+\frac{\delta}{2}\right)\rho\theta = m\int\int\left(\frac{C^2}{2}+e_{int}\right) f_{int} d\mathbf{c}dI = m\int\int\left(\frac{C^2}{2}+e_{int}\right) f d\mathbf{c}dI \ .\end{aligned} \tag{2.28b}$$

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

The remainder of this section is dedicated to prove the H-theorem for the proposed model. Multiplication of the kinetic equation (2.11a) 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

$$\begin{aligned}\sum = -k\int \ln f \ S d\mathbf{c}dI \\ = \frac{k}{\tau_{int}}\int\int \ln f(f-f_{int})d\mathbf{c}dI + \frac{k}{\tau_{tr}}\int\int \ln f(f-f_{tr})d\mathbf{c}dI \geqslant \mathbf{0} \ ,\end{aligned} \tag{2.29}$$

non-equality shows that the entropy generation ought to be non-negative. Right hand side of Eq. 2.29 have two terms, first we consider the first term.

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

$$\begin{aligned}\frac{k}{\tau_{int}}\int\int \ln f(f-f_{int})d\mathbf{c}dI = \frac{k}{\tau_{int}}\int\int \frac{\ln f}{\ln f_{int}}(f-f_{int})d\mathbf{c}dI \\ + \frac{k}{\tau_{int}}\int\int \ln f_{int}(f-f_{int})d\mathbf{c}dI \ .\end{aligned} \tag{2.30}$$

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

$$\begin{aligned}\ln f_{int} = \ln f_{int_0} + \big(b^{0,0} + b_i^{0,0}C_i + b^{1+1}\left(C^2+e_{int}\right) + b_{ij}^{0,0}C_{<i}C_{j>} \\ + b_i^{1,0}C_iC^2 + b_i^{0,1}C_ie_{int} + b^{1,1}C^2e_{int} + b^{2,0}C^2C^2\big) \ ;\end{aligned} \tag{2.31}$$

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

$$\int\int \ln f_{int_0}(f - f_{int})d\mathbf{c}dI =$$
$$\int\int \left[\ln\left[\frac{\rho}{m}\frac{1}{(2\pi)^{\frac{3}{2}}\,\theta^{3/2}}\frac{1}{\Gamma\left(1+\frac{\delta}{2}\right)}\right] - \frac{1}{\theta}\left(\frac{C^2}{2} + e_{int}\right)\right](f - f_{int})d\mathbf{c}dI = 0\ ,$$

$$\int b^{0,0}(f - f_{int})d\mathbf{c}dI = 0\ \ ,\quad \int b_i^{0,0}C_i(f - f_{int})d\mathbf{c}dI = 0\ , \tag{2.32}$$
$$\text{and}\quad \int b^{1+1}\left(C^2 + e_{int}\right)(f - f_{int})d\mathbf{c}dI = 0\ .$$

Therefore, remaining terms of first term of Eq. 2.29 are

$$\int\int b_i^{1,0}C_iC^2(f - f_{int})d\mathbf{c}de_{int} = b_i^{1,0}2R_{q_{tr}}q_{i,tr} = \frac{2R_{q_{tr}}\left(1 - R_{q_{tr}}\right)}{5\rho\theta^3}q^2_{i,tr}\ , \tag{2.33a}$$
$$\int\int b_i^{0,1}C_iI^{2/\delta}(f - f_{int})d\mathbf{c}de_{int} = b_i^{0,1}R_{q_{int}}q_{i,int} = \frac{2R_{q_{int}}\left(1 - R_{q_{int}}\right)}{\delta\rho\theta^3}q^2_{i,int}\ , \tag{2.33b}$$

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

$$A_1 = \int\int b^{2,0}C^2C^2(f - f_{int})d\mathbf{c}de_{int} = b^{2,0}\left[R_{u^{2,0}}\left(u^{2,0} - 15\rho\theta^2\right)\right] =$$
$$\frac{20\delta\left(6-\delta\right)R_{u^{2,0}}\left(1 - R_{u^{1,1}}\right)\left[u^{1,1} - \frac{3}{2}\delta\rho\theta^2\right]}{120\delta\rho\theta^4\left(30 + \delta\left(3+\delta\right)\right)}\left[u^{2,0} - 15\rho\theta^2\right]$$
$$+\frac{\delta\left(30 - \delta\left(7-\delta\right)\right)R_{u^{2,0}}\left(1 - R_{u^{2,0}}\right)}{120\delta\rho\theta^4\left(30 + \delta\left(3+\delta\right)\right)}\left[u^{2,0} - 15\rho\theta^2\right]^2\ ,$$

$$A_2 = \int\int b^{1,1}C^2I^{2/\delta}(f - f_{int})d\mathbf{c}de_{int} = b^{1,1}\left[R_{u^{1,1}}\left(u^{1,1} - \frac{3}{2}\delta\rho\theta^2\right)\right] =$$
$$= \frac{480\left(1+\delta\right)R_{u^{1,1}}\left(1 - R_{u^{1,1}}\right)}{120\delta\rho\theta^4\left(30 + \delta\left(3+\delta\right)\right)}\left[u^{1,1} - \frac{3}{2}\delta\rho\theta^2\right]^2$$
$$+\frac{20\delta\left(3-\delta\right)R_{u^{1,1}}\left(1 - R_{u^{2,0}}\right)}{120\delta\rho\theta^4\left(30 + \delta\left(3+\delta\right)\right)}\left[u^{2,0} - 15\rho\theta^2\right]\left(u^{1,1} - \frac{3}{2}\delta\rho\theta^2\right)\ .$$

It should be pointed out here that two relaxation parameters, $R_{q_{tr}}$ and $R_{q_{int}}$, are analogies to the Pr number and their typical values are around $0.6 - 0.8$. We use the

Onsager relation due to the coupling between these last two equations as

$$A_1 + A_2 = L_{AB} X_B . X_A \ , \tag{2.34a}$$

with Onsager phenomenological matrix,

$$L_{AB} = \begin{pmatrix} \frac{\delta(30-\delta(7-\delta))R_{u^{2,0}}\left(1-R_{u^{2,0}}\right)}{120\delta\rho\theta^4(30+\delta(3+\delta))} & \frac{20\delta(6-\delta)R_{u^{2,0}}\left(1-R_{u^{1,1}}\right)}{120\delta\rho\theta^4(30+\delta(3+\delta))} \\ \frac{20\delta(3-\delta)R_{u^{1,1}}\left(1-R_{u^{2,0}}\right)}{120\delta\rho\theta^4(30+\delta(3+\delta))} & \frac{480(1+\delta)R_{u^{1,1}}\left(1-R_{u^{1,1}}\right)}{120\delta\rho\theta^4(30+\delta(3+\delta))} \end{pmatrix} , \tag{2.34b}$$

and forces,

$$X_1 = u^{2,0} - 15\rho\theta^2 \quad \text{and} \qquad X_2 = u^{1,1} - \frac{3}{2}\delta\rho\theta^2 \ . \tag{2.34c}$$

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

$$b^{2,0}\left[R_{u^{2,0}}\left(u^{2,0} - 15\rho\theta^2\right)\right] + b^{1,1}\left[R_{u^{1,1}}\left(u^{1,1} - \frac{3}{2}\delta\rho\theta^2\right)\right] \geqslant 0 \ . \tag{2.34d}$$

The relaxation parameter, $R_{u^{2,0}}$, have values around 0.7 for monatomic gas as mentioned in table 2.1. Now that we proved that the first term in the right hand side of entropy production, Eq. 2.29, is non-negative, the second term is analyzed next.

We re-write the second term in the entropy production equation (2.29) which is related to translational exchange processes as,

$$\int \ln f (f - f_{tr}) d\mathbf{c} dI = \int \frac{\ln f}{\ln f_{tr}} (f - f_{tr}) d\mathbf{c} dI + \int \ln f_{tr} (f - f_{tr}) d\mathbf{c} dI \ . \tag{2.35}$$

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,

$$\begin{aligned} \ln f_{tr} = \ln f_{tr_0} + \big(& a^{0,0} + a_i^{0,0} C_i + a^{1,0} C^2 \\ & + a_i^{1,0} C_i C^2 + a_i^{0,1} C_i e_{int} + a^{2,0} C^2 C^2 + a^{1,1} C^2 e_{int}\big) \end{aligned} \tag{2.36a}$$

$$\ln f_{tr_0} = \ln\left[\frac{\rho_I}{m}\left(\frac{1}{2\pi\theta_{tr}}\right)^{\frac{3}{2}}\right] - \frac{1}{2\theta_{tr}} C^2 \tag{2.36b}$$

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

$$\int\int \ln f_{tr_0}(f-f_{tr})d\mathbf{c}dI = \int\int \left[\ln\left[\frac{\rho_I}{m}\left(\frac{1}{2\pi\theta_{tr}}\right)^{\frac{3}{2}}\right] - \frac{1}{2\theta_{tr}}C^2\right](f-f_{tr})d\mathbf{c}dI = 0\ ,$$

$$\int a^{0,0}(f-f_{tr})d\mathbf{c}dI = 0\ \ ,\ \ \int a_i^{0,0}C_i(f-f_{tr})d\mathbf{c}dI = 0 \tag{2.37}$$

$$\text{and}\quad \int a^{1,0}C^2(f-f_{tr})d\mathbf{c}dI = 0\ .$$

Therefore the remaining parts are,

$$\int a_i^{1,0}C_iC^2(f-f_{tr})d\mathbf{c}dI = \frac{2R_{q_{tr}}\left(1-R_{q_{tr}}\right)}{5\rho\theta_{tr}^3}q_{i,tr}^2\ , \tag{2.38a}$$

$$\int a_i^{0,1}C_iI^{2/\delta}(f-f_{tr})d\mathbf{c}dI = \frac{4R_{q_{int}}\left(1-R_{q_{int}}\right)}{\theta_{tr}\left[4u^{0,2}-\delta^2\rho\theta_{int}^2\right]}q_{i,int}^2\ , \tag{2.38b}$$

$$\int a^{2,0}C^2C^2(f-f_{tr})d\mathbf{c}dI = \frac{R_{u^{2,0}}\left(1-R_{u^{2,0}}\right)}{120\rho\theta_{tr}^4}\left(u^{2,0}-15\rho\theta_{tr}^2\right)^2\ , \tag{2.38c}$$

$$\int a^{1,1}C^2I^{2/\delta}(f-f_{tr})d\mathbf{c}dI = \frac{4R_{u^{1,1}}\left(1-R_{u^{1,1}}\right)}{15\theta_{tr}^2\left[4u^{0,2}-\delta^2\rho\theta_{int}^2\right]}\left(u^{1,1}-\frac{3}{2}\delta\rho\theta_{tr}\theta_{int}\right)^2\ , \tag{2.38d}$$

which are always positive for $\{R_{q_{tr}}, R_{q_{int}}, R_{u^{2,0}}, R_{u^{1,1}}\} \leq 1$. Here, based on the obtained G36 distribution function (3.9) we calculate the moment $u^{0,2}$ to be

$$u^{0,2}_{|G36} = \frac{1}{4}\left(2+\delta\right)\rho\theta\left[\left(6+\delta\right)\theta - 6\theta_{tr}\right]\ , \tag{2.39a}$$

$$\left[4u^{0,2}_{|G36} - \delta^2\rho\theta_{int}^2\right] = \rho\left[2\delta\theta^2 + 3\Delta\theta\left(4\theta - 3\Delta\theta\right)\right]\ . \tag{2.39b}$$

Therefore, both terms in entropy production inequality are non-negative. It follows from Eq. 2.29 that the H-theorem is fulfilled as,

$$\sum = -k\int \ln f\ Sd\mathbf{c}dI \geqslant 0\ \text{ for }\ \{R_{q_{tr}}, R_{q_{int}}, R_{u^{2,0}}, R_{u^{1,1}}\} \leq 1\ . \tag{2.40}$$

Therefore, 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 experimental and DSMC simulation data, as will be shown in Chapter 8.

Chapter 3

Moment equations

Do not fear to be eccentric in opinion, for every opinion now accepted was once eccentric.

Bertrand Russell

Moment methods replace the kinetic equation by a finite set of differential equations for the moments of the distribution function. Some of moments are interesting and we have physical meaning of them, e.g. heat flux and velocity. 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 [36].

3.1 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 (2.12) as

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_i}{\partial x_i} = 0\ , \tag{3.1a}$$

$$\frac{Dv_i}{Dt} + \frac{1}{\rho}\frac{\partial \sigma_{ij}}{\partial x_j} + \frac{\partial \theta_{tr}}{\partial x_i} + \frac{\theta_{tr}}{\rho}\frac{\partial \rho}{\partial x_i} = 0\ , \tag{3.1b}$$

$$\frac{3}{2}\rho\frac{D\theta_{tr}}{Dt} + \frac{\partial q_{i,tr}}{\partial x_i} + \sigma_{ij}\frac{\partial v_j}{\partial x_i} + \rho\theta_{tr}\frac{\partial v_i}{\partial x_i} = \frac{3\rho}{\tau_{int}}\frac{(\theta - \theta_{tr})}{2}\ , \tag{3.1c}$$

$$\rho\frac{D\frac{\delta}{2}\theta_{int}}{Dt} + \frac{\partial q_{i,int}}{\partial x_i} = -\frac{3\rho}{\tau_{int}}\frac{(\theta - \theta_{tr})}{2}\ . \tag{3.1d}$$

The time derivative and spatial derivative of internal heat capacity are

$$\frac{D\frac{\delta}{2}}{Dt} = \frac{\partial\frac{\delta}{2}}{\partial t} + v_i \frac{\partial\frac{\delta}{2}}{\partial x_i} = \frac{d\frac{\delta}{2}}{d\theta}\left[\frac{\partial\theta}{\partial t} + v_i \frac{\partial\theta}{\partial x_i}\right] = \frac{1}{2}\frac{d\delta}{d\theta}\frac{D\theta}{Dt} \ , \tag{3.2a}$$

$$\frac{\partial\frac{\delta}{2}}{\partial x_i} = \frac{1}{2}\frac{d\delta}{d\theta}\frac{\partial\theta}{\partial x_i} \ . \tag{3.2b}$$

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

$$\rho\frac{3+\delta+\theta\frac{d\delta}{d\theta}}{2}\frac{D\theta}{Dt} + \frac{\partial q_{i,int}}{\partial x_i} + \frac{\partial q_{i,tr}}{\partial x_i} + \sigma_{ij}\frac{\partial v_j}{\partial x_i} + \rho\left(\theta - \Delta\theta\right)\frac{\partial v_i}{\partial x_i} = 0 \ . \tag{3.3}$$

Here and later, we replace the translational temperature θ_{tr} as variable by its nonequilibrium part $\Delta\theta = \theta - \theta_{tr}$, named dynamic temperature,

$$\rho\frac{D\Delta\theta}{Dt} + \frac{2}{3+\delta+\theta\frac{d\delta}{d\theta}}\frac{\partial q_{i,int}}{\partial x_i} - \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\frac{\partial q_{i,tr}}{\partial x_i} - \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\sigma_{ij}\frac{\partial v_j}{\partial x_i}$$
$$- \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\rho\left(\theta-\Delta\theta\right)\frac{\partial v_i}{\partial x_i} = -\frac{\rho}{\tau_{int}}\Delta\theta \ . \tag{3.4}$$

The originally derived conservation laws above are coincide with the conservation laws obtained in References [70, 30].

3.2 Balance laws

Moment equations for stress tensor, $\sigma_{ij} = u_{ij}^{0,0}$, translational heat flux, $q_{i,tr} = \frac{1}{2}u_i^{1,0}$, and internal heat flux, $u_i^{0,1} = q_{i,int}$, which are present in the conservation laws, are obtained from the general moment equation (2.12), as

$$\frac{D\sigma_{ij}}{Dt} + \frac{\partial u_{ijk}^{0,0}}{\partial x_k} + \frac{4}{5}\frac{\partial q_{<i,tr}}{\partial x_{j>}} + 2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k}$$
$$+ 2\rho\left[\theta - \Delta\theta\right]\frac{\partial v_{<i}}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\sigma_{ij} \ , \tag{3.5}$$

$$\frac{Dq_{i,tr}}{Dt} - \frac{5}{2}\left[\theta - \Delta\theta\right]\left[\frac{\partial \sigma_{ij}}{\partial x_j} + \rho\frac{\partial \theta}{\partial x_i} - \rho\frac{\partial \Delta\theta}{\partial x_i}\right]
+ \sigma_{ik}\left[\frac{\partial \Delta\theta}{\partial x_k} - \frac{\partial \theta}{\partial x_k} - \left[\theta - \Delta\theta\right]\frac{\partial \ln\rho}{\partial x_k} - \frac{1}{\rho}\frac{\partial \sigma_{kj}}{\partial x_j}\right]
+ \frac{1}{2}\frac{\partial u_{ik}^{1,0}}{\partial x_k} + \frac{1}{6}\frac{\partial u^{2,0}}{\partial x_i} + u_{ijk}^{0,0}\frac{\partial v_j}{\partial x_k} + \frac{7}{5}q_{i,tr}\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_{k,tr}\frac{\partial v_i}{\partial x_k}
+ \frac{2}{5}q_{j,tr}\frac{\partial v_j}{\partial x_i} - \frac{5}{2}\left[\theta^2 - 2\theta\Delta\theta + \Delta\theta^2\right]\frac{\partial \rho}{\partial x_i} = -R_{q_{tr}}\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]q_{i,tr} \ , \quad (3.6)$$

$$\frac{Dq_{i,int}}{Dt} - \frac{\delta\theta + 3\Delta\theta}{2}\left[\frac{\partial \sigma_{ij}}{\partial x_j} + \rho\frac{\partial \theta}{\partial x_i} - \rho\frac{\partial \Delta\theta}{\partial x_i} + \rho\left[\theta - \Delta\theta\right]\frac{\partial \ln\rho}{\partial x_i}\right] + \frac{\partial u_{ik}^{0,1}}{\partial x_k}
+ \frac{1}{3}\frac{\partial u^{1,1}}{\partial x_i} + q_{k,int}\frac{\partial v_i}{\partial x_k} + q_{i,int}\frac{\partial v_k}{\partial x_k} = -R_{q_{int}}\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]q_{i,int} \ . \quad (3.7)$$

These equations contain higher moments $u_{ij}^{1,0}$, $u^{2,0}$, $u_{ijk}^{0,0}$, $u_{ij}^{0,1}$ and $u^{1,1}$ for which full moment equations can be obtained from Eq. (2.12) with the appropriate choices for ς and A. Choosing all moments mentioned so far as variables will construct a 36 moments set,

$$\left\{\rho, v_i, \theta, \Delta\theta, \sigma_{ij}, q_{i,tr}, q_{i,int}, u_{ij}^{1,0}, u^{2,0}, u_{ij}^{0,1}, u^{1,1}, u_{ijk}^{0,0}\right\} \ . \quad (3.8)$$

The obtained equations for these 36 moments contain higher moments in the fluxes which we have to obtain constitutive equations for $\left\{u_{ijk}^{1,0}, u_i^{2,0}, u_{ijkl}^{0,0}, u_{ijk}^{0,1}, u_i^{1,1}\right\}$, to close the set of equations. Grad's distribution function will be used to obtain constitutive equations for these higher moments as functions of the 36 variables and close the system of 36 equations.

3.3 Grad closure: 36 moments

Grad [62, 63] proposed a distribution function based on the expansion of the Maxwellian into a series of Hermite polynomials. It is convenient to consider the expansion with the trace free moments instead of regular moments, so that the generalized Grad distribution function based on the 36 variables is written as

$$f_{|36} = f_{int_0} \big(\lambda^{0,0} + \lambda_i^{0,0} C_i + \lambda^{1,0} C^2 + \lambda_{<ij>}^{0,0} C_{<i} C_{j>} + \lambda^{0,1} e_{int} \\ + \lambda_i^{1,0} C_i C^2 + \lambda_i^{0,1} C_i e_{int} + \lambda_{<ij>}^{1,0} C^2 C_{<i} C_{j>} + \lambda^{2,0} C^4 \\ + \lambda_{<ijk>}^{0,0} C_{<i} C_j C_{k>} + \lambda_{<ij>}^{0,1} C_{<i} C_{j>} e_{int} + \lambda^{1,1} C^2 e_{int} \big) \ , \tag{3.9}$$

where, $\lambda^{\varsigma,A}_{\langle i_1 i_2 \dots i_n \rangle}$ are expansion coefficients. Grad 36 distribution function should reproduce the set of 36 moments. This is done by choosing the coefficients λ based on the definition of 36 moments as,

$$u_A = m \int\int \Psi_A f_{|36} d\mathbf{c} dI \ , \tag{3.10a}$$

with

$$u_A = \{ \rho, \rho\theta_{tr}, \rho\theta_{int}, \sigma_{ij}, q_{i,tr}, q_{i,int}, u_{ij}^{1,0}, u^{2,0}, u_{ijk}^{0,0}, u_{ij}^{0,1}, u^{1,1} \} \ , \tag{3.10b}$$

$$\Psi_A = \Big\{ 1,\, C_i,\, \frac{C^2}{3},\, \frac{2}{\delta} e_{int},\, C_{<i} C_{j>},\, \frac{C_i C^2}{2},\, C_i e_{int}, \\ C_{<i} C_{j>} C^2,\, C^4,\, C_{<i} C_j C_{k>},\, C_{<i} C_{j>} e_{int},\, C^2 e_{int} \Big\} \ . \tag{3.10c}$$

The obtained coefficients are

$$\lambda^{0,0} = \frac{4u^{1,1} + u^{2,0}}{8\rho\theta^2} + \frac{5}{8} - \frac{3\,(2+\delta)\,\theta_{tr}}{4\theta} \quad , \tag{3.11a}$$

$$\lambda^{0,1} = -\frac{u^{1,1}}{\delta\rho\theta^3} + \frac{15}{2\delta\theta} - \frac{3\,(5-\delta)\,\theta_{tr}}{2\delta\theta^2} \ , \tag{3.11b}$$

$$\lambda^{1,0} = -\frac{2u^{1,1} + u^{2,0}}{12\rho\theta^3} - \frac{1}{\theta} + \frac{(9+\delta)\,\theta_{tr}}{4\theta^2} \quad , \tag{3.11c}$$

$$\lambda^{2,0} = \frac{u^{2,0}}{120\rho\theta^4} + \frac{1}{8\theta^2} - \frac{\theta_{tr}}{4\theta^3} \ , \tag{3.11d}$$

$$\lambda^{1,1} = \frac{u^{1,1}}{3\delta\rho\theta^4} - \frac{3}{2\delta\theta^2} + \frac{(9-\delta)\,\theta_{tr}}{6\delta\theta^3} \quad , \tag{3.11e}$$

$$\lambda_i^{0,0} = -\frac{q_{i,tr} + q_{i,int}}{\rho\theta^2} \ , \ \lambda_{<ij>}^{1,0} = \frac{u_{ij}^{1,0}}{28\rho\theta^4} - \frac{\sigma_{ij}}{4\rho\theta^3} \ , \tag{3.11f}$$

$$\lambda_i^{1,0} = \frac{q_{i,tr}}{5\rho\theta^3} \quad , \quad \lambda_i^{0,1} = \frac{2q_{i,int}}{\delta\rho\theta^3} \ , \tag{3.11g}$$

$$\lambda_{<ij>}^{0,0} = -\frac{2u_{ij}^{0,1} + u_{ij}^{1,0}}{4\rho\theta^3} + \frac{(9+\delta)\,\sigma_{ij}}{4\rho\theta^2} \ , \tag{3.11h}$$

$$\lambda_{<ijk>}^{0,0} = \frac{u_{ijk}^{0,0}}{6\rho\theta^3} \quad , \quad \lambda_{<ij>}^{0,1} = \frac{u_{ij}^{0,1}}{\delta\rho\theta^4} - \frac{\sigma_{ij}}{2\rho\theta^3} \ . \tag{3.11i}$$

Using the Grad distribution function (3.9), the constitutive equations are obtained as

$$\begin{aligned} u_{ijk}^{1,0} &= 9\theta u_{ijk}^{0,0} \quad , \quad u_i^{2,0} = 28\theta q_{i,tr} \quad , \quad u_{ijkl}^{0,0} = 0 \ , \\ u_{ijk}^{0,1} &= \frac{\delta}{2}\theta u_{ijk}^{0,0} \quad , \quad u_i^{1,1} = \left(5q_{i,int} + \delta q_{i,tr}\right)\theta \ . \end{aligned} \tag{3.12}$$

Substituting these equations into the 36 balance laws gives the closed set of equations. Therefore the balance laws for the moments $u^{1,0}_{ij}$, $u^{2,0}$, $u^{0,0}_{ijk}$, $u^{0,1}_{ij}$ and $u^{1,1}$ are

$$\begin{aligned}\frac{Du^{1,0}_{ij}}{Dt} - u^{0,0}_{ijk} 2\left[\theta - \Delta\theta\right]\frac{\partial \ln\rho}{\partial x_k} - \frac{28}{5}\left[\theta - \Delta\theta\right] q_{<i,tr}\frac{\partial \ln\rho}{\partial x_{j>}} \\ + 7u^{0,0}_{ijk}\frac{\partial\theta}{\partial x_k} + 2u^{0,0}_{ijk}\frac{\partial\Delta\theta}{\partial x_k} + \frac{28}{5}q_{<i,tr}\frac{\partial\theta}{\partial x_{j>}} \\ + \frac{28}{5}q_{<i,tr}\frac{\partial\Delta\theta}{\partial x_{j>}} + 9\theta\frac{\partial u^{0,0}_{ijk}}{\partial x_k} + \frac{2}{5}28\theta\frac{\partial q_{<i,tr}}{\partial x_{j>}} + \frac{6}{7}u^{1,0}_{<ij}\frac{\partial v_{k>}}{\partial x_k} \\ + \frac{4}{5}u^{1,0}_{j<i}\frac{\partial v_j}{\partial x_{j>}} + 2u^{1,0}_{k<i}\frac{\partial v_{j>}}{\partial x_k} + u^{1,0}_{ij}\frac{\partial v_k}{\partial x_k} + \frac{14}{15}u^{2,0}\frac{\partial v_{<i}}{\partial x_{j>}} \\ - 2\frac{1}{\rho}u^{0,0}_{ijk}\frac{\partial\sigma_{kl}}{\partial x_l} - \frac{28}{5}\frac{1}{\rho}q_{<i,tr}\frac{\partial\sigma_{j>l}}{\partial x_l} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]u^{1,0}_{ij} \ ,\end{aligned} \tag{3.13a}$$

$$\begin{aligned}\frac{Du^{2,0}}{Dt} - 8q_{k,tr}\left[\theta - \Delta\theta\right]\frac{\partial\ln\rho}{\partial x_k} + 28\theta\frac{\partial q_{k,tr}}{\partial x_k} - 8\frac{q_{k,tr}}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j} \\ + 20q_{k,tr}\frac{\partial\theta}{\partial x_k} + 8q_{k,tr}\frac{\partial\Delta\theta}{\partial x_k} + 4u^{1,0}_{kj}\frac{\partial v_j}{\partial x_k} + \frac{7}{3}u^{2,0}\frac{\partial v_k}{\partial x_k} \\ = \frac{R_{u^{2,0}}}{\tau_{tr}}\left[\left(15\rho\left[\theta^2 - 2\theta\Delta\theta + \Delta\theta^2\right]\right) - u^{2,0}\right] + \frac{R_{u^{2,0}}}{\tau_{int}}\left[\left(15\rho\theta^2\right) - u^{2,0}\right] \ ,\end{aligned} \tag{3.13b}$$

$$\begin{aligned}\frac{Du^{0,0}_{ijk}}{Dt} - 3\frac{\sigma_{<ij}}{\rho}\frac{\partial\sigma_{k>l}}{\partial x_l} + \frac{3}{7}\frac{\partial u^{1,0}_{<ij}}{\partial x_{k>}} - 3\sigma_{<ij}\frac{\partial\theta}{\partial x_{k>}} \\ - 3\left[\theta - \Delta\theta\right]\sigma_{<ij}\frac{\partial\ln\rho}{\partial x_{k>}} + 3\sigma_{<ij}\frac{\partial\Delta\theta}{\partial x_{k>}} + 3u^{0,0}_{l<ij}\frac{\partial v_{k>}}{\partial x_l} \\ + u^{0,0}_{ijk}\frac{\partial v_l}{\partial x_l} + \frac{12}{5}q_{<i,tr}\frac{\partial v_j}{\partial x_{k>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]u^{0,0}_{ijk} \ ,\end{aligned} \tag{3.13c}$$

$$
\begin{aligned}
\frac{Du^{0,1}_{ij}}{Dt} - 2q_{<i,int}\frac{1}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_k} - 2\frac{[\theta-\Delta\theta]}{\rho}q_{<i,int}\frac{\partial\rho}{\partial x_{ij>}} + \frac{\delta}{2}\theta\frac{\partial u^{0,0}_{ijk}}{\partial x_k}& \\
+ u^{0,0}_{ijk}\frac{\theta}{2}\frac{\partial\delta}{\partial x_k} + \frac{\delta}{2}u^{0,0}_{ijk}\frac{\partial\theta}{\partial x_k} + \frac{2\delta}{5}q_{<i,tr}\frac{\partial\theta}{\partial x_{j>}} + 2q_{<i,int}\frac{\partial\Delta\theta}{\partial x_{j>}}& \\
+ 2\theta\frac{\partial q_{<i,int}}{\partial x_{j>}} + \frac{2\delta}{5}\theta\frac{\partial q_{<i,tr}}{\partial x_{j>}} + \frac{2}{5}\theta q_{<i,tr}\frac{\partial\delta}{\partial x_{j>}} + 2u^{0,1}_{k<i}\frac{\partial v_{j>}}{\partial x_k}& \\
+ u^{0,1}_{ij}\frac{\partial v_k}{\partial x_k} + \frac{2}{3}u^{1,1}\frac{\partial v_{<i}}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]u^{0,1}_{ij}\ ,& \quad (3.13d)
\end{aligned}
$$

$$
\begin{aligned}
\frac{Du^{1,1}}{Dt} - 2\frac{q_{k,int}}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j} - 2q_{k,int}\left[\theta-\Delta\theta\right]\frac{\partial\ln\rho}{\partial x_k} + 2q_{k,int}\frac{\partial\Delta\theta}{\partial x_k}& \\
+ \left(3q_{k,int} + \delta q_{k,tr}\right)\frac{\partial\theta}{\partial x_k} + 5\theta\frac{\partial q_{k,int}}{\partial x_k} + \delta\theta\frac{\partial q_{k,tr}}{\partial x_k}& \\
+ \theta q_{k,tr}\frac{\partial\delta}{\partial x_k} + 2u^{0,1}_{kj}\frac{\partial v_j}{\partial x_k} + \frac{5}{3}u^{1,1}\frac{\partial v_k}{\partial x_k}& \\
= \frac{R_{u^{1,1}}}{\tau_{tr}}\left[3\rho\left[\frac{\delta}{2}\theta + \frac{3}{2}\Delta\theta\right]\left[\theta-\Delta\theta\right] - u^{1,1}\right] + \frac{R_{u^{1,1}}}{\tau_{int}}\left[\left(3\frac{\delta}{2}\rho\theta^2\right) - u^{1,1}\right]\ .& \quad (3.13e)
\end{aligned}
$$

Grad distribution function implies a relation between the internal state density, ρ_I, total density, ρ, and the temperatures, θ and $\Delta\theta = \theta - \theta_{tr}$, viz.

$$
\rho_I = \frac{\rho}{\theta^{1+\delta/2}\Gamma\left(1+\frac{\delta}{2}\right)}\left[\frac{I^{2/\delta}}{\delta}\frac{\theta\delta - (\delta-3)\,\Delta\theta}{\theta} + \frac{2\theta - 3\Delta\theta}{2}\right]\exp\left(-\frac{1}{\theta}I^{2/\delta}\right)\ . \quad (3.14)
$$

Chapter 4

Reconstructing Moments

Do not go where the path may lead, go instead where there is no path and leave a trail.

Waldo Emerson

Closed system of 36 moments is used in this chapter to optimize the moment definitions. The relation betwen two Kn numbers are explored at the beginning. Then, ordering in two Kn numbers by applying Chapman-Enskog expansion on system of raw moment equations, are used to obtain the first order of all 36 moments. Considering moments with linear dependent first order, new moment definitions are 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 least moment numbers possible. At the end, using the obtained optimized moment definitions, set of new moment equations are presented. It should be mentioned that all the work presented here are new and original, and to the best knowledge of the author there are no similar work done before for polyatomic gases.

4.1 Mean free times and Knudsen numbers

In the definition of Knudsen number, Eq. 2.4, the typical reference time scale τ_0 is defined as $L_0/\sqrt{\theta_0}$. For the proposed polyatomic model (2.11a) we have two different relaxation times, corresponding to two different mean free paths, and two distinct Knudsen numbers, $\mathrm{Kn}_{tr} = \frac{\tau_{tr}}{\tau_0}$ and $\mathrm{Kn}_{int} = \frac{\tau_{int}}{\tau_0}$. The Knudsen numbers measure the degree of rarefaction, and will be used for model reduction. The expansion parameter in the Chapman-Enskog method is the Knudsen number, of which we have two, Kn_{tr}

Gas	$T_0(K)$	μ (Pa · s) $\times 10^7$	v (Pa · s) $\times 10^6$	τ_{tr} (s)	τ_{int} (s)	τ_{tr}/τ_{int}
H_2	77.3	35.0	98	3.50×10^{-9}	3.30×10^{-6}	1.06×10^{-3}
	293	88.2	326	8.82×10^{-9}	1.26×10^{-6}	7×10^{-3}
D_2	77.3	48.2	174	4.82×10^{-9}	6.37×10^{-7}	7.57×10^{-3}
	293	123	271	1.23×10^{-8}	1.01×10^{-6}	0.012

Table 4.1: Shear and bulk viscosity values of Hydrogen and Deuterium for two temperature values and reference pressure of 10^3 Pa. Corresponding additional degrees of freedom and obtained values of relaxation times and their ratios.

and Kn_{int}, to account for translational and internal energy exchange. We rescale the microscopic time scales as

$$\tau_{tr} = \mathrm{Kn}_{tr}\tilde{\tau}_{tr} \quad \text{and} \quad \tau_{int} = \mathrm{Kn}_{int}\tilde{\tau}_{int} \; . \tag{4.1}$$

Here, $\tilde{\tau}_{tr}$ and $\tilde{\tau}_{int}$ are of the order of the macroscopic time scale τ_0. The notation used is chosen since it always indicates the type of collision (translational or internal) that gives rise to a term occurring in the equations below. After the expansion is done, the Knudsen numbers will be substituted back to microscopic time scales and the original equations will be recovered.

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 ε as

$$\mathrm{Kn}_{tr} = \epsilon \quad \text{and} \quad \mathrm{Kn}_{int} = \epsilon^{\alpha} \; . \tag{4.2}$$

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

$$\alpha = 1 - \frac{\ln \frac{\tau_{tr}}{\tau_{int}}}{\ln \mathrm{Kn}_{tr}} = \left(1 + \frac{\ln \frac{\tau_{tr}}{\tau_{int}}}{\ln \mathrm{Kn}_{int}}\right)^{-1} \; . \tag{4.3}$$

While the ratio of relaxation times $\frac{\tau_{tr}}{\tau_{int}}$ depends on the state of the gas, the ratio $\frac{\tau_{tr}}{\tau_0} = \epsilon = \mathrm{Kn}_{tr}$ depends on the relevant macroscopic time scale τ_0. Accordingly, the value of both α and $\epsilon = \mathrm{Kn}_{tr}$ depend on the chosen scale. To show some examples of the translational and internal relaxation times and their ratios, we used the experimental data on shear viscosity [83] and fitting data on bulk viscosity [38] of normal

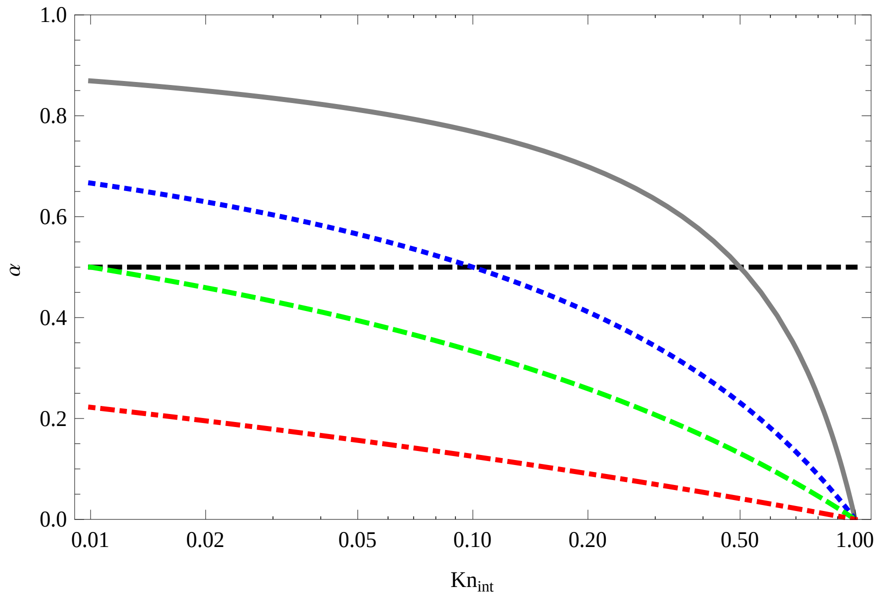

Figure 4.1: Knudsen number and four relaxation times ratio, $\tau_{tr}/\tau_{int} = 0.5$ (gray solid line), $\tau_{tr}/\tau_{int} = 10^{-1}$ (blue dots), $\tau_{tr}/\tau_{int} = 10^{-2}$ (green dashed line) and $\tau_{tr}/\tau_{int} = 10^{-7}$ (red dot-dashed line). The limit of $\alpha = 0.5$ is shown with black dashed line.

Hydrogen and Deuterium. As will be shown later, shear and bulk viscosity (5.16) becomes,

$$\mu = \tau_{tr}\rho_0\theta_0 = \tau_{tr}p_0 \; , \tag{4.4a}$$

$$v = \tau_{int}\frac{2\left(\delta + \theta_0 \frac{d\delta}{d\theta}\mid_0\right)}{3\left(3 + \delta + \theta_0 \frac{d\delta}{d\theta}\mid_0\right)}\, p_0. \tag{4.4b}$$

Values for the translational and internal relaxation times of normal Hydrogen and Deuterium for reference pressure of 10^3 Pa and reference temperature of 77.3 and 293 (K) are listed in the table 4.1 [83, 38]. Bulk viscosity values are obtained by assuming different values for specific heat based on the temperature, which are converted to corresponding values of δ, Eq. 5.78. The obtained relaxation times and their ratio, $\tau_{tr}/\tau_{int} = \mathrm{Kn}_{tr}/\mathrm{Kn}_{int}$, is at order of 10^{-2} and 10^{-3}.

Different values of α correspond to different values of internal or translational Knudsen number and ratios of the relaxation times, $\tau_{tr}/\tau_{int} = \mathrm{Kn}_{tr}/\mathrm{Kn}_{int}$, as shown in figure 4.1. For higher Knudsen numbers Kn_{int}, particularly near unity, mostly values of α less than 0.5 are relevant. The ratio of the relaxation times considered here covers both extreme cases, $\tau_{tr} \approx \tau_{int}$ ($\tau_{tr}/\tau_{int} = 0.5$) and $\tau_{tr} \ll \tau_{int}$ ($\tau_{tr}/\tau_{int} = 10^{-7}$), and the values in between.

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

4.2 Optimizing moment definitions

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

Order of magnitude method is performed in several steps. First step is applying Chapman-Enskog expansion on the moment equations which is done by expanding all the variables in smallness parameters, substituting these expansions back into set of equations and obtaining the first non-vanishing term of each variable. Next step is defining new linearly independent moment definition to substitute variables with linearly dependent first order terms. These two steps repeats until we have full optimized moments with linearly independent first order terms at all orders of accuracy. Model reduction which is the last step of order of magnitude method is presented in next chapter. The Chapman-Enskog expansion on the moment equations must be performed for both Knudsen numbers, that is for all powers of ϵ and ϵ^{α}. 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 $\mathrm{Kn}_{int}^2 \simeq \mathrm{Kn}_{tr}$, proper accounting to first order in Kn_{tr} might require consideration of *different* orders in the CE expansion: expansion to first order in Kn_{tr}, but to second order in Kn_{int}. The conserved variables, density, velocity and total temperature, have equilibrium values and hence are at zero order. The remaining variables are expanded in the smallness parameter as

$$\psi = \epsilon^{0\alpha}\left[\epsilon^0\psi^{(0,0)} + \epsilon^1\psi^{(0,1)} + \epsilon^2\psi^{(0,2)} + \epsilon^3\psi^{(0,3)} + \cdots\right] \\ + \epsilon^{1\alpha}\left[\epsilon^0\psi^{(1,0)} + \epsilon^1\psi^{(1,1)} + \epsilon^2\psi^{(1,2)} + \cdots\right] + \epsilon^{2\alpha}\left[\epsilon^0\psi^{(2,0)} + \epsilon^1\psi^{(2,1)} + \cdots\right] + \cdots \quad , \tag{4.5}$$

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

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

$$\mathcal{O}\left(\epsilon^0\right): \quad u^{2,0(0,0)} = 15\rho\theta^2 \ , \tag{4.6a}$$

$$\mathcal{O}\left(\epsilon^0\right): \quad u^{1,1(0,0)} = \frac{3\delta}{2}\rho\theta^2 \ , \tag{4.6b}$$

$$\mathcal{O}\left(\epsilon^\alpha\right): \quad \Delta\theta^{(1,0)} = \tilde{\tau}_{int}\frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}\theta\frac{\partial v_i}{\partial x_i} \ , \tag{4.6c}$$

$$\mathcal{O}\left(\epsilon^1\right): \quad q_{i,tr}^{(0,1)} = -\frac{\tilde{\tau}_{tr}}{R_{q_{tr}}}\frac{5}{2}\rho\theta\frac{\partial\theta}{\partial x_i} \ , \tag{4.6d}$$

$$\mathcal{O}\left(\epsilon^1\right): \quad u_{ij}^{1,0(0,1)} = -\tilde{\tau}_{tr}14\rho\theta^2\frac{\partial v_{<i}}{\partial x_{j>}} \ , \tag{4.6e}$$

$$\mathcal{O}\left(\epsilon^1\right): \quad u_{ij}^{0,1(0,1)} = -\tilde{\tau}_{tr}\delta\rho\theta^2\frac{\partial v_{<i}}{\partial x_{j>}} \ , \tag{4.6f}$$

$$\mathcal{O}\left(\epsilon^1\right): \quad \sigma_{ij}^{(0,1)} = -\tilde{\tau}_{tr}2\rho\theta\frac{\partial v_{<i}}{\partial x_{j>}} \ , \tag{4.6g}$$

$$\mathcal{O}\left(\epsilon^1\right): \quad q_{i,int}^{(0,1)} = -\frac{\tilde{\tau}_{tr}}{R_{q_{int}}}\frac{\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{2}\rho\theta\frac{\partial\theta}{\partial x_i} \ , \tag{4.6h}$$

$$\mathcal{O}\left(\epsilon^2\right): \quad u_{ijk}^{0,0(0,2)} = -\tilde{\tau}_{tr}\left(\frac{3}{7}\frac{\partial u_{<ij}^{1,0}}{\partial x_{k>}} - 3\sigma_{<ij}\frac{\partial\theta}{\partial x_{k>}} - 3\theta\sigma_{<ij}\frac{\partial\ln\rho}{\partial x_{k>}} + \frac{12}{5}q_{<i,tr}\frac{\partial v_j}{\partial x_{k>}}\right) \ . \tag{4.6i}$$

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

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

$$w^{2,0} = u^{2,0} - 15\rho\theta^2 \ , \tag{4.7a}$$

$$w^{1,1} = u^{1,1} - \frac{3}{2}\delta\rho\theta^2 \ . \tag{4.7b}$$

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

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

$$q_i = q_{i,tr} + q_{i,int} \ , \tag{4.8a}$$

and one unique higher order variable, heat flux difference,

$$\Delta q_i = q_{i,tr} - \frac{5R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} q_{i,int} \ . \tag{4.8b}$$

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

$$u_{ij}^{-} = u_{ij}^{1,0} - \frac{14}{\delta} u_{ij}^{0,1} \ , \tag{4.9a}$$

$$u_{ij}^{+} = u_{ij}^{1,0} + u_{ij}^{0,1} - \frac{(14+\delta)}{2}\theta\sigma_{ij} \ . \tag{4.9b}$$

The second order moment $u_{ijk}^{0,0}$ is the only 3-tensor in the equations and thus remains unchanged. After this first round of the reconstructing moments, we replaced the original 36 variables by the alternative set

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

The new moment equations are obtained from original moment equations, based on the definition of the new moments. The equations for $w^{2,0}$ and $w^{1,1}$ read

$$
\begin{aligned}
&\frac{Dw^{1,1}}{Dt} + \frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} \\
&\qquad [q_k-\Delta q_k]\left[3\frac{\partial\theta}{\partial x_k}+2\frac{\partial\Delta\theta}{\partial x_k}-2\left[\theta-\Delta\theta\right]\frac{\partial\ln\rho}{\partial x_k}-\frac{2}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right] \\
&\qquad + \frac{5\left(5-\delta\right)R_{q_{tr}}R_{q_{int}}}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)\theta\left(q_k-\Delta q_k\right)\frac{\partial\theta}{\partial x_k} \\
&\qquad + \left(\delta-3\frac{2\delta+\theta\frac{d\delta}{d\theta}}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} - \frac{\left(5-\delta\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial\Delta q_k}{\partial x_k} \\
&\qquad + \frac{5R_{q_{int}}q_k+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\Delta q_k}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\left[\delta+\theta\frac{d\delta}{d\theta}\right]\frac{\partial\theta}{\partial x_k} \\
&\qquad + \left(2-\frac{5\left(5-\delta\right)R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}+\frac{3\left(3-\delta\right)}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\theta\frac{\partial q_k}{\partial x_k} \\
&\qquad + \left[\left(\delta-3\frac{2\delta+\theta\frac{d\delta}{d\theta}}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\theta+3\frac{2\delta+\theta\frac{d\delta}{d\theta}}{3+\delta+\theta\frac{d\delta}{d\theta}}\Delta\theta\right]\rho\theta\frac{\partial v_i}{\partial x_i} \\
&\qquad - 2\left(\frac{\delta}{14+\delta}\right)\left[u_{ij}^{-}-u_{ij}^{+}\right]\frac{\partial v_j}{\partial x_i}+\frac{5}{3}w^{1,1}\frac{\partial v_k}{\partial x_k} \\
&\qquad = \frac{R_{u^{1,1}}}{\tau_{tr}}\left[3\rho\left[\frac{3-\delta}{2}\theta\Delta\theta-\frac{3}{2}\Delta\theta^2\right]-w^{1,1}\right]-\frac{R_{u^{1,1}}}{\tau_{int}}w^{1,1}\ . \qquad (4.10)
\end{aligned}
$$

$$
\begin{aligned}
&\frac{Dw^{2,0}}{Dt} + \left(\frac{140 R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}} - \frac{60}{3+\delta+\theta\frac{d\delta}{d\theta}} \right) \theta \frac{\partial q_i}{\partial x_i} \\
&\qquad + \frac{28\left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}} \theta \frac{\partial \Delta q_k}{\partial x_k} + \frac{4}{14+\delta}\left[\delta u^{-}_{ij} + 14 u^{+}_{ij}\right] \frac{\partial v_j}{\partial x_i} \\
&\quad + 4 \frac{5R_{q_{int}} q_k + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}} \Delta q_k}{5R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}} \left[5\frac{\partial \theta}{\partial x_k} + 2\frac{\partial \Delta\theta}{\partial x_k} - 2\left[\theta - \Delta\theta\right] \frac{\partial \ln\rho}{\partial x_k} - \frac{2}{\rho}\frac{\partial \sigma_{kj}}{\partial x_j} \right] \\
&\qquad - \frac{140 R_{q_{tr}} R_{q_{int}}}{\left(5R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)^2} \left(2\frac{d\delta}{d\theta} + \theta \frac{d^2\delta}{d\theta^2} \right) \theta \left(q_k - \Delta q_k\right) \frac{\partial \theta}{\partial x_k} \\
&\qquad\qquad + \frac{60}{3+\delta+\theta\frac{d\delta}{d\theta}} \rho\theta\Delta\theta \frac{\partial v_k}{\partial x_k} + 20 \frac{\delta + \theta\frac{d\delta}{d\theta}}{3+\delta+\theta\frac{d\delta}{d\theta}} \rho\theta^2 \frac{\partial v_k}{\partial x_k} \\
&\qquad\qquad + \left(28 - \frac{60}{3+\delta+\theta\frac{d\delta}{d\theta}} \right) \theta \sigma_{ij} \frac{\partial v_j}{\partial x_i} + \frac{7}{3} w^{2,0} \frac{\partial v_k}{\partial x_k} \\
&\qquad\qquad\quad = \frac{R_{u^{2,0}}}{\tau_{tr}} \left[\left(15\rho\left[-2\theta\Delta\theta + \Delta\theta^2\right] \right) - w^{2,0} \right] - \frac{R_{u^{2,0}}}{\tau_{int}} w^{2,0} \ ,
\end{aligned} \tag{4.11}
$$

