

Mathematical modeling of rarefied gas-mixtures

Von der Fakultät für Mathematik, Informatik und Naturwissenschaften
der RWTH Aachen University zur Erlangung des akademischen Grades
eines **Doktors der Naturwissenschaften** genehmigte Dissertation

vorgelegt von

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Tag der mündlichen Prüfung: 24 September 2015

Diese Dissertation ist auf den Internetseiten der Universitätsbibliothek
online verfügbar.

Acknowledgements

There are many people whom I wish to thank for their support during the course of my research. First and foremost, it is an honour for me to express my sincere gratitude to my research supervisor, *Prof. Dr. Manuel Torrilhon*. I thank him for his enlightening guidance and teaching, untiring interest, patience and accepting me as his (first) doctoral student. I have learned a lot from him and am really fortunate to have him as my research adviser.

I would like to extend my heartfelt gratitude to *Prof. Dr. Henning Struchtrup*, University of Victoria (UVic), for his generous support and valuable guidance during my visit to UVic. His guidance helped me understand the regularization of moment equations, which resulted into chapter 8 of this thesis.

My sincere thanks goes to *Prof. Dr. Martin Frank* and *Dr. Stephan Martin* for their help and suggestions. I am grateful to my previous advisers, *Prof. Dr. Premananda Bera* (IIT Roorkee) and *Prof. Dr. Meheboob Alam* (JNCASR), for their support and motivation throughout my research, to *Prof. Dr. Santosh Ansumali* (JNCASR) for his recommendation to join this research group, and to my teacher, *Mr. R. P. Giri*, for the wonderful teaching and inspiration. I am appreciative and grateful to *Dr. Anil Nemili and his wife*, *Prof. Dr. Anuj Sharma*, *Prof. Dr. K. R. Arun* and *Dr. Abhay A. Sagade* for their help and support during my stay in Aachen.

I am very thankful to my friend, *Dr. Anirudh Singh Rana*, for many fruitful discussions during the course of this thesis and his help in many ways. I also thank *Behnam* and *Ali* for their help and support during my visit to UVic.

I am grateful to my friend, *Prof. Dr. Priyanka Shukla* (IIT Madras), for her continuous motivation, encouragement and proof-reading of this thesis.

I express my deep gratitude to my parents for their love, blessings and endless support. I owe them more than I could possibly express. I also thank my sisters, brother-in-law and other family members for their support.

I thank *Satya sir*, *Anubhab dada*, *Ujjayan* for their help and motivation. I also thank my colleagues—*Armin*, *Birte*, *Desiree*, *Edgar*, *Emre*, *Graham*, *James*, *Julian*, *Kai*, *Kerstin*, *Kira*, *Neeraj*, *Pascal*, *Peter*, *Philipp*, *Dr. Rich*, *Roman*, *Teddy*, *Thomas*, *Tobias*, *Torsten* and *Zhenning*—for fruitful discussions and helping me in many ways. I extend my thanks to *Brijendra*, *Dinesh*, *Jagabandhu*, *Ram Keval*, *Triveni* and *Vikas* for providing me the papers, which were not accessible here.

I am ever grateful to my institute, **RWTH Aachen University** for providing the necessary infrastructure and financial support, including the travel supports for various conferences and support for visiting UVic.

Finally, I thank the almighty God for his blessings.

Abstract

A mathematical framework based on the higher order Grad's moment equations for studying processes in rarefied gas-mixtures is developed. The fully non-linear Grad's $N \times 13$ -moment ($N \times G13$) and Grad's $N \times 26$ -moment ($N \times G26$) equations for a gaseous mixture comprised of N monatomic-inert-ideal gases are derived. The strategy for computing the production terms (or Boltzmann collision integrals) associated with the moment equations for gaseous mixtures interacting with any interaction potential is presented. Employing this strategy, the explicit expressions of the non-linear production terms associated with the $N \times G13$ and $N \times G26$ equations are computed and presented for Maxwell as well as hard-sphere interaction potentials.