The equations for total heat flux and heat flux difference are

$$
\begin{aligned}
&\frac{Dq_i}{Dt} + \rho \left[\frac{5+\delta}{2}\theta - \Delta\theta \right] \frac{\partial \Delta\theta}{\partial x_i} - \sigma_{ik}\left[\theta - \Delta\theta\right] \frac{\partial \ln\rho}{\partial x_k} \\
&\qquad + \left[\frac{7+\delta}{2}\theta\Delta\theta - \Delta\theta^2 \right] \frac{\partial \rho}{\partial x_i} + \frac{1}{3}\frac{\partial w^{1,1}}{\partial x_i} + \frac{1}{6}\frac{\partial w^{2,0}}{\partial x_i} + u^{0,0}_{ijk}\frac{\partial v_j}{\partial x_k} \\
&\qquad - \frac{1}{\rho}\sigma_{ik}\frac{\partial \sigma_{kj}}{\partial x_j} + \left[\theta + \Delta\theta\right] \frac{\partial \sigma_{ij}}{\partial x_j} + \left[\theta\frac{d\delta}{d\theta} + 5 + \delta \right] \frac{\sigma_{ij}}{2} \frac{\partial \theta}{\partial x_j} \\
&\qquad - \frac{7}{(14+\delta)^2}\frac{d\delta}{d\theta}\left[u^{-}_{ij} - u^{+}_{ij}\right] \frac{\partial \theta}{\partial x_j} + \rho \left[\frac{5+\delta}{2}\theta + \frac{\theta^2}{2}\frac{d\delta}{d\theta} + \Delta\theta \right] \frac{\partial \theta}{\partial x_i} \\
&\qquad - \frac{\delta}{2(14+\delta)}\frac{\partial u^{-}_{ij}}{\partial x_j} + \frac{7+\delta}{14+\delta}\frac{\partial u^{+}_{ij}}{\partial x_j} + \frac{2R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}} q_k \frac{\partial v_k}{\partial x_i} \\
&\qquad + \sigma_{ik}\frac{\partial \Delta\theta}{\partial x_k} + \left(1 + \frac{2R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{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] \\
&\qquad + \frac{2\left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{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] \\
&= -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}} \right] \left[\frac{R_{q_{int}} R_{q_{tr}} \left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}} q_i + \frac{\left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}} \left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}} \Delta q_i \right] \ ,
\end{aligned} \tag{4.12}
$$

$$
\begin{aligned}
&\frac{D\Delta q_i}{Dt} - \frac{5}{2}\left[\theta - \Delta\theta\right]\left[\frac{\partial \sigma_{ij}}{\partial x_j} + \rho\frac{\partial \theta}{\partial x_i} - \rho\frac{\partial \Delta\theta}{\partial x_i}\right] \\
&\qquad + \sigma_{ik}\left[\frac{\partial \Delta\theta}{\partial x_k} - \frac{\partial \theta}{\partial x_k} - \left[\theta - \Delta\theta\right]\frac{\partial \ln\rho}{\partial x_k} - \frac{1}{\rho}\frac{\partial \sigma_{kj}}{\partial x_j}\right] \\
&\quad + \frac{5R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\delta\theta + 3\Delta\theta}{2}\left[\frac{\partial \sigma_{ij}}{\partial x_j} + \rho\frac{\partial \theta}{\partial x_i} - \rho\frac{\partial \Delta\theta}{\partial x_i} + \rho\left[\theta - \Delta\theta\right]\frac{\partial \ln\rho}{\partial x_i}\right] \\
&\quad + \frac{5R_{q_{int}}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)\left[q_i - \Delta q_i\right]}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\left[\left(\frac{2}{3 + \delta + \theta\frac{d\delta}{d\theta}}\right)\frac{\sigma_{ij}}{\rho}\frac{\partial v_j}{\partial x_i}\right. \\
&\qquad \left. + \left(\frac{2}{3 + \delta + \theta\frac{d\delta}{d\theta}}\right)\left(\theta - \Delta\theta\right)\frac{\partial v_i}{\partial x_i}\right] + \frac{1}{2}\frac{\partial u^{1,0}_{ik}}{\partial x_k} + u^{0,0}_{ijk}\frac{\partial v_j}{\partial x_k} \\
&\qquad - \frac{5R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\partial u^{0,1}_{ik}}{\partial x_k} + \frac{1}{6}\frac{\partial u^{2,0}}{\partial x_i} - \frac{5R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{1}{3}\frac{\partial u^{1,1}}{\partial x_i} \\
&\quad - \frac{5}{2}\left[\theta^2 - 2\theta\Delta\theta + \Delta\theta^2\right]\frac{\partial \rho}{\partial x_i} + \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\Delta q_j\frac{\partial v_j}{\partial x_i} \\
&\quad + \frac{10R_{q_{int}}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}\left[\frac{q_i}{\rho} - \frac{\Delta q_i}{\rho}\right]\frac{\partial q_i}{\partial x_i} \\
&\qquad + \left(\frac{25R_{q_{int}} + 7\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{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) \\
&\qquad + \frac{2R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{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[\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\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_i + \frac{5R^2_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R^2_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_i\right], \qquad (4.13)
\end{aligned}
$$

Finally equations for u^+_{ij} and u^-_{ij} are obtained as

$$
\begin{aligned}
&\frac{Du^+_{ij}}{Dt} + 2\theta\frac{\partial u^{0,0}_{ijk}}{\partial x_k} + \frac{14+\delta+\theta\frac{d\delta}{d\theta}}{2}u^{0,0}_{ijk}\frac{\partial\theta}{\partial x_k} + 2u^{0,0}_{ijk}\frac{\partial\Delta\theta}{\partial x_k} \\
&\quad + \left[\frac{6}{7}\frac{\delta}{14+\delta}u^-_{<ij} + \frac{12}{14+\delta}u^+_{<ij} + 6\theta\sigma_{<ij}\right]\frac{\partial v_{k>}}{\partial x_k} - 2\left[\theta-\Delta\theta\right]u^{0,0}_{ijk}\frac{\partial\ln\rho}{\partial x_k} \\
&\quad + u^+_{ij}\frac{\partial v_k}{\partial x_k} - 2\frac{u^{0,0}_{ijk}}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l} + \frac{4}{5}\left[\frac{\delta}{14+\delta}u^-_{k<i} + \frac{14}{14+\delta}u^+_{k<i} + 7\theta\sigma_{k<i}\right]\frac{\partial v_k}{\partial x_{j>}} \\
&\quad + \left[\frac{2R_{q_{int}}\left[14+\delta+\theta\frac{d\delta}{d\theta}\right]}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} - \frac{18R_{q_{int}}R_{q_{tr}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right]q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\
&\quad - \left(1+\frac{11}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\sigma_{ij}\left[\frac{1}{\rho}\frac{\partial q_k}{\partial x_k} + \frac{\sigma_{kl}}{\rho}\frac{\partial v_l}{\partial x_k} + (\theta-\Delta\theta)\frac{\partial v_k}{\partial x_k}\right] \\
&\quad + 2\left[\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left[14+\delta+\theta\frac{d\delta}{d\theta}\right]}{5\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)} + \frac{9R_{q_{int}}R_{q_{tr}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right]\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\
&\quad + \left(2\left[1+\frac{9R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right]q_{<i} + \frac{2}{5}\left[9-\frac{45R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right]\Delta q_{<i}\right) \\
&\quad \left[\frac{\partial\Delta\theta}{\partial x_{j>}} - \frac{\left[\theta-\Delta\theta\right]}{\rho}\frac{\partial\rho}{\partial x_{j>}} - \frac{1}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_k}\right] + 2u^+_{k<i}\frac{\partial v_{j>}}{\partial x_k} \\
&\quad + 2\frac{14R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_{<i}}{\partial x_{j>}} + \frac{18\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial\Delta q_{<i}}{\partial x_{j>}} \\
&\quad + \left[\frac{2}{3}w^{1,1} + \frac{14}{15}w^{2,0} + (14+\delta)\rho\theta\Delta\theta\right]\frac{\partial v_{<i}}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]u^+_{ij} \qquad (4.14)
\end{aligned}
$$

$$
\begin{aligned}
&\frac{Du^{-}_{ij}}{Dt} - 2u^{0,0}_{ijk}\left[[\theta-\Delta\theta]\frac{\partial\ln\rho}{\partial x_k} - \frac{\partial\Delta\theta}{\partial x_k} + \frac{1}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l}\right] \\
&\quad + 28\left(\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}} - \delta R_{q_{int}}}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}q_{<i} - \frac{(5+\delta)\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\Delta q_{<i}\right) \\
&\qquad\left[[\theta-\Delta\theta]\frac{\partial\ln\rho}{\partial x_{j>}} - \frac{\partial\Delta\theta}{\partial x_{j>}} + \frac{1}{\rho}\frac{\partial\sigma_{j>l}}{\partial x_l}\right] - \frac{7\theta}{\delta}\frac{d\delta}{d\theta}u^{0,0}_{ijk}\frac{\partial\theta}{\partial x_k} \\
&\qquad + 28\frac{\delta R_{q_{int}} - \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial q_{<i}}{\partial x_{j>}} + 2\theta\frac{\partial u^{0,0}_{ijk}}{\partial x_k} \\
&\qquad + \frac{28(5+\delta)\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial\Delta q_{<i}}{\partial x_{j>}} + 2u^{-}_{k<i}\frac{\partial v_{j>}}{\partial x_k} \\
&\qquad + \left[\frac{2R_{q_{int}}\left[14+\delta+\theta\frac{d\delta}{d\theta}\right]}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} - \frac{18\delta R_{q_{int}}R_{q_{tr}}\theta\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right. \\
&\left. -28R_{q_{int}}\frac{\theta\frac{d\delta}{d\theta}\left(5R_{q_{int}} + \delta R_{q_{tr}}\right) + \theta\left(\theta\left(\frac{d\delta}{d\theta}\right)^2 + (5+\delta)\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)\right)R_{q_{tr}}}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right]q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\
&+ 28\theta R_{q_{tr}}\left[\frac{(5+\delta)\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)R_{q_{int}}}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} - \frac{\frac{d\delta}{d\theta}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\right]\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\
&\qquad + \left[\frac{6}{7}\frac{\delta}{14+\delta}u^{-}_{<ij} + \frac{12}{14+\delta}u^{+}_{<ij} + 6\theta\sigma_{<ij}\right]\frac{\partial v_{k>}}{\partial x_k} \\
&\qquad + \frac{4}{5}\left[\frac{\delta}{14+\delta}u^{-}_{k<i} + \frac{14}{14+\delta}u^{+}_{k<i} + 7\theta\sigma_{k<i}\right]\frac{\partial v_k}{\partial x_{j>}} \\
&\quad + \frac{\frac{28}{\delta}\frac{d\delta}{d\theta}}{3+\delta+\theta\frac{d\delta}{d\theta}}\left[\frac{\theta\sigma_{ij}}{2} + \frac{u^{+}_{ij} - u^{-}_{ij}}{14+\delta}\right]\left[\frac{1}{\rho}\frac{\partial q_i}{\partial x_i} + \frac{\sigma_{ij}}{\rho}\frac{\partial v_j}{\partial x_i} + (\theta-\Delta\theta)\frac{\partial v_i}{\partial x_i}\right] \\
&\qquad + u^{-}_{ij}\frac{\partial v_k}{\partial x_k} + \frac{14}{15}\left(w^{2,0} - \frac{10}{\delta}w^{1,1}\right)\frac{\partial v_{<i}}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]u^{-}_{ij}\ , \qquad (4.15)
\end{aligned}
$$

The leading order terms of the new moments are found as the first non vanishing term in their expansion (4.5). Here, $\left\{\rho, v_i, \theta, q_i, \Delta q_i, \sigma_{ij}, u^{0,0}_{ijk}\right\}$ have linear independent leading order terms, thus, there will be no further change for these variables. The other variables have linearly dependent leading orders as

$$
\mathcal{O}\left(\epsilon^{\alpha}\right):\quad w^{2,0(1,0)} = -30\rho\theta\Delta\theta\ ,\qquad w^{1,1(1,0)} = \frac{3}{2}[3-\delta]\rho\theta\Delta\theta\ , \qquad (4.16a)
$$

$$
\mathcal{O}\left(\epsilon^{1+\alpha}\right):\quad u^{-(1,1)}_{ij} = \tilde{\tau}_{tr}14\frac{[3+\delta]}{\delta}\rho\theta\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}\ ,\qquad u^{+(1,1)}_{ij} = \tilde{\tau}_{tr}11\rho\theta\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}\ . \qquad (4.16b)
$$

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

$$z^{2,0} = w^{2,0} + 30\rho\theta\Delta\theta \ \ , \tag{4.17a}$$

$$z^{1,1} = w^{1,1} - \frac{3}{2}\left[3-\delta\right]\rho\theta\Delta\theta \ , \tag{4.17b}$$

$$B^-_{ij} = u^+_{ij} - \frac{11}{14}\frac{\delta}{\delta+3}u^-_{ij} \ \ , \tag{4.17c}$$

$$B^+_{ij} = u^+_{ij} + u^-_{ij} \ . \tag{4.17d}$$

The new moment equations for B^+_{ij} and B^-_{ij} are written using linear combination of

u_{ij}^{-} and u_{ij}^{+} equations as

$$\frac{DB_{ij}^{+}}{Dt}+\left[\frac{28}{15}z^{2,0}-\frac{2\left(14-\delta\right)}{3\delta}z^{1,1}-\frac{\left(42+25\delta\right)}{\delta}\rho\theta\Delta\theta\right]\frac{\partial v_{<i}}{\partial x_{j>}}$$
$$+2\left(\frac{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{\left(14-\delta\right)}{\delta}\right)\theta\frac{\partial q_{<i}}{\partial x_{j>}}+4\theta\frac{\partial u_{ijk}^{0,0}}{\partial x_{k}}$$
$$+\frac{2\left(70+23\delta\right)R_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial\Delta q_{<i}}{\partial x_{j>}}+B_{ij}^{+}\frac{\partial v_{k}}{\partial x_{k}}$$
$$+2R_{q_{tr}}\left[\frac{\delta\left[14+\delta+\theta\frac{d\delta}{d\theta}\right]-14\frac{d\delta}{d\theta}}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\left(\delta+\theta\frac{d\delta}{d\theta}\right)\right.$$
$$\left.+\frac{2R_{q_{tr}}R_{q_{int}}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^{2}\delta}{d\theta^{2}}\right)\left(70+\delta\left[14+9\theta\right]\right)}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^{2}}\right]\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}}+2R_{q_{int}}\left[\frac{\left[14+\delta+\theta\frac{d\delta}{d\theta}\right]}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right.$$
$$\left.-\theta\frac{10\left(7R_{q_{int}}+2\left(7+3\delta\right)R_{q_{tr}}\right)\frac{d\delta}{d\theta}+14R_{q_{tr}}\theta\left(\frac{d\delta}{d\theta}\right)^{2}+\left(70+23\delta\right)R_{q_{tr}}\theta\frac{d^{2}\delta}{d\theta^{2}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^{2}}\right]q_{<i}\frac{\partial\theta}{\partial x_{j>}}$$
$$+2\left(\frac{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{\left(14-\delta\right)}{\delta}\right)q_{<i}\left[\frac{\partial\Delta\theta}{\partial x_{j>}}-\frac{\left[\theta-\Delta\theta\right]}{\rho}\frac{\partial\rho}{\partial x_{j>}}-\frac{1}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_{k}}\right]$$
$$+\frac{2\left(70+23\delta\right)R_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\Delta q_{<i}\left[\frac{\partial\Delta\theta}{\partial x_{j>}}-\frac{\left[\theta-\Delta\theta\right]}{\rho}\frac{\partial\rho}{\partial x_{j>}}-\frac{1}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_{k}}\right]$$
$$-4u_{ijk}^{0,0}\left[\left[\theta-\Delta\theta\right]\frac{\partial\ln\rho}{\partial x_{k}}-\frac{\partial\Delta\theta}{\partial x_{k}}+\frac{1}{\rho}\frac{\partial\sigma_{kl}}{\partial x_{l}}\right]+\frac{14+\delta+\frac{\delta-14}{\delta}\theta\frac{d\delta}{d\theta}}{2}u_{ijk}^{0,0}\frac{\partial\theta}{\partial x_{k}}$$
$$+2B_{k<i}^{+}\frac{\partial v_{j>}}{\partial x_{k}}+\frac{8\left(14-\delta\right)\left(3+\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}\left[\frac{14}{5}B_{k<i}^{-}\frac{\partial v_{k}}{\partial x_{j>}}+3B_{<ij}^{-}\frac{\partial v_{k>}}{\partial x_{k}}\right]$$
$$+\frac{8\delta}{\left(42+25\delta\right)}\left[\frac{14}{5}B_{k<i}^{+}\frac{\partial v_{k}}{\partial x_{j>}}+3B_{<ij}^{+}\frac{\partial v_{k>}}{\partial x_{k}}\right]+4\theta\left[\frac{14}{5}\sigma_{k<i}\frac{\partial v_{k}}{\partial x_{j>}}+3\sigma_{<ij}\frac{\partial v_{k>}}{\partial x_{k}}\right]$$
$$+\frac{28\frac{d\delta}{d\theta}}{\delta\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\frac{28\left(3+\delta\right)B_{ij}^{-}-3\left(14+\delta\right)B_{ij}^{+}}{\left(14+\delta\right)\left(42+25\delta\right)}\left[\frac{1}{\rho}\frac{\partial q_{k}}{\partial x_{k}}+\frac{\sigma_{kl}}{\rho}\frac{\partial v_{l}}{\partial x_{k}}+\left(\theta-\Delta\theta\right)\frac{\partial v_{k}}{\partial x_{k}}\right]$$
$$+\frac{\left(14-\delta\right)\theta\frac{d\delta}{d\theta}-\delta\left(14+\delta\right)}{\delta\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\sigma_{ij}\left[\frac{1}{\rho}\frac{\partial q_{k}}{\partial x_{k}}+\frac{\sigma_{kl}}{\rho}\frac{\partial v_{l}}{\partial x_{k}}+\left(\theta-\Delta\theta\right)\frac{\partial v_{k}}{\partial x_{k}}\right]=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]B_{ij}^{+}\,, \tag{4.18}$$

$$
\begin{aligned}
&\frac{DB^{-}_{ij}}{Dt} - \frac{14+\delta}{3+\delta}\sigma_{ij}\left[\frac{1}{\rho}\frac{\partial q_k}{\partial x_k} + \frac{\sigma_{kl}}{\rho}\frac{\partial v_l}{\partial x_k} + (\theta-\Delta\theta)\frac{\partial v_k}{\partial x_k}\right] \\
&\quad - \frac{22\frac{d\delta}{d\theta}}{(3+\delta)(14+\delta)\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}B^{-}_{ij}\left[\frac{1}{\rho}\frac{\partial q_k}{\partial x_k} + \frac{\sigma_{lk}}{\rho}\frac{\partial v_k}{\partial x_l} + (\theta-\Delta\theta)\frac{\partial v_k}{\partial x_k}\right] \\
&\quad + 2B^{-}_{k<i}\frac{\partial v_{j>}}{\partial x_k} + B^{-}_{ij}\frac{\partial v_k}{\partial x_k} + \frac{14+\delta+\frac{14+\delta}{3+\delta}\theta\frac{d\delta}{d\theta}}{2}u^{0,0}_{ijk}\frac{\partial \theta}{\partial x_k} \\
&\quad + \frac{3(14+\delta)}{14(3+\delta)}\left[\frac{12(14-\delta)(3+\delta)}{(14+\delta)(42+25\delta)}B^{-}_{<ij} + \frac{12\delta}{(42+25\delta)}B^{+}_{<ij} + 6\theta\sigma_{<ij}\right]\frac{\partial v_{k>}}{\partial x_k} \\
&\quad + \frac{6(14+\delta)}{35(3+\delta)}\left[\frac{14(14-\delta)(3+\delta)}{(14+\delta)(42+25\delta)}B^{-}_{k<i} + \frac{14\delta}{(42+25\delta)}B^{+}_{k<i} + 7\theta\sigma_{k<i}\right]\frac{\partial v_k}{\partial x_{j>}} \\
&\quad + \frac{14+\delta}{3+\delta}\left[\frac{2}{3}z^{1,1} + \frac{1}{5}z^{2,0}\right]\frac{\partial v_{<i}}{\partial x_{j>}} + 2\frac{(14+\delta)R_{q_{tr}}}{(3+\delta)\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)} \\
&\quad \left[\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5}\left(3+\delta+\theta\frac{d\delta}{d\theta}\right) - \frac{2\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right]\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\
&\quad + \frac{2(14+\delta)R_{q_{int}}}{(3+\delta)\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\left(5R_{q_{int}}\left[3+\delta+\theta\frac{d\delta}{d\theta}\right]\right. \\
&\quad \left. + R_{q_{tr}}\left[(3+\delta)\delta + (7+2\delta)\theta\frac{d\delta}{d\theta} + \left(\left(\frac{d\delta}{d\theta}\right)^2 + 2\frac{d^2\delta}{d\theta^2}\right)\theta^2\right]\right)q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\
&\quad + \frac{2(14+\delta)\left[\left(3R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)q_{<i} - \frac{2}{5}\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\Delta q_{<i}\right]}{(3+\delta)\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)} \\
&\quad \left[\frac{\partial\Delta\theta}{\partial x_{j>}} - \frac{[\theta-\Delta\theta]}{\rho}\frac{\partial\rho}{\partial x_{j>}} - \frac{1}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_k}\right] + \frac{3(14+\delta)}{7(3+\delta)}\theta\frac{\partial u^{0,0}_{ijk}}{\partial x_k} \\
&\quad - \frac{3(14+\delta)}{7(3+\delta)}u^{0,0}_{ijk}\left[[\theta-\Delta\theta]\frac{\partial\ln\rho}{\partial x_k} - \frac{\partial\Delta\theta}{\partial x_k} + \frac{1}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l}\right] \\
&\quad + 2\frac{(14+\delta)\left(3R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{(3+\delta)\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial q_{<i}}{\partial x_{j>}} \\
&\quad + \frac{2(70+23\delta)\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial\Delta q_{<i}}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]B^{-}_{ij}\ . \qquad (4.19)
\end{aligned}
$$

There will be no further change in definition of moments B^{-}_{ij} and B^{+}_{ij}, since they have linearly independent leading order terms. Furthermore, equations for $z^{2,0}$ and $z^{1,1}$ are obtained as

$$
\begin{aligned}
&\frac{Dz^{2,0}}{Dt} + \frac{8\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial\Delta q_k}{\partial x_k} \\
&\quad + 8\frac{5R_{q_{int}}q_k+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\Delta q_k}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\left[\frac{\partial\Delta\theta}{\partial x_k}-\left[\theta-\Delta\theta\right]\frac{\partial\ln\rho}{\partial x_k}-\frac{1}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right] \\
&\quad + \frac{40R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_i}{\partial x_i} + \frac{60}{3+\delta+\theta\frac{d\delta}{d\theta}}\Delta\theta\frac{\partial q_i}{\partial x_i} + 8\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} \\
&\quad + 20R_{q_{tr}}\frac{2R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)+\left(\delta+\theta\frac{d\delta}{d\theta}\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\Delta q_k\frac{\partial\theta}{\partial x_k} \\
&\quad + 20R_{q_{int}}\frac{\left(25R_{q_{int}}+5\delta R_{q_{tr}}+R_{q_{tr}}\theta\left(\frac{d\delta}{d\theta}-2\theta\frac{d^2\delta}{d\theta^2}\right)\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}q_k\frac{\partial\theta}{\partial x_k} + \frac{7}{3}z^{2,0}\frac{\partial v_k}{\partial x_k} \\
&\quad + \left[\frac{60}{3+\delta+\theta\frac{d\delta}{d\theta}}-20\right]\rho\theta\Delta\theta\frac{\partial v_k}{\partial x_k} - 30\left(\frac{2}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\rho\Delta\theta^2\frac{\partial v_k}{\partial x_k} \\
&\quad + \left[\frac{56\left(14-\delta\right)\left(3+\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}B^{-}_{ij}+\frac{56\delta}{\left(42+25\delta\right)}B^{+}_{ij}\right]\frac{\partial v_j}{\partial x_i} + \frac{60}{3+\delta+\theta\frac{d\delta}{d\theta}}\Delta\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} \\
&\quad = \frac{R_{u^{2,0}}}{\tau_{tr}}\left[\left(15\rho\Delta\theta^2\right)-z^{2,0}\right] - \frac{1}{\tau_{int}}\left[R_{u^{2,0}}z^{2,0}+\left(1-R_{u^{2,0}}\right)30\rho\theta\Delta\theta\right]\ , \qquad (4.20)
\end{aligned}
$$

$$
\begin{aligned}
&\frac{Dz^{1,1}}{Dt} + \frac{6\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3+\delta+\theta\frac{d\delta}{d\theta}}\rho\theta\Delta\theta\frac{\partial v_i}{\partial x_i} \\
&\quad + \left[\frac{10R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} + \frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right] q_k\frac{\partial\theta}{\partial x_k} \\
&\quad + \left[\frac{\left(-3+\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} - \frac{10R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right]\Delta q_k\frac{\partial\theta}{\partial x_k} \\
&\quad + \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_k}{\partial x_k} + 3\frac{-3+\delta+\theta\frac{d\delta}{d\theta}}{3+\delta+\theta\frac{d\delta}{d\theta}}\Delta\theta\frac{\partial q_k}{\partial x_k} \\
&\quad - \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial\Delta q_k}{\partial x_k} - \frac{6\delta}{(42+25\delta)}B^{+}_{ij}\frac{\partial v_j}{\partial x_i} \\
&\quad + \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\left[q_k-\Delta q_k\right]\left[\frac{\partial\Delta\theta}{\partial x_k} - \left[\theta-\Delta\theta\right]\frac{\partial\ln\rho}{\partial x_k} - \frac{1}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right] \\
&\quad + \left[3-\delta-\theta\frac{d\delta}{d\theta}\right]\frac{3}{3+\delta+\theta\frac{d\delta}{d\theta}}\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i} + 3\frac{-3+\delta+\theta\frac{d\delta}{d\theta}}{3+\delta+\theta\frac{d\delta}{d\theta}}\Delta\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} \\
&\quad + \frac{56\delta(3+\delta)}{(14+\delta)(42+25\delta)}B^{-}_{ij}\frac{\partial v_j}{\partial x_i} + \frac{5}{3}z^{1,1}\frac{\partial v_k}{\partial x_k} \\
&= -\frac{R_{u^{1,1}}}{\tau_{tr}}\left[\frac{9}{2}\rho\Delta\theta^2 + z^{1,1}\right] - \frac{1}{\tau_{int}}\left(R_{u^{1,1}}z^{1,1} + \left(R_{u^{1,1}}-1\right)\frac{3\left[3-\delta\right]}{2}\rho\theta\Delta\theta\right)\ , \qquad (4.21)
\end{aligned}
$$

The leading order terms of $z^{2,0}$ and $z^{1,1}$ are linearly dependent as

$$
\mathcal{O}\left(\epsilon^{2\alpha}\right): \quad z^{1,1(2,0)} = -\frac{9}{2}\rho\Delta\theta^2\ , \qquad z^{2,0(2,0)} = 15\rho\Delta\theta^2\ . \qquad (4.22)
$$

Therefore, we construct new moments to have linearly independent leading orders which substitute $\{z^{2,0}, z^{1,1}\}$ as

$$
B^{+} = z^{1,1} - z^{2,0}\ , \qquad (4.23a)
$$

$$
B^{-} = z^{1,1} + \frac{3}{10}z^{2,0}\ . \qquad (4.23b)
$$

Using linear combination, the equations for new moments obtained as,

$$
\begin{aligned}
&\frac{DB^{-}}{Dt}+\frac{2}{5}\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial\Delta q_k}{\partial x_k}\\
&\quad+\left[\frac{196\left(6+\delta\right)\left(3+\delta\right)}{5\left(14+\delta\right)\left(42+25\delta\right)}B^{-}_{ij}+\frac{54\delta}{5\left(42+25\delta\right)}B^{+}_{ij}\right]\frac{\partial v_j}{\partial x_i}+\frac{71}{39}B^{-}\frac{\partial v_k}{\partial x_k}\\
&\quad+2\left(1+\frac{R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)q_k\left[\frac{\partial\Delta\theta}{\partial x_k}-\left[\theta-\Delta\theta\right]\frac{\partial\ln\rho}{\partial x_k}-\frac{1}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right]\\
&\quad+\frac{2}{5}\left(1-\frac{5R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\Delta q_k\left[\frac{\partial\Delta\theta}{\partial x_k}-\left[\theta-\Delta\theta\right]\frac{\partial\ln\rho}{\partial x_k}-\frac{1}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right]\\
&\quad+\left[\frac{\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}+\frac{2R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right]\Delta q_k\frac{\partial\theta}{\partial x_k}\\
&\quad+\frac{12R_{q_{int}}+2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_k}{\partial x_k}+3\Delta\theta\frac{\partial q_k}{\partial x_k}\\
&\quad+\left[\frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)+30R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}-\frac{2R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right]q_k\frac{\partial\theta}{\partial x_k}\\
&\quad-\frac{2}{13}B^{+}\frac{\partial v_k}{\partial x_k}-3\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i}+\frac{12}{5}\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i}+3\Delta\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i}\\
&=-\frac{1}{\tau_{tr}}\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^{+}+\frac{9\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{2}\rho\Delta\theta^2\right]\\
&-\frac{1}{\tau_{int}}\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^{+}+\frac{3}{2}\left(3+\delta+\left[3-\delta\right]R_{u^{1,1}}-6R_{u^{2,0}}\right)\rho\theta\Delta\theta\right],
\end{aligned}
\tag{4.24}
$$

$$
\begin{aligned}
&\frac{DB^+}{Dt} + \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}} - 40R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_k}{\partial x_k} \\
&\quad + \left[\frac{\left(-23+\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} - \frac{50R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right]\Delta q_k\frac{\partial\theta}{\partial x_k} \\
&\quad + \frac{5}{39}\left(17B^+ - 4B^-\right)\frac{\partial v_k}{\partial x_k} + \left(26 - \frac{78}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\rho\theta\Delta\theta\frac{\partial v_i}{\partial x_i} \\
&\quad + 3\frac{-23+\delta+\theta\frac{d\delta}{d\theta}}{3+\delta+\theta\frac{d\delta}{d\theta}}\Delta\theta\frac{\partial q_k}{\partial x_k} - \frac{10\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial \Delta q_k}{\partial x_k} \\
&\quad + \left[\frac{50R_{q_{int}}R_{q_{tr}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} + \frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right) - 100R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right]q_k\frac{\partial\theta}{\partial x_k} \\
&\quad - \left[\frac{112\left(7-\delta\right)\left(3+\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}B^-_{ij} + \frac{62\delta}{\left(42+25\delta\right)}B^+_{ij}\right]\frac{\partial v_j}{\partial x_i} \\
&\quad + \left[\left(2 - \frac{50R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)q_k - \frac{10\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_k\right] \\
&\quad \left[\frac{\partial\Delta\theta}{\partial x_k} - \left[\theta-\Delta\theta\right]\frac{\partial\ln\rho}{\partial x_k} - \frac{1}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right] + \frac{3\left(23-\delta-\theta\frac{d\delta}{d\theta}\right)}{3+\delta+\theta\frac{d\delta}{d\theta}}\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i} \\
&\quad - \frac{3\left(23-\delta-\theta\frac{d\delta}{d\theta}\right)}{3+\delta+\theta\frac{d\delta}{d\theta}}\Delta\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} - 8\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} \\
&= -\frac{1}{\tau_{tr}}\left[\frac{1}{13}\left(10\left[R_{u^{1,1}} - R_{u^{2,0}}\right]B^- + \left[3R_{u^{1,1}} + 10R_{u^{2,0}}\right]B^+\right) + \left(\frac{9}{2}R_{u^{1,1}} + 15R_{u^{2,0}}\right)\rho\Delta\theta^2\right] \\
&\quad - \frac{1}{\tau_{int}}\left[\frac{1}{13}\left(10\left[R_{u^{1,1}} - R_{u^{2,0}}\right]B^- + \left[3R_{u^{1,1}} + 10R_{u^{2,0}}\right]B^+\right)\right. \\
&\quad \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] \ . \qquad (4.25)
\end{aligned}
$$

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

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

By construction, these variables are linearly independent in their leading orders. This give us the least number of variables at each order of accuracy.

4.3 Orders and leading terms of optimized moments

The leading order contributions of all non-equilibrium variables are obtained from Chapman-Enskog expansion as described in previous section for proper accounting of the magnitude and later use of the expressions. The leading order terms of dynamic temperature and stress tensor are

$$\Delta\theta = \tau_{int} \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)} \theta \frac{\partial v_i}{\partial x_i} \ , \tag{4.26}$$

$$\sigma_{ij} = -\tau_{tr} 2\rho\theta \frac{\partial v_{<i}}{\partial x_{j>}} \ . \tag{4.27}$$

The leading order terms of heat fluxes are obtained by decoupling the equations for total heat flux and heat flux difference. At the leading order we have,

$$\begin{bmatrix} \frac{R_{q_{int}} R_{q_{tr}} \left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} & \frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}} \left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} \\ \frac{5R_{q_{int}} \left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} & \frac{5R^2_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R^2_{q_{tr}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} \end{bmatrix} \begin{bmatrix} q_i \\ \Delta q_i \end{bmatrix} = \begin{bmatrix} -\tau_{tr} \frac{5+\delta+\theta\frac{d\delta}{d\theta}}{2} \rho\theta \frac{\partial\theta}{\partial x_i} \\ -\tau_{tr} \frac{5}{2} \left[1 - \frac{R_{q_{int}}}{R_{q_{tr}}}\right] \rho\theta \frac{\partial\theta}{\partial x_i} \end{bmatrix} \tag{4.28}$$

which give us the first order contributions as

$$\mathcal{O}\left(\epsilon^1\right): \quad q_i = \tau_{tr} \frac{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{2R_{q_{int}} R_{q_{tr}}} \rho\theta \frac{\partial\theta}{\partial x_i} \qquad \text{and} \qquad \Delta q_i = 0 \ . \tag{4.29}$$

Therefore, the total heat flux is at first order and the heat flux difference is at $\mathcal{O}\left(\epsilon^{1+\alpha}\right)$. The leading order terms of Δq_i is obtained by decoupling the equations at order $\epsilon^{1+\alpha}$ as

$$\mathcal{O}\left(\epsilon^{1+\alpha}\right): \quad \Delta q_i = \tau_{tr} \frac{5\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}{2\left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} \rho\theta \frac{\partial\Delta\theta}{\partial x_i} \ . \tag{4.30}$$

The leading order terms of scalar moments B^+ and B^- are obtained by decoupling their equations. At the $\mathcal{O}\left(\epsilon^{2\alpha}\right)$ we have

$$\begin{bmatrix} \frac{3R_{u^{1,1}} + 10R_{u^{2,0}}}{13} & \frac{10R_{u^{1,1}} - 10R_{u^{2,0}}}{13} \\ \frac{3R_{u^{1,1}} - 3R_{u^{2,0}}}{13} & \frac{10R_{u^{1,1}} + 3R_{u^{2,0}}}{13} \end{bmatrix} \begin{bmatrix} B^+ \\ B^- \end{bmatrix} = \begin{bmatrix} \left(\frac{9}{2} R_{u^{1,1}} + 15 R_{u^{2,0}}\right) \rho\Delta\theta^2 \\ -\frac{9}{2}\left(R_{u^{1,1}} - R_{u^{2,0}}\right) \rho\Delta\theta^2 \end{bmatrix} , \tag{4.31}$$

which give us the leading order term of B^+ as,

$$\mathcal{O}\left(\epsilon^{2\alpha}\right): \quad B^+ = -\frac{39}{2}\rho\Delta\theta^2 \qquad \text{and} \qquad B^- = 0\,. \tag{4.32}$$

The leading order term of B^- is obtained by decoupling the equations at $\mathcal{O}\left(\epsilon^1\right)$ as

$$\mathcal{O}\left(\epsilon^{1}\right): \quad B^- = -\frac{3\tau_{tr}}{\tau_{int}}\left[\frac{3}{R_{u^{2,0}}} - \frac{3-\delta}{2R_{u^{1,1}}} - \frac{3+\delta}{2}\right]\rho\theta\Delta\theta\,. \tag{4.33}$$

The leading order terms for the remaining optimized moments B^+_{ij}, B^-_{ij} and $u^{0,0}_{ijk}$ are obtained by applying the Chapman-Enskog expansion on their equations as

$$\mathcal{O}\left(\epsilon^{1+\alpha}\right): \quad B^+_{ij} = \tau_{tr}\frac{42+25\delta}{\delta}\rho\theta\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}\ , \tag{4.34}$$

$$\begin{aligned}
\mathcal{O}\left(\epsilon^{2}\right): \quad B^-_{ij} = -\tau_{tr}\Bigg(&\frac{6\left(14+\delta\right)}{7\left(3+\delta\right)}\theta\left[\sigma_{k<j}\frac{\partial v_{j>}}{\partial x_k} + \sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}} - \frac{2}{3}\sigma_{ij}\frac{\partial v_k}{\partial x_k}\right] \\
&+\frac{2\left(14+\delta\right)R_{q_{int}}}{\left(3+\delta\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\Bigg(5R_{q_{int}}\left[3+\delta+\theta\frac{d\delta}{d\theta}\right] \\
&+R_{q_{tr}}\left[\left(3+\delta\right)\delta+\left(7+2\delta\right)\theta\frac{d\delta}{d\theta}+\left(\left(\frac{d\delta}{d\theta}\right)^2+2\frac{d^2\delta}{d\theta^2}\right)\theta^2\right]\Bigg)q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\
&-\frac{2\left(14+\delta\right)\left(3R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{\left(3+\delta\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta q_{<i}\frac{\partial\ln\rho}{\partial x_{j>}} \\
&+2\frac{\left(14+\delta\right)\left(3R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{\left(3+\delta\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial q_{<i}}{\partial x_{j>}}\Bigg)\ ,
\end{aligned} \tag{4.35}$$

$$\mathcal{O}\left(\epsilon^{2}\right): \quad u^{0,0}_{ijk} = -\tau_{tr}\left[3\theta\frac{\partial\sigma_{<ij}}{\partial x_{k>}} - 3\theta\sigma_{<ij}\frac{\partial\ln\rho}{\partial x_{k>}} + \frac{12R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_{<i}\frac{\partial v_j}{\partial x_{k>}}\right]\,. \tag{4.36}$$

Chapter 5

Model reduction

So many of our dreams at first seems impossible, then they seem improbable, and then, when we summon the will, they soon become inevitable.

Christopher Reeve

The last stage of order of magnitude method is model reduction which is discussed in this chapter. In this stage, the obtained orders of different moments are used to eliminate higher order terms and equations at different levels of accuracy. We presents set of equations at different orders up to order ϵ^3.

The explicit orders can be used for model reduction such that in each order under consideration only terms up to the corresponding power ϵ^x are kept, while all other higher terms can be ignored. We require the explicit order of all terms be clearly visible in the equations, so the orders are made explicit by ϵ^x. By the next section, ϵ will be substituted back to unity so that the original form of the equations is recovered. The introduced notation allows us to arrange all terms by their explicit ϵ-orders. In particular we have:

The conservation laws for mass, momentum and energy,

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

$$\frac{Dv_i}{Dt} + \theta\frac{\partial \ln\rho}{\partial x_i} + \frac{\partial\theta}{\partial x_i} - \epsilon^\alpha\left[\frac{\partial\Delta\theta}{\partial x_i} + \Delta\theta\frac{\partial\ln\rho}{\partial x_i}\right] + \epsilon^1\left[\frac{1}{\rho}\frac{\partial\sigma_{ij}}{\partial x_j}\right] = 0 \ , \tag{5.1b}$$

$$\frac{3+\delta+\theta\frac{d\delta}{d\theta}}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_i}{\partial x_i} - \epsilon^\alpha\left[\rho\Delta\theta\frac{\partial v_i}{\partial x_i}\right] + \epsilon^1\left[\frac{\partial q_i}{\partial x_i} + \sigma_{ij}\frac{\partial v_j}{\partial x_i}\right] = 0 \ ; \tag{5.1c}$$

and the balance laws for dynamic temperature $\Delta\theta$, stress tensor σ_{ij}, overall heat flux q_i, heat flux difference Δq_i:

$$\begin{aligned}
&\epsilon^\alpha\left[\rho\frac{D\Delta\theta}{Dt}+\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\rho\Delta\theta\frac{\partial v_i}{\partial x_i}\right]\\
&\qquad+\epsilon^1\left[\left(\frac{2}{3+\delta+\theta\frac{d\delta}{d\theta}}-\frac{10R_{q_{int}}}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\right)\frac{\partial q_i}{\partial x_i}\right]\\
&\qquad+\epsilon^1\left[\frac{10R_{q_{int}}R_{q_{tr}}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}q_i\frac{\partial\theta}{\partial x_i}-\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\sigma_{ij}\frac{\partial v_j}{\partial x_i}\right]\\
&-\epsilon^{1+\alpha}\left[\frac{10R_{q_{int}}R_{q_{tr}}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\Delta q_i\frac{\partial\theta}{\partial x_i}+\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_i}{\partial x_i}\right]\\
&\qquad-\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\rho\theta\frac{\partial v_i}{\partial x_i}=-\frac{\rho}{\tau_{int}}\Delta\theta\ ,
\end{aligned}\tag{5.2}$$

$$\begin{aligned}
&\epsilon^1\left[\frac{D\sigma_{ij}}{Dt}-\frac{4R_{q_{int}}R_{q_{tr}}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}q_{<i}\frac{\partial\theta}{\partial x_{j>}}\right]\\
&\qquad+\epsilon^1\left[\frac{4R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\partial q_{<i}}{\partial x_{j>}}+2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\sigma_{ij}\frac{\partial v_k}{\partial x_k}\right]\\
&\qquad-\epsilon^\alpha\left[2\rho\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}\right]+\epsilon^{1+\alpha}\left[\frac{4\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_{<i}}{\partial x_{j>}}\right]\\
&\qquad+\epsilon^{1+\alpha}\left[\frac{4R_{q_{int}}R_{q_{tr}}}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}}\right]\\
&\qquad+\epsilon^2\left[\frac{\partial u^{0,0}_{ijk}}{\partial x_k}\right]+2\rho\theta\frac{\partial v_{<i}}{\partial x_{j>}}=-\left[\frac{1}{\tau_{tr}}+\frac{\epsilon^{1-\alpha}}{\tau_{int}}\right]\sigma_{ij}\ ,
\end{aligned}\tag{5.3}$$

$$
\begin{aligned}
&\epsilon^1 \left[\frac{Dq_i}{Dt} + \theta \frac{\partial \sigma_{ik}}{\partial x_k} + \sigma_{ik} \left(\frac{5+\delta+\theta\frac{d\delta}{d\theta}}{2} \frac{\partial \theta}{\partial x_k} - \theta \frac{\partial \ln \rho}{\partial x_k} \right) \right] \\
&\quad + \epsilon^1 \left[\left(1 + \frac{2R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{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] \\
&\quad + \epsilon^1 \left[\frac{2R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{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] \\
&\quad - \epsilon^\alpha \left[\rho\theta \frac{\partial \Delta\theta}{\partial x_i} + \frac{5+\delta+\theta\frac{d\delta}{d\theta}}{2} \rho\Delta\theta \frac{\partial \theta}{\partial x_i} \right] \\
&\quad - \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] \\
&\quad + \epsilon^{1+\alpha} \left[\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{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] \\
&\quad + \epsilon^{1+\alpha} \left[\frac{168}{(42+25\delta)^2} B^+_{ij} \frac{d\delta}{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 \sigma_{ij}}{\partial x_j} \right] \\
&\quad + \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\frac{d\delta}{d\theta}}{2} \rho\theta \frac{\partial \theta}{\partial x_i} \\
&\quad + \epsilon^2 \left[7 \left(\frac{1}{(14+\delta)^2} - \frac{24}{(42+25\delta)^2} \right) B^-_{ij} \frac{d\delta}{d\theta} \frac{\partial \theta}{\partial x_j} - \frac{1}{\rho} \sigma_{ik} \frac{\partial \sigma_{kj}}{\partial x_j} \right] \\
&\quad + \epsilon^2 \left[\frac{7(3+\delta)(14+3\delta)}{(14+\delta)(42+25\delta)} \frac{\partial B^-_{ij}}{\partial x_j} + u^{0,0}_{ijk} \frac{\partial v_j}{\partial x_k} \right] = - \left[\frac{1}{\tau_{tr}} + \frac{\epsilon^{1-\alpha}}{\tau_{int}} \right] \\
&\left(\frac{R_{q_{int}} R_{q_{tr}} \left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} q_i + \epsilon^\alpha \left[\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}} \left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} \Delta q_i \right] \right) , \qquad (5.4)
\end{aligned}
$$

$$
\begin{aligned}
&\epsilon^1\left[\frac{D\Delta q_i}{Dt}+\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.\\
&\qquad+\frac{\delta}{(42+25\delta)}\varsigma_4\frac{\partial B^+_{ij}}{\partial x_j}+\frac{42}{(42+25\delta)^2}\varsigma_4\frac{d\delta}{d\theta}B^+_{ij}\frac{\partial\theta}{\partial x_j}\\
&\qquad-\varsigma_2\theta\Delta q_i\frac{\partial v_k}{\partial x_k}+\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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\sigma_{ij}}{\partial x_j}\\
&\qquad\left.+\left(\frac{25R_{q_{int}}+7\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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]\\
&\qquad-\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]\\
&\qquad+\epsilon^{1-\alpha}\left[\frac{5}{39}\left(1-\frac{10R_{q_{int}}}{\left(\delta+\theta\frac{d\delta}{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{d\delta}{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]+\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)\\
&\left.+\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}+u^{0,0}_{ijk}\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{d\delta}{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}-\varsigma_1\frac{d\delta}{d\theta}B^-_{ij}\frac{\partial\theta}{\partial x_j}\right]\\
&\qquad-\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]\left(\epsilon^{-\alpha}\left[\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_i\right]+\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R^2_{q_{tr}}+5R^2_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_i\right),
\end{aligned}
\tag{5.5a}
$$

where,

$$\varsigma_1 = 7\left(\frac{1}{(14+\delta)^2} + \frac{42}{(42+25\delta)^2} + \frac{10R_{q_{int}}}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\left[\frac{1}{(14+\delta)^2} + \frac{9}{(42+25\delta)^2}\right]\right) \ , \tag{5.5b}$$

$$\varsigma_2 = \frac{10R_{q_{int}}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)} \ , \tag{5.5c}$$

$$\varsigma_3 = \left(1+\frac{3R_{q_{int}}}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right) \ , \tag{5.5d}$$

$$\varsigma_4 = \left(7+\frac{15R_{q_{int}}}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right) \ ; \tag{5.5e}$$

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

$$\begin{aligned}
&\epsilon^1\left[\frac{DB^-}{Dt}+\frac{71}{39}B^-\frac{\partial v_k}{\partial x_k}+\frac{12}{5}\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i}\right] \\
&\quad +\epsilon^1\left[\varsigma_5 q_k\frac{\partial\theta}{\partial x_k}+\frac{12R_{q_{int}}+2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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] \\
&\quad -\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] \\
&\quad +\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] \\
&\quad +\epsilon^{1+\alpha}\left[3\Delta\theta\left(\frac{\partial q_k}{\partial x_k}+\sigma_{ij}\frac{\partial v_j}{\partial x_i}\right)+\frac{2}{5}\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial\Delta q_k}{\partial x_k}\right] \\
&\quad -\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] \\
&\quad +\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] \\
&\quad =-\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\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{13}B^+\right]\right) \\
&-\epsilon^{2\alpha-1}\left[\frac{1}{\tau_{tr}}\frac{9\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{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{5.6a}$$

$$
\begin{aligned}
&\epsilon^{1}\left[\frac{DB^{+}}{Dt}+\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\frac{d\delta}{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\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}+\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}\left(R_{u^{1,1}}-R_{u^{2,0}}\right)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(\left(3-\delta\right)R_{u^{1,1}}+20R_{u^{2,0}}-\left(23-\delta\right)\right)\rho\theta\Delta\theta\right],
\end{aligned}
\tag{5.6b}
$$

where,

$$\varsigma_5 = \left(\frac{\left(5R_{q_{int}} + 3R_{q_{tr}}\right)\left(\delta + \theta\frac{d\delta}{d\theta}\right) + 30R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} - \frac{2R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} \right) , \tag{5.6c}$$

$$\varsigma_6 = 1 + \frac{R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} , \tag{5.6d}$$

$$\varsigma_7 = \frac{\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} + \frac{2R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} , \tag{5.6e}$$

$$\varsigma_8 = \frac{2}{5}\left(1 - \frac{5R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right) , \tag{5.6f}$$

$$\varsigma_9 = \left(\frac{50R_{q_{int}}R_{q_{tr}}\theta\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} + \frac{\left(5R_{q_{int}} + 3R_{q_{tr}}\right)\left(\delta + \theta\frac{d\delta}{d\theta}\right) - 100R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} \right) , \tag{5.6g}$$

$$\varsigma_{10} = \left(2 - \frac{50R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right) , \tag{5.6h}$$

$$\varsigma_{11} = \frac{10\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} , \tag{5.6i}$$

$$\varsigma_{12} = \left(\frac{\left(-23 + \delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} - \frac{50R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} \right) , \tag{5.6j}$$

$$\varsigma_{13} = \frac{3\left(23 - \delta - \theta\frac{d\delta}{d\theta}\right)}{3 + \delta + \theta\frac{d\delta}{d\theta}} \tag{5.6k}$$

$$\varsigma_{14} = \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}} - 40R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} ; \tag{5.6l}$$

The equations for higher moments B_{ij}^{+}, B_{ij}^{-} and $u_{ijk}^{0,0}$,

$$
\begin{aligned}
&\epsilon^{1}\left[\frac{DB_{ij}^{+}}{Dt}+\frac{2\left(70+23\delta\right)R_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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}{\left(42+25\delta\right)}\left(\frac{14}{5}B_{k<i}^{+}\frac{\partial v_{k}}{\partial x_{j>}}+3B_{<ij}^{+}\frac{\partial v_{k>}}{\partial x_{k}}\right)-\frac{\left(14-\delta\right)\theta\frac{d\delta}{d\theta}-\delta\left(14+\delta\right)}{\delta\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\Delta\theta\sigma_{ij}\frac{\partial v_{k}}{\partial x_{k}}\right]\\
&-\epsilon^{1}\left[\left(\Gamma_{1}-1\right)B_{ij}^{+}\frac{\partial v_{k}}{\partial x_{k}}+\frac{2\left(70+23\delta\right)R_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{\left(14-\delta\right)}{\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\left(70+23\delta\right)R_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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_{1}B_{ij}^{+}\Delta\theta\frac{\partial v_{k}}{\partial x_{k}}\right]\\
&+\epsilon^{1-\alpha}\left[2\left(\frac{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{\left(14-\delta\right)}{\delta}\right)\theta\frac{\partial q_{<i}}{\partial x_{j>}}+\Gamma_{2}q_{<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}}+\sigma_{ij}\frac{\partial v_{k}}{\partial x_{k}}\right)+\frac{\left(14-\delta\right)\theta\frac{d\delta}{d\theta}-\delta\left(14+\delta\right)}{\delta\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\theta\sigma_{ij}\frac{\partial v_{k}}{\partial x_{k}}\right]\\
&-\epsilon^{1-\alpha}\left[2\left(\frac{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{\left(14-\delta\right)}{\delta}\right)\theta q_{<i}\frac{\partial\ln\rho}{\partial x_{j>}}-\frac{4\left(70-19\delta\right)}{39\delta}B^{-}\frac{\partial v_{<i}}{\partial x_{j>}}\right]\\
&+\epsilon^{2-\alpha}\left[u_{ijk}^{0,0}\left(\frac{14+\delta+\frac{\delta-14}{\delta}\theta\frac{d\delta}{d\theta}}{2}\frac{\partial\theta}{\partial x_{k}}-4\theta\frac{\partial\ln\rho}{\partial x_{k}}\right)+\frac{\left(14-\delta\right)\theta\frac{d\delta}{d\theta}-\delta\left(14+\delta\right)}{\delta\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\frac{\sigma_{ij}}{\rho}\frac{\partial q_{k}}{\partial x_{k}}\right]\\
&+\epsilon^{2-\alpha}\left[\frac{\left(14-\delta\right)\theta\frac{d\delta}{d\theta}-\delta\left(14+\delta\right)}{\delta\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\frac{\sigma_{ij}\sigma_{kl}}{\rho}\frac{\partial v_{l}}{\partial x_{k}}+\frac{784\left(3+\delta\right)\Gamma_{1}}{84\left(14+\delta\right)}B_{ij}^{-}\frac{\partial v_{k}}{\partial x_{k}}\right]\\
&-\epsilon^{2-\alpha}\left[2\left(\frac{\left(70+23\delta\right)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{\left(14-\delta\right)}{\delta}\right)\frac{q_{<i}}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_{k}}\right]\\
&+\epsilon^{2-\alpha}\left[\frac{8\left(14-\delta\right)\left(3+\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}\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\left(14+\delta\right)\theta}\left(3\left(14+\delta\right)\frac{B_{ij}^{+}}{\rho}\left[\frac{\partial q_{k}}{\partial x_{k}}-\sigma_{kl}\frac{\partial v_{l}}{\partial x_{k}}\right]+28\left(3+\delta\right)B_{ij}^{-}\Delta\theta\frac{\partial v_{k}}{\partial x_{k}}\right)\right]\\
&+\epsilon^{2}\left[4u_{ijk}^{0,0}\left[\Delta\theta\frac{\partial\ln\rho}{\partial x_{k}}+\frac{\partial\Delta\theta}{\partial x_{k}}\right]-\frac{2\left(70+23\delta\right)R_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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\left(3+\delta\right)\Gamma_{1}}{84\left(14+\delta\right)}\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{u_{ijk}^{0,0}}{\rho}\frac{\partial\sigma_{kl}}{\partial x_{l}}\right]\\
&-\epsilon^{\alpha}\left[\frac{2\left(42+25\delta\right)}{39\delta}B^{+}\frac{\partial v_{<i}}{\partial x_{j>}}\right]-\frac{\left(42+25\delta\right)}{\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}^{+}\ ,\qquad(5.7\text{a})
\end{aligned}
$$

$$
\begin{aligned}
&\epsilon^1\left[\frac{DB^-_{ij}}{Dt}-\frac{14+\delta}{3+\delta}\frac{\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\frac{d\delta}{d\theta}}{(3+\delta)(14+\delta)\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}B^-_{ij}\frac{\partial v_k}{\partial x_k}-\frac{14+\delta+\frac{14+\delta}{3+\delta}\theta\frac{d\delta}{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]u^{0,0}_{ijk}\frac{\partial\theta}{\partial x_k}\right]\\
&+\epsilon^1\left[B^-_{ij}\frac{\partial v_k}{\partial x_k}+\frac{3(14+\delta)}{7(3+\delta)}\theta\frac{\partial u^{0,0}_{ijk}}{\partial x_k}-\frac{3(14+\delta)}{7(3+\delta)}\theta u^{0,0}_{ijk}\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\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial\Delta q_{<i}}{\partial x_{j>}}+4\Gamma_4\theta\Delta q_{<i}\frac{\partial\ln\rho}{\partial x_{j>}}\right]\\
&+\epsilon^\alpha\left[\frac{10}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)}\Gamma_4\left(\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5}\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)-\frac{2\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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)}u^{0,0}_{ijk}\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\frac{d\delta}{d\theta}}{(3+\delta)(14+\delta)\left(3+\delta+\theta\frac{d\delta}{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{u^{0,0}_{ijk}}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l}\right]\\
&-\epsilon^2\left[\frac{22\frac{d\delta}{d\theta}}{(3+\delta)(14+\delta)\left(3+\delta+\theta\frac{d\delta}{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\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\left(5R_{q_{int}}\left[3+\delta+\theta\frac{d\delta}{d\theta}\right]\right.\\
&\left.+R_{q_{tr}}\left[(3+\delta)\delta+(7+2\delta)\theta\frac{d\delta}{d\theta}+\left(\left(\frac{d\delta}{d\theta}\right)^2+2\frac{d^2\delta}{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}\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{5.7b}
$$

$$\epsilon^1 \left[\frac{Du^{0,0}_{ijk}}{Dt} - 3\frac{\sigma_{<ij}}{\rho}\frac{\partial \sigma_{k>l}}{\partial x_l} + \frac{6\left(14-\delta\right)\left(3+\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}\frac{\partial B^-_{<ij}}{\partial x_{k>}} \right]$$

$$- \epsilon^1 \left[\left(\frac{6}{\left(14+\delta\right)^2} + \frac{252}{\left(42+25\delta\right)^2} \right) \frac{d\delta}{d\theta} B^-_{<ij}\frac{\partial \theta}{\partial x_{k>}} \right]$$

$$+ \epsilon^1 \left[u^{0,0}_{ijk}\frac{\partial v_l}{\partial x_l} + 3u^{0,0}_{l<ij}\frac{\partial v_{k>}}{\partial x_l} \right] + \epsilon^\alpha \left[\frac{6\delta}{42+25\delta}\frac{\partial B^+_{,<ij}}{\partial x_{k>}} \right]$$

$$+ \epsilon^\alpha \left[\frac{252\frac{d\delta}{d\theta}}{\left(42+25\delta\right)^2} B^+_{,<ij}\frac{\partial \theta}{\partial x_{k>}} + 3\sigma_{<ij}\left(\frac{\partial \Delta\theta}{\partial x_{k>}} + \Delta\theta \frac{\partial \ln \rho}{\partial x_{k>}} \right) \right]$$

$$+ \epsilon^\alpha \left[\frac{12\left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)} \Delta q_{<i}\frac{\partial v_j}{\partial x_{k>}} \right] + 3\theta \left(\frac{\partial \sigma_{<ij}}{\partial x_{k>}} - \sigma_{<ij}\frac{\partial \ln \rho}{\partial x_{k>}} \right)$$

$$+ \frac{12R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} q_{<i}\frac{\partial v_j}{\partial x_{k>}} = -\left[\frac{1}{\tau_{tr}} + \frac{\epsilon^{1-\alpha}}{\tau_{int}} \right] u^{0,0}_{ijk} \,. \quad (5.7c)$$

where,

$$\Gamma_1 = \frac{84\left(14+\delta\right)\theta\frac{d\delta}{d\theta}}{\delta\left(14+\delta\right)\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)\left(42+25\delta\right)} \,, \quad (5.7d)$$

$$\Gamma_2 = 2R_{q_{int}} \left(\frac{\left[14+\delta+\theta\frac{d\delta}{d\theta}\right]}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} - \theta \right.$$
$$\left. \frac{10\left(7R_{q_{int}} + 2\left(7+3\delta\right)R_{q_{tr}}\right)\frac{d\delta}{d\theta} + 14R_{q_{tr}}\theta\left(\frac{d\delta}{d\theta}\right)^2 + \left(70+23\delta\right)R_{q_{tr}}\theta\frac{d^2\delta}{d\theta^2}}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} \right) \,, \quad (5.7e)$$

$$\Gamma_3 = 2R_{q_{tr}} \left(\frac{\left(\delta\left[14+\delta+\theta\frac{d\delta}{d\theta}\right] - 14\frac{d\delta}{d\theta}\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)} \right.$$
$$\left. + \frac{2R_{q_{tr}}R_{q_{int}}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)\left(70+\delta\left[14+9\theta\right]\right)}{\delta\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} \right) \,, \quad (5.7f)$$

$$\Gamma_4 = \frac{\left(14+\delta\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(3+\delta\right)\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)} \,, \quad (5.7g)$$

$$\Gamma_5 = \frac{2\left(14+\delta\right)\left(3R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{\left(3+\delta\right)\left(5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)} \,. \quad (5.7h)$$

As it was discussed earlier, values of α less than 0.5 are relevant and will be considered from now on, unless stated otherwise. While the expansion series (4.5) contains all mixed powers of ϵ and ϵ^α, the final equations only contain some terms. In the following, we are interested in terms up to ϵ^3, and find only the following powers:

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

Their order depends on the value of α. For values of α below 0.5 the different sequence of orders are (up to ϵ^3)

$$\begin{aligned}
0 < \alpha < 0.25 &: \left\{\epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \epsilon^{1+2\alpha}, \epsilon^{1+3\alpha}, \epsilon^{2-\alpha}, \epsilon^2, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^{2+3\alpha}, \epsilon^3\right\} \\
0.25 < \alpha < 0.33 &: \left\{\epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \epsilon^{1+2\alpha}, \underline{\epsilon^{2-\alpha}, \epsilon^{1+3\alpha}}, \epsilon^2, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^{2+3\alpha}, \epsilon^3\right\} \\
0.33 < \alpha < 0.5 &: \left\{\epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \underline{\epsilon^{2-\alpha}, \epsilon^{1+2\alpha}, \epsilon^2, \epsilon^{1+3\alpha}}, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^3\right\}
\end{aligned} \tag{5.8}$$

Here, only the underlined terms are changing location between different values of α.

The following sections will discuss different sets of equations based on the desired order of accuracy in the powers of ϵ, and the different values of the exponent α, which determines the relative importance of contributions. For this, we will consider the increasing orders as laid out in (5.8) up to third order.

5.1 Zeroth order, ϵ^0: Euler equations

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

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_i}{\partial x_i} = 0 \,, \tag{5.9a}$$

$$\frac{Dv_i}{Dt} + \theta\frac{\partial \ln\rho}{\partial x_i} + \frac{\partial \theta}{\partial x_i} = 0 \,, \tag{5.9b}$$

$$\frac{3+\delta+\theta\frac{d\delta}{d\theta}}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_i}{\partial x_i} = 0 \,. \tag{5.9c}$$

These equations form a closed set of equations for the variables $\{\rho, v_i, \theta\}$ these are the the Euler equations for polyatomic gases [84].

5.2 Order ϵ^α: Dynamic temperature

The first non-equilibrium correction appears for α order, where the momentum and total energy balance equations in the conservation laws are corrected as

$$\frac{Dv_i}{Dt} + \theta\frac{\partial \ln\rho}{\partial x_i} + \frac{\partial\theta}{\partial x_i} - \epsilon^\alpha\left[\frac{\partial\Delta\theta}{\partial x_i} + \Delta\theta\frac{\partial\ln\rho}{\partial x_i}\right] = 0\ , \tag{5.10}$$

$$\frac{3+\delta+\theta\frac{d\delta}{d\theta}}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_i}{\partial x_i} - \epsilon^\alpha\left[\rho\Delta\theta\frac{\partial v_i}{\partial x_i}\right] = 0\ . \tag{5.11}$$

Hence, an additional equation for the dynamic temperature $\Delta\theta$ is required, which at this order is simply the leading term of Eq. 5.2,

$$\Delta\theta = \tau_{int}\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\theta\frac{\partial v_i}{\partial x_i}\ . \tag{5.12}$$

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*, $\Pi = -\rho\Delta\theta$, and obtain similar relation as Eq. 5.12 [37, 70].

5.3 Order $\epsilon^{2\alpha}$: Refined dynamic temperature

For all $\alpha < 0.5$, the next order appearing in (5.8) is $\epsilon^{2\alpha}$. The conservation laws do not contain terms of order 2α, hence they are unchanged from the previous case (order ε^α). While the next higher order terms of $\Delta\theta$, Eq. 5.2, which are of order ε^α and give overall contributions of order $\epsilon^{2\alpha}$, must be considered. This gives the closure by a full balance equation for $\Delta\theta$, while stress and heat flux can still be ignored,

$$\epsilon^\alpha\left[\rho\frac{D\Delta\theta}{Dt} + \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\rho\Delta\theta\frac{\partial v_i}{\partial x_i}\right] - \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\rho\theta\frac{\partial v_i}{\partial x_i} = -\frac{\rho}{\tau_{int}}\Delta\theta\ . \tag{5.13}$$

This is a set of 6 field equations with variables $\{\rho, v_i, \theta, \Delta\theta\}$.

5.4 Order ϵ^1: Refined Navier-Stokes-Fourier equations

For the first order, terms up to ϵ^1 order are considered in the conservation laws, for which now all terms are relevant, Eqs. 5.1,

$$\begin{aligned} \frac{D\rho}{Dt}+\rho\frac{\partial v_i}{\partial x_i}=0\ , \\ \rho\frac{Dv_i}{Dt}+\frac{\partial\rho\left(\theta-\Delta\theta\right)}{\partial x_i}+\frac{\partial\sigma_{ij}}{\partial x_j}=0\ , \\ \frac{3+\delta+\theta\frac{d\delta}{d\theta}}{2}\rho\frac{D\theta}{Dt}+\frac{\partial q_i}{\partial x_i}+\rho\left(\theta-\Delta\theta\right)\frac{\partial v_i}{\partial x_i}+\sigma_{ij}\frac{\partial v_j}{\partial x_i}=0\ ; \end{aligned} \tag{5.14}$$

In addition to the balance law for $\Delta\theta$ (5.13)in order to close the set of equations, the leading terms of the stress tensor, Eq. 5.3, and total heat flux, Eq. 5.4, are required as well,

$$\begin{aligned} \sigma_{ij}=-\tau_{tr}2\rho\theta\frac{\partial v_{<i}}{\partial x_{j>}}\ , \\ q_i=-\tau_{tr}\frac{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}\rho\theta\frac{\partial\theta}{\partial x_i}\ . \end{aligned} \tag{5.15}$$

These first order equations for σ_{ij} and q_i are the classical Navier–Stokes-Fourier (NSF) equations, which relate the stress deviator and heat flux to the gradients of velocity and temperature. The factors between them are the shear viscosity μ and the heat conductivity κ which we identify as

$$\mu=\tau_{tr}\rho\theta \qquad \text{and} \qquad \kappa=\tau_{tr}\frac{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}\rho\theta\ . \tag{5.16}$$

The obtained relation for the shear viscosity is identical to that of the monatomic gas. Internal degrees of freedom affect the heat conductivity, which differs from the monatomic gas as extra means of energy transport are present in the polyatomic gases. In the classical Navier-Stokes equations, the dynamic pressure has the form $\Pi=-\nu\frac{\partial v_i}{\partial x_i}$ where ν is the bulk viscosity. Comparing with the above, we identify a relation between relaxation time τ_{int} and the bulk viscosity,

$$\upsilon=\tau_{int}\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\rho\left(\theta-\Delta\theta\right)\ . \tag{5.17}$$

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

However, what we have obtained here at first order are not the classical NSF equations, since we have to use the full balance law (5.13) for $\Delta\theta$ (or dynamic pressure). The classical NSF equations is a five variables model for $\{\rho, v_i, \theta\}$. However, the refined Navier-Stokes-Fourier (RNSF) equations obtained have six independent field variables, $\{\rho, v_i, \theta, \Delta\theta\}$. This is a result of the scaling, where we assumed $\alpha < 0.5$. The classical Navier-Stokes-Fourier equations only arise for $0.5 < \alpha < 1$.

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

The next order of accuracy (for all $\alpha < 0.5$) is obtained by considering the next higher terms in the equations for $\Delta\theta, \sigma_{ij}$ and q_i, Eqs. 5.2,5.3,5.4,which are the contributions with factor ϵ^1 for the dynamic temperature, and contributions with factor ϵ^α for stress and total heat flux (which are themselves at order ϵ^1), so that at order $1+\alpha$, the conservation laws (5.14) must be closed by

$$\rho\frac{D\Delta\theta}{Dt} + \frac{10R_{q_{int}}R_{q_{tr}}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}q_i\frac{\partial\theta}{\partial x_i}$$
$$+\left(\frac{2}{3+\delta+\theta\frac{d\delta}{d\theta}} - \frac{10R_{q_{int}}}{3\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\right)\frac{\partial q_i}{\partial x_i}$$
$$+\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\rho\left(\Delta\theta-\theta\right)\frac{\partial v_i}{\partial x_i} - \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\sigma_{ij}\frac{\partial v_j}{\partial x_i} = -\frac{\rho}{\tau_{int}}\Delta\theta\ , \quad (5.18a)$$

$$\sigma_{ij} = -\tau_{tr}2\rho\left[\theta-\Delta\theta\right]\frac{\partial v_{<i}}{\partial x_{j>}}\ , \quad (5.18b)$$

$$q_i = -\tau_{tr}\rho\left(\frac{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}\left(\theta-\Delta\theta\right)\frac{\partial\theta}{\partial x_i} - \frac{5R_{q_{int}}-3R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}\theta\frac{\partial\Delta\theta}{\partial x_i}\right)\ . \quad (5.18c)$$

Additional corrections to the NSF equations occur due to the internal degrees of freedom. If we consider this correction to the NSF equations, shear viscosity and heat conductivity will be of the form,

$$\mu = \tau_{tr}\rho\left(\theta - \Delta\theta\right) \qquad \text{and} \qquad \kappa = \tau_{tr}\frac{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}\rho\left(\theta - \Delta\theta\right)\ . \tag{5.19}$$

5.6 Cases with $0 < \alpha < 0.25$

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

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

Close inspection shows that, the next higher terms in the balance for $\Delta\theta$, Eq. 5.2, add contributions to order $1 + 2\alpha$. Indeed, at this order the full balance law for dynamic temperature must be considered,

$$\begin{aligned}
&\rho\frac{D\Delta\theta}{Dt} + \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}\rho\Delta\theta\frac{\partial v_i}{\partial x_i} + \frac{2}{3 + \delta + \theta\frac{d\delta}{d\theta}}\frac{\partial q_i}{\partial x_i} \\
&\qquad - \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}\rho\theta\frac{\partial v_i}{\partial x_i} - \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}\sigma_{ij}\frac{\partial v_j}{\partial x_i} \\
&- \frac{10R_{q_{int}}}{3\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\left[\frac{\partial q_i}{\partial x_i} + \frac{R_{q_{tr}}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{3\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\left(\Delta q_i\frac{\partial\theta}{\partial x_i} - q_i\frac{\partial\theta}{\partial x_i}\right)\right] \\
&\qquad\qquad \underline{- \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{3\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_i}{\partial x_i}} = -\frac{\rho}{\tau_{int}}\Delta\theta\ .
\end{aligned} \tag{5.20}$$

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

$$\Delta q_i = \tau_{tr}\frac{5\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\rho\theta\frac{\partial\Delta\theta}{\partial x_i}\ . \tag{5.21}$$

This relates the heat flux difference at leading order to the gradients of dynamic temperature. We name the factors between them the dynamic heat conductivity κ_Δ which we identify as,

$$\kappa_\Delta = \tau_{tr}\frac{5\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\rho\theta\ . \tag{5.22}$$

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

$$q_i = \frac{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{R_{q_{int}} R_{q_{tr}} \left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)} \tau_{tr} \left[\frac{5 + \delta + \theta\frac{d\delta}{d\theta}}{2} \rho \left(\Delta\theta - \theta\right) \frac{\partial\theta}{\partial x_i} \right.$$
$$\left. + \rho \left(\theta + \Delta\theta\right) \frac{\partial\Delta\theta}{\partial x_i} + \Delta\theta^2 \frac{\partial\rho}{\partial x_i} + \frac{2}{39} \frac{\partial B^+}{\partial x_i} \right] - \frac{\left(\delta + \theta\frac{d\delta}{d\theta}\right) \left(R_{q_{tr}} - R_{q_{int}}\right)}{R_{q_{int}} \left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)} \Delta q_i \ . \quad (5.23)$$

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

$$B^+ = -\frac{39}{2} \rho \Delta\theta^2 \ . \quad (5.24)$$

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

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

The next order of accuracy is obtained by considering the conservation laws (5.14), the dynamic temperature equation (5.2), the constitutive equations for the heat flux (5.23) and stress (5.18b), and terms up to α order in the heat flux difference, Eq. 5.5a,as

$$\Delta q_i = \frac{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{5R_{q_{int}}^2 + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}^2} \frac{5}{2} \tau_{tr} \left[\left(1 + \frac{3R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} \right) \right.$$
$$\left(\rho \left(\theta + \Delta\theta\right) \frac{\partial\Delta\theta}{\partial x_i} + \Delta\theta^2 \frac{\partial\rho}{\partial x_i} + \frac{2}{39} \frac{\partial B^+}{\partial x_i} \right)$$
$$\left. + \frac{\left(R_{q_{int}} - R_{q_{tr}}\right)}{R_{q_{tr}}} \rho \left(\theta + \Delta\theta\right) \frac{\partial\theta}{\partial x_i} \right] - \frac{5R_{q_{int}} \left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}}^2 + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}^2} q_i \ , \quad (5.25)$$

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

The equations at order $2 - \alpha$ are the full conservation laws (5.14), the full dynamic temperature equation (5.2), and the following constitutive equations for heat flux and stress (considering terms up to $\epsilon^{1-\alpha}$ order in Eqs. 5.3 and 5.4),

$$\sigma_{ij} = -\frac{1}{\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]} 2\rho\left[\theta - \Delta\theta\right] \frac{\partial v_{<i}}{\partial x_{j>}} \ , \tag{5.26a}$$

$$q_i = -\frac{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{R_{q_{int}} R_{q_{tr}} \left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]} \left(\frac{5 + \delta + \theta\frac{d\delta}{d\theta}}{2} \rho\left(\theta - \Delta\theta\right) \frac{\partial\theta}{\partial x_i} - \frac{2}{39}\frac{\partial B^+}{\partial x_i} \right.$$
$$\left. -\rho\left(\theta + \Delta\theta\right)\frac{\partial\Delta\theta}{\partial x_i} - \Delta\theta^2\frac{\partial\rho}{\partial x_i}\right) - \frac{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\left(R_{q_{tr}} - R_{q_{int}}\right)}{R_{q_{int}}\left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)}\Delta q_i \ . \tag{5.26b}$$

The equations for the heat flux difference Δq_i and for B^+ remain the same as for the previous case, i.e., (5.25, 5.24).

5.6.4 Order ϵ^2: Refined Grad's 14 moment equations

Starting with the second order of accuracy, balance laws for stress σ_{ij} and heat flux q_i must be considered as it can be seen from Eqs. 5.3 and 5.4. At the second order of accuracy, they should be expressed with terms up to order ϵ^1 as

$$\frac{D\sigma_{ij}}{Dt} + \frac{4R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\partial q_{<i}}{\partial x_{j>}} - \frac{4R_{q_{int}}R_{q_{tr}}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} q_{<i}\frac{\partial\theta}{\partial x_{j>}}$$
$$+ 2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k} + 2\rho\left(\theta - \Delta\theta\right)\frac{\partial v_{<i}}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\sigma_{ij} \ , \tag{5.27}$$

$$\frac{Dq_i}{Dt} + \sigma_{ik}\left[\frac{5+\delta+\theta\frac{d\delta}{d\theta}}{2}\frac{\partial\theta}{\partial x_k} - \theta\frac{\partial \ln\rho}{\partial x_k}\right] \underline{-\frac{2}{39}\frac{\partial B^+}{\partial x_i} + \frac{5}{13}\frac{\partial B^-}{\partial x_i}}$$
$$+\left(1+\frac{2R_{q_{int}}}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\left[q_k\frac{\partial v_i}{\partial x_k} + q_i\frac{\partial v_k}{\partial x_k}\right]$$
$$+\frac{2R_{q_{int}}q_k}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\partial v_k}{\partial x_i} - \Delta\theta^2\frac{\partial\rho}{\partial x_i} + \theta\frac{\partial\sigma_{ik}}{\partial x_k}$$
$$-\rho\left(\theta+\Delta\theta\right)\frac{\partial\Delta\theta}{\partial x_i} + \frac{5+\delta+\theta\frac{d\delta}{d\theta}}{2}\rho\left(\theta-\Delta\theta\right)\frac{\partial\theta}{\partial x_i}$$
$$= -\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_i + \underline{\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_i}\right) . \tag{5.28}$$

The other relevant equations are the conservation laws (5.14), and the dynamic temperature equation (5.20). For closing the set of equations we need constitutive equations for B^+ and Δq_i up to order $\epsilon^{1-2\alpha}$ from Eqs. 5.6b and 5.5a, as

$$B^+ = -\frac{39}{2}\rho\Delta\theta^2 + \frac{3\tau_{tr}}{\tau_{int}}\left[\frac{10}{R_{u^{2,0}}} + \frac{3-\delta}{2R_{u^{1,1}}} - \frac{23-\delta}{2}\right]\rho\theta\Delta\theta , \tag{5.29}$$

$$\Delta q_i = \frac{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R^2_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R^2_{q_{tr}}}\frac{5}{2}\tau_{tr}\left[\left(1+\frac{3R_{q_{int}}}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\right.$$
$$\left(\rho\left(\theta+\Delta\theta\right)\frac{\partial\Delta\theta}{\partial x_i} + \Delta\theta^2\frac{\partial\rho}{\partial x_i} + \frac{2}{39}\frac{\partial B^+}{\partial x_i}\right)$$
$$\left.+\frac{\left(R_{q_{int}}-R_{q_{tr}}\right)}{R_{q_{tr}}}\rho\left(\theta+\Delta\theta\right)\frac{\partial\theta}{\partial x_i}\right] - \frac{\left[1+\frac{\tau_{tr}}{\tau_{int}}\right]5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R^2_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R^2_{q_{tr}}}q_i , \tag{5.30}$$

and for B^- at leading order from Eq. 5.6a as,

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

With balance laws for stress and heat flux, the second order equations form a set of PDEs for the 14 variables $\{\rho, v_i, \theta, \Delta\theta, \sigma_{ij}, q_i\}$. Other authors discuss a 14 moment set for polyatomic gases, [23, 37, 39] where the equations agree with ours when letting relaxation parameters $R_{u^{2,0}}$ and $R_{u^{1,1}}$ to be 1 and considering constant δ, but with some differences due to the ordering of terms for $\alpha < 0.5$. Indeed, our refined

Grad's 14 moment (RG14) equations contain additional terms of order $\epsilon^{1+2\alpha}$, which are the terms underlined here in the equations for overall heat flux and the dynamic temperature containing B^+, Δq_i and B^- along with their constitutive equations. The terms involved with B^+ and Δq_i would not appear for $\alpha > 0.5$, where they would give contributions of higher than second order in ϵ. Hence we can say that the mentioned 14 field theory are more relevant for the cases that $\alpha > 0.5$, but still not at second order accuracy.

The mentioned 14 field theory [23, 37, 39] contains three nonlinear terms in (5.4), which according to our analysis are of orders $\epsilon^{2+\alpha}$ and ϵ^3, respectively, and will be considered below in the appropriate accuracy with other corresponding terms at the considered order of accuracy. As will be seen below, if one wishes to have a theory at $\epsilon^{2+\alpha}$ and ϵ^3 orders, there will be additional terms that must be included too. It should be mentioned that no other theories presents at accuracy higher than second order. Therefore, different set of equations presented in the coming sections are derived here for the first time and there are no alternative macroscopic models at these orders of accuracy.

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

In the next order of accuracy, the terms up to order $\epsilon^{1+\alpha}$ should be added to the equations for heat flux (5.28) and stress (5.27) as

$$\begin{aligned}
\frac{D\sigma_{ij}}{Dt} &+ \frac{4R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}}\frac{\partial q_{<i}}{\partial x_{j>}} - \frac{4R_{q_{int}}R_{q_{tr}}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)^2} q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\
&+ \frac{4\left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)}\frac{\partial\Delta q_{<i}}{\partial x_{j>}} + 2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k} \\
&+ \frac{4R_{q_{int}}R_{q_{tr}}}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)^2}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}} \\
&+ 2\rho\left(\theta - \Delta\theta\right)\frac{\partial v_{<i}}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\sigma_{ij}\ , \quad (5.32)
\end{aligned}$$

$$
\begin{aligned}
&\frac{Dq_i}{Dt}+\sigma_{ik}\left[\frac{5+\delta+\theta\frac{d\delta}{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}\\
&\qquad+\left(1+\frac{2R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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]\\
&\qquad+\frac{2R_{q_{int}}q_k}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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}\\
&\qquad-\rho\left(\theta+\Delta\theta\right)\frac{\partial\Delta\theta}{\partial x_i}+\frac{5+\delta+\theta\frac{d\delta}{d\theta}}{2}\rho\left(\theta-\Delta\theta\right)\frac{\partial\theta}{\partial x_i}\\
&\qquad+\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{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]\\
&\qquad+\frac{168}{\left(42+25\delta\right)^2}B^+_{ij}\frac{d\delta}{d\theta}\frac{\partial\theta}{\partial x_j}+\frac{4\delta}{\left(42+25\delta\right)}\frac{\partial B^+_{ij}}{\partial x_j}+\Delta\theta\frac{\partial\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)\\
&=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_i+\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_i\right)\ ,
\end{aligned}
\tag{5.33}
$$

Together with the conservation laws (5.14) and the full balance law for dynamic temperature (5.2), we still have a set of PDEs for 14 variables, which is closed by the constitutive equations for Δq_i and B^+ up to $\epsilon^{1-\alpha}$ order from Eqs. 5.5a and 5.6b,

$$
\begin{aligned}
\Delta q_i=&\frac{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R^2_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R^2_{q_{tr}}}\frac{1}{\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]}\left[\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\right.\\
&\left(\rho\left(\theta+\Delta\theta\right)\frac{\partial\Delta\theta}{\partial x_i}+\Delta\theta^2\frac{\partial\rho}{\partial x_i}+\frac{2}{39}\frac{\partial B^+}{\partial x_i}\right)-\frac{5}{39}\left(1-\frac{10R_{q_{int}}}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^-}{\partial x_i}\\
&+\frac{5}{2}\frac{\left(R_{q_{int}}-R_{q_{tr}}\right)}{R_{q_{tr}}}\rho\left(\theta+\Delta\theta\right)\frac{\partial\theta}{\partial x_i}-\sigma_{ik}\left(\frac{5}{2}\left[1-\frac{R_{q_{int}}}{R_{q_{tr}}}\right]\frac{\partial\theta}{\partial x_k}-\theta\frac{\partial\ln\rho}{\partial x_k}\right)\\
&-\frac{10R_{q_{int}}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta q_i\frac{\partial v_k}{\partial x_k}-\theta\frac{\partial\sigma_{ik}}{\partial x_k}\\
&\left.-\frac{2R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\left(q_j\frac{\partial v_j}{\partial x_i}+q_i\frac{\partial v_k}{\partial x_k}+q_k\frac{\partial v_i}{\partial x_k}\right)\right]-\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R^2_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R^2_{q_{tr}}}q_i\ ,
\end{aligned}
\tag{5.34}
$$

$$B^{+}=-\frac{13}{3R_{u^{1,1}}+10R_{u^{2,0}}}\frac{1}{\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]}\left[\left(26-\frac{78}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\rho\theta\Delta\theta\frac{\partial v_i}{\partial x_i}\right.$$
$$+\frac{1}{\tau_{int}}\left(\frac{3}{2}\left[\left(3-\delta\right)R_{u^{1,1}}+20R_{u^{2,0}}-\left(23-\delta\right)\right]\rho\theta\Delta\theta\right)$$
$$\left.+\frac{1}{\tau_{tr}}\left(\frac{9}{2}R_{u^{1,1}}+15R_{u^{2,0}}\right)\rho\Delta\theta^{2}\right]-\frac{10\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{3R_{u^{1,1}}+10R_{u^{2,0}}}B^{-}\ , \quad (5.35)$$

$$B^{+}=-\frac{1}{\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]}\left(\frac{39}{2}\frac{\rho\Delta\theta^{2}}{\tau_{tr}}+\frac{26\delta}{3+\delta}\rho\theta\Delta\theta\frac{\partial v_k}{\partial x_k}\right)\ , \quad (5.36)$$

and the leading order contributions to B^{-}(5.31) and B_{ij}^{+}, Eq. ,

$$B_{ij}^{+}=\tau_{tr}\frac{42+25\delta}{\delta}\rho\theta\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}\ . \quad (5.37)$$

$$B_{ij}^{+}=\tau_{tr}\frac{42+25\delta}{\delta}\rho\theta\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}\ . \quad (5.38)$$

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

Increasing the accuracy to $2+2\alpha$, require the following equations: the conservation laws (5.14), the full equation for dynamic temperature (5.2), the equations for stress and heat flux (5.32, 5.33), and balance laws for Δq_i and B^{+} with terms up to order

ϵ^1 from Eqs. 5.5a and 5.6b,

$$
\begin{aligned}
&\frac{D\Delta q_i}{Dt} + \sigma_{ik}\left[\frac{\partial \Delta\theta}{\partial x_k} + \Delta\theta\frac{\partial \ln\rho}{\partial x_k}\right] - \frac{5}{2}\left(1 + \frac{3R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\rho\Delta\theta\frac{\partial\Delta\theta}{\partial x_i} \\
&\quad - \frac{10R_{q_{int}}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\Delta\theta q_i\frac{\partial v_k}{\partial x_k} \\
&\quad + \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\Delta q_j\frac{\partial v_j}{\partial x_i} + \frac{5}{2}\left(1 + \frac{3R_{q_{int}}}{R_{q_{tr}}\left(\delta + \theta\frac{d\delta}{d\theta}\right)}\right)\Delta\theta\frac{\partial\sigma_{ij}}{\partial x_j} \\
&\quad + \frac{\delta}{(42 + 25\delta)}\left(7 + \frac{15R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^+_{ij}}{\partial x_j} - \frac{5}{2}\left(1 + \frac{3R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\Delta\theta^2\frac{\partial\rho}{\partial x_i} \\
&\quad + \left(\frac{25R_{q_{int}} + 7\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{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\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{d\delta}{d\theta}B^+_{ij}\frac{\partial\theta}{\partial x_j} + \theta\frac{\partial\sigma_{ik}}{\partial x_k} \\
&\quad - \frac{10R_{q_{int}}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\Delta q_i\frac{\partial v_k}{\partial x_k} \\
&\quad + \frac{10R_{q_{int}}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta q_i\frac{\partial v_k}{\partial x_k} \\
&\quad + \frac{5}{39}\left(1 - \frac{10R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^-}{\partial x_i} - \frac{5\left[R_{q_{int}} - R_{q_{tr}}\right]}{2R_{q_{tr}}}\rho\theta\frac{\partial\theta}{\partial x_i} \\
&\quad - \frac{5}{39}\left(1 + \frac{3R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^+}{\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) \\
&\quad + \frac{2R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{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] \\
&\quad - \frac{5}{2}\rho\left(\left[1 + \frac{3R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right]\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) \\
&= -\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\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_i + \frac{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R^2_{q_{tr}} + 5R^2_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_i\right)\,, \qquad (5.39)
\end{aligned}
$$

$$\frac{DB^{+}}{Dt}+\frac{85}{39}B^{+}\frac{\partial v_k}{\partial x_k}+\frac{3\left(23-\delta-\theta\frac{d\delta}{d\theta}\right)}{3+\delta+\theta\frac{d\delta}{d\theta}}\rho\Delta\theta^{2}\frac{\partial v_i}{\partial x_i}+\left(26-\frac{78}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\rho\theta\Delta\theta\frac{\partial v_i}{\partial x_i}$$
$$=-\frac{1}{\tau_{tr}}\left(\frac{9}{2}R_{u^{1,1}}+15R_{u^{2,0}}\right)\rho\Delta\theta^{2}-\frac{1}{\tau_{int}}\left[\frac{3}{2}\left(\left(3-\delta\right)R_{u^{1,1}}+20R_{u^{2,0}}-\left(23-\delta\right)\right)\rho\theta\Delta\theta\right]$$
$$-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{3R_{u^{1,1}}+10R_{u^{2,0}}}{13}B^{+}+\frac{10}{13}\left(R_{u^{1,1}}-R_{u^{2,0}}\right)B^{-}\right)\ . \quad (5.40)$$

Closure of this set of equations requires constitutive equations for B_{ij}^{+} (up to α order from Eq. 5.7a) and B^{-} (up to 2α order from Eq. 5.6a), which read,

$$B_{ij}^{+}=\tau_{tr}\left[\frac{42+25\delta}{\delta}\left(\rho\theta\Delta\theta+\frac{2}{39}B^{+}\right)\frac{\partial v_{<i}}{\partial x_{j>}}\right]\ , \quad (5.41)$$

$$B^{-}=\frac{13}{10R_{u^{1,1}}+3R_{u^{2,0}}}\left[\frac{9\left(R_{u^{2,0}}-R_{u^{1,1}}\right)}{2}\rho\Delta\theta^{2}\right.$$
$$+\tau_{tr}\left(-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\frac{3\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{13}B^{+}+\frac{2}{13}B^{+}\frac{\partial v_k}{\partial x_k}\right.$$
$$\left.\left.+3\rho\Delta\theta^{2}\frac{\partial v_i}{\partial x_i}-\frac{1}{\tau_{int}}\frac{3}{2}\left[3+\delta+\left[3-\delta\right]R_{u^{1,1}}-6R_{u^{2,0}}\right]\rho\theta\Delta\theta\right)\right]\ . \quad (5.42)$$

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

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

At the next order, $2+3\alpha$, the equations are the same as for $2+2\alpha$, only that now terms up to order $\epsilon^{1+\alpha}$ must be added to equation (5.39),

$$\frac{D\Delta q_i}{Dt}+...+\frac{10R_{q_{int}}\left(2\frac{d\delta}{d\theta}+\theta\frac{d^{2}\delta}{d\theta^{2}}\right)}{\left(\delta+\theta\frac{d\delta}{d\theta}\right)\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\Delta\theta\Delta q_i\frac{\partial v_k}{\partial x_k}+...$$
$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_i+\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}^{2}+5R_{q_{int}}^{2}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_i\right) \quad (5.43)$$

5.6.8 Order ϵ^3: Regularized 19 (R19) equations

Finally, we present the equations at third order of accuracy, which are: the conservation laws (5.14); the full equation for the dynamic temperature (5.2); The equation for heat flux difference (5.43), the equations (5.32, 5.33, 5.40) for stress, heat flux, and B^+ with added terms as

$$\begin{aligned}
\frac{D\sigma_{ij}}{Dt} &+ \frac{4R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} \frac{\partial q_{<i}}{\partial x_{j>}} - \frac{4R_{q_{int}} R_{q_{tr}} \left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)^2} q_{<i} \frac{\partial \theta}{\partial x_{j>}} \\
&+ \frac{4\left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)} \frac{\partial \Delta q_{<i}}{\partial x_{j>}} + 2\sigma_{k<i} \frac{\partial v_{j>}}{\partial x_k} + \sigma_{ij} \frac{\partial v_k}{\partial x_k} \\
&+ \frac{4R_{q_{int}} R_{q_{tr}}}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)^2} \left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right) \Delta q_{<i} \frac{\partial \theta}{\partial x_{j>}} + \frac{\partial u^{0,0}_{ijk}}{\partial x_k} \\
&+ 2\rho\left(\theta - \Delta\theta\right) \frac{\partial v_{<i}}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right] \sigma_{ij} \ , \qquad (5.44)
\end{aligned}$$

$$\begin{aligned}
\frac{Dq_i}{Dt} &+ ... + 7\left(\frac{1}{\left(14+\delta\right)^2} - \frac{24}{\left(42+25\delta\right)^2}\right) \frac{d\delta}{d\theta} B^-_{ij} \frac{\partial \theta}{\partial x_j} \\
&+ \frac{7\left(3+\delta\right)\left(14+3\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)} \frac{\partial B^-_{ij}}{\partial x_j} + u^{0,0}_{ijk} \frac{\partial v_j}{\partial x_k} - \frac{\sigma_{ik}}{\rho} \frac{\partial \sigma_{kj}}{\partial x_j} \\
= -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right] &\left(\frac{R_{q_{int}} R_{q_{tr}} \left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} q_i + \frac{\left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}} \left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right) R_{q_{tr}}} \Delta q_i\right) \ , \qquad (5.45)
\end{aligned}$$

$$\frac{DB^{+}}{Dt}-8\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i}+\frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}-40R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_k}{\partial x_k}$$
$$+\left(\frac{50R_{q_{int}}R_{q_{tr}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}+\frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)-100R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)q_k\frac{\partial\theta}{\partial x_k}$$
$$-\left(2-\frac{50R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\theta q_k\frac{\partial\ln\rho}{\partial x_k}-\frac{20}{39}B^{-}\frac{\partial v_k}{\partial x_k}$$
$$+\frac{85}{39}B^{+}\frac{\partial v_k}{\partial x_k}+\frac{3\left(23-\delta-\theta\frac{d\delta}{d\theta}\right)}{3+\delta+\theta\frac{d\delta}{d\theta}}\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i}+\left(26-\frac{78}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\rho\theta\Delta\theta\frac{\partial v_i}{\partial x_i}$$
$$=-\frac{1}{\tau_{tr}}\left(\frac{9}{2}R_{u^{1,1}}+15R_{u^{2,0}}\right)\rho\Delta\theta^2-\frac{1}{\tau_{int}}\left[\frac{3}{2}\left(\left(3-\delta\right)R_{u^{1,1}}+20R_{u^{2,0}}-\left(23-\delta\right)\right)\rho\theta\Delta\theta\right]$$
$$-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{3R_{u^{1,1}}+10R_{u^{2,0}}}{13}B^{+}+\frac{10}{13}\left(R_{u^{1,1}}-R_{u^{2,0}}\right)B^{-}\right)\ ,\quad(5.46)$$

and the balance law for B^{-}

$$\frac{DB^{-}}{Dt}+\frac{12}{5}\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i}+\frac{12R_{q_{int}}+2\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\frac{\partial q_k}{\partial x_k}-\frac{2}{13}B^{+}\frac{\partial v_k}{\partial x_k}$$
$$+\left(\frac{\left(5R_{q_{int}}+3R_{q_{tr}}\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)+30R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}-\frac{2R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right)q_k\frac{\partial\theta}{\partial x_k}$$
$$-2\left(1+\frac{R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\theta q_k\frac{\partial\ln\rho}{\partial x_k}-3\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i}+\frac{71}{39}B^{-}\frac{\partial v_k}{\partial x_k}$$
$$=-\frac{1}{\tau_{tr}}\frac{9\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{2}\rho\Delta\theta^2-\frac{1}{\tau_{int}}\left(\frac{3}{2}\left(3+\delta+\left[3-\delta\right]R_{u^{1,1}}-6R_{u^{2,0}}\right)\rho\theta\Delta\theta\right)$$
$$-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{10R_{u^{1,1}}+3R_{u^{2,0}}}{13}B^{-}+\left[\frac{3\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{13}B^{+}\right]\right)\ .\quad(5.47)$$

These 19 PDEs are closed with the constitutive equations for B^{+}_{ij} up to $1-\alpha$ order,

$$\begin{aligned}
B^{+}_{ij} = &-\frac{1}{\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]}\left[2\left(\frac{(70+23\delta)\,R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{14-\delta}{\delta}\right)\theta\frac{\partial q_{<i}}{\partial x_{j>}}\right.\\
&-\frac{4\,(70-19\delta)}{39\delta}B^{-}\frac{\partial v_{<i}}{\partial x_{j>}}+\frac{(14-\delta)\,\theta\frac{d\delta}{d\theta}-\delta\,(14+\delta)}{\delta\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\theta\sigma_{ij}\frac{\partial v_k}{\partial x_k}\\
&-2\left(\frac{(70+23\delta)\,R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{14-\delta}{\delta}\right)\theta q_{<i}\frac{\partial\ln\rho}{\partial x_{j>}}\\
&-\frac{2\,(42+25\delta)}{39\delta}B^{+}\frac{\partial v_{<i}}{\partial x_{j>}}+2R_{q_{int}}\left(\frac{14+\delta+\theta\frac{d\delta}{d\theta}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right.\\
&\left.-\theta\frac{10\,(7R_{q_{int}}+2\,(7+3\delta)\,R_{q_{tr}})\,\frac{d\delta}{d\theta}+14R_{q_{tr}}\theta\left(\frac{d\delta}{d\theta}\right)^2+(70+23\delta)\,R_{q_{tr}}\theta\frac{d^2\delta}{d\theta^2}}{\delta\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right)q_{<i}\frac{\partial\theta}{\partial x_{j>}}\\
&\left.+4\theta\left(2\sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}}+2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\sigma_{ij}\frac{\partial v_k}{\partial x_k}\right)-\frac{(42+25\delta)}{\delta}\rho\theta\Delta\theta\frac{\partial v_{<i}}{\partial x_{j>}}\right]\ ,
\end{aligned}\tag{5.48}$$

and for $u^{0,0}_{ijk}$ and B^{-}_{ij} at their leading orders,

$$u^{0,0}_{ijk} = -\tau_{tr}\left[3\theta\frac{\partial\sigma_{<ij}}{\partial x_{k>}}-3\theta\sigma_{<ij}\frac{\partial\ln\rho}{\partial x_{k>}}+\frac{12R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_{<i}\frac{\partial v_j}{\partial x_{k>}}\right]\ ,\tag{5.49}$$

$$\begin{aligned}
B^{-}_{ij} = &-\tau_{tr}\left[\frac{6\,(14+\delta)}{7\,(3+\delta)}\theta\left(\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}}-\frac{2}{3}\sigma_{ij}\frac{\partial v_k}{\partial x_k}\right)\right.\\
&+\frac{2\,(14+\delta)\,R_{q_{int}}}{(3+\delta)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\left(5R_{q_{int}}\left[3+\delta+\theta\frac{d\delta}{d\theta}\right]\right.\\
&\left.+R_{q_{tr}}\left[(3+\delta)\,\delta+(7+2\delta)\,\theta\frac{d\delta}{d\theta}+\left(\left(\frac{d\delta}{d\theta}\right)^2+2\frac{d^2\delta}{d\theta^2}\right)\theta^2\right]\right)q_{<i}\frac{\partial\theta}{\partial x_{j>}}\\
&+\frac{2\,(14+\delta)}{3\,(3+\delta)}B^{-}\frac{\partial v_{<i}}{\partial x_{j>}}-\frac{2\,(14+\delta)\left(3R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{(3+\delta)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta q_{<i}\frac{\partial\ln\rho}{\partial x_{j>}}\\
&\left.+2\frac{(14+\delta)\left(3R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{(3+\delta)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\theta\frac{\partial q_{<i}}{\partial x_{j>}}\right]\ .
\end{aligned}\tag{5.50}$$

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 constitutive equations to replace Eqs. (5.48,5.49,5.50) in the set of R19 equations. New forms eliminates some derivatives with stress tensor, heat flux and dynamic temperature and makes the set of equations more suitable to solve while keeping the order of accuracy.