The boundary conditions complementing the $N \times G13$ and $N \times G26$ equations are derived by extending the Maxwell's accommodation model for a single gas to a gaseous mixture. The moment equations and the boundary conditions are then restricted to binary gas mixtures and the linear stability analysis is performed to conclude that the Grad's 2×13 -moment ($2 \times G13$) and Grad's 2×26 -moment ($2 \times G26$) equations for a binary gas-mixture are linearly stable for both Maxwell as well as hard-sphere interaction potentials.

Next, the $2 \times G13$ and $2 \times G26$ equations, specialized to Maxwell and hard-sphere interaction potentials, along with the boundary conditions are exploited to study some benchmark problems of fluid mechanics in simple geometries. The heat transfer in a binary gas-mixture confined between two infinite plates having different temperatures is analyzed with all four types of moment systems ($2 \times G13$ and $2 \times G26$ equations, both with Maxwell and hard-sphere interaction potentials) and the results are compared with those existing in the literature. Furthermore, a one-dimensional problem of binary gas-mixture having one component infinitely diluted is solved *analytically* with all four types of moment systems in order to study the flow of the diluted component in the mixture.

The numerical method based on finite differences for solving the aforementioned moment systems is demonstrated and employed to various problems in order to study the convergence of the numerical method. The convergence is analyzed for the above one-dimensional problems as well as for the standard two-dimensional problems of bottom-heated and lid-driven square cavities. The preliminary results on heat transfer for the latter two problems are also presented. However, the detailed comparison of the results with those obtained with highly accurate (particle based) methods is left for the future.

Moreover, for model reduction, the Grad's moment equations for a binary gas-mixture with Maxwell interaction potential are regularized by employing the order of magnitude method and the regularized 17-moment (R17) equations for a binary gas-mixture with Maxwell interaction potential are derived; the R17 equations are third order accurate in the Knudsen number. The linear stability of R17 equations is analyzed and it is concluded empirically that the R17 equations are linearly stable for binary gas-mixtures with small and moderate mass differences while unstable for those with large mass differences.

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Chapter 1

Introduction

The accurate and efficient modeling of non-equilibrium processes in gases is a real challenge, especially when gases are rarefied. The conventional fluid dynamical descriptions of processes in gases rely on the underlying assumption that the mean-free-path is sufficiently small in comparison to a macroscopic length scale pertaining to the geometry of the problem [18, 62, 102]. This assumption is characterized by a dimensionless parameter, the Knudsen number (Kn), which is defined as the ratio of mean-free-path (λ) to a macroscopic length scale (L) in the system. A gas is said to be in equilibrium when $\text{Kn} \ll 1$ or, in other words, when the mean-free-path is very small in comparison to a macroscopic length scale pertaining to the problem. Thus, the conventional fluid dynamical description of processes in a gas—e.g., by Euler equations or by Navier–Stokes and Fourier (NSF) equations—is valid only when the gas is in local equilibrium or very close to equilibrium, i.e., the Knudsen number is very close to zero.

For rarefied gases, the mean-free-path is not sufficiently small in comparison to the macroscopic length scale. Thus, the fundamental assumption of fluid dynamics extirpates for rarefied gas flows. Consequently, the conventional fluid dynamical equations—e.g., Euler equations or NSF equations—are inadequate for describing non-equilibrium processes in rarefied gases, and therefore more sophisticated models are required for describing them. The typical examples of the non-equilibrium rarefied gas flows are atmospheric re-entry flows and high altitude flights in the outer atmosphere of the earth, and gas flows in complex conduits of micro devices—commonly known as micro flows. In the outer atmosphere of the earth, the density of gases is so low that the mean-free-path ranges in several meters and, therefore, it becomes comparable to a macroscopic length scale (e.g., the length of vehicle) resulting into a large Knudsen number. On the other hand, the size of a micro device is so small that the macroscopic length scale (e.g., the size of device) becomes comparable with the mean-free-path even under standard conditions, again resulting into a large Knudsen number.

1.1 Flow regimes and rarefaction

Depending on the Knudsen number, gas flows can be classified into different regimes [24, 55, 70, 80, 102, 125]:

- (a) Hydrodynamic regime ($\text{Kn} \lesssim 0.01$): Gases in the hydrodynamic regime are close to equilibrium, and therefore processes in this regime can be well-described by the traditional fluid dynamical equations, e.g. by NSF equations.
- (b) Slip flow regime ($0.01 \lesssim \text{Kn} \lesssim 0.1$): Processes in the slip flow regime may still be described with the NSF equations, however they must be furnished with appropriate velocity slip and temperature jump boundary conditions.