Transformation of equations The balance laws of B^+ and B^-, and constitutive equations in the set of R19 equations could be rewritten using the leading order heat flux difference, Navier-Stokes-Fourier stress, and viscosities as

$$\sigma_{ij}^{NSF} = -2\mu\frac{\partial v_{<i}}{\partial x_{j>}} = \sigma_{ij} + \mathcal{O}\left(\epsilon^{1+\alpha}\right) + ... \quad , \tag{5.51a}$$

$$q_i^{NSF} = -\kappa\frac{\partial \theta}{\partial x_i} = q_i + \mathcal{O}\left(\epsilon^{1+\alpha}\right) + ... \quad , \tag{5.51b}$$

$$\kappa_\Delta\frac{\partial \Delta\theta}{\partial x_i} = \Delta q_i + \mathcal{O}\left(\epsilon^{1+2\alpha}\right) + ... \quad , \tag{5.51c}$$

$$\Delta\theta^{NSF} = \frac{\upsilon}{\rho}\frac{\partial v_i}{\partial x_i} = \Delta\theta + \mathcal{O}\left(\epsilon^{2\alpha}\right) + ... \quad , \tag{5.51d}$$

and still keep the proper order of accuracy. The balance laws take the form of

$$\begin{aligned}
&\frac{DB^+}{Dt} - 2\frac{20R_{q_{int}} - \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\left[\frac{\partial q_k}{\partial x_k} - q_k\frac{\partial \ln\rho\left(\theta - \Delta\theta\right)}{\partial x_k}\right] \\
&+ \left[\left(26 - \frac{78}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\rho\theta\Delta\theta + \frac{3\left(23-\delta-\theta\frac{d\delta}{d\theta}\right)}{3+\delta+\theta\frac{d\delta}{d\theta}}\rho\Delta\theta^2 + \frac{85}{39}B^+ - \frac{20}{39}B^-\right]\frac{\partial v_k}{\partial x_k} \\
&- \left(\frac{50R_{q_{int}}R_{q_{tr}}\theta\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} + \frac{\left(5R_{q_{int}} + 3R_{q_{tr}}\right)\left(\delta + \theta\frac{d\delta}{d\theta}\right) - 100R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{q_k q_k}{\kappa} \\
&\qquad + 2\frac{20R_{q_{int}} - \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\theta}{\theta - \Delta\theta}\left[\frac{q_k q_k}{\kappa} + \frac{q_k\Delta q_k}{\kappa_\Delta}\right] + 4\theta\frac{\sigma_{ij}\sigma_{ij}}{\mu} \\
&= -\frac{1}{\tau_{tr}}\left(\frac{9}{2}R_{u^{1,1}} + 15R_{u^{2,0}}\right)\rho\Delta\theta^2 - \frac{1}{\tau_{int}}\left[\frac{3}{2}\left(\left(3-\delta\right)R_{u^{1,1}} + 20R_{u^{2,0}} - \left(23-\delta\right)\right)\rho\theta\Delta\theta\right] \\
&\qquad - \left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\left(\frac{3R_{u^{1,1}} + 10R_{u^{2,0}}}{13}B^+ + \frac{10}{13}\left(R_{u^{1,1}} - R_{u^{2,0}}\right)B^-\right) \quad ,
\end{aligned} \tag{5.52}$$

$$
\begin{aligned}
&\frac{DB^-}{Dt} - 2\frac{6R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\theta}{(\theta - \Delta\theta)}\left[\frac{q_k q_k}{\kappa} + \frac{q_k \Delta q_k}{\kappa_\Delta}\right] \\
&\quad - \left(\frac{(5R_{q_{int}} + 3R_{q_{tr}})\left(\delta + \theta\frac{d\delta}{d\theta}\right) + 30R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} - \frac{2R_{q_{tr}}R_{q_{int}}\theta\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right)\frac{q_k q_k}{\kappa} \\
&\qquad - \frac{6}{5}\theta\frac{\sigma_{ij}\sigma_{ij}}{\mu} - \left(3\rho\Delta\theta^2 - \frac{71}{39}B^- + \frac{2}{13}B^+\right)\frac{\partial v_k}{\partial x_k} \\
&\qquad + 2\frac{6R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\theta\left[\frac{\partial q_k}{\partial x_k} - q_k\frac{\partial \ln\rho\,(\theta - \Delta\theta)}{\partial x_k}\right] \\
&\quad = -\frac{1}{\tau_{tr}}\frac{9\left(R_{u^{1,1}} - R_{u^{2,0}}\right)}{2}\rho\Delta\theta^2 - \frac{1}{\tau_{int}}\left(\frac{3}{2}\left(3 + \delta + [3 - \delta]\,R_{u^{1,1}} - 6R_{u^{2,0}}\right)\rho\theta\Delta\theta\right) \\
&\qquad - \left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\left(\frac{10R_{u^{1,1}} + 3R_{u^{2,0}}}{13}B^- + \left[\frac{3\left(R_{u^{1,1}} - R_{u^{2,0}}\right)}{13}B^+\right]\right)\ . \qquad (5.53)
\end{aligned}
$$

The new constitutive equations for B_{ij}^+, B_{ij}^- and $u_{ijk}^{0,0}$ in the set of R19 equations after some manipulations become

$$
\begin{aligned}
B_{ij}^+ = &-\frac{1}{\left[1 + \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)\mu}{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)v}\right]\rho\theta}\left(\frac{2\,(70 - 19\delta)\,B^- + (42 + 25\delta)\,B^+}{39\delta}\sigma_{ij}\right. \\
&\quad + \frac{(42 + 25\delta)}{2\delta}\rho\theta\Delta\theta\sigma_{ij} - 2R_{q_{int}}\left[\frac{14 + \delta + \theta\frac{d\delta}{d\theta}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right. \\
&\left. -\theta\frac{10\left(7R_{q_{int}} + 2\,(7 + 3\delta)\,R_{q_{tr}}\right)\frac{d\delta}{d\theta} + 14R_{q_{tr}}\theta\left(\frac{d\delta}{d\theta}\right)^2 + (70 + 23\delta)\,R_{q_{tr}}\theta\frac{d^2\delta}{d\theta^2}}{\delta\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right]\frac{\mu}{\kappa}q_{<i}q_{j>} \\
&\quad \left. + \left[\frac{(14 - \delta)\,\theta\frac{d\delta}{d\theta} - \delta\,(14 + \delta)}{\delta\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)} + \frac{28}{3}\right]\frac{\mu}{v}\rho\theta\Delta\theta\sigma_{ij} - 8\theta\sigma_{k<i}\sigma_{j>k}\right) \\
&+ \frac{2\mu}{1 + \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)\mu}{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)v}}\left(\frac{(70 + 23\delta)\,R_{q_{int}}}{\delta\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)} - \frac{14 - \delta}{\delta}\right)\frac{q_{<i}}{\rho\,(\theta - \Delta\theta)}\left[\frac{q_{j>}}{\kappa} + \frac{\Delta q_{j>}}{\kappa_\Delta}\right] \\
&- \frac{2}{\frac{1}{\mu} + \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)v}}\left(\frac{(70 + 23\delta)\,R_{q_{int}}}{\delta\left(5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)} - \frac{14 - \delta}{\delta}\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]\ , \qquad (5.54)
\end{aligned}
$$

$$
\begin{aligned}
B^-_{ij} = -\frac{1}{\rho\theta}\Bigg[& -\frac{6\left(14+\delta\right)}{7\left(3+\delta\right)}\theta\sigma_{k<i}\sigma_{j>k} - \frac{\left(14+\delta\right)}{3\left(3+\delta\right)}B^-\sigma_{ij} \\
& - \frac{2\left(14+\delta\right)R_{q_{int}}}{\left(3+\delta\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\left(5R_{q_{int}}\left[3+\delta+\theta\frac{d\delta}{d\theta}\right]\right. \\
& \left. +R_{q_{tr}}\left[\left(3+\delta\right)\delta+\left(7+2\delta\right)\theta\frac{d\delta}{d\theta}+\left(\left(\frac{d\delta}{d\theta}\right)^2+2\frac{d^2\delta}{d\theta^2}\right)\theta^2\right]\right)\frac{\mu}{\kappa}q_{<i}q_{j>}\Bigg] \\
& + \mu\frac{2\left(14+\delta\right)\left(3R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{\left(3+\delta\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{q_{<i}}{\rho\left(\theta-\Delta\theta\right)}\left[\frac{q_{j>}}{\kappa}+\frac{\Delta q_{j>}}{\kappa_\Delta}\right] \\
& - \mu\frac{2\left(14+\delta\right)\left(3R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{\left(3+\delta\right)\left(5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{1}{\rho}\left(\frac{\partial q_{<i}}{\partial x_{j>}}-q_{<i}\frac{\partial\ln\rho\left(\theta-\Delta\theta\right)}{\partial x_{j>}}\right) \ , \quad (5.55)
\end{aligned}
$$

$$
\begin{aligned}
u^{0,0}_{ijk} = & \frac{6R_{q_{int}}}{5R_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{q_{<i}\sigma_{jk>}}{\rho\theta} + 3\mu\frac{\sigma_{<ij}}{\rho\left(\theta-\Delta\theta\right)}\left[\frac{q_{k>}}{\kappa}+\frac{\Delta q_{k>}}{\kappa_\Delta}\right] \\
& - 3\frac{\mu}{\rho}\left(\frac{\partial\sigma_{<ij}}{\partial x_{k>}}-\sigma_{<ij}\frac{\partial\ln\rho\left(\theta-\Delta\theta\right)}{\partial x_{k>}}\right) \ , \quad (5.56)
\end{aligned}
$$

where the microscopic time scales are substituted by

$$
\tau_{int} = \frac{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}\frac{\upsilon}{\rho\theta} \quad \text{and} \quad \tau_{tr} = \frac{\mu}{\rho\theta} \ . \quad (5.57)
$$

The following relations were used for more compact notation:

$$
\sigma_{k<i}\frac{\partial v_{<j>}}{\partial x_{k>}} = \frac{1}{2}\sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}} + \frac{1}{2}\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k} - \frac{1}{3}\sigma_{ij}\frac{\partial v_l}{\partial x_l} \ , \quad (5.58a)
$$

$$
\sigma_{<ij}\frac{\partial v_{k>}}{\partial x_k} = \frac{1}{3}\sigma_{ij}\frac{\partial v_k}{\partial x_k} + \frac{1}{3}\sigma_{ik}\frac{\partial v_j}{\partial x_k} + \frac{1}{3}\sigma_{kj}\frac{\partial v_i}{\partial x_k} - \frac{2}{15}\sigma_{lj}\frac{\partial v_l}{\partial x_i} - \frac{2}{15}\sigma_{il}\frac{\partial v_l}{\partial x_j} - \frac{2}{15}\sigma_{kl}\frac{\partial v_l}{\partial x_k}\delta_{ij} \ , \quad (5.58b)
$$

$$
\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k} = \frac{1}{2}\sigma_{ki}\frac{\partial v_j}{\partial x_k} + \frac{1}{2}\sigma_{kj}\frac{\partial v_i}{\partial x_k} - \frac{1}{3}\sigma_{kl}\frac{\partial v_l}{\partial x_k}\delta_{ij} \ , \quad (5.58c)
$$

$$
\sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}} = \frac{1}{2}\sigma_{ki}\frac{\partial v_k}{\partial x_j} + \frac{1}{2}\sigma_{kj}\frac{\partial v_k}{\partial x_i} - \frac{1}{3}\sigma_{kl}\frac{\partial v_l}{\partial x_k}\delta_{ij} \ , \quad (5.58d)
$$

$$\frac{14}{5}\sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}} + 3\sigma_{<ij}\frac{\partial v_{k>}}{\partial x_k} = \sigma_{ki}\frac{\partial v_k}{\partial x_j} + \sigma_{kj}\frac{\partial v_k}{\partial x_i} - \frac{2}{3}\sigma_{kl}\frac{\partial v_l}{\partial x_k}\delta_{ij}$$
$$+ \sigma_{ik}\frac{\partial v_j}{\partial x_k} + \sigma_{kj}\frac{\partial v_i}{\partial x_k} - \frac{2}{3}\sigma_{kl}\frac{\partial v_l}{\partial x_k}\delta_{ij} + \sigma_{ij}\frac{\partial v_k}{\partial x_k}\ , \quad (5.58e)$$

$$2\sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}} + 2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k} = 4\sigma_{k<i}\frac{\partial v_{<j>}}{\partial x_{k>}} + \frac{7}{3}\sigma_{ij}\frac{\partial v_k}{\partial x_k}\ . \quad (5.58f)$$

5.7 Cases with $0.25 < \alpha < 0.33$

The ordering of terms depends on the value of α, as outlined in Eq. (5.8). Above, we considered the model reduction for $\alpha < 0.25$, which gave a hierarchical sequence of equations. When we consider slightly larger values of α, those in the interval $0.25 < \alpha < 0.33$, the ordering of contributions changes. Specifically, only two orders change position in the ordering sequence (5.8), namely $\epsilon^{2-\alpha}$ and $\epsilon^{1+3\alpha}$. The difference is relatively small: all set of equations corresponding to orders

$$\left\{\epsilon^0, \epsilon^\alpha, \epsilon^{2\alpha}, \epsilon^1, \epsilon^{1+\alpha}, \epsilon^{1+2\alpha}, \epsilon^2, \epsilon^{2+\alpha}, \epsilon^{2+2\alpha}, \epsilon^{2+3\alpha}, \epsilon^3\right\}$$

are the same as those in previous section. The two changed sets of equations are discussed below.

5.7.1 Order $\epsilon^{2-\alpha}$

The $2-\alpha$ order of accuracy requires the full conservation laws (5.14), the dynamic temperature equation (5.2), the constitutive equations for the heat flux and stress (5.26b), the heat flux difference (5.21), and the leading term of B^+ (5.24). To save space, we will not show the equations in detail.

5.7.2 Order $\epsilon^{1+3\alpha}$

At order $1 + 3\alpha$ one must consider the full conservation laws (5.14), the dynamic temperature equation (5.2), the constitutive equations for the heat flux and stress (5.26b), the leading order of B^+ (5.24), and the equation for heat flux difference (5.25).

5.8 Cases with $0.33 < \alpha < 0.5$

At even larger values of α, in the range of $0.33 < \alpha < 0.5$, four orders change position in the ordering sequence (5.8), viz. $\epsilon^{2-\alpha}$, $\epsilon^{1+2\alpha}$, ϵ^{2} and $\epsilon^{1+3\alpha}$. Moreover, the $2+3\alpha$ order is greater than third order and is not further considered. The changed sets of equations are presented below, the equations at all other orders remain same as those of previous Section.

5.8.1 Order $\epsilon^{2-\alpha}$

The $2-\alpha$ order of accuracy is gained by considering the full conservation laws (5.14), the dynamic temperature equation with terms up to order $2-2\alpha$ (5.18a), and terms up to $1-\alpha$ order in the heat flux and stress tensor,

$$\sigma_{ij} = -\frac{1}{\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]} 2\rho \left[\theta - \Delta\theta\right] \frac{\partial v_{<i}}{\partial x_{j>}} \ , \tag{5.59a}$$

$$\begin{aligned} q_i = \frac{1}{\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]} \rho \Bigg(& \frac{-10 R_{q_{int}} R_{q_{tr}} \left(\delta + \theta \frac{d\delta}{d\theta}\right)}{2 R_{q_{int}} R_{q_{tr}} \left(5 R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)} \Delta\theta \frac{\partial \theta}{\partial x_i} \\ & + \frac{\left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}^2 \left(10 + \delta + \theta \frac{d\delta}{d\theta}\right) + 5 R_{q_{int}}^2 \left(5 + 2\delta + 2\theta \frac{d\delta}{d\theta}\right)}{2 R_{q_{int}} R_{q_{tr}} \left(5 R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)} \Delta\theta \frac{\partial \theta}{\partial x_i} \\ & - \frac{5 R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}}{2 R_{q_{int}} R_{q_{tr}}} \theta \frac{\partial \theta}{\partial x_i} + \frac{5 R_{q_{int}} - 3 R_{q_{tr}}}{2 R_{q_{int}} R_{q_{tr}}} \theta \frac{\partial \Delta\theta}{\partial x_i} \Bigg) \ . \end{aligned} \tag{5.59b}$$

5.8.2 Order $\epsilon^{1+2\alpha}$

At order $1+2\alpha$ the polyatomic gas must be described by the conservation laws (5.14), the dynamic temperature equation (5.2), the constitutive equations for the heat flux difference (5.21), and the following equations for stress (5.59a) and heat flux:

$$\begin{aligned} q_i = & \frac{5 R_{q_{int}} + \left(\delta + \theta \frac{d\delta}{d\theta}\right) R_{q_{tr}}}{R_{q_{int}} R_{q_{tr}} \left(5 + \delta + \theta \frac{d\delta}{d\theta}\right) \left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]} \Bigg[\frac{5 + \delta + \theta \frac{d\delta}{d\theta}}{2} \rho \left(\Delta\theta - \theta\right) \frac{\partial \theta}{\partial x_i} \\ & + \rho \left(\theta + \Delta\theta\right) \frac{\partial \Delta\theta}{\partial x_i} + \Delta\theta^2 \frac{\partial \rho}{\partial x_i} + \frac{2}{39} \frac{\partial B^+}{\partial x_i} \Bigg] - \frac{\left(\delta + \theta \frac{d\delta}{d\theta}\right) \left(R_{q_{tr}} - R_{q_{int}}\right)}{R_{q_{int}} \left(5 + \delta + \theta \frac{d\delta}{d\theta}\right)} \Delta q_i \ . \end{aligned} \tag{5.60}$$

For closing the set of equations, the leading order term of B^+ (5.24) is required.

5.8.3 Order ϵ^2

The second order of accuracy requires all terms in the stress and heat flux balance up to factors ϵ^1, which are Eqs. (5.27, 5.28), as well as the conservation laws (5.14), the dynamic temperature equation (5.2), and the constitutive equations for B^+ (5.24) and the equation for heat flux difference as

$$\Delta q_i = \tau_{tr}\frac{5}{2}\frac{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}^2 + 5R_{q_{int}}^2}\rho\left(\left[1 + \frac{3R_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right]\theta\frac{\partial\Delta\theta}{\partial x_i}\right.$$
$$\left. + \frac{\left[R_{q_{int}} - R_{q_{tr}}\right]}{R_{q_{tr}}}\left(\theta + \Delta\theta\right)\frac{\partial\theta}{\partial x_i}\right) - \frac{\left[1 + \frac{\tau_{tr}}{\tau_{int}}\right]5R_{q_{int}}\left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}}^2 + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}^2}q_i\,. \quad (5.61)$$

The second order equations form a set of PDEs for the 14 variables $\{\rho, v_i, \theta, \Delta\theta, \sigma_{ij}, q_i\}$.

5.8.4 Order $\epsilon^{1+3\alpha}$

In $1+3\alpha$ order of accuracy, almost all equations are the same as at second order, only that, in order to include the proper higher order terms, the constitutive equation for heat flux difference must be replaced by (5.30).

5.8.5 Order ϵ^3

In the third order of accuracy corresponds to the $0.33 < \alpha < 0.5$, the only change from the set of R19 equations at lower α ($0 < \alpha < 0.33$) is the balance law for the heat flux difference, which now takes the form of Eq. (5.39).

5.9 Classical Navier-Stokes-Fourier equations, $0.5 < \alpha < 1$

The classical Navier-Stokes-Fourier equations arise only for cases with $0.5 < \alpha < 1$, where they are the appropriate system at order ε^1. Here, the powers ε^0, ε^α and ε^1 are required, while the corrections to dynamic temperature of order $\epsilon^{2\alpha}$ and higher must be discarded. Accordingly, the proper first order set are the conservation laws

(5.14), together with the stress and heat flux as given in (5.15), while the equation for dynamic temperature is (5.12),

$$\Delta\theta = \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}\tau_{int}\theta\frac{\partial v_i}{\partial x_i} \ . \tag{5.62}$$

The classical NSF equations give a five variables model for $\{\rho, v_i, \theta\}$. As discussed before, α will assume values *below* 0.5 for rarefied flows. Thus, the classical Navier-Stokes-Fourier equations have rather limited applicability in the rarefied regime. As was shown earlier, for $0 < \alpha < 0.5$, the refined NSF equations are the appropriate model at first order in ε. These use the full balance law for dynamic temperature (5.13) instead of (5.12), and have the six independent field variables, $\{\rho, v_i, \theta, \Delta\theta\}$.

5.10 The Prandtl number

The Prandtl number is defined as the dimensionless ratio of specific heat and shear viscosity over heat conductivity [76],

$$\mathrm{Pr} = \frac{5 + \delta + \theta\frac{d\delta}{d\theta}}{2}\frac{\mu}{k}. \tag{5.63}$$

This is a measure of the importance of momentum over thermal diffusivity. Based on the obtained shear viscosity and heat conductivity definitions (5.16), the Prandtl number is

$$\mathrm{Pr} = \frac{\left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{int}}R_{q_{tr}}}{5R_{q_{int}} + \left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}} \ . \tag{5.64}$$

$$R_{q_{int}} = \frac{\mathrm{Pr}\left(\delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{\left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)R_{q_{tr}} - 5\,\mathrm{Pr}} \tag{5.65}$$

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 Pr number. Viscosity and heat conductivity values could be used to determine 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 numerical data for rarefied flows, such as damping of ultrasound, light scattering experiments, or shockwave structure.

5.11 Intermediate Summary

The relaxation of the internal degrees of freedom leads to various ordering sequences for different values of α, 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 α and the accuracy under consideration, needs great care.

At the first order of accuracy, a refined version of the classical Navier-Stokes-Fourier equations is obtained, which includes *the balance law* for the dynamic temperature (Sec. 5.4).

At the second order, a refined variant of Grad's 14 moment equations is obtained, which includes some corrections and three extra constitutive equations for Δq_i, B^- and B^+. We note that the higher order terms in the dynamic temperature introduce higher space derivatives into these equations, which are not present in the typical Grad 14 moment system. [23, 37]

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

Finally at the third order, the regularized 19 moment equations (R19) are obtained which consists of 19 PDEs and three constitutive equations, and contribute regularizing terms similar to what appears in the R13 equations for monatomic gases [44].

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 ϵ^{α} and low power in ϵ; these are models with corrections to the NSF equations, i.e., the set of $1 + 3\alpha$ order equations, Sec. 5.8.4. 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 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, Sec. 5.6.8.

5.12 BGK model equations

The resulting set of 36 Grad's equations from the BGK kinetic equation can be obtained from above equations by setting all relaxation parameters ($R_{q_{int}}$, $R_{q_{tr}}$, $R_{u^{2,0}}$ and $R_{u^{1,1}}$) to unity. The final form of the closed set of 36 optimized moment equations from BGK kinetic equation is

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_i}{\partial x_i} = 0 \ , \tag{5.66}$$

$$\frac{Dv_i}{Dt} + \frac{1}{\rho}\frac{\partial \sigma_{ij}}{\partial x_j} + \frac{1}{\rho}\frac{\partial \rho\left(\theta - \Delta\theta\right)}{\partial x_i} = 0 \ , \tag{5.67}$$

$$\frac{3+\delta+\theta\frac{d\delta}{d\theta}}{2}\rho\frac{D\theta}{Dt} + \frac{\partial q_i}{\partial x_i} + \sigma_{ij}\frac{\partial v_j}{\partial x_i} + \rho\left(\theta-\Delta\theta\right)\frac{\partial v_i}{\partial x_i} = 0 \ , \tag{5.68}$$

$$\begin{aligned}\rho\frac{D\Delta\theta}{Dt} &+ \frac{10}{3\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2}\left(q_i - \Delta q_i\right)\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)\frac{\partial\theta}{\partial x_i} \\ &- \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\rho\left(\theta-\Delta\theta\right)\frac{\partial v_i}{\partial x_i} - \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(5+\left(\delta+\theta\frac{d\delta}{d\theta}\right)\right)}\frac{\partial \Delta q_i}{\partial x_i} \\ - \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{3\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\sigma_{ij}\frac{\partial v_j}{\partial x_i} &+ \left(\frac{2}{3+\delta+\theta\frac{d\delta}{d\theta}} - \frac{10}{3\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}\right)\frac{\partial q_i}{\partial x_i} = -\frac{\rho}{\tau_{int}}\Delta\theta \ .\end{aligned} \tag{5.69}$$

$$\begin{aligned}\frac{D\sigma_{ij}}{Dt} &+ \frac{4}{5+\left(\delta+\theta\frac{d\delta}{d\theta}\right)}\frac{\partial q_{<i}}{\partial x_{j>}} + \frac{4}{5}\frac{\delta+\theta\frac{d\delta}{d\theta}}{5+\delta+\theta\frac{d\delta}{d\theta}}\frac{\partial \Delta q_{<i}}{\partial x_{j>}} \\ &+ \frac{\partial u^{0,0}_{ijk}}{\partial x_k} + 2\sigma_{k<i}\frac{\partial v_{j>}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k} + 2\rho\left[\theta-\Delta\theta\right]\frac{\partial v_{<i}}{\partial x_{j>}} \\ + \frac{4}{\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2}&\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)\left[\Delta q_{<i} - q_{<i}\right]\frac{\partial\theta}{\partial x_{j>}} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\sigma_{ij} \ ,\end{aligned} \tag{5.70}$$

$$\begin{aligned}
&\frac{Dq_i}{Dt} + \sigma_{ik}\frac{\partial \Delta\theta}{\partial x_k} - \sigma_{ik}\left[\theta - \Delta\theta\right]\frac{\partial \ln\rho}{\partial x_k} - \Delta\theta^2\frac{\partial \rho}{\partial x_i} + \frac{5}{13}\frac{\partial B^-}{\partial x_i} - \frac{2}{39}\frac{\partial B^+}{\partial x_i} \\
&\quad - \rho\left[\theta + \Delta\theta\right]\frac{\partial \Delta\theta}{\partial x_i} + \left[\theta + \Delta\theta\right]\frac{\partial \sigma_{ij}}{\partial x_j} + \frac{5+\delta+\theta\frac{d\delta}{d\theta}}{2}\sigma_{ij}\frac{\partial \theta}{\partial x_j} \\
&\quad + \frac{168}{\left(42+25\delta\right)^2}B^+_{ij}\frac{d\delta}{d\theta}\frac{\partial \theta}{\partial x_j} + 7\left(\frac{1}{\left(14+\delta\right)^2} - \frac{24}{\left(42+25\delta\right)^2}\right)B^-_{ij}\frac{d\delta}{d\theta}\frac{\partial \theta}{\partial x_j} \\
&\quad + u^{0,0}_{ijk}\frac{\partial v_j}{\partial x_k} + \frac{4\delta}{\left(42+25\delta\right)}\frac{\partial B^+_{ij}}{\partial x_j} + \frac{7\left(3+\delta\right)\left(14+3\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}\frac{\partial B^-_{ij}}{\partial x_j} \\
&\quad + \left(1 + \frac{2}{5+\left(\delta+\theta\frac{d\delta}{d\theta}\right)}\right)\left[q_k\frac{\partial v_i}{\partial x_k} + q_i\frac{\partial v_k}{\partial x_k}\right] - \frac{1}{\rho}\sigma_{ik}\frac{\partial \sigma_{kj}}{\partial x_j} \\
&\quad + \frac{2}{5+\delta+\theta\frac{d\delta}{d\theta}}q_k\frac{\partial v_k}{\partial x_i} + \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\left(5+\delta+\theta\frac{d\delta}{d\theta}\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] \\
&\quad + \frac{5+\delta+\theta\frac{d\delta}{d\theta}}{2}\rho\left(\theta - \Delta\theta\right)\frac{\partial \theta}{\partial x_i} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\frac{\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}{5+\left(\delta+\theta\frac{d\delta}{d\theta}\right)}q_i\ , \qquad (5.71)
\end{aligned}$$

$$
\begin{aligned}
&\frac{D\Delta q_i}{Dt} + \sigma_{ik}\left[\frac{\partial \Delta\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{5\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)[q_i - \Delta q_i]}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)}\left[\left(\frac{2}{3 + \delta + \theta\frac{d\delta}{d\theta}}\right)\frac{\sigma_{ij}}{\rho}\frac{\partial v_j}{\partial x_i} + \left(\frac{2}{3 + \delta + \theta\frac{d\delta}{d\theta}}\right)(\theta - \Delta\theta)\frac{\partial v_i}{\partial x_i}\right] \\
&\qquad - \frac{5}{2}\left(1 + \frac{3}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)}\right)\left[\Delta\theta\left(\Delta\theta\frac{\partial\rho}{\partial x_i} + \rho\frac{\partial\Delta\theta}{\partial x_i}\right) + \rho\theta\frac{\partial\Delta\theta}{\partial x_i}\right] \\
&\qquad + \frac{5}{39}\left[1 - \frac{10}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)}\right]\frac{\partial B^-}{\partial x_i} - \frac{5}{39}\left(1 + \frac{3}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)}\right)\frac{\partial B^+}{\partial x_i} \\
&\qquad + \frac{1}{(42 + 25\delta)}\left[7 + \frac{15}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)}\right]\left(\delta\frac{\partial B^+_{ij}}{\partial x_j} + \frac{42}{(42 + 25\delta)}\frac{d\delta}{d\theta}B^+_{ij}\frac{\partial\theta}{\partial x_j}\right) \\
&\quad - 7\left[\frac{1}{(14 + \delta)^2} + \frac{42}{(42 + 25\delta)^2} + \frac{10}{\delta + \theta\frac{d\delta}{d\theta}}\left(\frac{1}{(14 + \delta)^2} + \frac{9}{(42 + 25\delta)^2}\right)\right]\frac{d\delta}{d\theta}B^-_{ij}\frac{\partial\theta}{\partial x_j} \\
&\qquad + \frac{7(3 + \delta)}{(14 + \delta)(42 + 25\delta)}\left[14 - \delta - \frac{20\delta}{\delta + \theta\frac{d\delta}{d\theta}}\right]\frac{\partial B^-_{ij}}{\partial x_j} \\
&\qquad + \left[\theta + \frac{5}{2}\left(1 + \frac{3}{\delta + \theta\frac{d\delta}{d\theta}}\right)\Delta\theta\right]\frac{\partial\sigma_{ij}}{\partial x_j} + \frac{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{5\left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)}\Delta q_j\frac{\partial v_j}{\partial x_i} \\
&\qquad + \frac{10\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right)}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}\left[\frac{q_i}{\rho} - \frac{\Delta q_i}{\rho}\right]\frac{\partial q_i}{\partial x_i} \\
&\qquad + \left(\frac{25 + 7\left(\delta + \theta\frac{d\delta}{d\theta}\right)}{5\left(5 + \delta + \theta\frac{d\delta}{d\theta}\right)}\right)\left(\Delta q_i\frac{\partial v_k}{\partial x_k} + \Delta q_k\frac{\partial v_i}{\partial x_k}\right) + u^{0,0}_{ijk}\frac{\partial v_j}{\partial x_k} \\
&\qquad + \frac{2}{5 + \left(\delta + \theta\frac{d\delta}{d\theta}\right)}\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[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\Delta q_i\ , \qquad (5.72)
\end{aligned}
$$

$$
\begin{aligned}
\frac{DB^{+}}{Dt} &+ \left[\frac{\left(-23+\delta+\theta\frac{d\delta}{d\theta}\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5+\delta+\theta\frac{d\delta}{d\theta}} - \frac{50\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2}\right]\Delta q_k\frac{\partial\theta}{\partial x_k} \\
&+ \left(26-\frac{78}{3+\delta+\theta\frac{d\delta}{d\theta}}\right)\rho\theta\Delta\theta\frac{\partial v_i}{\partial x_i} - \frac{10\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5+\delta+\theta\frac{d\delta}{d\theta}}\theta\frac{\partial\Delta q_k}{\partial x_k} \\
&+ \frac{2\left(\delta+\theta\frac{d\delta}{d\theta}\right)-40}{5+\left(\delta+\theta\frac{d\delta}{d\theta}\right)}\theta\frac{\partial q_k}{\partial x_k} + 3\frac{-23+\delta+\theta\frac{d\delta}{d\theta}}{3+\delta+\theta\frac{d\delta}{d\theta}}\Delta\theta\frac{\partial q_k}{\partial x_k} \\
&+ \left[\frac{50\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2} + \frac{8\left(\delta+\theta\frac{d\delta}{d\theta}\right)-100}{5+\delta+\theta\frac{d\delta}{d\theta}}\right] q_k\frac{\partial\theta}{\partial x_k} \\
&- \left[\frac{112\,(7-\delta)\,(3+\delta)}{(14+\delta)\,(42+25\delta)}B^{-}_{ij} + \frac{62\delta}{(42+25\delta)}B^{+}_{ij}\right]\frac{\partial v_j}{\partial x_i} \\
&+ \left[\left(2-\frac{50}{5+\delta+\theta\frac{d\delta}{d\theta}}\right)q_k - \frac{10\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5+\delta+\theta\frac{d\delta}{d\theta}}\Delta q_k\right]\left[\frac{\partial\Delta\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{3\left(23-\delta-\theta\frac{d\delta}{d\theta}\right)}{3+\delta+\theta\frac{d\delta}{d\theta}}\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i} - \frac{3\left(23-\delta-\theta\frac{d\delta}{d\theta}\right)}{3+\delta+\theta\frac{d\delta}{d\theta}}\Delta\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} - 8\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} \\
&+ \frac{5}{39}\left(17B^{+}-4B^{-}\right)\frac{\partial v_k}{\partial x_k} = -\frac{1}{\tau_{tr}}\left[B^{+}+\frac{39}{2}\rho\Delta\theta^2\right] - \frac{1}{\tau_{int}}B^{+}\ . \qquad (5.73)
\end{aligned}
$$

$$
\begin{aligned}
\frac{DB^{-}}{Dt} &+ \frac{2}{5}\frac{\delta+\theta\frac{d\delta}{d\theta}}{5+\delta+\theta\frac{d\delta}{d\theta}}\theta\frac{\partial\Delta q_k}{\partial x_k} + \left[\frac{196\,(6+\delta)\,(3+\delta)}{5\,(14+\delta)\,(42+25\delta)}B^{-}_{ij} + \frac{54\delta}{5\,(42+25\delta)}B^{+}_{ij}\right]\frac{\partial v_j}{\partial x_i} \\
&+ 2\frac{6+\delta+\theta\frac{d\delta}{d\theta}}{5+\delta+\theta\frac{d\delta}{d\theta}}\theta\frac{\partial q_k}{\partial x_k} + 3\Delta\theta\frac{\partial q_k}{\partial x_k} + \frac{71}{39}B^{-}\frac{\partial v_k}{\partial x_k} - \frac{2}{13}B^{+}\frac{\partial v_k}{\partial x_k} \\
&+ 2\left[\left(1+\frac{1}{5+\delta+\theta\frac{d\delta}{d\theta}}\right)q_k + \left(1-\frac{5}{5+\delta+\theta\frac{d\delta}{d\theta}}\right)\frac{\Delta q_k}{5}\right] \\
&\left[\frac{\partial\Delta\theta}{\partial x_k} - [\theta-\Delta\theta]\frac{\partial\ln\rho}{\partial x_k} - \frac{1}{\rho}\frac{\partial\sigma_{kj}}{\partial x_j}\right] - 3\rho\Delta\theta^2\frac{\partial v_i}{\partial x_i} \\
&+ \left[\frac{\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5+\delta+\theta\frac{d\delta}{d\theta}} + \frac{2\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2}\right]\Delta q_k\frac{\partial\theta}{\partial x_k} \\
&+ \left[\frac{8\left(\delta+\theta\frac{d\delta}{d\theta}\right)+30}{5+\delta+\theta\frac{d\delta}{d\theta}} - \frac{2\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2}\right] q_k\frac{\partial\theta}{\partial x_k} \\
&+ \frac{12}{5}\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} + 3\Delta\theta\sigma_{ij}\frac{\partial v_j}{\partial x_i} = -\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]B^{-}\ , \qquad (5.74)
\end{aligned}
$$

$$\frac{Du_{ijk}^{0,0}}{Dt} - 3\frac{\sigma_{<ij}}{\rho}\frac{\partial\sigma_{k>l}}{\partial x_l} + 3\theta\frac{\partial\sigma_{<ij}}{\partial x_{k>}} + \frac{6\left(14-\delta\right)\left(3+\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}\frac{\partial B_{<ij}^{-}}{\partial x_{k>}} + u_{ijk}^{0,0}\frac{\partial v_l}{\partial x_l}$$
$$+\frac{d\delta}{d\theta}\left(\frac{252}{\left(42+25\delta\right)^2}B_{,<ij}^{+} - \left[\frac{6}{\left(14+\delta\right)^2} + \frac{252}{\left(42+25\delta\right)^2}\right]B_{<ij}^{-}\right)\frac{\partial\theta}{\partial x_{k>}}$$
$$+\frac{6\delta}{42+25\delta}\frac{\partial B_{,<ij}^{+}}{\partial x_{k>}} + 3\sigma_{<ij}\frac{\partial\Delta\theta}{\partial x_{k>}} - 3\left[\theta-\Delta\theta\right]\sigma_{<ij}\frac{\partial\ln\rho}{\partial x_{k>}} + 3u_{l<ij}^{0,0}\frac{\partial v_{k>}}{\partial x_l}$$
$$+\frac{12}{5}\left[\frac{5}{5+\delta+\theta\frac{d\delta}{d\theta}}q_{<i} + \frac{\delta+\theta\frac{d\delta}{d\theta}}{5+\delta+\theta\frac{d\delta}{d\theta}}\Delta q_{<i}\right]\frac{\partial v_j}{\partial x_{k>}} = -\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]u_{ijk}^{0,0}\,, \quad (5.75)$$

$$\frac{DB_{ij}^{+}}{Dt} - \left[\frac{4\left(70-19\delta\right)}{39\delta}B^{-} + \frac{2\left(42+25\delta\right)}{39\delta}B^{+} + \frac{\left(42+25\delta\right)}{\delta}\rho\theta\Delta\theta\right]\frac{\partial v_{<i}}{\partial x_{j>}}$$
$$+\frac{2}{\delta}\left(\frac{70+23\delta}{5+\delta+\theta\frac{d\delta}{d\theta}} - 14+\delta\right)\theta\frac{\partial q_{<i}}{\partial x_{j>}} + \frac{2\left(70+23\delta\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}\theta\frac{\partial\Delta q_{<i}}{\partial x_{j>}}$$
$$+\frac{2}{\delta}\left[\frac{\delta\left[14+\delta+\theta\frac{d\delta}{d\theta}\right]-14\frac{d\delta}{d\theta}}{5\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}\left(\delta+\theta\frac{d\delta}{d\theta}\right) + \frac{2\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)\left(70+\delta\left[14+9\theta\right]\right)}{\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2}\right]\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}}$$
$$+2\left[\frac{14+\delta+\theta\frac{d\delta}{d\theta}}{5+\delta+\theta\frac{d\delta}{d\theta}} - \theta\frac{30\left(7+2\delta\right)\frac{d\delta}{d\theta}+14\theta\left(\frac{d\delta}{d\theta}\right)^2+\left(70+23\delta\right)\theta\frac{d^2\delta}{d\theta^2}}{\delta\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2}\right]q_{<i}\frac{\partial\theta}{\partial x_{j>}}$$
$$+\left[\frac{2}{\delta}\left(\frac{\left(70+23\delta\right)}{5+\delta+\theta\frac{d\delta}{d\theta}} - 14+\delta\right)q_{<i} + \frac{2\left(70+23\delta\right)\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}\Delta q_{<i}\right]$$
$$\left[\frac{\partial\Delta\theta}{\partial x_{j>}} - \frac{\left[\theta-\Delta\theta\right]}{\rho}\frac{\partial\rho}{\partial x_{j>}} - \frac{1}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_k}\right] + 4\theta\frac{\partial u_{ijk}^{0,0}}{\partial x_k} + B_{ij}^{+}\frac{\partial v_k}{\partial x_k}$$
$$-4u_{ijk}^{0,0}\left[\left[\theta-\Delta\theta\right]\frac{\partial\ln\rho}{\partial x_k} - \frac{\partial\Delta\theta}{\partial x_k} + \frac{1}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l}\right] + \frac{14+\delta+\frac{\delta-14}{\delta}\theta\frac{d\delta}{d\theta}}{2}u_{ijk}^{0,0}\frac{\partial\theta}{\partial x_k}$$
$$+2B_{k<i}^{+}\frac{\partial v_{j>}}{\partial x_k} + \frac{8\left(14-\delta\right)\left(3+\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}\left[\frac{14}{5}B_{k<i}^{-}\frac{\partial v_k}{\partial x_{j>}} + 3B_{<ij}^{-}\frac{\partial v_{k>}}{\partial x_k}\right]$$
$$+\frac{8\delta}{\left(42+25\delta\right)}\left[\frac{14}{5}B_{k<i}^{+}\frac{\partial v_k}{\partial x_{j>}} + 3B_{<ij}^{+}\frac{\partial v_{k>}}{\partial x_k}\right] + 4\theta\left[\frac{14}{5}\sigma_{k<i}\frac{\partial v_k}{\partial x_{j>}} + 3\sigma_{<ij}\frac{\partial v_{k>}}{\partial x_k}\right]$$
$$+\frac{28\frac{d\delta}{d\theta}\left[28\left(3+\delta\right)B_{ij}^{-} - 3\left(14+\delta\right)B_{ij}^{+}\right]}{\delta\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)\left(14+\delta\right)\left(42+25\delta\right)}\left[\frac{1}{\rho}\frac{\partial q_k}{\partial x_k} + \frac{\sigma_{kl}}{\rho}\frac{\partial v_l}{\partial x_k} + \left(\theta-\Delta\theta\right)\frac{\partial v_k}{\partial x_k}\right]$$
$$+\frac{\left(14-\delta\right)\theta\frac{d\delta}{d\theta} - \delta\left(14+\delta\right)}{\delta\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}\sigma_{ij}\left[\frac{1}{\rho}\frac{\partial q_k}{\partial x_k} + \frac{\sigma_{kl}}{\rho}\frac{\partial v_l}{\partial x_k} + \left(\theta-\Delta\theta\right)\frac{\partial v_k}{\partial x_k}\right] = -\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]B_{ij}^{+}\,,$$
$$(5.76)$$

$$
\begin{aligned}
&\frac{DB^{-}_{ij}}{Dt}-\frac{14+\delta}{3+\delta}\sigma_{ij}\left[\frac{1}{\rho}\frac{\partial q_k}{\partial x_k}+\frac{\sigma_{kl}}{\rho}\frac{\partial v_l}{\partial x_k}+(\theta-\Delta\theta)\frac{\partial v_k}{\partial x_k}\right]\\
&\quad-\frac{22\frac{d\delta}{d\theta}}{(3+\delta)(14+\delta)\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}B^{-}_{ij}\left[\frac{1}{\rho}\frac{\partial q_k}{\partial x_k}+\frac{\sigma_{lk}}{\rho}\frac{\partial v_k}{\partial x_l}+(\theta-\Delta\theta)\frac{\partial v_k}{\partial x_k}\right]\\
&\quad+\frac{3(14+\delta)}{14(3+\delta)}\left[\frac{12(14-\delta)(3+\delta)}{(14+\delta)(42+25\delta)}B^{-}_{<ij}+\frac{12\delta}{(42+25\delta)}B^{+}_{<ij}+6\theta\sigma_{<ij}\right]\frac{\partial v_{k>}}{\partial x_k}\\
&\quad+\frac{6(14+\delta)}{35(3+\delta)}\left[\frac{14(14-\delta)(3+\delta)}{(14+\delta)(42+25\delta)}B^{-}_{k<i}+\frac{14\delta}{(42+25\delta)}B^{+}_{k<i}+7\theta\sigma_{k<i}\right]\frac{\partial v_k}{\partial x_{j>}}\\
&\quad+B^{-}_{ij}\frac{\partial v_k}{\partial x_k}+2\frac{14+\delta}{3+\delta}\left[\frac{\delta+\theta\frac{d\delta}{d\theta}}{5}\frac{3+\delta+\theta\frac{d\delta}{d\theta}}{5+\delta+\theta\frac{d\delta}{d\theta}}-\frac{2\theta\left(2\frac{d\delta}{d\theta}+\theta\frac{d^2\delta}{d\theta^2}\right)}{\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2}\right]\Delta q_{<i}\frac{\partial\theta}{\partial x_{j>}}\\
&+\frac{2(14+\delta)\left(5\left[3+\delta+\theta\frac{d\delta}{d\theta}\right]+\left[(3+\delta)\delta+(7+2\delta)\theta\frac{d\delta}{d\theta}+\left(\left(\frac{d\delta}{d\theta}\right)^2+2\frac{d^2\delta}{d\theta^2}\right)\theta^2\right]\right)}{(3+\delta)\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)^2}q_{<i}\frac{\partial\theta}{\partial x_{j>}}\\
&\quad-\frac{3(14+\delta)}{7(3+\delta)}u^{0,0}_{ijk}\left[[\theta-\Delta\theta]\frac{\partial\ln\rho}{\partial x_k}-\frac{\partial\Delta\theta}{\partial x_k}+\frac{1}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l}\right]+\frac{14+\delta+\frac{14+\delta}{3+\delta}\theta\frac{d\delta}{d\theta}}{2}u^{0,0}_{ijk}\frac{\partial\theta}{\partial x_k}\\
&+\frac{2(14+\delta)\left[\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)q_{<i}-\frac{2}{5}\left(\delta+\theta\frac{d\delta}{d\theta}\right)\Delta q_{<i}\right]}{(3+\delta)\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}\left[\frac{\partial\Delta\theta}{\partial x_{j>}}-\frac{[\theta-\Delta\theta]}{\rho}\frac{\partial\rho}{\partial x_{j>}}-\frac{1}{\rho}\frac{\partial\sigma_{j>k}}{\partial x_k}\right]\\
&\quad+2B^{-}_{k<i}\frac{\partial v_{j>}}{\partial x_k}+\frac{2(14+\delta)}{3(3+\delta)}B^{-}\frac{\partial v_{<i}}{\partial x_{j>}}+2\frac{(14+\delta)\left(3+\delta+\theta\frac{d\delta}{d\theta}\right)}{(3+\delta)\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}\theta\frac{\partial q_{<i}}{\partial x_{j>}}\\
&\quad+\frac{2(70+23\delta)\left(\delta+\theta\frac{d\delta}{d\theta}\right)}{5\delta\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}\theta\frac{\partial\Delta q_{<i}}{\partial x_{j>}}+\frac{3(14+\delta)}{7(3+\delta)}\theta\frac{\partial u^{0,0}_{ijk}}{\partial x_k}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]B^{-}_{ij}\ . \qquad (5.77)
\end{aligned}
$$

Applying order of magnitude on these set of equations produce different results than the results showed above for our proposed S-model. This is due to the fact that the leading order term of B^{-} from BGK theory is at order $\epsilon^{1+2\alpha}$, while it is at order ϵ^{1} from proposed S-model. Due to this difference in leading order of B^{-}, terms and equations that are presented at different orders of accuracy will change. This will reduce the number of full balance laws required at third order from R19 of S-model to R18 of BGK model. Full discussion and different set of equations obtained from BGK model are given in Ref. [77, 85] and they are not shown here due to lack of space.

Gas	C_0	$C_1 \times 10^6$	$C_2 \times 10^{11}$	$C_3 \times 10^{17}$
N_2	2.7399	−5.4490	3.6718	−5.4125
H_2	2.2638	0.27047	−0.00977	0.0013103
CO	2.7037	−5.2149	3.8171	−5.8349
CO_2	1.3822	46.8007	−18.8412	30.6293
CH_4	1.3153	12.0982	0.53867	−0.98386

Table 5.1: Constants of specific heats for various gases.

5.13 Properties of different diatomic and polyatomic gases

In this section we present data for temperature dependent specific heat, and translational and internal relaxation times for CO_2, CO, H_2, N_2 and CH_4.

Total specific heat is the sum of translational and internal DoF contributions. A third order formula gives us a valid approximation of specific heat in the temperature range between 250 to 1200 $°K$ [86] as,

$$C_v = \frac{3 + \delta + \theta \frac{d\delta}{d\theta}}{2} = C_0 + C_1\theta + C_2\theta^2 + C_3\theta^3 \ , \tag{5.78}$$

the four constants for different gases are given in table 5.1. Based on the obtained formula for specific heat we have

$$\frac{dC_v}{d\theta} = \frac{1}{2}\left(2\frac{d\delta}{d\theta} + \theta\frac{d^2\delta}{d\theta^2}\right) = C_1 + 2C_2\theta + 3C_3\theta^2 \ , \tag{5.79a}$$

$$\theta^2\frac{d^2\delta}{d\theta^2} = 2\left(\theta\frac{dC_v}{d\theta} - \theta\frac{d\delta}{d\theta}\right) \ , \tag{5.79b}$$

$$\delta + \theta\frac{d\delta}{d\theta} = 2C_v - 3 \ . \tag{5.79c}$$

We use measured data of bulk and shear viscosity of non-rarefied flows obtained based on classical hydrodynamics and apply them to identify the relaxation times, τ_{tr} and τ_{int}, in our kinetic model, Eq. 2.11. The relaxation times present in our model have direct relation at N-S-F level to the measured viscosities, and translational and internal relaxation times are calculated based on them. This is done through the shear and bulk viscosity definitions, Eqs. 5.16 and 5.17 as,

Gas	n_{υ}	$\frac{\mu_0}{\upsilon_0}$
N_2	1.376	1.3038
H_2	1	0.0346
CO_2	-1.353	2.5974×10^{-4}
CH_4	1.295	0.7874

Table 5.2: Bulk viscosity temperature exponent and ratio of reference viscosities at 295 K for various gases.

$$\tau_{tr} = \frac{\mu}{\rho\left(\theta - \Delta\theta\right)}, \tag{5.80a}$$

$$\tau_{int} = \frac{3\left(3 + \delta + \theta\frac{d\delta}{d\theta}\right)}{2\left(\delta + \theta\frac{d\delta}{d\theta}\right)}\frac{\upsilon}{\rho\left(\theta - \Delta\theta\right)}\ . \tag{5.80b}$$

For power law potentials with temperature exponent $0.5 \leq n_\mu \leq 1$, the viscosity is given by [87]

$$\mu = \mu_0\left(\frac{p/\rho}{p_0/\rho_0}\right)^{n_\mu}\ ; \tag{5.81a}$$

bulk viscosity can also be represented by power law formula as,

$$\upsilon = \upsilon_0\left(\frac{p/\rho}{p_0/\rho_0}\right)^{n_\upsilon}\ , \tag{5.81b}$$

where, pressure is $p = \rho\left(\theta - \Delta\theta\right)$, and temperature exponents are given in table 5.2 for different gases [79]. CH_4 gas bulk viscosity is best fitted to power law formula at temperature range between $77 - 293\ K$. At higher temperatures, bulk viscosity experimental data is best fitted with exponential function through internal relaxation time, Eq. 5.80b, as [79]

$$\tau_{int} = \frac{429.3 \times 10^{-5}}{\rho\left(\theta - \Delta\theta\right)\frac{m}{k}}Exp[\frac{21.07}{\left(\frac{m}{k}\theta\right)^{\frac{1}{3}}}]\ , \tag{5.82}$$

m and k are mass of molecule and Boltzmann constant.

Using the dimensionless parameters,

$$\bar{\tau}_{int} = \frac{\tau_{int}}{\tau_{int0}} \ , \ \bar{\tau}_{tr} = \frac{\tau_{tr}}{\tau_{int0}} \ , \ \bar{\rho} = \frac{\rho}{\rho_0} - 1 \ ,$$
$$\bar{\theta} = \frac{\theta}{\theta_0} - 1 \ , \ \Delta\bar{\theta} = \frac{\Delta\theta}{\theta_0} \ , \tag{5.83}$$

the dimensionless relaxation times becomes,

$$\tau_{tr} = \frac{\mu_0}{\upsilon_0}\frac{2C_v - 3}{3C_v}\frac{(1+\theta-\Delta\theta)^{n_\mu - 1}}{1+\rho} \ , \tag{5.84a}$$
$$\tau_{int} = \frac{3C_v}{2C_v - 3}\frac{2C_{v0} - 3}{3C_{v0}}\frac{(1+\theta-\Delta\theta)^{n_v - 1}}{1+\rho} \ , \tag{5.84b}$$

and for CH_4 gas at high temperatures,

$$\tau_{int} = \frac{1}{(1+\rho)(1+\theta-\Delta\theta)}\frac{Exp[\frac{21.07}{\left(\frac{m}{k}\theta_0(1+\theta)\right)^{\frac{1}{3}}}]}{Exp[\frac{21.07}{\left(\frac{m}{k}\theta_0\right)^{\frac{1}{3}}}]} \ , \tag{5.84c}$$

where the bars are dropped for simplicity. Therefore, the values of dimensionless relaxation times or Kn numbers as discussed in Sec. 4.1 are obtained based on experimental data of viscosities and specific heat.

Chapter 6

Linear wave analysis

There is nothing more genuine than breaking away from the chorus to learn the sound of your own voice.

Po Bronson

As a first application of the above models, we study the phase speed and damping of one-dimensional linear waves as forecasted in the obtained different orders of equations. We compare the predictions of the various equations in the hierarchies among each other as well as to those of the classical Navier-Stokes-Fourier equations, and its modification containing the balance law for the dynamic temperature. Moreover, we study the influence of excitations of the internal degrees of freedom by comparing with results for monatomic gases, where we will highlight the influence of the ratio of collision times, τ_{tr}/τ_{int}. For simplicity, all relaxation parameters ($R_{u^{1,1}}$, $R_{u^{2,0}}$, $R_{q_{int}}$ and $R_{q_{tr}}$) are considered to be 1 and specific heat is constant with $\delta = 2$.

6.1 Linearized equations

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

$$\rho = \rho_0 + \hat{\rho},\ \theta = \theta_0 + \hat{\theta},\ v_i = \hat{v}_i,\ \Delta\theta = \Delta\hat{\theta},\ \sigma_{ij} = \hat{\sigma}_{ij},\ q_i = \hat{q}_i,$$
$$\Delta q_i = \Delta\hat{q}_i,\ B_{ij}^{+} = \hat{B}_{ij}^{+},\ B^{-} = \hat{B}^{-},\ B_{ij}^{-} = \hat{B}_{ij}^{-},\ B^{-} = \hat{B}^{-},\ u_{ijk}^{0,0} = \hat{u}_{ijk}^{0,0}\,. \tag{6.1}$$

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

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

$$\bar{x}_i = \frac{x_i}{\tau_0\sqrt{\theta_0}} \ , \ \bar{t} = \frac{t}{\tau_0} \ , \ \bar{\tau}_{int} = \frac{\tau_{int}}{\tau_0} \ , \ \bar{\tau}_{tr} = \frac{\tau_{tr}}{\tau_0} \ , \ \bar{\rho} = \frac{\rho}{\rho_0} - 1 \ ,$$
$$\bar{\theta} = \frac{\theta}{\theta_0} - 1 \ , \ \Delta\bar{\theta} = \frac{\Delta\theta}{\theta_0} \ , \ \bar{v}_i = \frac{v_i}{\sqrt{\theta_0}} \ , \ \bar{\sigma}_{ij} = \frac{\sigma_{ij}}{\rho_0\theta_0} \ , \ \bar{q}_i = \frac{q_i}{\rho_0\sqrt{\theta_0}^3} \ , \ \Delta\bar{q}_i = \frac{\Delta q_i}{\rho_0\sqrt{\theta_0}^3} \ , \tag{6.2}$$
$$\bar{u}^{0,0}_{ijk} = \frac{u^{0,0}_{ijk}}{\rho_0\sqrt{\theta_0}^3} \ , \ \bar{B}^+_{ij} = \frac{B^+_{ij}}{\rho_0\theta_0^2} \ , \ \bar{B}^-_{ij} = \frac{B^-_{ij}}{\rho_0\theta_0^2} \ , \ \bar{B}^+ = \frac{B^+}{\rho_0\theta_0^2} \ , \ \bar{B}^- = \frac{B^-}{\rho_0\theta_0^2} \ .$$

Here, τ_0 and L are characteristics time and length scales. Note that the dimensionless relaxation times , $\bar{\tau}_{int}$ and $\bar{\tau}_{tr}$, are the Knudsen numbers. In order to do the one-dimensional wave analysis, all variables should depend only on time and x-direction. For simplicity we use the following notation for the relevant elements of vectors and tensors:

$$v_1 = v, \ \sigma_{11} = \sigma, \ q_1 = q, \ \Delta q_1 = \Delta q, \ u^{0,0}_{111} = u^{0,0} \ . \tag{6.3}$$

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

6.2 One-dimensional linear dimensionless equations

In the below set of G36 equations, first, second and third order set of equations are obtained by zeroing the corresponding underlined terms, e.g. zeroing the double and triple underlined terms reproduce the second order set of equations. For having the

Grad's 36 moment equations, the linearized, dimensionless conservation laws read,

$$\frac{\partial \rho}{\partial t} + \frac{\partial v}{\partial x} = 0 \; , \tag{6.4a}$$

$$\frac{\partial v}{\partial t} + \frac{\partial \rho}{\partial x} + \frac{\partial \theta}{\partial x} + \frac{\partial \sigma}{\partial x} - \frac{\partial \Delta\theta}{\partial x} = 0 \; , \tag{6.4b}$$

$$\frac{\partial \theta}{\partial t} + \frac{2}{3+\delta}\frac{\partial v}{\partial x} + \frac{2}{3+\delta}\frac{\partial q}{\partial x} = 0 \; , \tag{6.4c}$$

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

$$\frac{\partial \Delta\theta}{\partial t} - \frac{2\delta}{3\,(3+\delta)}\frac{\partial v}{\partial x} \underline{- \frac{4\delta}{3\,(3+\delta)\,(5+\delta)}\frac{\partial q}{\partial x} - \frac{2\delta}{3\,(5+\delta)}\frac{\partial \Delta q}{\partial x}} = -\frac{\Delta\theta}{\tau_{int}} \; , \tag{6.4d}$$

$$\underline{\frac{\partial \sigma}{\partial t}} + \frac{4}{3}\frac{\partial v}{\partial x} + \underline{\frac{8}{3\,(5+\delta)}\frac{\partial q}{\partial x}} + \underline{\underline{\frac{8\delta}{15\,(5+\delta)}\frac{\partial \Delta q}{\partial x} + \frac{\partial u^{0,0}}{\partial x_k}}} = -\left[\underline{\frac{1}{\tau_{int}}} + \frac{1}{\tau_{tr}}\right]\sigma \; , \tag{6.4e}$$

$$\begin{aligned} \underline{\frac{\partial q}{\partial t}} + \frac{5+\delta}{2}\frac{\partial \theta}{\partial x} + \underline{\frac{\partial \sigma}{\partial x} - \frac{\partial \Delta\theta}{\partial x}} + \underline{\underline{\frac{4\delta}{25\delta+42}\frac{\partial B_{11}^{+}}{\partial x} - \frac{2}{39}\frac{\partial B^{+}}{\partial x}}} & \\ \underline{\underline{+\frac{7\,(14+3\delta)\,(3+\delta)}{(14+\delta)\,(42+25\delta)}\frac{\partial B_{11}^{-}}{\partial x} + \frac{5}{13}\frac{\partial B^{-}}{\partial x}}} &= -\left[\underline{\frac{1}{\tau_{int}}} + \frac{1}{\tau_{tr}}\right] q \; , \end{aligned} \tag{6.4f}$$

must be considered along with balance laws,

$$\begin{aligned} \underline{\underline{\frac{\partial \Delta q}{\partial t}}} - \underline{\frac{5\,(3+\delta)}{2\delta}\frac{\partial \Delta\theta}{\partial x}} + \underline{\underline{\frac{\partial \sigma}{\partial x} + \frac{15+7\delta}{42+25\delta}\frac{\partial B_{11}^{+}}{\partial x} - \frac{5\,(3+\delta)}{39\delta}\frac{\partial B^{+}}{\partial x_i}}} & \\ \underline{\underline{+\frac{5\,(\delta-10)}{39\delta}\frac{\partial B^{-}}{\partial x}}} - \underline{\underline{\underline{7\frac{3+\delta}{14+\delta}\frac{\delta+6}{42+25\delta}\frac{\partial B_{11}^{-}}{\partial x}}}} &= -\left[\underline{\underline{\frac{1}{\tau_{int}}}} + \underline{\frac{1}{\tau_{tr}}}\right]\underline{\Delta q} \; , \end{aligned} \tag{6.4g}$$

$$\underline{\underline{\frac{\partial B^{+}}{\partial t} - \frac{240-\delta\,(47-\delta)}{2\,(3+\delta)\,(5+\delta)}\frac{\partial q}{\partial x}}} - \underline{\underline{\frac{10\delta}{5+\delta}\frac{\partial \Delta q}{\partial x}}} = \underline{\underline{-\left[\frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}}\right] B^{+}}} \; , \tag{6.4h}$$

$$\underline{\underline{\underline{\frac{\partial B_{11}^{+}}{\partial t}}}} + \underline{\underline{\frac{4\,(14+\delta)}{3\,(5+\delta)}\frac{\partial q}{\partial x}}} + \underline{\underline{\underline{4\frac{\partial u^{0,0}}{\partial x} + \frac{4\,(70+23\delta)}{15\,(5+\delta)}\frac{\partial \Delta q}{\partial x}}}} = \underline{\underline{-\left[\frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}}\right] B_{11}^{+}}} \; , \tag{6.4i}$$

$$\underline{\underline{\underline{\frac{\partial u^{0,0}}{\partial t}}}} + \underline{\underline{\frac{9}{5}\frac{\partial \sigma}{\partial x}}} + \underline{\underline{\underline{\frac{18\delta}{5\,(25\delta+42)}\frac{\partial B^{+}_{11}}{\partial x} + \frac{18\,(14-\delta)\,(3+\delta)}{5\,(14+\delta)\,(42+25\delta)}\frac{\partial B^{-}_{11}}{\partial x}}}}$$
$$= -\left[\frac{1}{\underline{\underline{\underline{\tau_{int}}}}} + \frac{1}{\underline{\underline{\tau_{tr}}}}\right]\underline{\underline{u^{0,0}}}\,, \tag{6.4j}$$

$$\underline{\underline{\underline{\frac{\partial B^{-}}{\partial t}}}} + \underline{\underline{\frac{2\,(6+\delta)}{5+\delta}\frac{\partial q}{\partial x}}} + \underline{\underline{\underline{\frac{2\delta}{5\,(5+\delta)}\frac{\partial \Delta q}{\partial x}}}} = -\left[\frac{1}{\underline{\underline{\underline{\tau_{int}}}}} + \frac{1}{\underline{\underline{\tau_{tr}}}}\right]\underline{\underline{B^{-}}}\,, \tag{6.4k}$$

$$\underline{\underline{\underline{\frac{\partial B^{-}_{11}}{\partial t}}}} + \underline{\underline{\frac{4\,(14+\delta)}{3\,(5+\delta)}\frac{\partial q}{\partial x}}} + \underline{\underline{\underline{\frac{3\,(14+\delta)}{7\,(3+\delta)}\frac{\partial u^{0,0}}{\partial x} - \frac{8\delta\,(14+\delta)}{15\,(3+\delta)\,(5+\delta)}\frac{\partial \Delta q}{\partial x}}}}$$
$$= -\left[\frac{1}{\underline{\underline{\underline{\tau_{int}}}}} + \frac{1}{\underline{\underline{\tau_{tr}}}}\right]\underline{\underline{B^{-}_{11}}}\,. \tag{6.4l}$$

6.3 Plane harmonic waves

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

$$A_{AB}\frac{\partial u_B}{\partial t} + C_{AB}\frac{\partial u_B}{\partial x} = L_{AB}u_B\ , \tag{6.5}$$

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

$$u^{[14]} = \{\rho, v_i, \theta, \sigma_{ij}, \Delta\theta, q_i\} \qquad \text{first and second order,} \tag{6.6a}$$

$$u^{[36]} = \{\rho, v_i, \theta, \sigma_{ij}, \Delta\theta, q_i, \Delta q_i, B^{+}, B^{-}, u^{0,0}_{ijk}, B^{+}_{ij}, B^{-}_{ij}\} \quad \text{third order and G36.} \tag{6.6b}$$

Making the harmonic wave ansatz,

$$u_A(x,t) = \breve{u}_A \exp[i(\omega t - kx)]\ , \tag{6.7}$$

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

$$\left[i\omega A_{AB} - ikC_{AB} - L_{AB}\right]\breve{u}_B = 0\ . \tag{6.8}$$

Non-trivial solutions for this equation are obtained when the determinant of the complex matrix inside the bracket becomes zero, which gives the dispersion relation. For different set of equations, the dispersion relation has different numbers of branches, hence several solutions.

6.4 Phase velocity and damping factor

The phase velocity and damping factor are defined as

$$v_{ph} = \frac{\omega}{k_r} \text{ and } \phi = -k_i \ . \tag{6.9}$$

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

The frequency is made dimensionless such that it can be considered as a Knudsen number, [88]

$$\bar{\omega} = \omega\tau_0 = \mathrm{Kn} \ . \tag{6.10}$$

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

Figure 6.1 shows the branches associated with the lowest damping, this is the sound wave [88], for the different sets of equations, where only one branch is plotted. The dimensionless inverse phase velocity and the reduced damping factor ϕ/ω for a wide range of dimensionless frequency and two different ratios of Knudsen numbers, 10^{-2} and 10^{-3}, are shown as functions of inverse frequency.

All sets of equations agree for low frequency (i.e., small Knudsen number). However, as the Knudsen number rises (i.e., for smaller inverse frequency), first the refined NSF equations starts to deviate, followed by the second order set of equations. The third order equations, R19, have agreement with the full set of 36 equations up to higher Knudsen numbers. Therefore, the range of validity for the set of R19 equations is near $1/\omega\tau_{int} = \mathrm{Kn}_{tr}/\mathrm{Kn}_{int}$; this value of dimensionless frequency corresponds to the case of $\mathrm{Kn}_{tr} = 1$. Based on the Fig. 6.1, the expected validity of the R19 is up to $\mathrm{Kn}_{tr} = 0.6$.

A comparison between the refined and classical NSF equations is made in Fig.

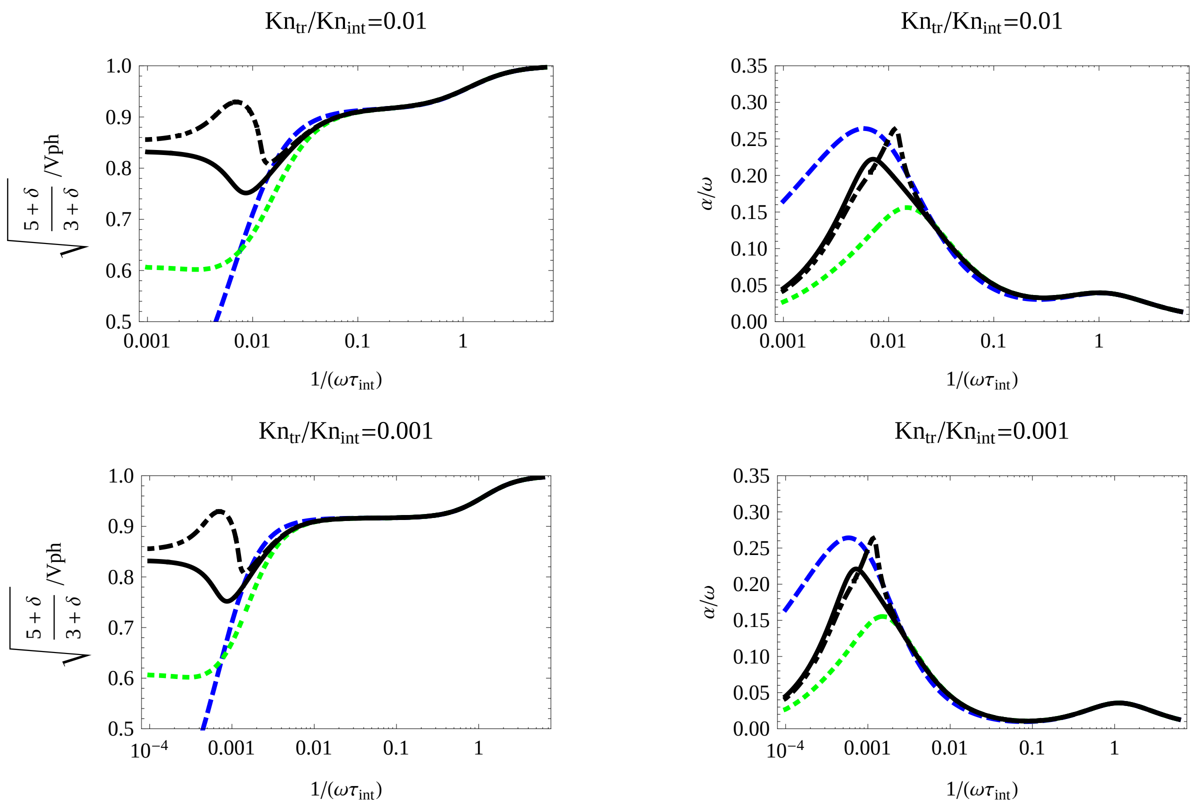

Figure 6.1: Inverse dimensionless phase velocity $\sqrt{(5+\delta)\,/\,(3+\delta)}/v_{ph}$ (left) and reduced damping α/ω (right) as functions of inverse frequency $1/\omega$ for various Knudsen number ratios and different sets of equations: refined NSF (blue dashed), second order (green dotted), R19 (black continuous), G36 (black dash-dotted).

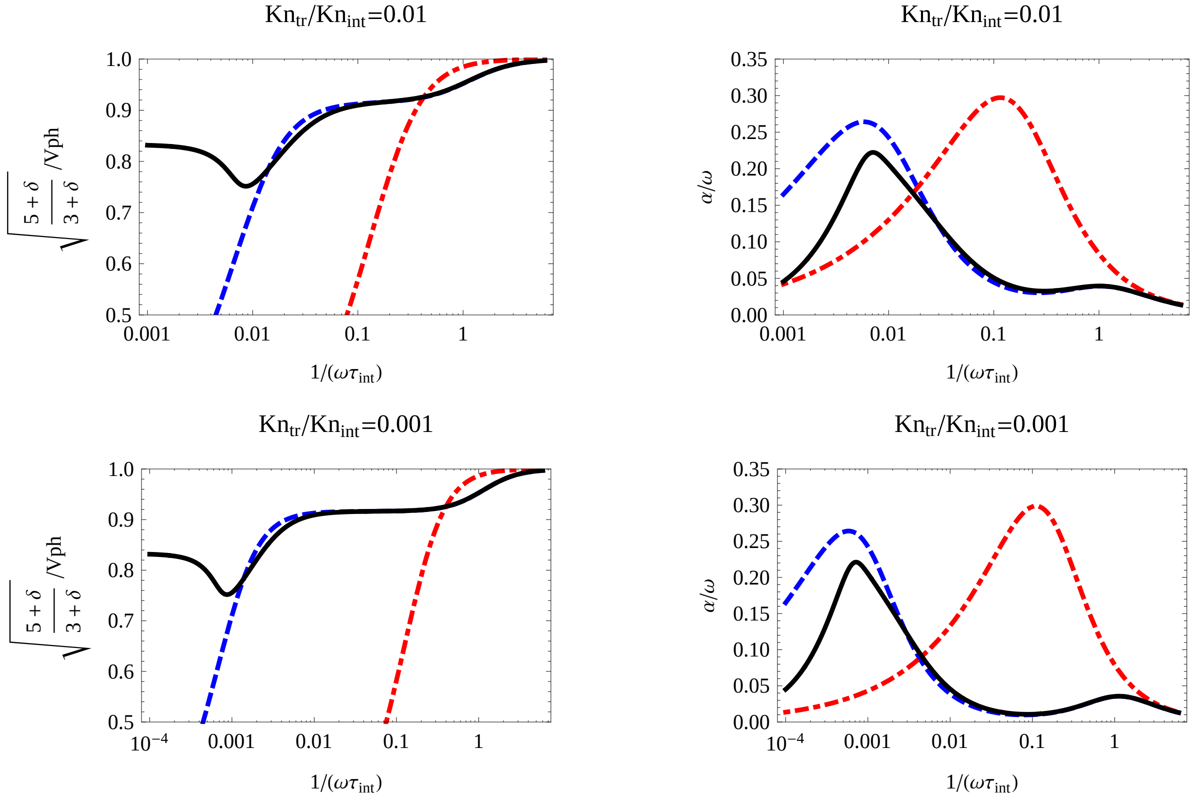

Figure 6.2: Inverse dimensionless phase velocity $\sqrt{(5+\delta)\,/\,(3+\delta)}/v_{ph}$ (left) and reduced damping α/ω (right) as functions of inverse frequency $1/\omega$ for two Knudsen number ratios and different sets of equations: R19 (black continuous), classical NSF (red dash-dotted), refined NSF (orange dashed).

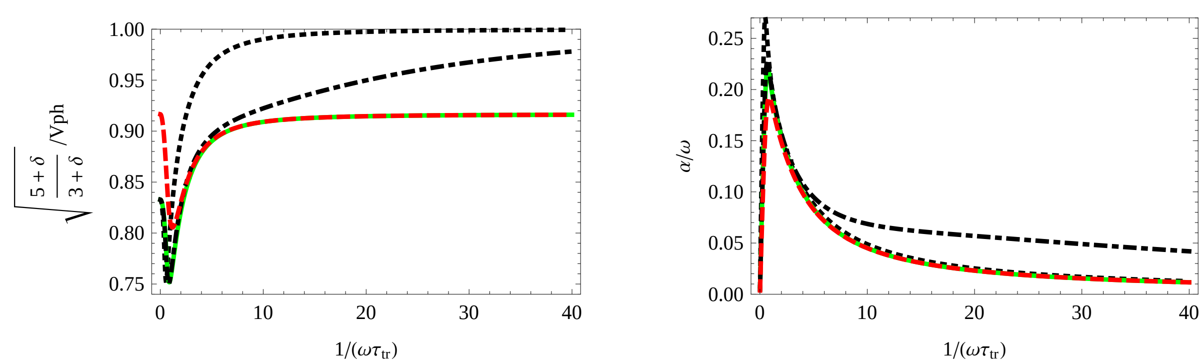

Figure 6.3: Inverse dimensionless phase velocity $\sqrt{(5+\delta)\,/\,(3+\delta)}/v_{ph}$ (left) and reduced damping α/ω (right) as functions of inverse frequency $1/\omega$ for set of R19 equations for Knudsen number ratios, 0.5 (black dotted), 0.05 (black dash-dotted), 10^{-5} (red dashed), and for the set of R13 equations corresponds to the monatomic gas (green continuous).

6.2. The difference between the two sets is simply the time derivative $\frac{\partial \Delta\theta}{\partial t}$ in Eq. (6.4d), which is there for the refined case, but not for the classical NSF equations. Original NSF deviates from R19 for almost all frequencies plotted, while refined NSF agrees to R19 for dimensionless inverse frequencies $1/\left(\omega\tau_{int}\right)$ down to the values of $\mathrm{Kn}_{tr}/\mathrm{Kn}_{int}$. Considering the proposed refined version of the NSF equations, Sec. 5.4, instead of the classical one, will extend the range of validity of the NSF equations considerably.

6.5 Monatomic limit

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

For convenience, now the translational Knudsen number is set to unity, $Kn_{tr} = 1$, so that the reference time scale is the translational mean free time, $\tau_0 = \tau_{tr}$. This means frequency is a measure of the translational Knudsen number. In Fig. 6.3 results from the R19 equations for three different relaxation times ratios are compared with the result from monatomic counterpart, which are the R13 equations [44]. The three relaxation times considered here corresponds to two extreme cases, excited ($\tau_{tr} \approx \tau_{int}$) and frozen ($\tau_{int} \gg \tau_{tr}$) internal degrees of freedom, and one case in between: $\tau_{tr}/\tau_{int} = 0.5, 0.05, 10^{-5}$. The case with $\tau_{tr}/\tau_{int} = 10^{-5}$ corresponds to the frozen internal state and exhibits a good agreement with the monatomic results from the R13 equations. A polyatomic gas with $\delta = 2$ behaves like a monatomic gas with $\delta = 0$, if the internal degrees of freedom are frozen. This behavior is seen for polyatomic gases with higher internal degrees of freedom too. For intermediate values of τ_{tr}/τ_{int}, the speed of sound is strongly dependent on frequency. If the frequency is small (large $1/\omega\tau$), the internal degrees of freedom have time to relax, and the speed of sound is that for $\delta = 2$, but for larger frequency, the internal degree of freedom does not have sufficient time to relax, which results in an increased speed of sound.

Here, we reproduce the monatomic gas behavior as an asymptotic solution of the equations, without setting the internal degrees of freedom to zero, as was done in Ref. [40].

Chapter 7

Theory of boundary condition

One sign that you are pushing boundaries is a lot of failures.
Ben Silbermann

In this chapter, we introduce a microscopic boundary condition using same idea that we used to model two distinguished exchanged processes, internal and translational. In next two chapters, we use this microscopic boundary condition to obtain the corresponding macroscopic boundary conditions. Having the macroscopic boundary condition enable us to solve different boundary value problems, e.g. stationary heat transfer and Couette flow, using proposed macroscopic models above.

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 condition for boundary is the Maxwell's accommodation model [89]. Maxwell proposed that the gas particles are reflected from the wall specularly or diffusivity. A portion of the particles hit the wall and accommodate at the wall so that they being reflected with the equilibrium distribution of the wall. The other portion 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, $f^*(\mathbf{c}) = f(\mathbf{c} - \mathbf{2}(\mathbf{n}.\mathbf{c})\,\mathbf{n})$.

For polyatomic particles that are diffusively reflected, we have two Maxwellian type equilibrium distribution functions, Eqs. (2.21, 2.25) corresponding to only translational energy equilibrium and total energy equilibrium. We adopt the generalized Grad's 36 distribution function (3.9) and its corresponding form as the phase density (f^*) for incoming and specularly reflected particles. Therefore we introduce the wall boundary condition as the velocity distribution function in the infinitesimal precinct of the wall,

$$\tilde{f}\left(c\right)=\begin{cases}\chi\left[\left(1-\zeta\right)f_{tr,w}\left(\mathbf{c}\right)+\zeta f_{int,w}\left(\mathbf{c}\right)\right]+\left(1-\chi\right)f^{*}_{|36}\left(\mathbf{c}\right) & \mathbf{n}.\left(\mathbf{c}-\mathbf{v}_{w}\right)\succ 0\ ,\\ f_{|36}\left(\mathbf{c}\right) & \mathbf{n}.\left(\mathbf{c}-\mathbf{v}_{w}\right)\prec 0\ ,\end{cases} \tag{7.1}$$

where the two wall accommodation coefficients, ζ and χ, 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 $\zeta = 0$ and $\chi = 0$. Moreover, $\mathbf{n}$ 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 [90].The above is a variant of Maxwell boundary conditions, and obeys these requirements. Normalization implies that the number of particles conserved, and this is ensured here by adjusting the densities for the wall Maxwellians, $f_{tr,w}$ and $f_{int,w}$, accordingly, see Eq. 8.17 in Sec. 8.2. The distribution used on the wall are Maxwellian distribution which are normalized and the Grad's distribution is an expansion on the Maxwellian distribution, which are designed to ensure conserved particles number as will be seen in Eq. 8.17. This means the kernel is normalized and number of particles hitting the wall are same as reflecting particles and the normalization condition is satisfied [90].

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 $\left(\tilde{f}\right)$ by corresponding velocity and internal parameter function, Ψ, and take the integral of it over velocity and internal parameter space. This will give us the relations between the macroscopic properties at the wall to the wall properties given in the wall equilibrium distribution functions, $f_{tr,w}$ and $f_{int,w}$. We define two peculiar velocities based on average velocity, $\mathbf{C} = \mathbf{c} - \mathbf{V}_{gas}$, and based on the wall velocity, $\mathbf{C}_w = \mathbf{c} - \mathbf{V}_w$. This will give us the integral of the weighted wall distribution function as,

$$\int \Psi(\mathbf{C},\mathbf{I})\,\tilde{f}(\mathbf{C})\,d\mathbf{C}d\mathbf{I} =$$
$$\int\int_{\mathbf{C}.\mathbf{n}\prec 0} \left[\Psi(\mathbf{C},\mathbf{I}) + (1-\chi)\,\Psi(\mathbf{C}-\mathbf{2}\,(\mathbf{n}.\mathbf{C})\,\mathbf{n},\mathbf{I})\right] f_{|36}(\mathbf{C},\mathbf{I})\,d\mathbf{C}dI$$
$$+\chi\left[\int\int_{\mathbf{C}.\mathbf{n}\succ 0} \Psi(\mathbf{C}_w - V_s, I)\left[(1-\zeta)\,f_{tr,w}(\mathbf{C}_w, I) + \zeta f_{int,w}(\mathbf{C}_w, I)\right] d\mathbf{C}_w dI\right], \quad (7.2)$$

where the slip velocity is $V_s = \mathbf{V}_{gas} - \mathbf{V}_w$.

The choice of the velocity and internal parameter function $\Psi(\mathbf{C},\mathbf{I})$ is restricted by Grad's finding based on the argument of specular reflection that the velocity function should be odd in the normal component of the particle velocity [62]. This is due to the fact that the even polynomials at the wall boundary condition will produce identity and are uncontrollable. Also, we only prescribe fluxes and not the variables based on the theory of balance laws which states that at the boundary we need to prescribe fluxes, not variables [47].

In next two chapters, we model and solve two boundary value problems, heat conduction and Couette flow, using above proposed models. Based on the model formulation of each problem, corresponding velocity and internal parameter function $\Psi(\mathbf{C},\mathbf{I})$ is obtained and macroscopic boundary conditions are derived using Eq. 7.2.

Chapter 8

One dimensional stationary heat conduction

But heat can also be produced by the friction of liquids, in which there could be no question of changes in structure, or of the liberation of latent heat.

Hermann von Helmholtz

As the first boundary value problem, one dimensional heat transfer within the stationary polyatomic gas is studied, using numerical and analytical methods to solve non-linear and linear systems. Two sets of equations are used in this chapter, the R19 and the refined NSF equations. We consider an unsteady heat conduction which is homogeneous in y and z directions. The gas is confined between two infinite plates and is stationary, as shown in Fig. 8.1. The walls are at different temperatures and the flow properties and variables depend only on 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

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

Note that the dimensionless relaxation times , $\bar{\tau}_{int}$ and $\bar{\tau}_{tr}$, are the Knudsen num-

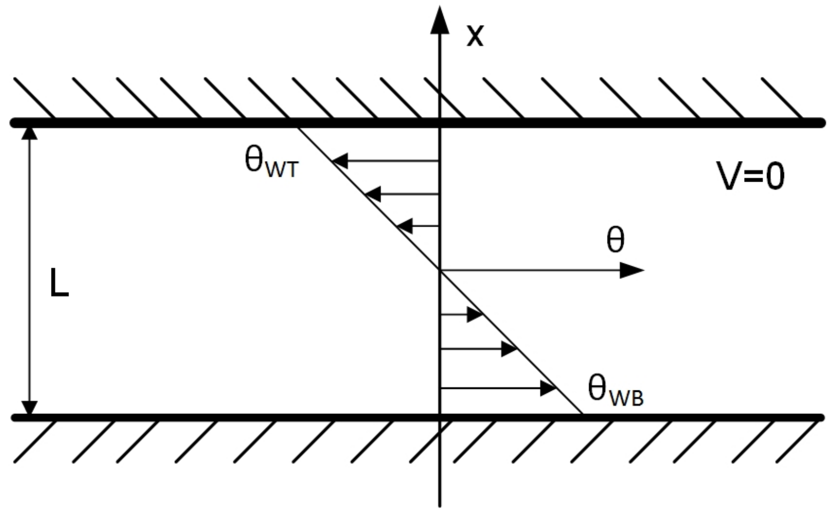

Figure 8.1: General stationary heat conduction schematic. Top and bottom walls are at different temperatures.

bers. To avoid complexity, the over bars and hats are dropped in the following dimensionless set of R19 equations describing the considered problem:

energy and momentum conservations and the balance laws for dynamic temperature $\Delta\theta$, stress tensor σ_{ij},

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

$$\frac{3+\delta+(1+\theta)\frac{d\delta}{d\theta}}{2}\left(1+\rho\right)\frac{\partial\theta}{\partial t}+\frac{\partial q}{\partial x}=0\;; \tag{8.3}$$

$$\begin{aligned}(1+\rho)\frac{\partial\Delta\theta}{\partial t}&+\left(\frac{2}{3+\delta+(1+\theta)\frac{d\delta}{d\theta}}-\frac{10R_{q_{int}}}{3\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\right)\frac{\partial q}{\partial x}\\&-\frac{2\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{3\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q}{\partial x}\\&+\frac{10R_{q_{int}}R_{q_{tr}}\left(2\frac{d\delta}{d\theta}+(1+\theta)\frac{d^2\delta}{d\theta^2}\right)}{3\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\left(q-\Delta q\right)\frac{\partial\theta}{\partial x}=-\frac{(1+\rho)}{\tau_{int}}\Delta\theta\;,\end{aligned} \tag{8.4}$$

$$\begin{aligned}\frac{\partial\sigma_{11}}{\partial t}&+\frac{2}{3}\frac{4R_{q_{int}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\partial q}{\partial x}+\frac{2}{3}\frac{4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q}{\partial x}\\&+\frac{2}{3}\frac{4R_{q_{int}}R_{q_{tr}}\left(2\frac{d\delta}{d\theta}+(1+\theta)\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\left(\Delta q-q\right)\frac{\partial\theta}{\partial x}+\frac{\partial u^{0,0}_{111}}{\partial x}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\sigma_{11}\;,\end{aligned} \tag{8.5}$$

overall heat flux q, heat flux difference Δq,

$$\frac{\partial q}{\partial t}+\left(1+\theta+\Delta\theta-\frac{1}{\rho}\sigma_{11}\right)\frac{\partial\sigma_{11}}{\partial x}+\frac{5+\delta+(1+\theta)\frac{d\delta}{d\theta}}{2}\left[(1+\rho)\left[1+\theta-\Delta\theta\right]+\sigma_{11}\right]\frac{\partial\theta}{\partial x}$$
$$+\frac{168}{(42+25\delta)^2}B_{11}^{+}\frac{d\delta}{d\theta}\frac{\partial\theta}{\partial x}+\frac{4\delta}{(42+25\delta)}\frac{\partial B_{11}^{+}}{\partial x}-\frac{2}{39}\frac{\partial B^{+}}{\partial x}+\frac{5}{13}\frac{\partial B^{-}}{\partial x}$$
$$+\frac{7(3+\delta)(14+3\delta)}{(14+\delta)(42+25\delta)}\frac{\partial B_{11}^{-}}{\partial x}+\left[\sigma_{11}-(1+\rho)\left[1+\theta+\Delta\theta\right]\right]\frac{\partial\Delta\theta}{\partial x}$$
$$-\left[\frac{(1+\theta-\Delta\theta)\,\sigma_{11}}{(1+\rho)}+\Delta\theta^2\right]\frac{\partial\rho}{\partial x}+7\left(\frac{1}{(14+\delta)^2}-\frac{24}{(42+25\delta)^2}\right)B_{11}^{-}\frac{d\delta}{d\theta}\frac{\partial\theta}{\partial x}$$
$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q+\frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q\right)\,, \tag{8.6}$$

$$\frac{\partial\Delta q}{\partial t}+\left[\sigma_{11}-\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)(1+\rho)(1+\theta+\Delta\theta)\right]\frac{\partial\Delta\theta}{\partial x}$$
$$+\left[\frac{(\Delta\theta-1-\theta)}{1+\rho}\sigma_{11}-\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\Delta\theta^2\right]\frac{\partial\rho}{\partial x}$$
$$+\left[1+\theta+\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{R_{q_{tr}}\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}\right)\Delta\theta\right]\frac{\partial\sigma_{11}}{\partial x}-\frac{5}{39}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{+}}{\partial x}$$
$$+\frac{5}{39}\left(1-\frac{10R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{-}}{\partial x}+\frac{\delta}{(42+25\delta)}\left(7+\frac{15R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B_{11}^{+}}{\partial x}$$
$$+\left(\frac{5}{2}\left[1-\frac{R_{q_{int}}}{R_{q_{tr}}}\right]\left[\sigma_{11}+(1+\rho)(1+\theta+\Delta\theta)\right]+\frac{42\left(7+\frac{15R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)}{(42+25\delta)^2}\frac{d\delta}{d\theta}B_{11}^{+}\right)\frac{\partial\theta}{\partial x}$$
$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q+\frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}^2+5R_{q_{int}}^2}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q\right)\,, \tag{8.7}$$

and higher moments B^+ and B^-,

$$
\begin{aligned}
&\frac{\partial B^+}{\partial t} - 2\left(1+\theta\right)\left[\frac{\partial q}{\partial x} - \frac{q}{\left(1+\rho\right)\left(1+\theta-\Delta\theta\right)}\frac{\partial \rho\left(\theta-\Delta\theta\right)}{\partial x}\right] \\
&\qquad = \frac{5R_{q_{int}} + \left(\delta + \left(1+\theta\right)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{20R_{q_{int}} - \left(\delta + \left(1+\theta\right)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\left[-\frac{1}{\tau_{tr}}\left(\frac{9}{2}R_{u^{1,1}} + 15R_{u^{2,0}}\right)\left(1+\rho\right)\Delta\theta^2\right. \\
&\quad - \frac{1}{\tau_{int}}\left(\frac{3}{2}\left(\left(3-\delta\right)R_{u^{1,1}} + 20R_{u^{2,0}} - \left(23-\delta\right)\right)\left(1+\rho\right)\left(1+\theta\right)\Delta\theta\right) - 6\left(1+\theta\right)\frac{\sigma_{11}\sigma_{11}}{\mu} \\
&+ \left(\frac{50R_{q_{int}}R_{q_{tr}}\left(1+\theta\right)\left(2\frac{d\delta}{d\theta} + \left(1+\theta\right)\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta+\left(1+\theta\right)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2} + \frac{\left(5R_{q_{int}} + 3R_{q_{tr}}\right)\left(\delta + \left(1+\theta\right)\frac{d\delta}{d\theta}\right) - 100R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \left(1+\theta\right)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{qq}{\kappa} \\
&\quad - \left.\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\left(\frac{3R_{u^{1,1}} + 10R_{u^{2,0}}}{13}B^+ + \frac{10}{13}\left(R_{u^{1,1}} - R_{u^{2,0}}\right)B^-\right)\right] - \frac{2\left(1+\theta\right)}{1+\theta-\Delta\theta}\left[\frac{qq}{\kappa} + \frac{q\Delta q}{\kappa_\Delta}\right],
\end{aligned}
\tag{8.8}
$$

$$
\begin{aligned}
&\frac{\partial B^-}{\partial t} + 2\left(1+\theta\right)\left[\frac{\partial q}{\partial x} - \frac{q}{\left(1+\rho\right)\left(1+\theta-\Delta\theta\right)}\frac{\partial \rho\left(\theta-\Delta\theta\right)}{\partial x}\right] \\
&\qquad = \frac{5R_{q_{int}} + \left(\delta + \left(1+\theta\right)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{6R_{q_{int}} + \left(\delta + \left(1+\theta\right)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\left[-\frac{1}{\tau_{tr}}\frac{9\left(R_{u^{1,1}} - R_{u^{2,0}}\right)}{2}\left(1+\rho\right)\Delta\theta^2\right. \\
&\quad - \frac{1}{\tau_{int}}\left(\frac{3}{2}\left(3+\delta+\left[3-\delta\right]R_{u^{1,1}} - 6R_{u^{2,0}}\right)\left(1+\rho\right)\left(1+\theta\right)\Delta\theta\right) + \frac{9}{5}\left(1+\theta\right)\frac{\sigma_{11}\sigma_{11}}{\mu} \\
&+ \left(\frac{\left(5R_{q_{int}} + 3R_{q_{tr}}\right)\left(\delta + \left(1+\theta\right)\frac{d\delta}{d\theta}\right) + 30R_{q_{int}}}{5R_{q_{int}} + \left(\delta + \left(1+\theta\right)\frac{d\delta}{d\theta}\right)R_{q_{tr}}} - \frac{2R_{q_{tr}}R_{q_{int}}\left(1+\theta\right)\left(2\frac{d\delta}{d\theta} + \left(1+\theta\right)\frac{d^2\delta}{d\theta^2}\right)}{\left(5R_{q_{int}} + \left(\delta+\left(1+\theta\right)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right)\frac{qq}{\kappa} \\
&\qquad - \left.\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]\left(\frac{10R_{u^{1,1}} + 3R_{u^{2,0}}}{13}B^- + \frac{3\left(R_{u^{1,1}} - R_{u^{2,0}}\right)}{13}B^+\right)\right] \\
&\qquad\qquad + 2\frac{\left(1+\theta\right)}{\left(1+\theta-\Delta\theta\right)}\left[\frac{qq}{\kappa} + \frac{q\Delta q}{\kappa_\Delta}\right],
\end{aligned}
\tag{8.9}
$$

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

$$\begin{aligned}
&\frac{(1+\rho)(1+\theta)}{\frac{(70+23\delta)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{14-\delta}{\delta}}\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]B^+_{11}=\frac{4}{3}\frac{(1+\theta)q}{(1+\theta-\Delta\theta)}\left[\frac{q}{\kappa}+\frac{\Delta q}{\kappa_\Delta}\right]\\
&\quad-\frac{4}{3}(1+\theta)\left[\frac{\partial q}{\partial x}-\frac{q}{(1+\rho)(1+\theta-\Delta\theta)}\frac{\partial\rho(\theta-\Delta\theta)}{\partial x}\right]\\
&\quad-\frac{1}{\left(\frac{(70+23\delta)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{14-\delta}{\delta}\right)}\left(\frac{2(70-19\delta)B^-+(42+25\delta)B^+}{\mu 39\delta}\sigma_{11}\right.\\
&+\frac{(42+25\delta)}{\mu 2\delta}(1+\rho)(1+\theta)\Delta\theta\sigma_{11}-\frac{4\sigma_{11}\sigma_{11}}{(1+\rho)\tau_{tr}}-\frac{4}{3}R_{q_{int}}\frac{qq}{\kappa}\left[\frac{14+\delta+(1+\theta)\frac{d\delta}{d\theta}}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right.\\
&-\left.\frac{10\left(7R_{q_{int}}+2(7+3\delta)R_{q_{tr}}\right)(1+\theta)\frac{d\delta}{d\theta}+14R_{q_{tr}}\left((1+\theta)\frac{d\delta}{d\theta}\right)^2+(70+23\delta)R^2_{q_{tr}}(1+\theta)\frac{d^2\delta}{d\theta^2}}{\delta\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\right]\\
&\quad\left.+\left[\frac{(14-\delta)(1+\theta)\frac{d\delta}{d\theta}-\delta(14+\delta)}{\delta\left(3+\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}+\frac{28}{3}\right]\frac{3\left(3+\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}{2\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\tau_{int}}\Delta\theta\sigma_{11}\right), \quad (8.10)
\end{aligned}$$

$$\begin{aligned}
&\frac{(3+\delta)\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{(14+\delta)\left(3R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{B^-_{11}}{\tau_{tr}}=\frac{4}{3}\frac{(1+\theta)q}{(1+\theta-\Delta\theta)}\left[\frac{q}{\kappa}+\frac{\Delta q}{\kappa_\Delta}\right]\\
&\quad-\frac{4}{3}(1+\theta)\left(\frac{\partial q}{\partial x}-\frac{q}{(1+\rho)(1+\theta-\Delta\theta)}\frac{\partial\rho(\theta-\Delta\theta)}{\partial x}\right)\\
&\quad-\frac{(3+\delta)\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{(14+\delta)\left(3R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{1}{(1+\rho)(1+\theta)\tau_{tr}}\\
&\quad\left[-\frac{3(14+\delta)}{7(3+\delta)}(1+\theta)\sigma_{11}\sigma_{11}-\frac{(14+\delta)}{3(3+\delta)}B^-\sigma_{11}-4(14+\delta)R_{q_{int}}\right.\\
&\frac{5R_{q_{int}}\left[3+\delta+(1+\theta)\frac{d\delta}{d\theta}\right]+R_{q_{tr}}\left[(3+\delta)\delta+(7+2\delta)(1+\theta)\frac{d\delta}{d\theta}+\left(\left(\frac{d\delta}{d\theta}\right)^2+2\frac{d^2\delta}{d\theta^2}\right)(1+\theta)^2\right]}{3(3+\delta)\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)^2}\\
&\quad\left.\frac{2R_{q_{int}}R_{q_{tr}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}qq\right], \quad (8.11)
\end{aligned}$$

$$\frac{u_{111}^{0,0}}{\tau_{tr}} = \frac{9}{5} \frac{(1+\theta)\,\sigma_{11}}{(1+\theta-\Delta\theta)} \left[\frac{q}{\kappa} + \frac{\Delta q}{\kappa_\Delta}\right] + \frac{18 R_{q_{int}}}{5\left(5R_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)} \frac{q\sigma_{11}}{(1+\rho)\,(1+\theta)\,\tau_{tr}} - \frac{9}{5}(1+\theta)\left(\frac{\partial \sigma_{11}}{\partial x} - \frac{\sigma_{11}}{(1+\rho)\,(1+\theta-\Delta\theta)} \frac{\partial \rho\,(\theta-\Delta\theta)}{\partial x}\right) . \tag{8.12}$$

8.1 Refined NSF equations

The corresponding first order equations, refined Navier Stokes Fourier (RNSF), to the stationary heat conduction problem under consideration are,

$$\frac{\partial \rho}{\partial x} + \frac{\partial \theta}{\partial x} = 0 , \tag{8.13a}$$

$$\frac{3+\delta+(1+\theta)\frac{d\delta}{d\theta}}{2}(1+\rho)\frac{\partial \theta}{\partial t} + \frac{\partial q}{\partial x} = 0 , \tag{8.13b}$$

$$q = -\tau_{tr} \frac{5R_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{2R_{q_{int}} R_{q_{tr}}} (1+\rho)\,(1+\theta)\,\frac{\partial \theta}{\partial x} . \tag{8.13c}$$

Where, the stress tensor and dynamic temperature are obtained to be zero at this order, for the problem under consideration.