- (c) Transition regime ($0.1 \lesssim \text{Kn} \lesssim 10$): Due to strong non-equilibrium, the NSF equations are inadequate for describing processes in the transition regime and a particle based treatment—e.g. by the direct simulation Monte Carlo (DSMC) method [9] or by the *Boltzmann equation*, which is the fundamental equation in kinetic theory—is required for the flow description.
- (d) Free molecular flow regime ($\text{Kn} \gtrsim 10$): In this regime, gas molecules move in free flight without interacting with each other. Therefore, the collisions among the molecules can be neglected in this regime and the flow is governed mainly by the collisions of molecules with walls. Molecular dynamic simulations can be employed to describe processes in this regime.

The transition regime can further be split into two parts: $0.1 \lesssim \text{Kn} \lesssim 1$ and $1 \lesssim \text{Kn} \lesssim 10$. The latter part (regime with $1 \lesssim \text{Kn} \lesssim 10$) is sometimes referred to as the kinetic regime [115]. In the kinetic regime, non-equilibrium is so strong that it becomes indispensable either to solve the Boltzmann equation directly or to use the DSMC method for describing a process, even though both the methods are computationally expensive. Nevertheless, in the former part of the transition regime (regime with $0.1 \lesssim \text{Kn} \lesssim 1$), processes can still be described macroscopically by considering larger set of field variables. Moreover, direct solutions of the Boltzmann equation or DSMC method are increasingly expensive in this regime.

In terms of the above classification of flow regimes, a gas is said to be rarefied when it is outside the hydrodynamic regime, i.e., when the NSF equations, usually, start losing their validity [102]. The rarefied gases exhibit several interesting effects, such as velocity slip and temperature jump [24, 25, 51, 95, 127], Knudsen layers [63, 94, 95, 107], thermal creep or transpiration [53, 55, 76, 77, 91], thermal stress [92, 94, 96], heat flux without temperature gradients [2, 3, 79, 112], etc. These effects are referred to as the non-equilibrium effects and they are solely the manifestation of rarefaction. Although, the thermal creep and the velocity slip and temperature jump can be construed by the NSF equations when supplemented with the appropriate boundary conditions, the other rarefaction effects cannot be captured by NSF equations and, therefore, more sophisticated models are required to capture these effects.

1.2 Elements of kinetic theory

1.2.1 Single gases

It is generally accepted that processes in rarefied gases can be described by means of kinetic theory based on the statistical description of the gas. The fundamental quantity in kinetic theory is the velocity distribution function (also referred to as the phase density or just the distribution function) of the gas. The governing equation for the velocity distribution function is the Boltzmann equation [12], which is capable of describing processes in all flow regimes [19, 46, 102, 105, 125]. Nevertheless, it is not easy to deal with the Boltzmann equation due to the presence of the Boltzmann collision operator (the right-hand side of the Boltzmann equation), which incorporates the collisions among gas molecules and have very involved mathematical structure that renders the Boltzmann equation to become a non-linear integro-differential equation. For the mathematical details and treatment of the Boltzmann equation the reader is referred to the textbook [22] and the treatise [121]. Owing to the mathematical structure

of the Boltzmann collision operator, obtaining the exact solution of the Boltzmann equation is a chimera whereas its direct numerical solutions are forbiddingly expensive, especially in the transition regime.

Alternatively, kinetic theory offers the approximate solutions of the Boltzmann equation. Aiming to simplify the formidable Boltzmann collision operator—which is essentially the main source of difficulty in dealing with the Boltzmann equation—while retaining its basic attributes, few simplified models for the Boltzmann collision operator were introduced in the literature. These models are generically referred to as the *kinetic models*. One of the oldest kinetic model which replaces the Boltzmann collision operator in the Boltzmann equation with a simple integral-free relaxation model is the well-known *Bhatnagar-Gross-Krook (BGK) model* [8]. The BGK model retains some of the basic properties of the Boltzmann collision operator (e.g., conservation laws and H -theorem), but fails to yield the correct value of the Prandtl number for monatomic gases [20, 60, 102]. Nevertheless, the BGK model has been extensively used in the literature, since it preserves the basic features of the Boltzmann equation reasonably well. There exist other popular kinetic models, e.g., ES-BGK model [50], S-model [85], etc., in the literature which produce the correct value of the Prandtl number for monatomic gases, nonetheless these kinetic models usually exhibit very different behaviour from the realistic one in the transition regime and are beyond the scope of this thesis.