8.2 Boundary conditions

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

$$\Phi = \left\{\theta, \Delta\theta, q, \Delta q, B^+, B^-, B_{11}^+, B_{11}^-, \rho, \sigma_{11}, u_{111}^{0,0}\right\} \ ,$$

and write the system of equations as

$$B\,(\Phi)\,\frac{\partial \Phi}{\partial y} = P\,(\Phi)\,\Phi . \tag{8.14}$$

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 $A\,(\Phi)$ [47]. This is due to the fact that the left zero eigenvectors associated with the zero eigenvalues in Eq.(8.14) are acting like constraint on the variable vector

Φ and reduces the dimension of the system by the number of zero eigenvalues. Calculation of the eigenvalues shows that the matrix $A(\Phi)$ possesses a zero eigenvalue with multiplicity of 4. Therefore, we need to prescribe a total number of 7 boundary conditions for regularized 19 equations. Using the eigenvectors associated with the zero eigenvalues, we obtain relations for

$$\left\{B^{+}, B^{-}, B_{11}^{+}, B_{11}^{-}\right\} . \tag{8.15}$$

These relations are used to eliminate the depending variables and reduce the system from 11 independent variables to a system of 7 independent variables. Based on this reduced 7 field of variables of Φ, we have the velocity and internal energy parameter function corresponding to the odd fluxes of the variables as,

$$\Psi = \left\{C_1,\, C_1\left(\frac{C^2}{2} + I^{2/\delta}\right),\, C_1\left(\frac{C^2}{2} - \frac{5\,\mathrm{Pr}_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}} I^{2/\delta}\right),\, C_1\left(C_1C_1 - \frac{3}{5}C^2\right)\right\} . \tag{8.16}$$

The microscopic boundary condition along with Ψ function, Eq. 7.2, are used to obtain macroscopic boundary conditions. We obtained from the first term in Ψ,

$$\begin{aligned}\rho_w\sqrt{\theta_w} = -\frac{(14-\delta)(3+\delta)}{2(14+\delta)(42+25\delta)\theta^{\frac{3}{2}}}B_{11}^{-} + \frac{1}{156}\frac{B^{+}-B^{-}}{\theta^{\frac{3}{2}}} - \frac{\delta}{2(42+25\delta)\theta^{\frac{3}{2}}}B_{11}^{+} \\ + \frac{1}{2}\frac{\sigma_{11}}{\sqrt{\theta}} + \frac{1}{2\sqrt{\theta}}\rho(2\theta - \Delta\theta) = \Upsilon .\end{aligned} \tag{8.17}$$

The boundary condition for total heat flux is obtained by second term in Ψ as,

$$\begin{aligned}q = -n_y\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\Bigg[\frac{(56-\delta(1-\zeta))}{312}B^{-} + (3+\delta)\frac{(140+\delta(32+\delta)+(14-\delta)\delta\zeta)}{4(14+\delta)(42+25\delta)}B_{11}^{-} \\ + \frac{[(1-\zeta)\delta - 4]}{312}B^{+} + \frac{\delta(4-\delta(1-\zeta))}{4(42+25\delta)}B_{11}^{+} - \frac{(2+\delta(1-\zeta))}{4}\theta(\rho\Delta\theta - \sigma_{11}) \\ + \frac{\delta(1-\zeta)}{2}\rho\theta^2 + \frac{\Upsilon}{2}\sqrt{\theta}\left[(4+\delta\zeta)(\theta-\theta_w) - (1-\zeta)(\delta\theta + 3\Delta\theta)\right]\Bigg] .\end{aligned} \tag{8.18}$$

From third term in Ψ, boundary condition for heat flux difference is obtained as,

$$\Delta q = n_y \frac{\chi}{(2-\chi)\,\mathrm{Pr}_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{5\,(40-\delta)\,\mathrm{Pr}_{q_{int}} - 12\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{312}B^{-}\right.$$
$$+\frac{5\,(12+\delta)\,\mathrm{Pr}_{q_{int}} + 12\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{312}B^{+} + \frac{10\delta\,\mathrm{Pr}_{q_{int}} - 8\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4}\rho\theta^{2}$$
$$+\left[3+\delta\right]\frac{5\delta\,(42+\delta)\,\mathrm{Pr}_{q_{int}} - 6\,(14-\delta)\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4\,(14+\delta)\,(42+25\delta)}B_{11}^{-}$$
$$+\frac{5\delta\,\mathrm{Pr}_{q_{int}} - 6\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4}\theta\sigma_{yy} + \frac{5\,(6-\delta)\,\mathrm{Pr}_{q_{int}} + 12\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4}\rho\theta\Delta\theta$$
$$-\delta\frac{5\,(6+\delta)\,\mathrm{Pr}_{q_{int}} + 6\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4\,(42+25\delta)}B_{11}^{+} + \frac{\Upsilon}{2}\sqrt{\theta}\left[\left(\delta+\theta\frac{d\delta}{d\theta}\right)\underset{q_{tr}}{\mathrm{Pr}}\,V_s^2 - 15\underset{q_{int}}{\mathrm{Pr}}\,(1-\zeta)\,\Delta\theta\right.$$
$$\left.\left.-\left(5\delta\underset{q_{int}}{\mathrm{Pr}} - 4\left(\delta+\theta\frac{d\delta}{d\theta}\right)\underset{q_{tr}}{\mathrm{Pr}}\right)\theta + \left(5\delta\zeta\underset{q_{int}}{\mathrm{Pr}} - 4\left(\delta+\theta\frac{d\delta}{d\theta}\right)\underset{q_{tr}}{\mathrm{Pr}}\right)(\theta-\theta_W)\right]\right]\ , \quad (8.19)$$

Finally, last term in Ψ give us boundary condition for $u_{yyy}^{0,0}$ as,

$$u_{111}^{0,0} = n_y \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{(-14+\delta)\,(3+\delta)}{(14+\delta)\,(42+25\delta)}B_{11}^{-} - \frac{\delta B_{11}^{+}}{42+25\delta} - \frac{2\,(B^{+}-B^{-})}{195}\right.$$
$$\left.-\frac{7\sigma_{11}+2\rho\Delta\theta}{5}\theta + \Upsilon\frac{2}{5}\sqrt{\theta}\left[\theta-\theta_W\right]\right]\ . \quad (8.20)$$

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

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} \rho dx = \rho_0 L\ . \quad (8.21)$$

If the gas was not stationary and velocity component towards the wall was non-zero, the balance of mass would replace this condition.

Also, the boundary condition for the RNSF equations along with the prescribe mass condition is the temperature jump condition obtained from Eq. 8.18 at order ε^1as,

$$\theta - \theta_w = n_y \tau_{tr}\frac{(2-\chi)}{\chi}\sqrt{\frac{\pi\theta}{2}}\frac{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{(4+\delta\zeta)\,R_{q_{int}}R_{q_{tr}}}\frac{\partial\theta}{\partial x}\ . \quad (8.22)$$

8.3 Numerical scheme

The finite difference method is used to discretize our system of equations

$$A\left(\Phi^{n}\right)\frac{\partial\Phi}{\partial t}+B\left(\Phi^{n}\right)\frac{\partial\Phi^{n}}{\partial y}=P\left(\Phi^{n}\right)\Phi^{n}\ . \tag{8.23}$$

with second order accuracy in spatial discretization as,

$$\frac{\partial\Phi}{\partial y}=\frac{\Phi_{i+1}-\Phi_{i-1}}{2\Delta x}\ , \tag{8.24}$$

and first order discretization in time as,

$$\frac{\partial\Phi}{\partial t}=\frac{\Phi_{i}^{n+1}-\Phi_{i}^{n}}{\Delta t}\ . \tag{8.25}$$

Where, superscript $n+1$ denotes next time step values while variables with superscript n are at current time step. Spatial nodes are shown by subscript i with $0\leq i\leq m$, where m is number of grid nodes.

The above set of equations along with the boundary conditions are solved at each time step to obtain the next time step values, starting from the initial conditions. This procedure continuous until we reach steady state and the steady state condition is satisfied,

$$\frac{\left|\theta_{m/2}^{n+1}-\theta_{m/2}^{n}\right|}{\left|\theta_{m/2}^{n}\right|}\leq 10^{-6}\ . \tag{8.26}$$

The initial conditions are the reference equilibrium state $\{\rho_0,\theta_0\}$ with all non-equilibrium values are equal to zero. The dimensionless boundary conditions are as follows:

boundary condition for total heat flux,

$$\begin{aligned}q=-n_{y}\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\left(1+\theta\right)}}&\left[\frac{\left(56-\delta\left(1-\zeta\right)\right)}{312}B^{-}+\left(3+\delta\right)\frac{\left(140+\delta\left(32+\delta\right)+\left(14-\delta\right)\delta\zeta\right)}{4\left(14+\delta\right)\left(42+25\delta\right)}B_{11}^{-}\right.\\&+\frac{\left[\left(1-\zeta\right)\delta-4\right]}{312}B^{+}+\frac{\delta\left(4-\delta\left(1-\zeta\right)\right)}{4\left(42+25\delta\right)}B_{11}^{+}-\frac{\left(2+\delta\left(1-\zeta\right)\right)}{4}\left(1+\theta\right)\left(\left(1+\rho\right)\Delta\theta-\sigma_{11}\right)\\&\left.+\frac{\delta\left(1-\zeta\right)}{2}\left(1+\rho\right)\left(1+\theta\right)^{2}+\frac{\Upsilon}{2}\sqrt{\left(1+\theta\right)}\left[\left(4+\delta\zeta\right)\left(\theta-\theta_{w}\right)-\left(1-\zeta\right)\left(\delta\left(1+\theta\right)+3\Delta\theta\right)\right]\right]\ ,\end{aligned} \tag{8.27}$$

for heat flux difference,

$$\begin{aligned}
\Delta q = n_y \frac{\chi}{(2-\chi)\,\mathrm{Pr}_{q_{tr}}\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}\sqrt{\frac{2}{\pi(1+\theta)}}
&\left[\frac{5(40-\delta)\,\mathrm{Pr}_{q_{int}} - 12\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{312}B^-\right.\\
&+\frac{5(12+\delta)\,\mathrm{Pr}_{q_{int}} + 12\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{312}B^+\\
&-\delta\frac{5(6+\delta)\,\mathrm{Pr}_{q_{int}} + 6\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4(42+25\delta)}B^+_{11}\\
&+[3+\delta]\frac{5\delta(42+\delta)\,\mathrm{Pr}_{q_{int}} - 6(14-\delta)\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4(14+\delta)(42+25\delta)}B^-_{11}\\
&+\frac{5(6-\delta)\,\mathrm{Pr}_{q_{int}} + 12\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4}(1+\rho)(1+\theta)\Delta\theta\\
&+\frac{10\delta\,\mathrm{Pr}_{q_{int}} - 8\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4}(1+\rho)(1+\theta)^2\\
&+\frac{5\delta\,\mathrm{Pr}_{q_{int}} - 6\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4}(1+\theta)\sigma_{yy} + \frac{\Upsilon}{2}\sqrt{(1+\theta)}\\
&\left[-15\underset{q_{int}}{\mathrm{Pr}}(1-\zeta)\Delta\theta - \left(5\delta\underset{q_{int}}{\mathrm{Pr}} - 4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\underset{q_{tr}}{\mathrm{Pr}}\right)(1+\theta)\right.\\
&\left.\left.+\left(5\delta\zeta\underset{q_{int}}{\mathrm{Pr}} - 4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\underset{q_{tr}}{\mathrm{Pr}}\right)(\theta-\theta_W)\right]\right] \ , \qquad (8.28)
\end{aligned}$$

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

$$\begin{aligned}
u^{0,0}_{111} = n_y \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi(1+\theta)}}&\left[\frac{(-14+\delta)(3+\delta)}{(14+\delta)(42+25\delta)}B^-_{11} - \frac{\delta B^+_{11}}{42+25\delta} - \frac{2(B^+-B^-)}{195}\right.\\
&\left.-\frac{7\sigma_{11}+2(1+\rho)\Delta\theta}{5}(1+\theta) + \Upsilon\frac{2}{5}\sqrt{(1+\theta)}\,[\theta-\theta_W]\right] \ . \qquad (8.29)
\end{aligned}$$

The prescribed mass condition along with Eq. 8.2,

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} \rho dx = 0 \ , \qquad (8.30)$$

is solved by trapezoidal rule to obtain the density. Here we are interested in only stationary heat conduction, therefore all the velocities are set to zero. And the prescribed mass condition along with conservation of momentum is solved to gain distribution of mass at each time step. 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 wall would replace the prescribed mass condition.

For RNSF's temperature jump boundary condition, Eq. 8.22, the second order backward and forward finite difference discretization are used, e.g. for lower wall we have

$$\theta_i^{n+1} - \theta_w = \tau_{tr} \frac{(2-\chi)}{\chi} \sqrt{\frac{\pi\left(1+\theta_i^n\right)}{2}} \frac{5R_{q_{int}} + \left(\delta_i^n + 1 + \theta_i^n \frac{d\delta_i^n}{d\theta_i^n}\right) R_{q_{tr}}}{\left(4 + \delta_i^n \zeta\right) R_{q_{int}} R_{q_{tr}}} \frac{-\theta_{i+2}^n + 4\theta_{i+1}^n - 3\theta_i^{n+1}}{2\Delta x} \ . \tag{8.31}$$

8.4 Linear and steady Case

In this section, we study the steady linearized set of equations with small disturbances from an equilibrium ground state $\{\rho_0, v_i^0 = 0, \theta_0\}$. First, we write all variables in terms of their ground state values plus a small deviation, denoted by a hat, as

$$\begin{gathered}\rho = \rho_0 + \hat{\rho},\ \theta = \theta_0 + \hat{\theta},\ v_i = \hat{v}_i,\ \Delta\theta = \Delta\hat{\theta},\ \sigma_{ij} = \hat{\sigma}_{ij},\ q_i = \hat{q}_i, \\ \Delta q_i = \Delta\hat{q}_i,\ B_{ij}^{+} = \hat{B}_{ij}^{+},\ B^{-} = \hat{B}^{-},\ B_{ij}^{-} = \hat{B}_{ij}^{-},\ B^{-} = \hat{B}^{-},\ u_{ijk}^{0,0} = \hat{u}_{ijk}^{0,0} \ . \end{gathered} \tag{8.32}$$

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

the conservation laws,

$$\frac{\partial q}{\partial x} = 0 \ , \tag{8.33}$$

$$\frac{\partial \rho}{\partial x} + \frac{\partial\left(\theta - \Delta\theta\right)}{\partial x} + \frac{\partial \sigma_{11}}{\partial x} = 0 \ , \tag{8.34}$$

balance laws for dynamic temperature and stress tensor,

$$\left(\frac{2}{3 + \delta + (1+\theta)\frac{d\delta}{d\theta}} - \frac{10R_{q_{int}}}{3\left(5R_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\right)\frac{\partial q}{\partial x} - \frac{2\left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{3\left(5R_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial \Delta q}{\partial x} = -\frac{\Delta\theta}{\tau_{int}} \ , \tag{8.35}$$

$$\frac{2}{3}\frac{4R_{q_{int}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\partial q}{\partial x}+\frac{\partial u_{111}^{0,0}}{\partial x}$$
$$+\frac{2}{3}\frac{4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q}{\partial x}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\sigma_{11}\ , \quad (8.36)$$

balance laws for heat fluxes,

$$\frac{\partial\sigma_{11}}{\partial x}+\frac{5+\delta+(1+\theta)\frac{d\delta}{d\theta}}{2}\frac{\partial\theta}{\partial x}-\frac{\partial\Delta\theta}{\partial x}-\frac{2}{39}\frac{\partial B^{+}}{\partial x}$$
$$+\frac{4\delta}{(42+25\delta)}\frac{\partial B_{11}^{+}}{\partial x}+\frac{7(3+\delta)(14+3\delta)}{(14+\delta)(42+25\delta)}\frac{\partial B_{11}^{-}}{\partial x}+\frac{5}{13}\frac{\partial B^{-}}{\partial x}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]$$
$$\left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q+\frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q\right)\ , \quad (8.37)$$

$$\frac{5}{2}\left[1-\frac{R_{q_{int}}}{R_{q_{tr}}}\right]\frac{\partial\theta}{\partial x}-\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial\Delta\theta}{\partial x}$$
$$-\frac{5}{39}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{+}}{\partial x}+\frac{5}{39}\left(1-\frac{10R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{-}}{\partial x}$$
$$+\frac{\delta}{(42+25\delta)}\left(7+\frac{15R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B_{11}^{+}}{\partial x}+\frac{\partial\sigma_{11}}{\partial x}$$
$$=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q+\frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}^{2}+5R_{q_{int}}^{2}}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q\right)\ , \quad (8.38)$$

balance laws for B^{+} and B^{-},

$$-2\frac{\partial q}{\partial x}=\frac{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{20R_{q_{int}}-\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\left[-\frac{1}{\tau_{int}}\frac{3}{2}\left((3-\delta)R_{u^{1,1}}+20R_{u^{2,0}}-(23-\delta)\right)\Delta\theta\right.$$
$$\left.-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{3R_{u^{1,1}}+10R_{u^{2,0}}}{13}B^{+}+\frac{10}{13}\left(R_{u^{1,1}}-R_{u^{2,0}}\right)B^{-}\right)\right]\ , \quad (8.39)$$

$$2\frac{\partial q}{\partial x}=\frac{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{6R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\left[-\frac{1}{\tau_{int}}\frac{3}{2}\left(3+\delta+[3-\delta]R_{u^{1,1}}-6R_{u^{2,0}}\right)\Delta\theta\right.$$
$$\left.-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\left(\frac{10R_{u^{1,1}}+3R_{u^{2,0}}}{13}B^{-}+\frac{3\left(R_{u^{1,1}}-R_{u^{2,0}}\right)}{13}B^{+}\right)\right]\;,\quad(8.40)$$

and constitutive equations,

$$\frac{u_{111}^{0,0}}{\tau_{tr}}=-\frac{9}{5}\frac{\partial\sigma_{11}}{\partial x}\;,\tag{8.41}$$

$$\frac{1+\frac{2\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mu}{3\left(3+\delta+(1+\theta)\frac{d\delta}{d\theta}\right)v}}{\frac{(70+23\delta)R_{q_{int}}}{\delta\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}-\frac{14-\delta}{\delta}}\frac{B_{11}^{+}}{\mu}=-\frac{4}{3}\frac{\partial q}{\partial x}=0\;\Rightarrow B_{11}^{+}=0\;,\tag{8.42}$$

$$\frac{(3+\delta)\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{(14+\delta)\left(3R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{B_{11}^{-}}{\mu}=-\frac{4}{3}\frac{\partial q}{\partial x}=0\;\Rightarrow B_{11}^{-}=0.\tag{8.43}$$

8.4.1 Linear solution

The above set of equations are reduced to 5 coupled equations for $\Phi=\{\Delta q,\ q,\ u_{111}^{0,0},\ \sigma_{11},\ \Delta\theta\}$ and the rest of the variables $\{\rho,\ \theta,\ B^{+},\ B^{-}\}$ are functions of them. The solution of set of coupled equations, $A_{5\times5}\frac{\partial\Phi}{\partial x}=B_{5\times5}\Phi$,is obtained using the eigenvalue method as

$$\Phi(x)=\sum_{n=1}^{5}C_n\vartheta_n e^{\lambda_n x}\;,\tag{8.44}$$

where, λ and ϑ are eigenvalues and eigenvectors of the coefficient matrix, $A^{-1}B$. Substituting new normalized coefficients,

$$\begin{aligned}C_2'&=(C_2+C_3)\sinh(\lambda_3/2)\;,\\C_3'&=(C_3-C_2)\cosh(\lambda_3/2)\;,\\C_4'&=(C_4+C_5)\sinh(\lambda_5/2)\;,\\C_5'&=-(C_4-C_5)\cosh(\lambda_5/2)\;,\end{aligned}$$

into the above set of equations, results in the final form of the solution obtained as,

$$\Delta q(x)=C_1\vartheta_{1,1}+C_3'\vartheta_{1,3}\frac{\cosh(\lambda_3 x)}{\cosh(\lambda_3/2)}+C_2'\vartheta_{1,3}\frac{\sinh(\lambda_3 x)}{\sinh(\lambda_3/2)}$$
$$+C_5'\vartheta_{1,5}\frac{\cosh(\lambda_5 x)}{\cosh(\lambda_5/2)}+C_4'\vartheta_{1,5}\frac{\sinh(\lambda_5 x)}{\sinh(\lambda_5/2)}\;,\quad(8.45a)$$

$$u_{111}^{0,0}(x) = C_3'\vartheta_{2,3}\frac{\cosh(\lambda_3 x)}{\cosh(\lambda_3/2)} + C_2'\vartheta_{2,3}\frac{\sinh(\lambda_3 x)}{\sinh(\lambda_3/2)} + C_5'\vartheta_{2,5}\frac{\cosh(\lambda_5 x)}{\cosh(\lambda_5/2)} + C_4'\vartheta_{2,5}\frac{\sinh(\lambda_5 x)}{\sinh(\lambda_5/2)} \ , \tag{8.45b}$$

$$\sigma_{11}(x) = C_2'\vartheta_{3,3}\frac{\cosh(\lambda_3 x)}{\sinh(\lambda_3/2)} + C_3'\vartheta_{3,3}\frac{\sinh(\lambda_3 x)}{\cosh(\lambda_3/2)} + C_4'\vartheta_{3,5}\frac{\cosh(\lambda_5 x)}{\sinh(\lambda_5/2)} + C_5'\vartheta_{3,5}\frac{\sinh(\lambda_5 x)}{\cosh(\lambda_5/2)} \ , \tag{8.45c}$$

$$\Delta\theta(x) = C_2'\vartheta_{4,3}\frac{\cosh(\lambda_3 x)}{\sinh(\lambda_3/2)} + C_3'\vartheta_{4,3}\frac{\sinh(\lambda_3 x)}{\cosh(\lambda_3/2)} + C_4'\vartheta_{4,5}\frac{\cosh(\lambda_5 x)}{\sinh(\lambda_5/2)} + C_5'\vartheta_{4,5}\frac{\sinh(\lambda_5 x)}{\cosh(\lambda_5/2)} \ , \tag{8.45d}$$

$$q = \mathbf{C}_1 \ . \tag{8.45e}$$

The solution for the remaining variables are

$$B^+ = -\frac{1}{\tau_{int}\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]}\frac{13\left(3+\delta+[3-\delta]R_{u^{1,1}} - 6R_{u^{2,0}}\right)}{2\left(R_{u^{1,1}} - R_{u^{2,0}}\right)}\Delta\theta \ , \tag{8.46}$$

$$B^- = -\frac{1}{\tau_{int}\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]}\frac{169\left([3-\delta+[3+\delta]R_{u^{1,1}}]R_{u^{2,0}} - 6R_{u^{1,1}}\right)}{20\left(R_{u^{1,1}} - R_{u^{2,0}}\right)^2}\Delta\theta \ , \tag{8.47}$$

$$\begin{aligned}\frac{5+\delta+\theta\frac{d\delta}{d\theta}}{2}\theta = \Delta\theta + \frac{2}{39}B^+ - \frac{5}{13}B^- + \frac{5}{9}\frac{u_{111}^{0,0}}{\tau_{tr}}x - \left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right] \\ \left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+\theta\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q + \frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}} + \left(\delta+\theta\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q\right)x + C_6 \ ,\end{aligned} \tag{8.48}$$

and,

$$\rho = -(\theta - \Delta\theta) - \sigma_{11} + C_7 \ . \tag{8.49}$$

8.4.2 Linear boundary conditions

The boundary conditions for the dimensionless linear case become,

boundary condition for total heat fluxes,

$$\begin{aligned}q_y = -\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi}}\left[\frac{7}{39}B^- - \frac{1}{78}B^+ - \frac{1}{2}(\Delta\theta - \sigma_{yy})\right. \\ \left. + \frac{1}{2}\left[(4+\delta\zeta)(\theta-\theta_w) - (1-\zeta)3\Delta\theta\right]\right] \ ,\end{aligned} \tag{8.50}$$

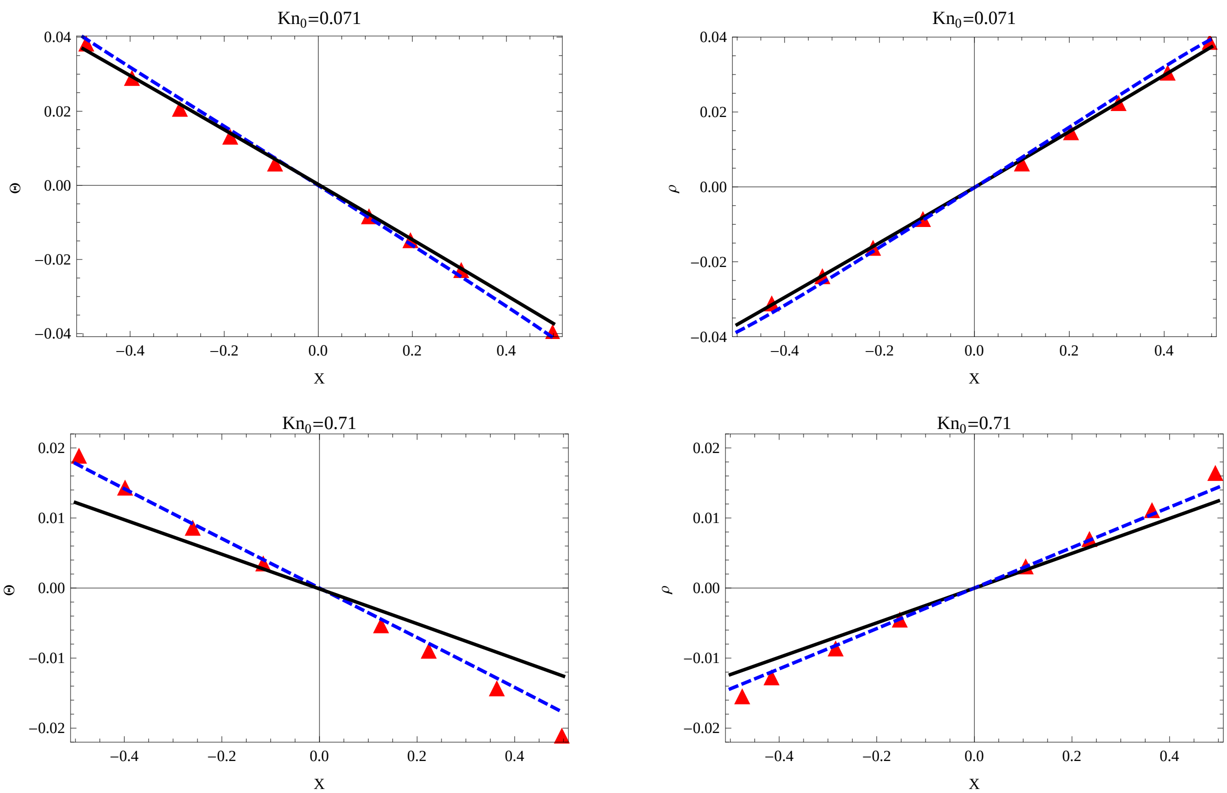

Figure 8.2: Comparison of temperature and density profiles for Kn numbers equal to 0.071 and 0.71. Results shown are obtained from: set of R19 equations, blue dashed; set of RNSF equations, black line; DSMC method, red triangles.

for heat fluxes difference,

$$\Delta q_y = \frac{\chi}{(2-\chi)\,\mathrm{Pr}_{q_{tr}}\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}\sqrt{\frac{2}{\pi}}\left[\frac{25\,\mathrm{Pr}_{q_{int}} - 2\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{39}B^- \right.$$
$$+\frac{15\,\mathrm{Pr}_{q_{int}} + 4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{78}B^+$$
$$-\frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{2}\sigma_{yy}+\frac{15\,\mathrm{Pr}_{q_{int}} + 4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{2}\Delta\theta$$
$$\left.-\frac{1}{2}\left[15\underset{q_{int}}{\mathrm{Pr}}(1-\zeta)\,\Delta\theta-\left(5\delta\zeta\underset{q_{int}}{\mathrm{Pr}}-4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\underset{q_{tr}}{\mathrm{Pr}}\right)(\theta-\theta_W)\right]\right]\ , \tag{8.51}$$

for $u^{0,0}_{yyy}$,

$$u^{0,0}_{111} = \frac{\chi}{5\,(2-\chi)}\sqrt{\frac{2}{\pi}}\left[\frac{2\,(B^- - B^+)}{39} + 2\left([\theta-\theta_W]-\Delta\theta\right) - 7\sigma_{11}\right]\ , \tag{8.52}$$

and the last one is prescribed mass condition,

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} \rho dx = 0\ . \tag{8.53}$$

8.5 Results

We first compare the results of our proposed models with the Direct Simulation Monte Carlo method results [91]. Comparison between numerical solution of the R19, the RNSF equations and DSMC results are shown in Fig. 8.2. Dimensionless wall temperatures are at ± 0.0476 and reference temperature at 350 K. DSMC data is obtained by considering equivalent translational and rotational relaxation rates, therefore we have equivalent internal and translational Kn numbers. We investigate two different reference Kn numbers, 0.071 and 0.71, which represents slip and transition flow regimes, respectively. We use the values for Maxwell molecules of relaxation parameters for pure translational moments, $R_{u^{2,0}}$ and $R_{q_{tr}}$, from Table 2.1. Prandtl number is set to 0.73 and based on Eq. 5.64, $R_{q_{int}}$ is calculated. We extend this relation between $R_{q_{tr}}$ and $R_{q_{int}}$ to $R_{u^{2,0}}$ and $R_{u^{1,1}}$, and obtained $R_{u^{1,1}}$ value. These procedures for calculating relaxation parameters are used from now on, unless otherwise stated. Also, excited internal degrees of freedom is set to 2. It is evident from Fig. 8.2 that there is a good agreement between the DSMC and the R19 results. However in transition

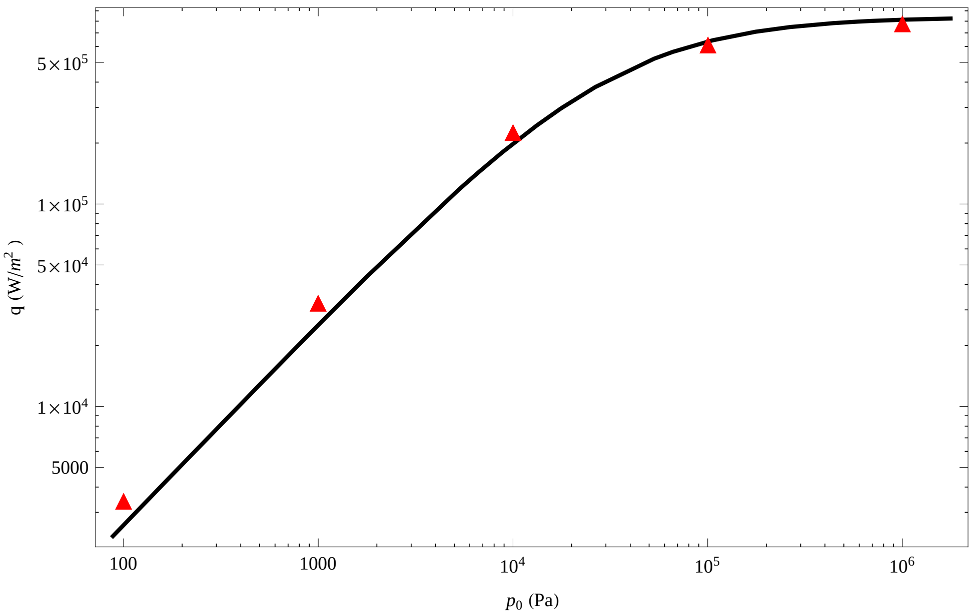

Figure 8.3: Comparison of total heat flux as a function of reference pressure, ranging from continuum to free molecular regime. Results shown are obtained from: set of R19 equations, black line; DSMC method, red triangles.

regime, there is a considerable deviation of Refined Navier–Stokes–Fourier equations results from DSMC results and first order set of equations fails to accurately model the problem.

We compare obtained total heat flux values from R19 equations with DSMC data [92] at various reference pressure, ranging from Continuum to free molecular regime in Fig 8.3. The simulation case is a channel with $1\mu m$ width and wall temperatures at 285 and 315 K. The Prandtl number is set to 0.71, and relaxation parameters are obtained based on Eq. 5.64 and fitting to DSMC data. The reference temperature and reference shear viscosity is 300 K and 1.775 $Pa.s$, respectively. The gas under consideration is N_2 with $\delta+\theta\frac{d\delta}{d\theta}$ equal to 2.015. Also, full accommodation coefficients are considered. Reference pressure of $10^6, 10^4$ *and* 100 Pa are corresponding to reference Kn_{tr} equal to 0.005, 0.5 and 50. As it is depicted in Fig. 8.3, there is good agreement between our data and DSMC data up to Knudsen number 0.5. Results start to deviate at the end of the transition regime and beginning of the free molecular regime. 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.

The developing profiles from equilibrium ground state initial condition $\{\rho_0, \theta_0\}$ to steady state condition are presented for H_2 in Fig. 8.4. Prandtl number is set to 0.69, reference temperature is at 300 K and dimensionless wall temperatures are ± 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 Eq. 5.84 we have

$$\begin{cases} Kn_{tr} = 0.0091 \\ Kn_{int} = 1 \end{cases} . \tag{8.54}$$

The results presented in Fig. 8.4 are obtained from numerical solution of R19 set of equations with the initial conditions of the reference equilibrium state $\{\rho_0, \theta_0\}$ and all non-equilibrium values are equal to zero. It is depicted that total temperature and density is rising from zero starting from regions near walls and gradually in time moving towards central region. Other variables, which all are non-equilibrium ones, starts from zero at initial state and jump to their maximum value immediately and then start to decay over time to reach their steady state profiles. The speed of these decays is not constant and their values keep reducing in time. The values of nonequilibrium variables at the beginning of the process are order of magnitude higher than their values in steady state.

Now, we analyze N_2 gas. The reference time scale is chosen so that based on Eq. 5.84, we have

$$\begin{cases} Kn_{tr} = 0.062 \\ Kn_{int} = 0.2 \end{cases} . \tag{8.55}$$

This implies the need of a set of equations with both high order accuracy in Kn_{tr} and Kn_{int}, that is the set of R19 equations. The reference temperature is at 400 K and dimensionless temperature at walls are ± 0.3. Shear viscosity temperature exponent is set to 0.74 and Prandtl number is 0.69. Figure 8.5 illustrates the steady state profiles obtained numerically from full set of R19 and RNSF equations, and analytically from linear R19 equations. Results from RNSF equations are not in agreement with the R19 profiles and they are not a good set of equations to be used under these conditions with mentioned Kn numbers. Also, it is evident that the non-linear and temperature dependent properties effects are more dominant in profiles associated with internal variables ($\Delta\theta$ and Δq) and differ the analytical from numerical results.

The effects of different range of temperatures are studied on N_2 gas in Fig. 8.6. We investigate two cases with upper dimensionless wall temperature at 0.5 and 2.5. The lower wall temperature and reference temperature are kept fixed at 300 K and

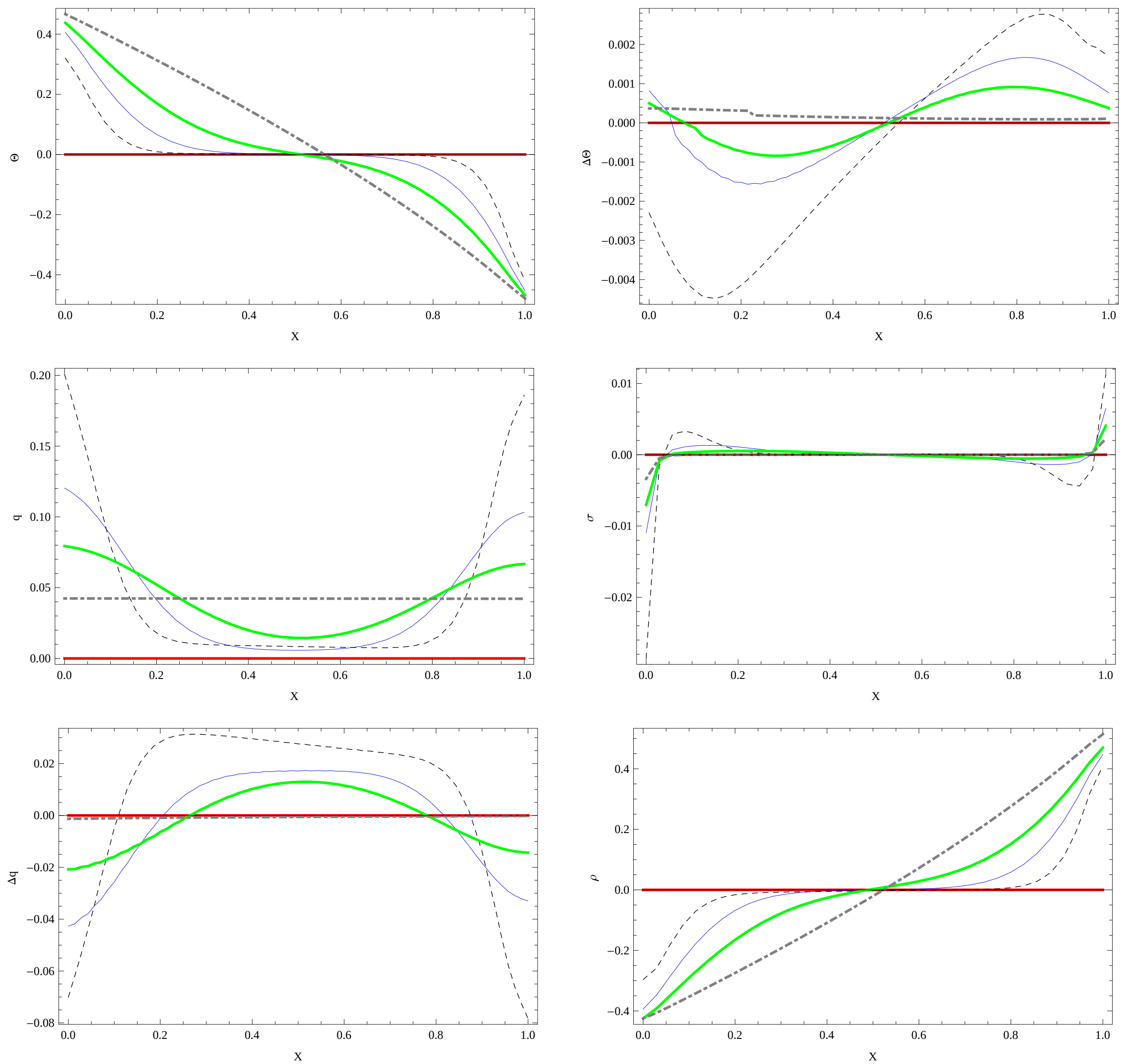

Figure 8.4: Numerical results of stationary heat conduction from set of R19 equations. Red line is at t=0 s; black-dashed is at t=0.2 s; blue-thin line is at t=0.6 s; green-thick is at t=1.5 s; gray-dotdashed is at t=29 s.

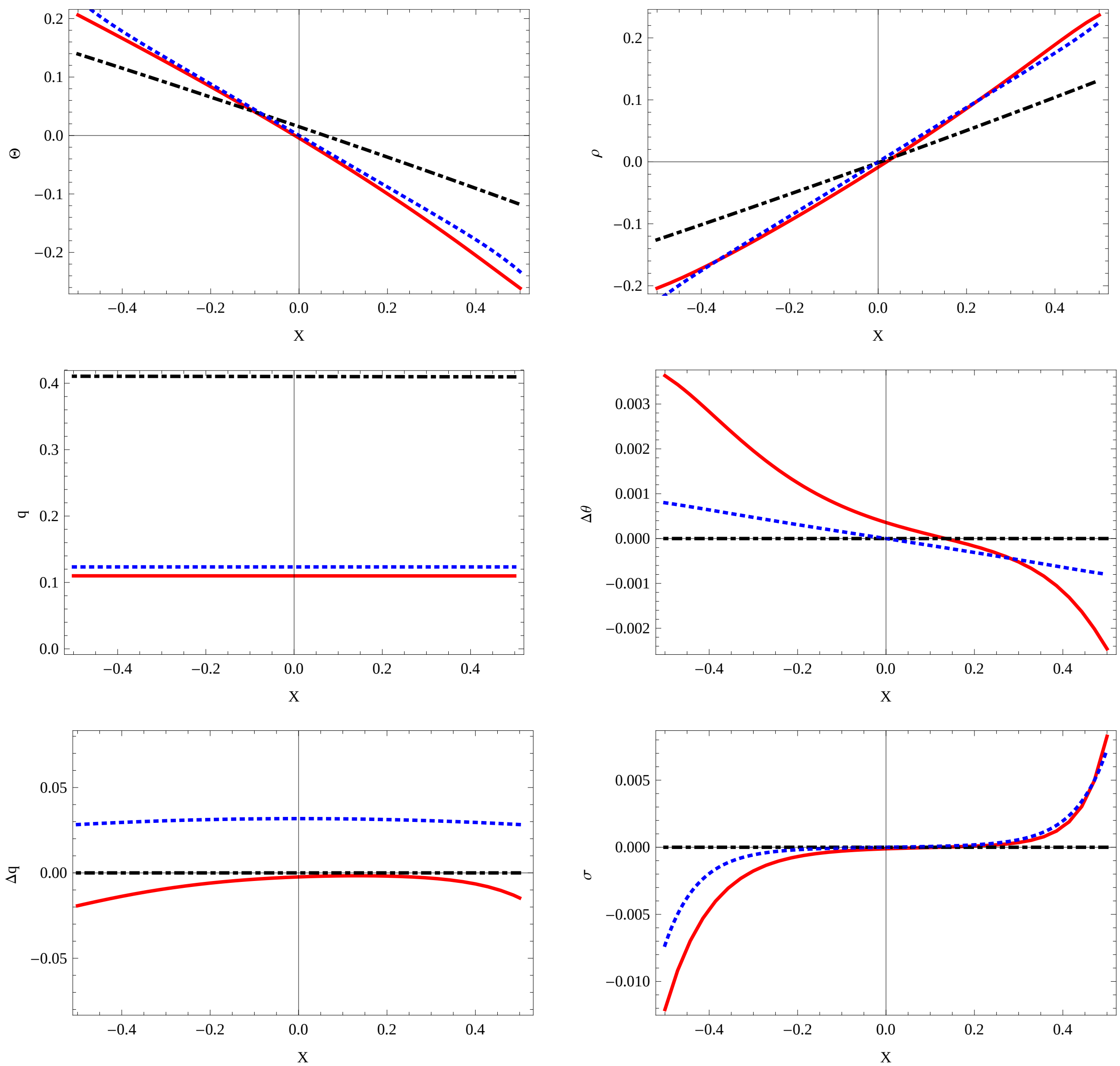

Figure 8.5: Steady state profiles of N_2 gas obtained from numerical and analytical methods. Red line: R19-numerical; black-dotdashed: RNSF-numerical; blue-dotted: R19-analytical.

referenced Kn numbers are fixed at $Kn_{tr} = 0.077$ and $Kn_{int} = 0.2$ for two cases under study. As it can be seen, the main effect here is promoting 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 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 Fig. 8.7. Reference and wall's 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 Eq. 5.84 to be

$$Kn_{int} = \begin{cases} N_2: & 0.158 \\ H_2: & 3.78 \\ CH_4: & 10 \end{cases} . \tag{8.56}$$

Number of excited internal degrees of freedom at reference temperature of these gases are

$$\delta + \theta \frac{d\delta}{d\theta} = \begin{cases} N_2: & 2.41 \\ H_2: & 2.09 \\ CH_4: & 8.89 \end{cases} . \tag{8.57}$$

H_2 and CH_4 gases both have large differences between internal and translational relaxation times. However, internal and translational relaxation times of N_2 gas have comparable values. On the other hand, H_2 and N_2 gases both have similar excited internal degrees of freedom. Nonetheless, excited internal DoF of CH_4 gas is higher than the other two gases. The effects of having internal and translational relaxation times at the same order are seen in profiles of moments corresponding to deviations from total values, $\Delta\theta$ and Δq, which are derived by translational-internal interactions. These effects are towards promoting the temperature dependency of the profiles, which now covers a larger range of values between two walls. The effects of different internal DoF is most seen in total heat flux and stress tensor. CH_4 gas with higher DoF gains higher total heat flux and lower stress tensor in comparison with other two gases. Effects of the reference temperature on variables is studied in Fig. 8.8. 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,

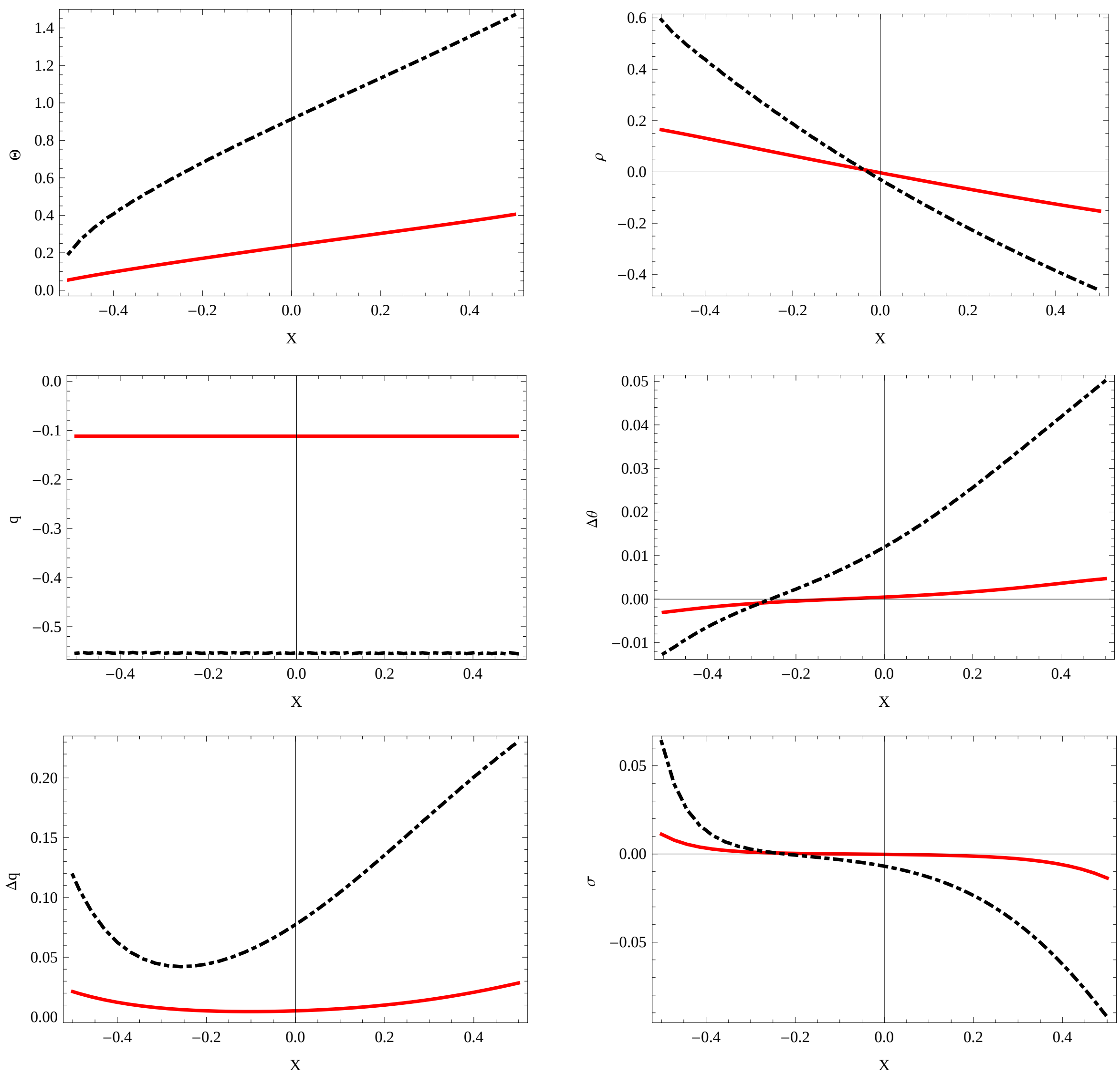

Figure 8.6: Steady state profiles of N_2 gas obtained from numerical method with $\theta_{WB} = 0$ and Red line: $\theta_{WT} = 0.5$; black-dotdashed: $\theta_{WT} = 2.5$.

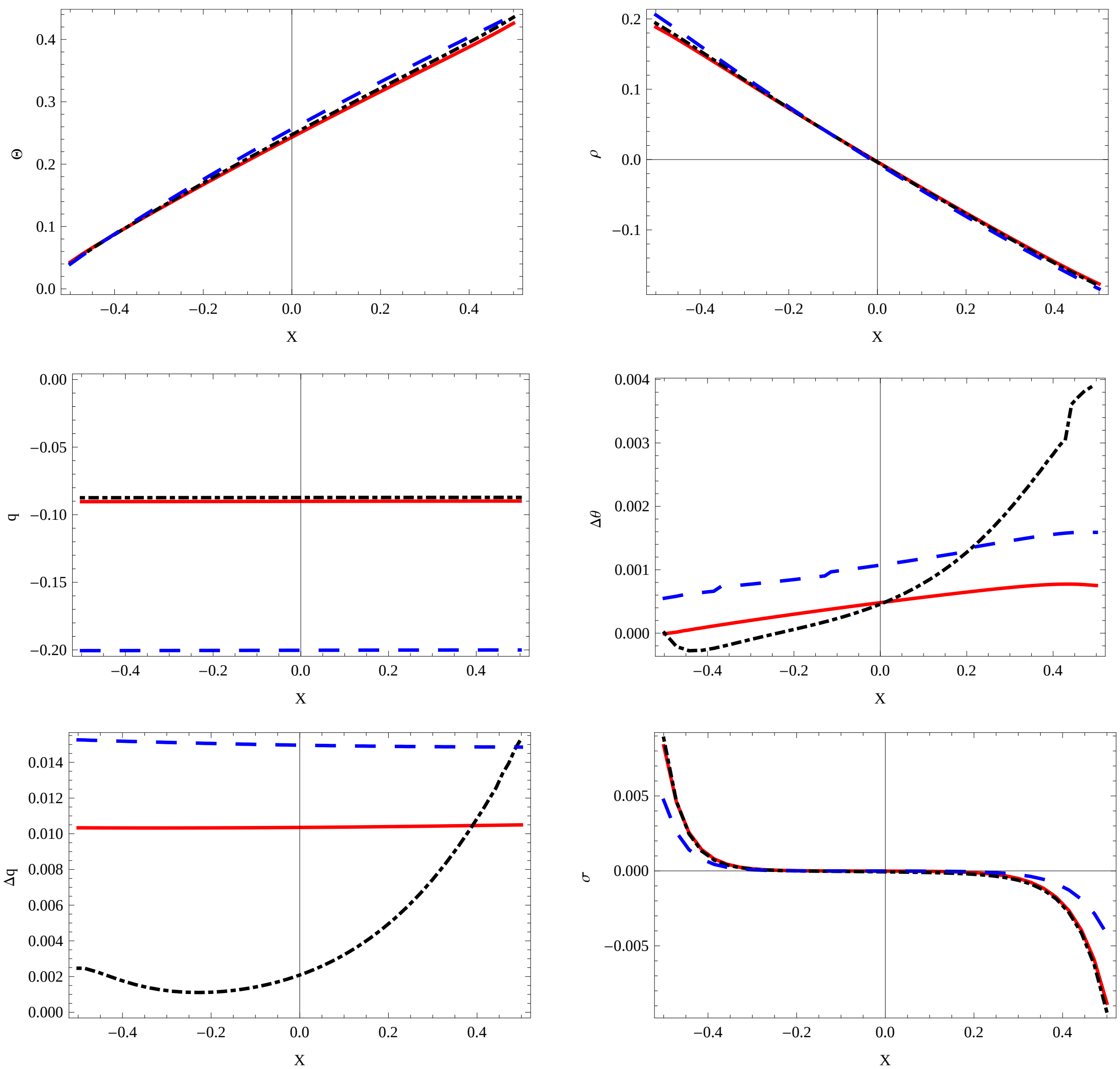

Figure 8.7: Steady state profiles of different gases obtained from numerical solution of the R19 equations. Red line: H_2; black-dotdashed: N_2; blue-dashed: CH_4.

respectively. As it is depicted in Fig. 8.8, the case with higher reference temperature, which means more excited internal degrees of freedom, have higher heat flux value and more flatter deviation moments, $\Delta\theta$ and Δq, profiles in comparison with lower reference temperature. Also there is slightly higher temperature jump, especially on bottom wall , in case of higher reference temperature in comparison with the lower one case.

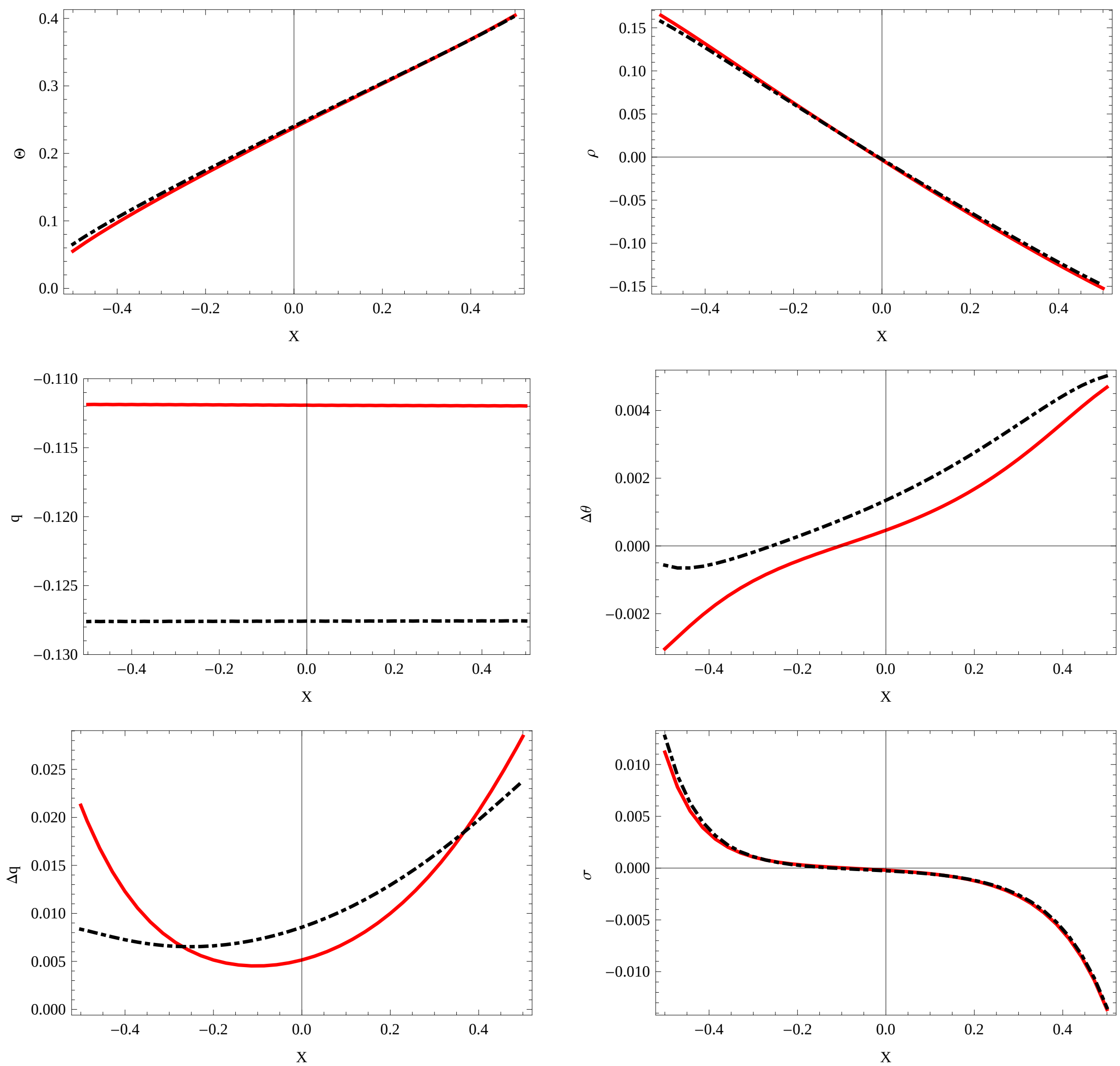

Figure 8.8: Steady state profiles of N_2 gas obtained from numerical method of the R19 equations with $\theta_{WB} = 0$ and $\theta_{WT} = 0.5$. Red line: $T_0 = 300$; black-dotdashed: $T_0 = 700$.

Chapter 9

Couette flow

Yes, we have to divide up our time like that, between our politics and our equations. But to me our equations are far more important, for politics are only a matter of present concern. A mathematical equation stands forever.

Albert Einstein

Shear flow like Couette flow, is a multi-dimensional phenomenon. As an application of a boundary value problem with moving gas, we analyze the steady linear Couette flow and model different gases with R19 and RNSF equations. We consider a steady state flow which is homogeneous in z direction. The gas is confined between two infinite plates and its movement is only at x-direction, $\mathbf{v}(x,y,z) = (v_x(y), 0, 0)$, as shown in Fig. 9.1.The walls are at different temperatures and move with different x-velocities as

$$\begin{cases} \text{Top wall:} \quad \theta_{wt} = 0.05, \;\; v_{wt} = -0.05 \\ \text{Bottom wall:} \quad \theta_{wb} = -0.05, \;\; v_{wb} = 0.05 \end{cases} . \tag{9.1}$$

Taking into account the homogeneity of flow in z-direction we have the total heat flux, heat flux difference and trace-free stress tensor as,

$$\mathbf{q} = (q_x, q_y, 0), \quad \mathbf{\Delta q} = (\Delta q_x, \Delta q_y, 0), \quad \sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & -(\sigma_{xx} + \sigma_{yy}) \end{pmatrix}. \tag{9.2}$$

First, we show the linear set of R19 and RNSF equations for the considered problem. Then, the linear system is solved analytically. Finally, the obtained results for different gases are shown and discussed.

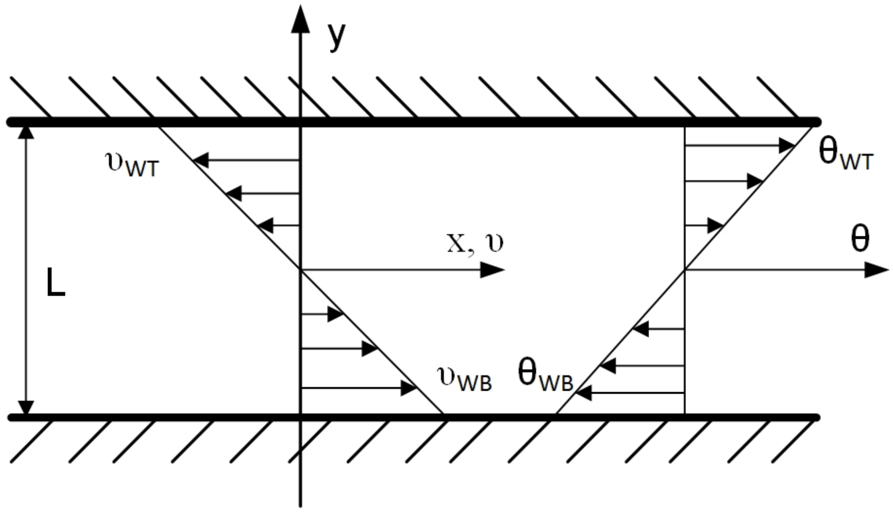

Figure 9.1: General Couette flow schematic. Top and bottom walls are at different temperatures and moving with different velocities.

9.1 Linear Couette flow

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

$$\bar{x}_i = \frac{x_i}{\tau_0\sqrt{\theta_0}} = \frac{x_i}{L}\ ,\ \bar{t} = \frac{t}{\tau_0}\ ,\ \bar{\tau}_{int} = \frac{\tau_{int}}{\tau_0}\ ,\ \bar{\tau}_{tr} = \frac{\tau_{tr}}{\tau_0}\ ,\ \bar{\rho} = \frac{\rho}{\rho_0} - 1\ ,$$
$$\bar{\theta} = \frac{\theta}{\theta_0} - 1\ ,\ \Delta\bar{\theta} = \frac{\Delta\theta}{\theta_0}\ ,\ \bar{v}_i = \frac{v_i}{\sqrt{\theta_0}}\ ,\ \bar{\sigma}_{ij} = \frac{\sigma_{ij}}{\rho_0\theta_0}\ ,\ \bar{q}_i = \frac{q_i}{\rho_0\sqrt{\theta_0}^3}\ ,\ \Delta\bar{q}_i = \frac{\Delta q_i}{\rho_0\sqrt{\theta_0}^3}\ , \tag{9.3}$$

$$\bar{u}^{0,0}_{ijk} = \frac{u^{0,0}_{ijk}}{\rho_0\sqrt{\theta_0}^3}\ ,\ \bar{B}^+_{ij} = \frac{B^+_{ij}}{\rho_0\theta_0^2}\ ,\ \bar{B}^-_{ij} = \frac{B^-_{ij}}{\rho_0\theta_0^2}\ ,\ \bar{B}^+ = \frac{B^+}{\rho_0\theta_0^2}\ ,\ \bar{B}^- = \frac{B^-}{\rho_0\theta_0^2}\ ,\ \bar{F} = \frac{\tau_0}{\sqrt{\theta_0}}F\ .$$

Linearized set of equations with small disturbances from an equilibrium ground state $\{\rho_0, v_i^0 = 0, \theta_0\}$ are studied in this section. Reference time scale, τ_0, is chosen such that the Kn_{int} be controlled as will be shown in the results section. First, we write all variables in terms of their ground state values plus a small deviation, denoted by a hat, as

$$\rho = \rho_0 + \hat{\rho},\ \theta = \theta_0 + \hat{\theta},\ v_i = \hat{v}_i,\ \Delta\theta = \Delta\hat{\theta},\ \sigma_{ij} = \hat{\sigma}_{ij},\ q_i = \hat{q}_i,$$
$$\Delta q_i = \Delta\hat{q}_i,\ B^+_{ij} = \hat{B}^+_{ij},\ B^- = \hat{B}^-,\ B^-_{ij} = \hat{B}^-_{ij},\ B^- = \hat{B}^-,\ u^{0,0}_{ijk} = \hat{u}^{0,0}_{ijk}\ . \tag{9.4}$$

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

The set of full R19 equations for this setting consists of 13 independent variables, namely

$$\left\{\rho, v_x, \theta, \Delta\theta, \sigma_{xx}, \sigma_{yy}, \sigma_{xy}, q_x, \Delta q_x, q_y, \Delta q_y, B^+, B^-\right\};$$

and, seven constitutive equations for $\left\{B^{+}_{xy}, B^{-}_{xy}, B^{+}_{yy}, B^{-}_{yy}, u^{0,0}_{xxy}, u^{0,0}_{xyy}, u^{0,0}_{yyy}\right\}$. Set of linear steady equations consists of 8 coupled equations and 12 uncoupled equations. System of 8 coupled equations, after dropping the hats are,

$$-\frac{2\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{3\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_y}{\partial y}=-\frac{\Delta\theta}{\tau_{int}}\ , \tag{9.5}$$

$$-\frac{4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{15\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_y}{\partial y}+\frac{\partial u^{0,0}_{xxy}}{\partial y}=-\left(\frac{1}{\tau_{int}}+\frac{1}{\tau_{tr}}\right)\sigma_{xx}\ , \tag{9.6}$$

$$\frac{8\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{15\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial\Delta q_y}{\partial y}+\frac{\partial u^{0,0}_{yyy}}{\partial y}=-\left(\frac{1}{\tau_{int}}+\frac{1}{\tau_{tr}}\right)\sigma_{yy}\ , \tag{9.7}$$

$$\begin{gathered}\frac{4\delta}{25\delta+42}\frac{\partial B^{+}_{xy}}{\partial y}+\frac{7(3+\delta)(14+3\delta)}{(14+\delta)(42+25\delta)}\frac{\partial B^{-}_{xy}}{\partial y}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\\ \left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_x+\frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_x\right)\end{gathered} \tag{9.8}$$

$$\begin{gathered}\frac{5}{2}\left(1-\frac{R_{q_{int}}}{R_{q_{tr}}}\right)\frac{\partial\theta}{\partial y}-\frac{5}{2}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial\Delta\theta}{\partial y}\\ +\frac{\partial\sigma_{yy}}{\partial y}-\frac{5}{39}\left(1+\frac{3R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{+}}{\partial y}\\ +\frac{5}{39}\left(1-\frac{10R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^{-}}{\partial y}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\\ \left(\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_y+\frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R^2_{q_{tr}}+5R^2_{q_{int}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_y\right)\ ,\end{gathered} \tag{9.9}$$

$$B^{-}_{xy}=-\frac{(14+\delta)\left(3R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}{(3+\delta)\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\tau_{tr}\frac{\partial q_x}{\partial y}\ , \tag{9.10}$$

$$u^{0,0}_{xxy}=-\tau_{tr}\left(\frac{\partial\sigma_{xx}}{\partial y}-\frac{2}{5}\frac{\partial\sigma_{yy}}{\partial y}\right)\ , \tag{9.11}$$

$$u^{0,0}_{yyy}=-\frac{9}{5}\tau_{tr}\frac{\partial\sigma_{yy}}{\partial x_y}\ . \tag{9.12}$$

Uncoupled equations, which depends on the variables in the above coupled equations, are,

$$\frac{\partial \rho}{\partial y}+\frac{\partial \theta}{\partial y}-\frac{\partial \Delta\theta}{\partial y}+\frac{\partial \sigma_{yy}}{\partial y}=0\ , \tag{9.13}$$

$$\frac{\partial \sigma_{xy}}{\partial y}=0\ , \tag{9.14}$$

$$\frac{\partial q_y}{\partial y}=0\ , \tag{9.15}$$

$$\begin{aligned}\frac{\partial v_x}{\partial y}&+\frac{2R_{q_{int}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\frac{\partial q_x}{\partial y}\\ &+\frac{2\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}{5\left(5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)}\frac{\partial \Delta q_x}{\partial y}=-\left(\frac{1}{\tau_{int}}+\frac{1}{\tau_{tr}}\right)\sigma_{xy}\ ,\end{aligned} \tag{9.16}$$

$$B^+_{xy}=\frac{(3+\delta)\left(28\delta R_{q_{int}}-(14-\delta)\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)\tau_{int}}{\delta\,(14+\delta)\left(3R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\right)(\tau_{tr}+\tau_{int})}B^-_{xy}\ , \tag{9.17}$$

$$\begin{aligned}&\frac{\delta}{(42+25\delta)}\left(7+\frac{15R_{q_{int}}}{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\right)\frac{\partial B^+_{xy}}{\partial y}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\\ &\left(\frac{5R_{q_{int}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_x+\frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R^2_{q_{tr}}+5R^2_{q_{int}}}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_x\right)\ ,\end{aligned} \tag{9.18}$$

$$\begin{aligned}&\frac{5+\delta+(1+\theta)\frac{d\delta}{d\theta}}{2}\frac{\partial \theta}{\partial y}-\frac{\partial \Delta\theta}{\partial y}+\frac{\partial \sigma_{yy}}{\partial y}\\ &\qquad-\frac{2}{39}\frac{\partial B^+}{\partial y}+\frac{5}{13}\frac{\partial B^-}{\partial y}=-\left[\frac{1}{\tau_{tr}}+\frac{1}{\tau_{int}}\right]\\ &\left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}q_y+\frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(R_{q_{tr}}-R_{q_{int}}\right)}{5R_{q_{int}}+\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_y\right)\ ,\end{aligned} \tag{9.19}$$

$$B^{-} = -\left[\frac{3\left(3-\delta\right)}{2} - \frac{9R_{u^{2,0}} - \frac{3(3+\delta)}{2}}{R_{u^{1,1}}}\right]\frac{\tau_{tr}}{\tau_{tr}+\tau_{int}}\Delta\theta \ , \tag{9.20}$$

$$B^{+} = -3\tau_{tr}\frac{15+5\delta(1-R_{u^{1,1}})+184R_{u^{1,1}}-30R_{u^{2,0}}-\frac{169R_{u^{1,1}}\left(10+3R_{u^{1,1}}\right)}{3R_{u^{1,1}}+10R_{u^{2,0}}}}{10R_{u^{1,1}}\left(\tau_{tr}+\tau_{int}\right)}\Delta\theta \ , \tag{9.21}$$

$$B^{+}_{yy} = 0 \ , \tag{9.22}$$

$$B^{-}_{yy} = 0 \ , \tag{9.23}$$

$$u^{0,0}_{xyy} = 0 \ . \tag{9.24}$$

Also, the linear dimensionless form of RNSF equations corresponding to the considered problem is,

$$\frac{\partial\rho}{\partial y} + \frac{\partial\theta}{\partial y} = 0 \ , \tag{9.25}$$

$$\frac{\partial\sigma_{xy}}{\partial y} = 0 \ , \tag{9.26}$$

$$\frac{\partial q_y}{\partial y} = 0 \ , \tag{9.27}$$

$$\sigma_{xy} = -\tau_{tr}\frac{\partial v_x}{\partial y} \ , \tag{9.28}$$

$$q_y = -\tau_{tr}\frac{5R_{q_{int}} + \left(\delta + \frac{d\delta}{d\theta}\right)R_{q_{tr}}}{2R_{q_{int}}R_{q_{tr}}}\frac{\partial\theta}{\partial y} \ . \tag{9.29}$$

where, $\Delta\theta$ and σ_{yy} found to be zero from the linear RNSF equations in the problem under consideration.

9.2 Solution

Solution for the set of 8 coupled equations,

$$A_{8\times8}\frac{\partial\Phi}{\partial x} = B_{8\times8}\Phi \ ,$$

$\Phi = \{\Delta q_y, B^{-}_{xy}, \Delta\theta, u^{0,0}_{xxy}, u^{0,0}_{yyy}, q_x, \sigma_{yy}, \sigma_{xx}\}$, is obtained using the eigenvalue method as,

$$\Phi\left(x\right) = \sum_{n=1}^{5} C_n\vartheta_n e^{\lambda_n x} \ , \tag{9.30}$$

where, λ and ϑ are eigenvalues and eigenvectors of the coefficient matrix, $A^{-1}B$. After some mathematical manipulations we found,

$$\Delta q_y(x) = C_3'\vartheta_{1,4}\frac{\sinh(\lambda_4 x)}{\sinh(\lambda_4/2)} + C_4'\vartheta_{1,4}\frac{\cosh(\lambda_4 x)}{\cosh(\lambda_4/2)} + C_5'\vartheta_{1,6}\frac{\sinh(\lambda_6 x)}{\sinh(\lambda_6/2)} + C_6'\vartheta_{1,6}\frac{\cosh(\lambda_6 x)}{\cosh(\lambda_6/2)} \ ,$$

$$B_{xy}^{-}(x) = C_1'\vartheta_{2,2}\frac{\sinh(\lambda_2 x)}{\sinh(\lambda_2/2)} + C_2'\vartheta_{2,2}\frac{\cosh(\lambda_2 x)}{\cosh(\lambda_2/2)} \ , \tag{9.31}$$

$$\Delta\theta(x) = C_3'\vartheta_{3,4}\frac{\cosh(\lambda_4 x)}{\sinh(\lambda_4/2)} + C_4'\vartheta_{3,4}\frac{\sinh(\lambda_4 x)}{\cosh(\lambda_4/2)} + C_5'\vartheta_{3,6}\frac{\cosh(\lambda_6 x)}{\sinh(\lambda_6/2)} + C_6'\vartheta_{3,6}\frac{\sinh(\lambda_6 x)}{\cosh(\lambda_6/2)} \ , \tag{9.32}$$

$$u_{xxy}^{0,0}(x) = C_3'\vartheta_{4,4}\frac{\sinh(\lambda_4 x)}{\sinh(\lambda_4/2)} + C_4'\vartheta_{4,4}\frac{\cosh(\lambda_4 x)}{\cosh(\lambda_4/2)} + C_5'\vartheta_{4,6}\frac{\sinh(\lambda_6 x)}{\sinh(\lambda_6/2)} + C_6'\vartheta_{4,6}\frac{\cosh(\lambda_6 x)}{\cosh(\lambda_6/2)} + C_7'\vartheta_{4,8}\frac{\sinh(\lambda_4 x)}{\sinh(\lambda_4/2)} + C_8'\vartheta_{4,8}\frac{\cosh(\lambda_4 x)}{\cosh(\lambda_4/2)} \ , \tag{9.33}$$

$$u_{yyy}^{0,0}(x) = C_3'\vartheta_{5,4}\frac{\sinh(\lambda_4 x)}{\sinh(\lambda_4/2)} + C_4'\vartheta_{5,4}\frac{\cosh(\lambda_4 x)}{\cosh(\lambda_4/2)} + C_5'\vartheta_{5,6}\frac{\sinh(\lambda_6 x)}{\sinh(\lambda_6/2)} + C_6'\vartheta_{5,6}\frac{\cosh(\lambda_6 x)}{\cosh(\lambda_6/2)} \ , \tag{9.34}$$

$$q_x(x) = C_1'\frac{\cosh(\lambda_2 x)}{\sinh(\lambda_2/2)} + C_2'\frac{\sinh(\lambda_2 x)}{\cosh(\lambda_2/2)} \ , \tag{9.35}$$

$$\sigma_{yy}(x) = C_3'\vartheta_{7,4}\frac{\cosh(\lambda_4 x)}{\sinh(\lambda_4/2)} + C_4'\vartheta_{7,4}\frac{\sinh(\lambda_4 x)}{\cosh(\lambda_4/2)} + C_5'\vartheta_{7,6}\frac{\cosh(\lambda_6 x)}{\sinh(\lambda_6/2)} + C_6'\vartheta_{7,6}\frac{\sinh(\lambda_6 x)}{\cosh(\lambda_6/2)} \ , \tag{9.36}$$

$$\sigma_{xx}(x) = C_3'\frac{\cosh(\lambda_4 x)}{\sinh(\lambda_4/2)} + C_4'\frac{\sinh(\lambda_4 x)}{\cosh(\lambda_4/2)} + C_5'\frac{\cosh(\lambda_6 x)}{\sinh(\lambda_6/2)} + C_6'\frac{\sinh(\lambda_6 x)}{\cosh(\lambda_6/2)} + C_7'\frac{\cosh(\lambda_8 x)}{\sinh(\lambda_8/2)} + C_8'\frac{\sinh(\lambda_8 x)}{\cosh(\lambda_8/2)} \ , \quad (9.37)$$

where,

$$\begin{aligned}
C_1' &= (C_1 + C_2)\sinh(\lambda_2/2)\,;\; C_2' = (C_2 - C_1)\cosh(\lambda_2/2) \ , \\
C_3' &= (C_3 + C_4)\sinh(\lambda_4/2)\,;\; C_4' = (C_4 - C_3)\cosh(\lambda_4/2) \ , \\
C_5' &= (C_6 + C_5)\sinh(\lambda_6/2)\,;\; C_6' = (C_6 - C_5)\cosh(\lambda_6/2) \ , \\
C_7' &= (C_8 + C_7)\sinh(\lambda_8/2)\,;\; C_8' = (C_8 - C_7)\cosh(\lambda_8/2) \ .
\end{aligned}$$

Also, for the dependent variables we have,

$$\sigma_{xy} = C_{12} \ , \quad (9.38)$$

$$q_y = C_{11} \ , \quad (9.39)$$

$$\theta = \frac{2}{5+\delta+(1+\theta)\frac{d\delta}{d\theta}}\left(\Delta\theta - \sigma_{yy} + \frac{2}{39}B^+ - \frac{5}{13}B^- + C_9 - \left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right] y \left(\frac{R_{q_{int}}R_{q_{tr}}\left(5+\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}{5R_{q_{int}} + \left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}} q_y + \frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}\left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}} + \left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)R_{q_{tr}}}\Delta q_y\right)\right] \ , \quad (9.40)$$

$$\rho = -\theta + \Delta\theta - \sigma_{yy} + C_{10} \ , \quad (9.41)$$

$$B^- = -\left[\frac{3(3-\delta)}{2} - \frac{9R_{u^{2,0}} - \frac{3(3+\delta)}{2}}{R_{u^{1,1}}}\right]\frac{\tau_{tr}}{\tau_{tr}+\tau_{int}}\Delta\theta \ , \quad (9.42)$$

$$B^+ = -\frac{3\left[15 + 5\delta(1 - R_{u^{1,1}}) + 184R_{u^{1,1}} - 30R_{u^{2,0}} - \frac{169R_{u^{1,1}}\left(10+3R_{u^{1,1}}\right)}{3R_{u^{1,1}}+10R_{u^{2,0}}}\right]}{10R_{u^{1,1}}}\frac{\tau_{tr}}{\tau_{tr}+\tau_{int}}\Delta\theta \ , \quad (9.43)$$

$$v_x = -\frac{2R_{q_{int}}}{5R_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}} q_x - \frac{2\left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}}{5\left(5R_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)} \Delta q_x$$
$$- u^{0,0}_{xyy} - \left(\frac{1}{\tau_{int}} + \frac{1}{\tau_{tr}}\right) \sigma_{xy} y + C13 \ , \quad (9.44)$$

$$B^+_{xy} = \frac{(3+\delta)\left(28\delta R_{q_{int}} + (14-\delta)\left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)\tau_{int}}{\delta(14+\delta)\left(3R_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}\right)(\tau_{tr} + \tau_{int})} B^-_{xy} \ , \quad (9.45)$$

$$\frac{\delta}{(42+25\delta)} \left(7 + \frac{15R_{q_{int}}}{\left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}}\right) \frac{\partial B^+_{xy}}{\partial y} = -\left[\frac{1}{\tau_{tr}} + \frac{1}{\tau_{int}}\right]$$
$$\left(\frac{5R_{q_{int}}\left(R_{q_{tr}} - R_{q_{int}}\right)}{5R_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}} q_x + \frac{\left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R^2_{q_{tr}} + 5R^2_{q_{int}}}{5R_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right) R_{q_{tr}}} \Delta q_x\right) \ , \quad (9.46)$$

$$B^+_{yy} = 0 \ , \quad (9.47)$$
$$B^-_{yy} = 0 \ , \quad (9.48)$$
$$u^{0,0}_{xyy} = 0 \ . \quad (9.49)$$

9.3 Boundary conditions

The above set of equations has 20 independent variables

$$\Phi = \left\{\rho, v_x, \theta, \Delta\theta, q_x, \Delta q_x, q_y, \Delta q_y, \sigma_{xx}, \sigma_{xy}, \sigma_{yy}, B^+_{xy}, B^-_{xy}, B^+_{yy}, B^-_{yy}, u^{0,0}_{xxy}, u^{0,0}_{xyy}, u^{0,0}_{yyy}, B^+, B^-\right\} \ .$$

First we write the system of equations as

$$A(\Phi) \frac{\partial \Phi}{\partial y} = P(\Phi)\Phi \ . \quad (9.50)$$

The number of boundary conditions which should be described equals the number of the variables of the system (20 for one dimensional R19) minus the number of multiplicity of the zero eigenvalues of the matrix $A(\Phi)$. This is due to the fact that the left zero eigenvectors in Eq.(9.50) associated with the zero eigenvalues are acting like constraints on the variable vector Φ and reduce the dimension of the system by the number of zero eigenvalues. Calculation of the eigenvalues shows that the matrix $A(\Phi)$ possesses a zero eigenvalue with multiplicity of 7. Therefore, we need to prescribe a total number of 13 boundary conditions for regularized 19 equations. Using the null-space of coefficient matrix, we obtain relations for

$$\left\{u^{0,0}_{xyy}, B^{+}_{xy}, B^{+}, B^{-}, B^{+}_{yy}, B^{-}_{yy}\right\} \ . \tag{9.51}$$

These relations are used to eliminate the depending variables and reduce the system. The definition of remaining variables are used to obtain the velocity function Ψ corresponding to the field of variables Φ. The choice of the velocity and internal parameter function $\Psi(\mathbf{C}, \mathbf{I})$ is restricted by Grad's finding based on the argument of specular reflection that the velocity function should be odd in the normal component of the particle velocity [62]. This is due to the fact that the even polynomials at the wall boundary condition will produce identity and are uncontrollable. Also, we only prescribe fluxes and not the variables based on the theory of balance laws which states that at the boundary we need to prescribe fluxes, not variables [47]. Therefore, the corresponding velocity and internal parameter function obtained as,

$$\begin{aligned}\Psi = \Bigg\{ & C_y,\, C_xC_y,\, C_y\left(\frac{C^2}{2} + I^{2/\delta}\right), \\ & C_xC_y\left(\left[1 - \frac{11}{14}\frac{\delta}{\delta+3}\right]C^2 + \left[1 + \frac{11}{\delta+3}\right]I^{2/\delta} - \frac{14+\delta}{2}\theta\right), \\ & C_y\left(\frac{C^2}{2} - \frac{5\,\mathrm{Pr}_{q_{int}}}{\left(\delta + \theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}I^{2/\delta}\right),\, C_y\left(C_yC_y - \frac{3}{5}C^2\right),\, C_y\left(C_xC_x - \frac{1}{5}C^2\right)\Bigg\} \ ,\end{aligned} \tag{9.52}$$

We consider that $\mathbf{n} = (0, 1, 0)$ and $\mathbf{V}_w = (V_w, 0, 0)$. The general boundary condition, Eq. 7.2, is used here to obtain macroscopic boundary conditions for different functions in Ψ. The first condition is obtained by considering $\Psi = C_y$. For this we rewrite the part representing incoming particles as

$$f_{|36}(\mathbf{c}) = \chi\left[(1-\zeta)\, f_{|36}(\mathbf{c}) + \zeta f_{|36}(\mathbf{c})\right] + (1-\chi)\, f_{|36}(\mathbf{c})\,. \tag{9.53}$$

So, we have three identity relations which state that the flux of molecules towards the wall is the same as those leaving for all three reflection types, pure specular, partial accommodation and full accommodation,

$$-\left(1-\chi\right)\int\int_{\mathbf{C}.\mathbf{n}\prec 0} C_y f_{|36} d\mathbf{C}d\mathbf{I} = \left(1-\chi\right)\int\int_{\mathbf{C}.\mathbf{n}\succ 0} C_y f^{*}_{|36} d\mathbf{C}d\mathbf{I}\ , \tag{9.54a}$$

$$-\chi\left(1-\zeta\right)\int_{\mathbf{C}.\mathbf{n}\prec 0} C_y f_{|36} d\mathbf{C} = \chi\left(1-\zeta\right)\int_{\mathbf{C}.\mathbf{n}\succ 0} C_y f_{tr,w} d\mathbf{C}\ , \tag{9.54b}$$

$$-\chi\zeta\int\int_{\mathbf{C}.\mathbf{n}\prec 0} C_y f_{|36} d\mathbf{C}d\mathbf{I} = \chi\zeta\int\int_{\mathbf{C}.\mathbf{n}\succ 0} C_y f_{int,w} d\mathbf{C}d\mathbf{I}\ . \tag{9.54c}$$

The first identity is always true based on the definition of $f^{*}_{|36}$ and $f_{|36}$. The second identity give us a relation for $\rho_{I,w}$ as,

$$\begin{aligned}\rho_{I,w}\sqrt{\theta_w} = &-\frac{\exp\left[-\frac{I^{2/\delta}}{\theta_w}\right]}{\Gamma\left(1+\frac{\delta}{2}\right)840\delta\sqrt{2}\theta^{(\delta+5)/2}}\Bigg[\frac{70\sqrt{2}\delta}{13}\theta\Big(21B^{-}+5B^{+}\\ &+78\left[\frac{\left(3+\delta\right)\left(14+27\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}B^{-}_{yy}-\frac{2\delta}{42+25\delta}B^{+}_{yy}\right.\\ &\left.+\frac{\left(\delta+\theta\frac{d\delta}{d\theta}\right)\sqrt{2\pi\theta}\,\mathrm{Pr}_{q_{tr}}}{\left(5\,\mathrm{Pr}_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)}\left(\Delta q_y-q_y\right)+\theta\left(2\rho\left[2\Delta\theta-\theta\right]-\sigma_{yy}\right)\right]\Big)\\ &-140I^{2/\delta}\Bigg(\frac{12\left(\delta+\theta\frac{d\delta}{d\theta}\right)\sqrt{\pi}\,\mathrm{Pr}_{q_{tr}}}{\left(5\,\mathrm{Pr}_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)}\sqrt{\theta}\left(\Delta q_y-q_y\right)+\frac{168\sqrt{2}\delta\left(3+\delta\right)}{\left(14+\delta\right)\left(42+25\delta\right)}B^{-}_{yy}\\ &+\frac{20\sqrt{2}}{13}B^{-}+\frac{6\sqrt{2}}{13}B^{+}-\frac{18\sqrt{2}\delta}{\left(42+25\delta\right)}B^{+}_{yy}+\frac{18\sqrt{2}}{\left(42+25\delta\right)}\rho\theta\Delta\theta\Bigg)\Bigg]\ ,\end{aligned} \tag{9.55}$$

and the third one give us,

$$\begin{aligned}\rho_w\sqrt{\theta_w} = &-\frac{\left(14-\delta\right)\left(3+\delta\right)}{2\left(14+\delta\right)\left(42+25\delta\right)\theta^{\frac{3}{2}}}B^{-}_{yy}+\frac{1}{156}\frac{B^{+}-B^{-}}{\theta^{\frac{3}{2}}}\\ &-\frac{\delta}{2\left(42+25\delta\right)\theta^{\frac{3}{2}}}B^{+}_{yy}+\frac{1}{2}\frac{\sigma_{yy}}{\sqrt{\theta}}+\frac{1}{2\sqrt{\theta}}\rho\left(2\theta-\Delta\theta\right)=\Upsilon\ .\end{aligned} \tag{9.56}$$

Furthermore, we obtain boundary condition for stress tensor,

$$\sigma_{xy} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi}}\left[\Upsilon V_s+\frac{5\,\mathrm{Pr}_{q_{int}}\,q_x+\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\,\Delta q_x}{5\left(5\,\mathrm{Pr}_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)\sqrt{\theta}}+\frac{u^{0,0}_{xyy}}{2\sqrt{\theta}}\right]\ , \tag{9.57}$$

boundary condition for total heat flux,

$$q_y = -\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{\Upsilon}{2}\sqrt{\theta}\left[(4+\delta\zeta)(\theta-\theta_w)-(1-\zeta)(\delta\theta+3\Delta\theta)-V_s^2\right]\right.$$
$$+(3+\delta)\frac{(140+\delta(32+\delta)+(14-\delta)\delta\zeta)}{4(14+\delta)(42+25\delta)}B_{yy}^- + \frac{[(1-\zeta)\delta-4]}{312}B^+$$
$$+\frac{\delta(4-\delta(1-\zeta))}{4(42+25\delta)}B_{yy}^+ - \frac{(2+\delta(1-\zeta))}{4}\theta(\rho\Delta\theta-\sigma_{yy})$$
$$\left.+\frac{(56-\delta(1-\zeta))}{312}B^- + \frac{\delta(1-\zeta)}{2}\rho\theta^2\right] \quad , \quad (9.58)$$

boundary condition for heat flux difference Δq_y,

$$\Delta q_y = \frac{\chi}{(2-\chi)\,\mathrm{Pr}_{q_{tr}}\left(\delta+\theta\frac{d\delta}{d\theta}\right)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{5(40-\delta)\,\mathrm{Pr}_{q_{int}}-12\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{312}B^-\right.$$
$$+\frac{5(12+\delta)\,\mathrm{Pr}_{q_{int}}+12\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{312}B^+$$
$$+\frac{5\delta\,\mathrm{Pr}_{q_{int}}-6\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4}\theta\sigma_{yy} - \delta\frac{5(6+\delta)\,\mathrm{Pr}_{q_{int}}+6\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4(42+25\delta)}B_{yy}^+$$
$$+\frac{10\delta\,\mathrm{Pr}_{q_{int}}-8\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4}\rho\theta^2 + \frac{5(6-\delta)\,\mathrm{Pr}_{q_{int}}+12\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4}\rho\theta\Delta\theta$$
$$+[3+\delta]\frac{5\delta(42+\delta)\,\mathrm{Pr}_{q_{int}}-6(14-\delta)\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{4(14+\delta)(42+25\delta)}B_{yy}^-$$
$$+\frac{\Upsilon}{2}\sqrt{\theta}\left[\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}V_s^2 - 15\,\mathrm{Pr}_{q_{int}}(1-\zeta)\Delta\theta\right.$$
$$\left.\left.-\left(5\delta\,\mathrm{Pr}_{q_{int}}-4\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)\theta + \left(5\delta\zeta\,\mathrm{Pr}_{q_{int}}-4\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)(\theta-\theta_W)\right]\right] \quad , \quad (9.59)$$

boundary condition for B_{xy}^- is

$$B_{xy}^- = \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi}}\frac{3(14+\delta)}{14(3+\delta)}\left(\frac{37\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{15\left(5\,\mathrm{Pr}_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)}\sqrt{\theta}\Delta q_x\right.$$
$$-\frac{14\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}+33\,\mathrm{Pr}_{q_{int}}}{3\left(5\,\mathrm{Pr}_{q_{int}}+\left(\delta+\theta\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)}\sqrt{\theta}q_x - \frac{1}{2}\sqrt{\theta}u_{xyy}^{0,0}$$
$$\left.-\Upsilon V_s\left(V_s^2-\theta+7(1-\zeta)\Delta\theta-\frac{(18+7\zeta\delta)}{3}[\theta-\theta_W]\right)\right) \quad , \quad (9.60)$$

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

$$u^{0,0}_{yyy} = \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{(-14+\delta)(3+\delta)}{(14+\delta)(42+25\delta)}B^{-}_{yy} - \frac{\delta B^{+}_{yy}}{42+25\delta} - \frac{2(B^{+}-B^{-})}{195}\right.$$
$$\left. - \frac{7\sigma_{yy}+2\rho\Delta\theta}{5}\theta - \Upsilon\frac{\sqrt{\theta}}{5}\left(3V_s^2 - 2\left[\theta-\theta_W\right]\right)\right] , \quad (9.61)$$

and for $u^{0,0}_{xxy}$,

$$u^{0,0}_{xxy} = \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{(-14+\delta)(3+\delta)}{(14+\delta)(42+25\delta)}B^{-}_{xx} - \frac{\delta B^{+}_{xx}}{42+25\delta} + \frac{(B^{+}-B^{-})}{195}\right.$$
$$\left. + \frac{\theta}{5}(\rho\Delta\theta + \sigma_{yy} - 5\sigma_{xx}) + \Upsilon\frac{\sqrt{\theta}}{5}\left(4V_s^2 - \left[\theta-\theta_W\right]\right)\right] . \quad (9.62)$$

9.3.1 Linear boundary condition

The boundary conditions in the dimensionless linear form are
stress tensor,

$$\sigma_{xy} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi}}\left[V_s + \frac{5\,\mathrm{Pr}_{q_{int}}\,q_x + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\,\Delta q_x}{5\left(5\,\mathrm{Pr}_{q_{int}} + \left(\delta + (1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)} + \frac{u^{0,0}_{xyy}}{2}\right] , \quad (9.63)$$

total heat flux,

$$q_y = -\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi}}\left[\frac{1}{2}\left[(4+\delta\zeta)(\theta-\theta_w) - (1-\zeta)\,3\Delta\theta\right]\right.$$
$$\left. + \frac{7}{39}B^{-} - \frac{1}{78}B^{+} - \frac{1}{2}(\Delta\theta - \sigma_{yy})\right] , \quad (9.64)$$

heat flux difference Δq_y,

$$\Delta q_y = \frac{\chi}{(2-\chi)\,\mathrm{Pr}_{q_{tr}}\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)}\sqrt{\frac{2}{\pi}}\left[\frac{25\,\mathrm{Pr}_{q_{int}} - 2\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{39}B^- \right.$$
$$+\frac{15\,\mathrm{Pr}_{q_{int}} + 4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{78}B^+ - \frac{\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{2}\sigma_{yy}$$
$$+\frac{15\,\mathrm{Pr}_{q_{int}} + 4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{2}\Delta\theta$$
$$\left. +\frac{1}{2}\left[-15\underset{q_{int}}{\mathrm{Pr}}(1-\zeta)\,\Delta\theta + \left(5\delta\zeta\underset{q_{int}}{\mathrm{Pr}} - 4\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\underset{q_{tr}}{\mathrm{Pr}}\right)(\theta-\theta_W)\right]\right] \ , \tag{9.65}$$

and boundary conditions for B^-_{xy}, $u^{0,0}_{yyy}$ and $u^{0,0}_{xxy}$,

$$B^-_{xy} = \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi}}\frac{3\,(14+\delta)}{14\,(3+\delta)}\left(\frac{37\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}}{15\left(5\,\mathrm{Pr}_{q_{int}} + \left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)}\Delta q_x \right.$$
$$\left. -\frac{14\left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}} + 33\,\mathrm{Pr}_{q_{int}}}{3\left(5\,\mathrm{Pr}_{q_{int}} + \left(\delta+(1+\theta)\frac{d\delta}{d\theta}\right)\mathrm{Pr}_{q_{tr}}\right)}q_x - \frac{1}{2}u^{0,0}_{xyy} + V_s\right) \ , \tag{9.66}$$

$$u^{0,0}_{yyy} = \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi}}\left[-\frac{2\,(B^+-B^-)}{195} - \frac{7\sigma_{yy}+2\Delta\theta}{5} + \frac{2}{5}(\theta-\theta_W)\right] \ , \tag{9.67}$$

$$u^{0,0}_{xxy} = \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi}}\left[\frac{(B^+-B^-)}{195} + \frac{1}{5}(\Delta\theta+\sigma_{yy}-5\sigma_{xx}) - \frac{1}{5}[\theta-\theta_W]\right] \ . \tag{9.68}$$

Also, boundary conditions for the set of RNSF equations are

$$\sigma_{xy} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi}}V_s \ , \tag{9.69}$$

$$q_y = -\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi}}\left[\frac{1}{2}\left[(4+\delta\zeta)(\theta-\theta_w)\right]\right] \ . \tag{9.70}$$

9.4 Results

In this section we investigate the effects of Kn numbers, internal degrees of freedom, Pr number, and accommodation coefficients on the behavior of the Couette flow.

First we investigate the N_2 gas and compare the results obtained from the RNSF and R19 equations. Reference time scale, τ_0, along with reference temperature of 300

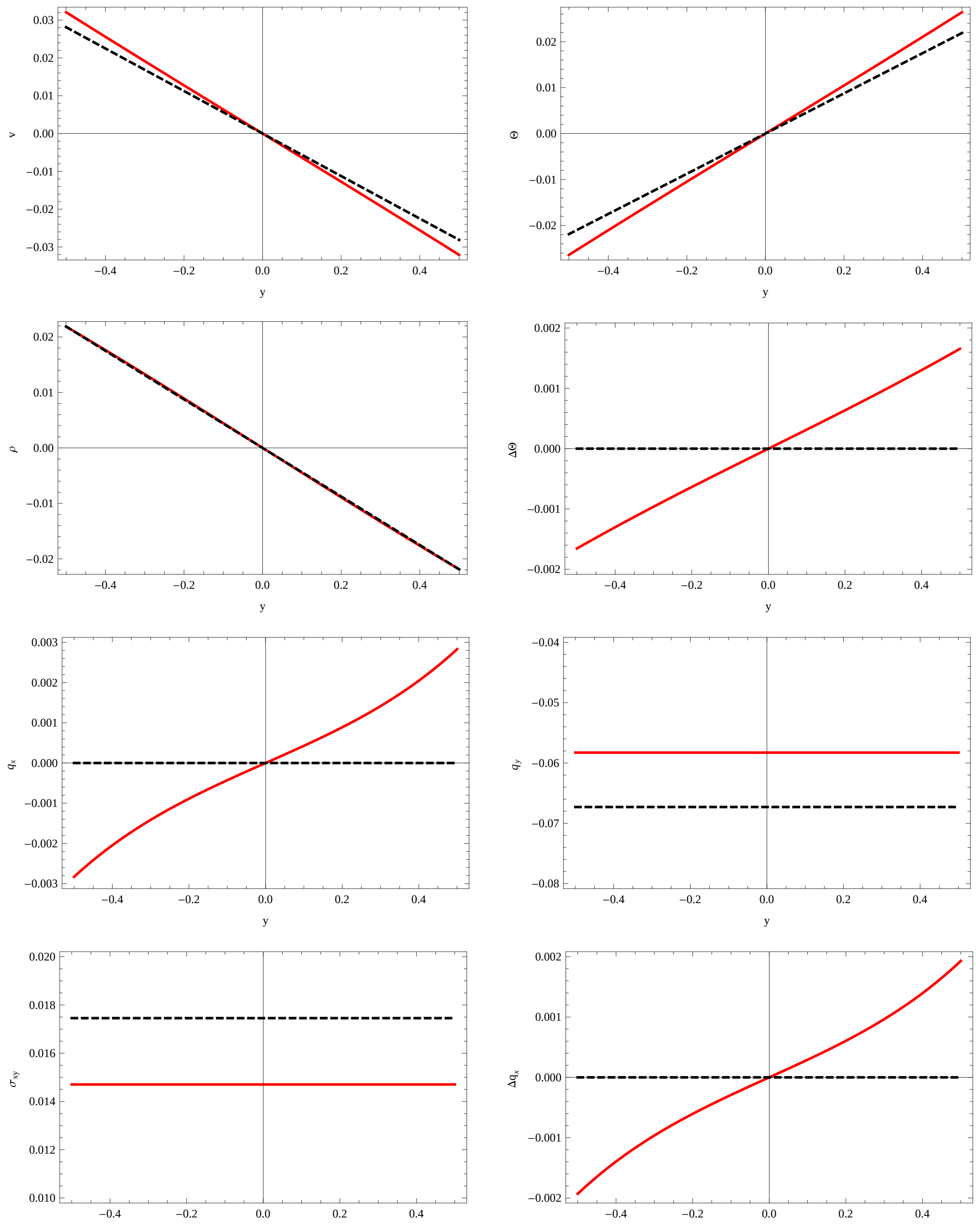

Figure 9.2: Couette flow profiles obtained from set of R19 (red solid line) and RNSF (black dashed) equations of N_2 gas with $Kn_{tr} = 0.31$.

K are chosen such that the $Kn_{int} = 1$ and $Kn_{tr} = 0.31$. Figure 9.2 illustrates profiles obtained from RNSF and R19 equations. Results from R19 and RNSF equations are different and again this is shown that the set of refined NSF equations can not predict accurate results. Temperature gradient on the walls are higher for R19 equations. However normal heat flux is higher for RNSF equations. This is due to the effects of the gradients of dynamic temperature and σ_{yy}, which act in opposition to the gradient of temperature and reduces the total heat flux, Eq. 9.19. Also based on Eq. 9.64, low heat flux value effect on reducing temperature jump is promoted by the effects of $\Delta\theta$ and σ_{yy} and result in lower temperature jump of R19 equations compare to RNSF equations. Also the same trend is seen for σ_{xy}, Eq. 9.16, which have higher value for RNSF equations while the velocity gradient is higher for R19 equations. This is due to the effects of gradient of q_x and Δq_x. Furthermore, low stress tensor, q_x and Δq_x effects give lower velocity slip for R19, Eq. 9.63, compare to RNSF equations.

Now we investigate the effects of the relation between two Kn numbers on flow. Two cases are investigated in Fig. 9.3. The translational Knudsen number is fixed at 0.5 and internal Knudsen number is set to 0.5 for case #1 and 50 for case #2. Also, internal degrees of freedom is fixed at 2. It is seen that effects of increasing internal Knudsen number is strong on all the variables. The case with higher internal Kn number has higher temperature jump and velocity slip. Due to the lower internal relaxation times and more active internal exchange processes in case 1, value of dynamic temperature is slightly higher compare to case 1. Also, less active internal exchange processes of case 2 produced higher heat fluxes and stress tensor. This strong effects of different ratios of Kn numbers are diminished at low translational Knudsen number.

Internal degrees of freedom effects on flow is investigated in Fig. 9.4. Two cases are studied, both with same Knudsen number, $Kn_{tr} = 0.5$ and $Kn_{int} = 1$. Internal degrees of freedom of Case #1 is 10 and of Case #2 is 2. There is no effects on velocity field, density and stress tensor. Normal components of heat fluxes are increased by increasing internal DoF, this reduces the parallel components of the heat fluxes. Also, the dynamic temperature, which is a non-equilibrium variable illustrating internal-translational exchanges are increased with increasing internal degrees of freedom. Increasing the internal degrees of freedom, slightly decreases the temperature jump by increasing normal heat flux and dynamic temperature.

Furthermore, the influence of Pr number on flow is investigated in Fig. 9.5. We use the values for Maxwell molecules of relaxation parameters for pure translational

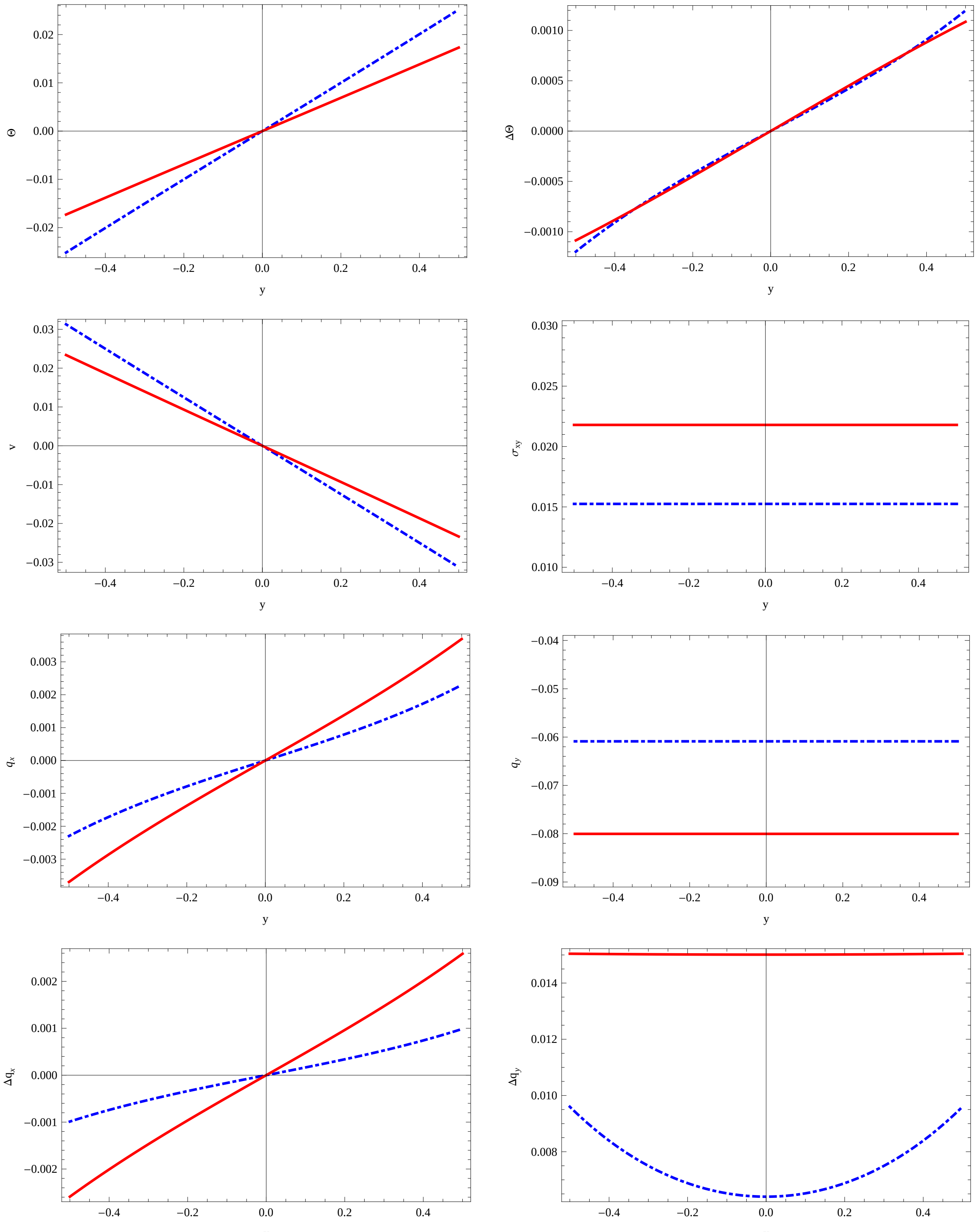

Figure 9.3: Couette flow profiles obtained from set of R19 equations with fixed internal degrees of freeedom and translational Knudsen number, $Kn_{tr} = 0.5$. Internal Knudsen number is set to $Kn_{int} = 50$ (red line) and $Kn_{int} = 0.5$ (blue dot-dashed line).

moment, $R_{q_{tr}}$, from Table 2.1 and calculate $R_{q_{int}}$ based on specified Prandtl numbers, Eq. 5.64, which are 0.7 and 0.8, meaning $R_{q_{int}}$ is equal to 0.73 and 0.96, respectively. Two other relaxation parameter, $R_{u^{2,0}}$ and $R_{u^{1,1}}$, and degrees of freedom are fixed. Also, the Knudsen numbers are fixed at $Kn_{tr} = 0.5$ and $Kn_{int} = 1$. Changing Prandtl numbers has no effects on velocity filed, density and stress tensor. Here, specific heat and viscosity are fixed. Therefore, higher Pr number means lower heat conductivity, Eq. 5.63. So, the normal component of total heat flux and temperature jump are higher for the case with lower Pr number. Consequently, the parallel part of the total heat flux is lower for the case with lower Pr number. The difference between relaxation times of translational and internal heat fluxes is more for the case with higher Pr number. Therefore, the heat flux differences and dynamic temperature values, which are an illustration of internal-translational interactions, are higher for the case with higher Pr number.

Effects of the accommodation coefficients are investigated in Fig. 9.6. Three cases are shown with different accommodation coefficients as

$$\begin{cases} \text{case \#1: } \chi = 1 \text{ and } \zeta = 1 \\ \text{case \#2: } \chi = 0.5 \text{ and } \zeta = 1 \\ \text{case \#3: } \chi = 1 \text{ and } \zeta = 0.5 \end{cases} .$$

Case #1 is the case with full accommodation. Case #2 and 3 are partial accommodations with full internal and half internal-translational accommodations, respectively. Heat flux parallel to the walls are almost unaffected by the change in accommodation coefficients. Partial accommodation with full internal accommodation, case #2, shows lower temperature and velocity gradient, normal heat flux and stress tensor in compare with fully accommodated case (#1). Comparing case #1 and 3 shows that the effects of half internal-translational accommodation are only on temperature, dynamic temperature, normal heat fluxes. Its effects are towards lower temperature gradient and normal heat flux. The drastic changes in dynamic temperature between case #1 and 3 are due to differences of gradient of Δq_y. Velocity, density and stress tensor is unaffected by half internal-translational accommodation.

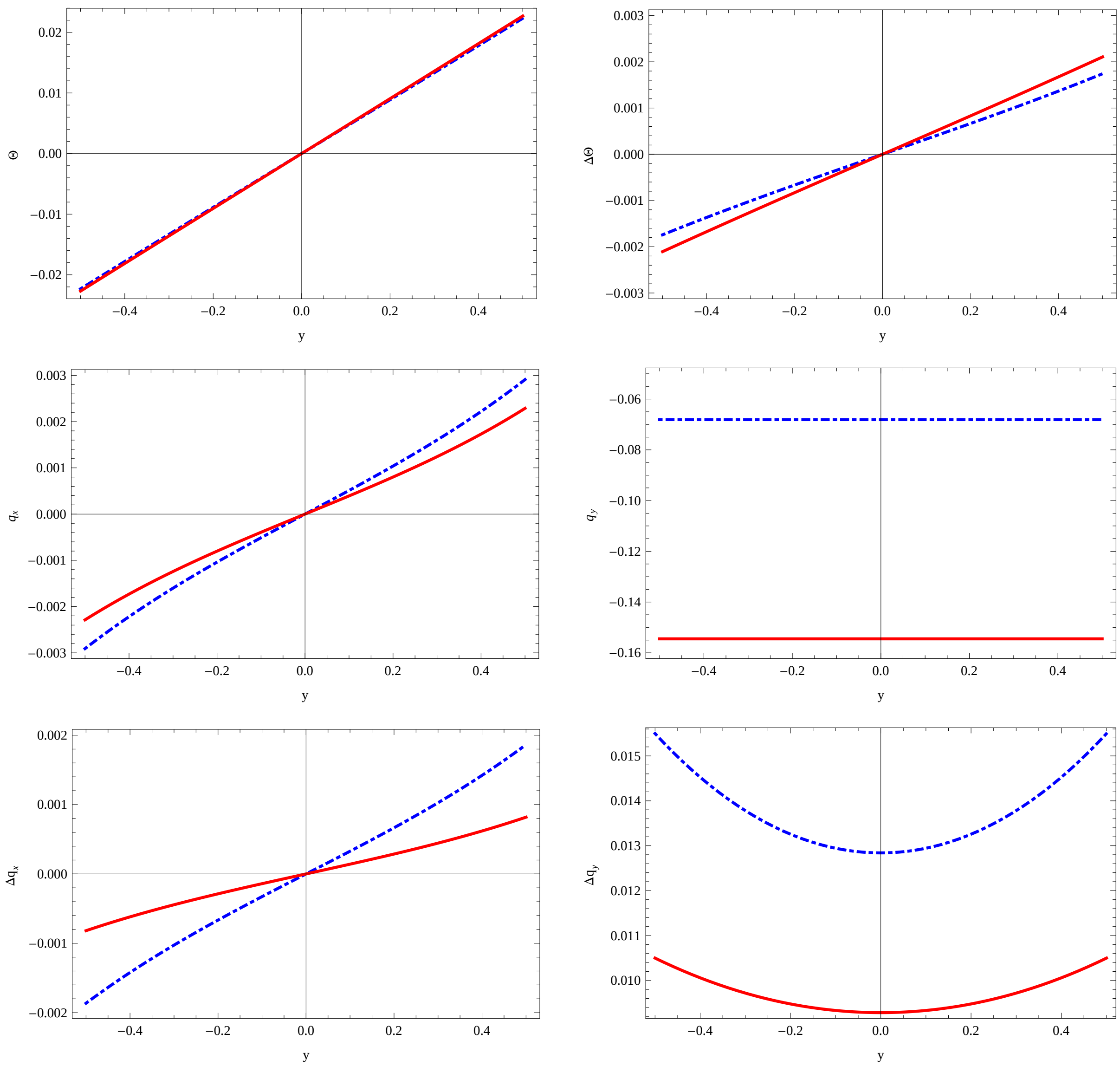

Figure 9.4: Couette flow profiles obtained from set of R19 equations with fixed Knudsen numbers. Internal degrees of freedom is set to 10 (red line) and 2 (blue dot-dashed line).

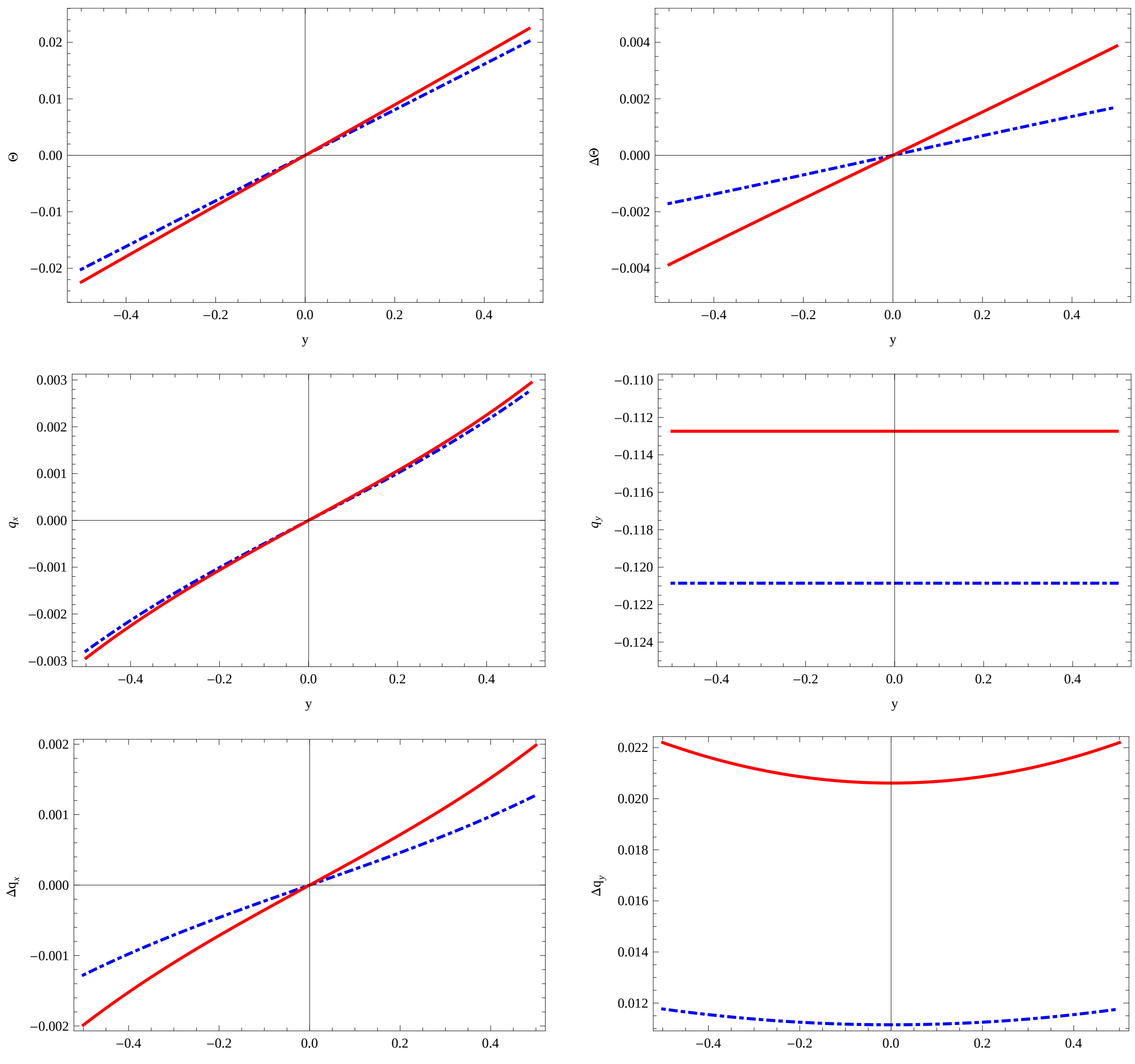

Figure 9.5: Couette flow profiles obtained from set of R19 equations with fixed Knudsen numbers and internal degrees of freedom. the Prandtl number is set to 0.8 (red line) and 0.7 (blue dot-dashed line).

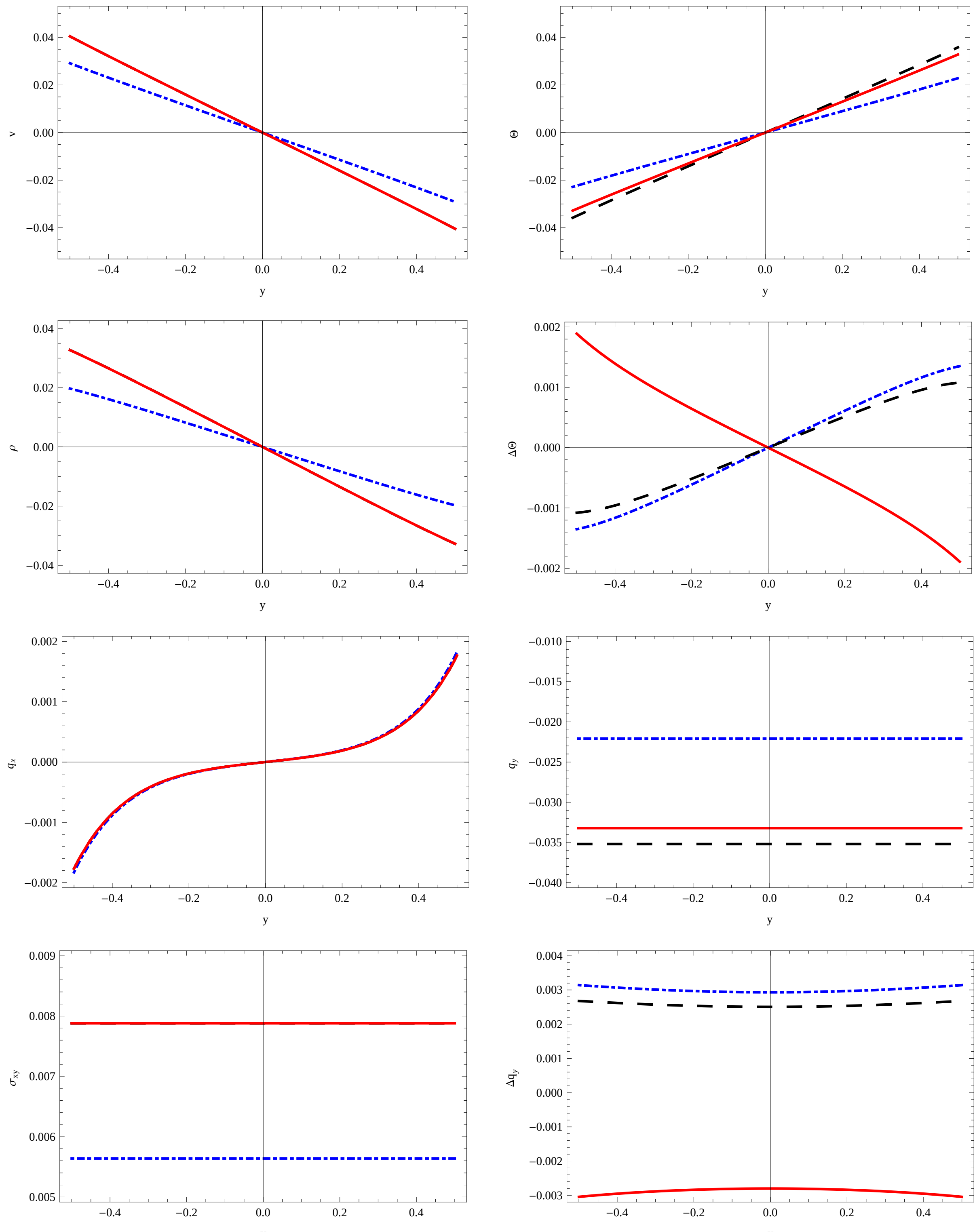

Figure 9.6: Couette flow profiles obtained from set of R19 equations of H_2 gas with $Kn_{tr} = 10^{-1}$ and $Kn_{int} = 10$. black dashed: $\chi = 1$ and $\zeta = 1$; red line: $\chi = 1$ and $\zeta = 0.5$; blue dotdashed: $\chi = 0.5$ and $\zeta = 1$.

Chapter 10

Conclusions and recommendations

This book has come to end but there is still story to be told.
Saadi

The present study introduced a modified kinetic model and new macroscopic models 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 [71]. It was shown that the proposed model offer accurate results and the ability to interpret the sometimes surprising details, caused by rarefaction, in the results in terms of macroscopic quantities. This is achieved with much less computational cost compared to that required for the DSMC simulations. The emphasis of the present thesis is on the derivation of the equations and introducing a comprehensive model for polyatomic gases in the transition regime. As the first applications of the newly introduced model, we studied the linear wave analysis, stationary heat conduction and Couette flow.

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:

1. The model predicts correct relaxation times of higher moments and Pr number.

2. The correct relaxation of the model towards equilibrium phase densities for different exchanged processes was shown.

3. We proved that the model conserves the collision invariants.

4. The H-theorem for the proposed model was proven.

Moment equations for 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 which was used to obtain constitutive equations to close the set of 36 moments equations.

The closed system of 36 moments was used to optimize the moment definitions based on Knudsen numbers. The relation between internal and translational Knudsen numbers were explored by introducing a smallness parameter, ϵ, and a magnifying parameter, α. We obtained orders of all 36 moments in two Kn numbers by applying Chapman-Enskog expansion on the original system of moment equations. Optimized moment definitions for polyatomic gases were found 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 number of moments possible.

After optimization, all moments have a clear order in the smallness parameter, ϵ, which were used for model reduction of the set of 36 moment equations and 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 different orders of accuracy up to order ϵ^3 were obtained. Based on ordering in two different Knudsen numbers, 13 different set of equations were obtained and a recipe of which set is suitable for different problems based on Knudsen numbers was given. At the first order of accuracy, a refined version of the classical Navier-Stokes-Fourier equations was obtained, which includes *the full balance law* for the dynamic temperature (Sec. 5.4). 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 Δq_i, B^- and B^+. At order $2+2\alpha$, a refined variant of Grad's 18 moment equations was obtained which consists of 18 PDEs and two constitutive equations. Finally, at the third order, the regularized 19 moment equations (R19) were obtained which consist of 19 PDEs and three constitutive equations. Also, temperature dependent internal degrees of freedom 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.

As a first application of the proposed model, we studied the phase speed and damping of one-dimensional linear waves as forecasted in the obtained different orders of equations. We compared the predictions of the various equations in the hierarchies among each other as well as to those of the classical Navier-Stokes-Fourier equations, and its modification containing the balance law for the dynamic temperature. Moreover, we studied the influence of excitations of the internal degrees of freedom by comparing with results for monatomic gases, where we highlighted the influence of the ratio of collision times, τ_{tr}/τ_{int}, and reproduced the monatomic gas behavior by freezing the internal exchange processes. It was shown that the classical Navier-Stokes-Fourier equations can not produce accurate results.

We introduced a microscopic boundary condition using same idea that we used to model 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 being 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, Eqs. (2.21, 2.25) corresponding to only translational energy equilibrium and total energy equilibrium. Macroscopic boundary conditions could be obtained from introduced microscopic boundary condition for different problems.

We solved unsteady one-dimensional stationary heat conduction numerically and analytically with set of the R19 and RNSF equations and compared the results with DSMC simulations. It was shown that the Navier-Stokes-Fourier equations were not accurate in transition regime. The results from set of R19 equations was in a good agreement with DSMC simulations up to translational Knudsen number of 0.5. The values of nonequilibrium variables at the beginning of the unsteady process found to be an order of magnitude higher than their values in steady state. Effects of non-linearity and temperature dependent properties were more dominant in profiles associated with translational-internal variables ($\Delta\theta$ and Δq). 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 at the same order found to be on moments corresponding to deviations from total values, $\Delta\theta$ and Δq, which are derived by translational-internal interactions. These effects were towards promoting the temperature dependency effects and obtained profiles covered a larger range of values. The effects of different internal DoF were most seen in total heat flux and stress tensor, where gas with higher DoF gains higher total heat flux and lower stress tensor in comparison with gas with lower DoF. Higher reference temperature, which means more excited internal degrees of freedom, produced higher heat flux value and flatter deviation moments, $\Delta\theta$ and Δq, profiles in comparison with lower reference temperature case.

Linear Couette flow was investigated by solving the set of R19 and RNSF equations analytically. This was shown that the set of refined NSF equations could not predict accurate results. Increasing Kn number ratio with fixed Kn_{tr} produced higher temperature jump, velocity slip, heat fluxes and stress tensor values. This strong effects of different ratios of Kn numbers were diminished at low translational Knudsen number. Increasing the internal degrees of freedom, decreased the temperature jump and increased the normal heat fluxes. Also, the dynamic temperature values were increased with increasing internal DoF. Heat flux parallel to the walls were almost unaffected by the change in accommodation coefficients. Partial accommodation with full internal accommodation showed lower temperature and velocity gradient, normal heat flux and stress tensor compare to fully accommodated case. Effects of half internal-translational accommodation were found to be only on temperature, dynamic temperature, normal heat flux and parallel heat flux difference.

Based on the results obtained, rarefied gas flows in early transition region could be modeled accurately using the proposed model. During the course of PhD studies, different issues and ideas were encountered. However due to lack of time, some of these ideas remained for future research. We divide the future works recommendations in two parts, first the recommendations for usage of the current proposed model and second modifications to the proposed model. The recommendations regarding the utilization of the proposed models are listed below:

1. Solving the multi-dimensional problems by applying finite volume or finite element numerical methods on the set of R19 equations. This will allow to investigate more complicated physical phenomena.

2. A very interesting idea for future work is to extend the proposed model to cover polyatomic gas mixtures.

3. Exploring more boundary conditions problems, especially in/out flow and open boundary conditions.

We listed the recommendations on modifying the proposed kinetic model next.

1. We used a continuous internal states model. Implementing a discretized internal states model will produce more accurate results in gases with internal DoF states distanced from each other.

2. In this dissertation, we have considered a simple BGK-type model. Implementing more complicated collision terms and molecular interaction potentials will allow to produce more accurate results.

The recommendations in part one are feasible. However, the recommendations given in part two are more challenging, considering that the macroscopic model should be derived from the modified kinetic model.

Bibliography

[1] J. C. Maxwell, "On the dynamical theory of gases," *Philosophical Transactions of the Royal Society of London*, vol. 157, pp. 49–88, 1867.

[2] L. Boltzmann, "Weitere studien über das wärmegleichgewicht unter gasmolekülen," in *Kinetische Theorie II*, vol. 67 of *WTB Wissenschaftliche Taschenbücher*, pp. 115–225, Vieweg+Teubner Verlag, 1970.

[3] S. Chapman, "On the law of distribution of molecular velocities, and on the theory of viscosity and thermal conduction, in a non-uniform simple monatomic gas," *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, vol. 216, no. 538-548, pp. 279–348, 1916.

[4] S. Chapman, "On the kinetic theory of a gas. part ii: A composite monatomic gas: Diffusion, viscosity, and thermal conduction," *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, vol. 217, no. 549-560, pp. 115–197, 1918.

[5] D. Enskog, *Kinetische Theorie der Vorgänge in mässig verdünnten Gasen. 1. Allgemeiner Teil.* Almqvist & Wiksells, 1917.

[6] A. Eucken, "Über das Wärmeleitvermögen, die spezifische wärme und die innere Reibung der Gase," *Physik. Z*, vol. 14, no. 8, pp. 324–332, 1913.

[7] W. Chang and G. E. Uhlenbeck, "Transport phenomena in polyatomic gases," 1951.

[8] C. W. Chang, G. Uhlenbeck, and J. De Boer, "The heat conductivity and viscosity of polyatomic gases," *Studies in statistical mechanics*, vol. 2, pp. 243–268, 1964.

[9] E. A. Mason and L. Monchick, “Heat conductivity of polyatomic and polar gases,” *The Journal of Chemical Physics*, vol. 36, no. 6, pp. 1622–1639, 1962.

[10] L. Monchick, K. Yun, and E. Mason, “Relaxation effects in the transport properties of a gas of rough spheres,” *The Journal of Chemical Physics*, vol. 38, no. 6, pp. 1282–1287, 1963.

[11] L. Monchick, K. Yun, and E. Mason, “Formal kinetic theory of transport phenomena in polyatomic gas mixtures,” *The Journal of Chemical Physics*, vol. 39, no. 3, pp. 654–669, 1963.

[12] L. Monchick, A. Pereira, and E. Mason, “Heat conductivity of polyatomic and polar gases and gas mixtures,” *The Journal of Chemical Physics*, vol. 42, no. 9, pp. 3241–3256, 1965.

[13] L. Monchick, R. Munn, and E. Mason, “Thermal diffusion in polyatomic gases: A generalized stefanmaxwell diffusion equation,” *The Journal of Chemical Physics*, vol. 45, no. 8, pp. 3051–3058, 1966.

[14] T. Morse, “Kinetic model for gases with internal degrees of freedom,” *Physics of Fluids (1958-1988)*, vol. 7, no. 2, pp. 159–169, 1964.

[15] F. Hanson and T. Morse, “Kinetic models for a gas with internal structure,” *Physics of Fluids (1958-1988)*, vol. 10, no. 2, pp. 345–353, 1967.

[16] F. McCourt and R. Snider, “Thermal conductivity of a gas with rotational states,” *The Journal of Chemical Physics*, vol. 41, no. 10, pp. 3185–3194, 1964.

[17] R. F. Snider, “Quantum-mechanical modified boltzmann equation for degenerate internal states,” *The Journal of Chemical Physics*, vol. 32, no. 4, pp. 1051–1060, 1960.

[18] L. Monchick, “Small periodic disturbances in polyatomic gases,” *Physics of Fluids (1958-1988)*, vol. 7, no. 6, pp. 882–896, 1964.

[19] A. Kogan, “Derivation of grad’s type equations and study of their relaxation properties by the method of maximization of entropy,” *Journal of Applied Mathematics and Mechanics*, vol. 29, no. 1, pp. 130–142, 1965.

[20] V. Zhdanov, "On the kinetic theory of a polyatomic gas," *Zh. Eksp. Teor. Fiz*, vol. 53, 1968.

[21] F. J. McCormack, "Kinetic equations for polyatomic gases: The 17-moment approximation," *Physics of Fluids (1958-1988)*, vol. 11, no. 12, pp. 2533–2543, 1968.

[22] J.-F. Bourgat, L. Desvillettes, P. Le Tallec, and B. Perthame, "Microreversible collisions for polyatomic gases and boltzmann's theorem," *European journal of mechanics. B, Fluids*, vol. 13, no. 2, pp. 237–254, 1994.

[23] F. Mallinger, "Generalization of the Grad theory to polyatomic gases," 1998.

[24] L. Desvillettes, R. Monaco, and F. Salvarani, "A kinetic model allowing to obtain the energy law of polytropic gases in the presence of chemical reactions," *European Journal of Mechanics-B/Fluids*, vol. 24, no. 2, pp. 219–236, 2005.

[25] E. Kustova and E. Nagnibeda, "Strong nonequilibrium effects on specific heats and thermal conductivity of diatomic gas," *Chemical physics*, vol. 208, no. 3, pp. 313–329, 1996.

[26] A. Chikhaoui, J. Dudon, E. Kustova, and E. Nagnibeda, "Transport properties in reacting mixture of polyatomic gases," *Physica A: Statistical Mechanics and its Applications*, vol. 247, no. 1, pp. 526–552, 1997.

[27] E. Kustova and E. Nagnibeda, "Transport properties of a reacting gas mixture with strong vibrational and chemical nonequilibrium," *Chemical physics*, vol. 233, no. 1, pp. 57–75, 1998.

[28] E. Kustova, E. Nagnibeda, and A. Chauvin, "State-to-state nonequilibrium reaction rates," *Chemical Physics*, vol. 248, no. 2, pp. 221–232, 1999.

[29] A. Chikhaoui, J. Dudon, S. Genieys, E. Kustova, and E. Nagnibeda, "Multitemperature kinetic model for heat transfer in reacting gas mixture flows," *Physics of Fluids (1994-present)*, vol. 12, no. 1, pp. 220–232, 2000.

[30] E. Nagnibeda and E. Kustova, *Non-equilibrium reacting gas flows: kinetic theory of transport and relaxation processes*. Springer Science & Business Media, 2009.

[31] P. Andries, P. L. Tallec, J.-P. Perlat, and B. Perthame, "The Gaussian-BGK model of Boltzmann equation with small Prandtl number," *European Journal of Mechanics - B/Fluids*, vol. 19, no. 6, pp. 813 – 830, 2000.

[32] S. Brull and J. Schneider, "On the ellipsoidal statistical model for polyatomic gases," *Continuum Mechanics and Thermodynamics*, vol. 20, no. 8, pp. 489–508, 2009.

[33] Z. Cai and R. Li, "The NRxx method for polyatomic gases," *Journal of Computational Physics*, vol. 267, pp. 63–91, 2014.

[34] Z. Cai, R. Li, and Y. Wang, "An efficient nrxx method for boltzmann-bgk equation," *Journal of Scientific Computing*, vol. 50, no. 1, pp. 103–119, 2012.

[35] Z. Cai, R. Li, and Y. Wang, "Numerical regularized moment method for high mach number flow," *arXiv preprint arXiv:1011.5787*, 2010.

[36] I. Müller and T. Ruggeri, *Rational extended thermodynamics*, vol. 37. Springer Science & Business Media, 2013.

[37] T. Arima, S. Taniguchi, T. Ruggeri, and M. Sugiyama, "Extended thermodynamics of dense gases," *Continuum Mechanics and Thermodynamics*, vol. 24, no. 4-6, pp. 271–292, 2012.

[38] T. Arima, S. Taniguchi, T. Ruggeri, and M. Sugiyama, "Dispersion relation for sound in rarefied polyatomic gases based on extended thermodynamics," *Continuum Mechanics and Thermodynamics*, vol. 25, no. 6, pp. 727–737, 2013.

[39] M. Pavić, T. Ruggeri, and S. Simić, "Maximum entropy principle for rarefied polyatomic gases," *Physica A: Statistical Mechanics and its Applications*, vol. 392, no. 6, pp. 1302–1317, 2013.

[40] T. Arima, S. Taniguchi, T. Ruggeri, and M. Sugiyama, "Monatomic rarefied gas as a singular limit of polyatomic gas in extended thermodynamics," *Physics Letters A*, vol. 377, no. 34, pp. 2136–2140, 2013.

[41] H. Struchtrup and P. Taheri, "Macroscopic transport models for rarefied gas flows: a brief review," *IMA Journal of Applied Mathematics*, vol. 76, no. 5, pp. 672–697, 2011.

[42] H. Struchtrup and M. Torrilhon, "Regularization of grads 13 moment equations: derivation and linear analysis," *Physics of Fluids (1994-present)*, vol. 15, no. 9, pp. 2668–2680, 2003.

[43] H. Struchtrup, "Stable transport equations for rarefied gases at high orders in the knudsen number," *Physics of Fluids (1994-present)*, vol. 16, no. 11, pp. 3921–3934, 2004.

[44] H. Struchtrup, *Macroscopic transport equations for rarefied gas flows*. Springer, 2005.

[45] H. Struchtrup, "Failures of the Burnett and super-Burnett equations in steady state processes," *Continuum Mechanics and Thermodynamics*, vol. 17, no. 1, pp. 43–50, 2005.

[46] M. Torrilhon and H. Struchtrup, "Regularized 13-moment equations: Shock structure calculations and comparison to Burnett models," *Journal of Fluid Mechanics*, vol. 513, pp. 171–198, 2004.

[47] M. Torrilhon and H. Struchtrup, "Boundary conditions for regularized 13-moment-equations for micro-channel-flows," *Journal of Computational Physics*, vol. 227, no. 3, pp. 1982–2011, 2008.

[48] P. Taheri, M. Torrilhon, and H. Struchtrup, "Couette and Poiseuille microflows: analytical solutions for regularized 13-moment equations," *Physics of Fluids (1994-present)*, vol. 21, no. 1, p. 017102, 2009.

[49] P. Taheri and H. Struchtrup, "Effects of rarefaction in microflows between coaxial cylinders," *Physical Review E*, vol. 80, no. 6, p. 066317, 2009.

[50] P. Taheri and H. Struchtrup, "An extended macroscopic transport model for rarefied gas flows in long capillaries with circular cross section," *Physics of Fluids (1994-present)*, vol. 22, no. 11, p. 112004, 2010.

[51] P. Taheri and H. Struchtrup, "Poiseuille flow of moderately rarefied gases in annular channels," *International Journal of Heat and Mass Transfer*, vol. 55, no. 4, pp. 1291–1303, 2012.

[52] P. Taheri and H. Struchtrup, "Rarefaction effects in thermally-driven microflows," *Physica A: Statistical Mechanics and its Applications*, vol. 389, no. 16, pp. 3069–3080, 2010.

[53] H. Struchtrup and T. Thatcher, "Bulk equations and Knudsen layers for the regularized 13 moment equations," *Continuum Mechanics and Thermodynamics*, vol. 19, no. 3-4, pp. 177–189, 2007.

[54] X.-j. Gu and D. R. Emerson, "A high-order moment approach for capturing non-equilibrium phenomena in the transition regime," *Journal of Fluid Mechanics*, vol. 636, pp. 177–216, 2009.

[55] X. J. Gu, D. R. Emerson, and G.-H. Tang, "Analysis of the slip coefficient and defect velocity in the knudsen layer of a rarefied gas using the linearized moment equations," *Physical Review E*, vol. 81, no. 1, p. 016313, 2010.

[56] X.-J. Gu, D. R. Emerson, and G.-H. Tang, "Kramers problem and the Knudsen minimum: a theoretical analysis using a linearized 26-moment approach," *Continuum Mechanics and Thermodynamics*, vol. 21, no. 5, pp. 345–360, 2009.

[57] A. Rana, M. Torrilhon, and H. Struchtrup, "Heat transfer in micro devices packaged in partial vacuum," in *Journal of Physics: Conference Series*, vol. 362, p. 012034, IOP Publishing, 2012.

[58] A. Rana, M. Torrilhon, and H. Struchtrup, "A robust numerical method for the r13 equations of rarefied gas dynamics: Application to lid driven cavity," *Journal of Computational Physics*, vol. 236, pp. 169–186, 2013.

[59] H. Struchtrup and M. Torrilhon, "Regularized 13 moment equations for hard sphere molecules: Linear bulk equations," *Physics of Fluids (1994-present)*, vol. 25, no. 5, p. 052001, 2013.

[60] A. Bobylev, "The Chapman-Enskog and Grad methods for solving the Boltzmann equation," in *Akademiia Nauk SSSR Doklady*, vol. 262, pp. 71–75, 1982.

[61] Y. Zheng and H. Struchtrup, "Burnett equations for the ellipsoidal statistical bgk model," *Continuum Mechanics and Thermodynamics*, vol. 16, no. 1-2, pp. 97–108, 2004.

[62] H. Grad, "On the kinetic theory of rarefied gases," *Communications on pure and applied mathematics*, vol. 2, no. 4, pp. 331–407, 1949.

[63] H. Grad, "Principles of the kinetic theory of gases," in *Thermodynamik der Gase/Thermodynamics of Gases*, pp. 205–294, Springer, 1958.

[64] P. L. Bhatnagar, E. P. Gross, and M. Krook, "A model for collision processes in gases. i. small amplitude processes in charged and neutral one-component systems," *Physical Review*, vol. 94, no. 3, p. 511, 1954.

[65] E. Shakhov, "Generalization of the krook kinetic relaxation equation," *Fluid Dynamics*, vol. 3, no. 5, pp. 95–96, 1968.

[66] V. Rykov, "A model kinetic equation for a gas with rotational degrees of freedom," *Fluid Dynamics*, vol. 10, no. 6, pp. 959–966, 1975.

[67] H. Struchtrup, "Derivation of 13 moment equations for rarefied gas flow to second order accuracy for arbitrary interaction potentials," *Multiscale Modeling & Simulation*, vol. 3, no. 1, pp. 221–243, 2005.

[68] H. Struchtrup, "Unique moment set from the order of magnitude method," *Kinet. Relat. Models*, vol. 5, pp. 417–440, 2012.

[69] R. P. Feynman, R. B. Leighton, and M. L. Sands, *Mainly mechanics, radiation, and heat*, vol. 1. Addison Wesley Publishing Company, 1963.

[70] G. M. Kremer, *An introduction to the Boltzmann equation and transport processes in gases.* Springer Science & Business Media, 2010.

[71] M. Gad-el Hak, *The MEMS handbook.* CRC press, 2001.

[72] H. Niazmand and B. Rahimi, "Mixed convective slip flows in a vertical parallel plate microchannel with symmetric and asymmetric wall heat fluxes," *Transactions of the Canadian Society for Mechanical Engineering*, vol. 36, no. 3, pp. 207–218, 2012.

[73] B. Rahimi and H. Niazmand, "Effects of high order slip/jump, thermal creep and variable thermo-physical properties on natural convection in microchannels with constant wall heat fluxes," *Heat Transfer Engineering*, vol. 35, no. 18, pp. 1528–1538, 2014.

[74] H. Niazmand and B. Rahimi, "Mixed convective rarefied flows with symmetric and asymmetric heated walls," *Computational Thermal Sciences*, vol. 5, no. 4, pp. 261–272, 2013.

[75] L. H. Holway, "New statistical models for kinetic theory: Methods of construction," *Physics of Fluids*, vol. 9, no. 9, 1966.

[76] B. Rahimi and H. Struchtrup, "Kinetic model and moment method for polyatomic gases," *AIP Conference Proceedings*, vol. 1628, no. 1, 2014.

[77] B. Rahimi and H. Struchtrup, "Capturing non-equilibrium phenomena in rarefied polyatomic gases: A high-order macroscopic model," *Physics of Fluids*, vol. 26, no. 5, 2014.

[78] C. Truesdell and R. Muncaster, "Fundamentals of maxwell's kinetic theory of a simple monatomic gas," *Academic, New York*, 1980.

[79] M. S. Cramer, "Numerical estimates for the bulk viscosity of ideal gases," *Physics of Fluids*, vol. 24, no. 6, 2012.

[80] F. J. Uribe, E. A. Mason, and J. Kestin, "Thermal conductivity of nine polyatomic gases at low density," *Journal of Physical and Chemical Reference Data*, vol. 19, no. 5, pp. 1123–1136, 1990.

[81] W. Dreyer, "Maximisation of the entropy in non-equilibrium," *Journal of Physics A: Mathematical and General*, vol. 20, no. 18, p. 6505, 1987.

[82] M. Kogan, "On the principle of maximum entropy," in *Rarefied Gas Dynamics, Volume 1*, vol. 1, p. 359, 1967.

[83] C. Sluijter, H. Knaap, and J. Beenakker, "Determination of rotational relaxation times of hydrogen isotopes by sound absorption measurements at low temperatures. i," *Physica*, vol. 30, no. 4, pp. 745–762, 1964.

[84] T. Ruggeri and M. Sugiyama, *Rational Extended Thermodynamics beyond the Monatomic Gas*. Springer, 2015.

[85] B. Rahimi and H. Struchtrup, "Refined navier-stokes-fourier equations for rarefied polyatomic gases," in *ASME 2014 12th International Conference on Nanochannels, Microchannels, and Minichannels collocated with the ASME*

2014 4th Joint US-European Fluids Engineering Division Summer Meeting, pp. V001T01A001–V001T01A001, American Society of Mechanical Engineers, 2014.

[86] C. Borgnakke and R. E. Sonntag, *Fundamentals of thermodynamics*. Wiley, 2009.

[87] B. E. Poling, J. M. Prausnitz, J. P. O'connell, *et al.*, *The properties of gases and liquids*, vol. 5. McGraw-Hill New York, 2001.

[88] H. Struchtrup, "Resonance in rarefied gases," *Continuum Mechanics and Thermodynamics*, vol. 24, no. 4-6, pp. 361–376, 2012.

[89] J. C. Maxwell, "On stresses in rarified gases arising from inequalities of temperature," *Philosophical Transactions of the royal society of London*, pp. 231–256, 1879.

[90] F. Sharipov, "Application of the cercignanilampis scattering kernel to calculations of rarefied gas flows. ii. slip and jump coefficients," *European Journal of Mechanics - B/Fluids*, vol. 22, no. 2, pp. 133 – 143, 2003.

[91] C. Tantos, D. Valougeorgis, and A. Frezzotti, "Conductive heat transfer in rarefied polyatomic gases confined between parallel plates via various kinetic models and the {DSMC} method," *International Journal of Heat and Mass Transfer*, vol. 88, pp. 636 – 651, 2015.

[92] M. Gallis, J. Torczynski, and D. Rader, "A computational investigation of noncontinuum gas-phase heat transfer between a heated microbeam and the adjacent ambient substrate," *Sensors and Actuators A: Physical*, vol. 134, no. 1, pp. 57 – 68, 2007.