In kinetic theory, the two most celebrated and classical techniques—which consider the full Boltzmann equation—for finding the approximate solutions of the Boltzmann equation are the *Chapman-Enskog expansion method* [13, 23, 28, 40, 65] and the *Grad's method of moments* [35, 36, 71]. Both these methods can be found in the standard textbooks, e.g., [18, 19, 33, 49, 57, 60, 102, 119].

The Chapman-Enskog expansion method is applicable to processes, which are close to equilibrium ($\text{Kn} \rightarrow 0$). The method relies on an asymptotic analysis in powers of the Knudsen number. In this method, the velocity distribution function is expanded in powers of the Knudsen number around the velocity distribution function in equilibrium (also termed as equilibrium distribution function). The expansion for the velocity distribution function is substituted into the Boltzmann equation and the coefficients of each power of the Knudsen number are compared on both sides of the equation. The procedure leads to the constitutive relations of different orders for the well-known conservation laws of fluid dynamics. At zeroth order, the method gives the Euler equations; at first order, it yields the classical NSF equations; at second order, it results into Burnett equations; at third order, it leads to the so-called super-Burnett equations and so on. The super-Burnett equations are already so involved that the full super-Burnett equations do not seem to exist in present day literature. Besides the complex structure due to presence of the higher order derivatives, the Burnett equations are known to suffer from inherent (linear) instabilities [10, 11, 120]. Additionally, the Burnett equations lack the proper boundary conditions [102].

In the Grad's method of moments, the Boltzmann equation is supplanted by a system of first order partial differential equations, referred to as *moment equations*. Moment equations are the evolution equations for the quantities, called *moments*, which are directly related to the velocity distribution function. Furthermore, moment equations form an infinite set of coupled

first order partial differential equations, which is not closed. The Grad’s method of moments truncates this infinite set at a certain level and to close the set at this level, it approximates the velocity distribution function by an expansion in orthogonal polynomials—usually, Hermite polynomials—in (peculiar) velocity of the molecule and the unknown coefficients in the expansion are obtained by satisfying the definition of the moments considered at that level. The moment equations resulting from the Grad’s method of moments (in case of single gases) are always linearly stable [10]. Unfortunately, the Grad’s method of moments does not, a priori, grant the touchstone on which and how many moments need to be considered for describing a process with a given Knudsen number. However, it can be stated empirically that the number of moments considered ought to be increased with increasing Knudsen number [106]. Furthermore, due to their hyperbolic nature, the well-known Grad’s 13-moment (G13) equations obtained via Grad’s method of moments manifest the non-physical sub-shocks for flows with Mach numbers above 1.65 [71, 122] and do not capture the Knudsen boundary layers [99, 101]. Nevertheless, by considering more moments, the Knudsen boundary layers can be captured [82, 99] and the smooth shock structure can be obtained for higher Mach numbers [122].

In order to surmount the deficiencies inherent to both Chapman–Enskog expansion method and Grad’s method of moments, Struchtrup and Torrilhon [106] introduced a new method, often referred to as the regularized moment method, which regularizes the original G13 equations by means of a Chapman–Enskog expansion around a pseudo-equilibrium leading to the regularized 13-moment (R13) equations. The method has been developed initially for Maxwell interaction potential as well as for BGK model [100, 102, 106] and subsequently also for hard-sphere interaction potential [108]. The R13 equations retain the enviable features of both the Chapman–Enskog expansion method and the Grad’s method of moments while avert their shortcomings. The R13 equations are always linearly stable and engender to smooth shock structures for all Mach numbers [106, 117]. Since their derivation, the R13 equations have been successfully employed to describe several rarefaction effects, see e.g., [39, 79, 81, 89, 109–111, 113, 114, 116, 117, 123].

There are other models—for instance, the maximum-entropy model [54, 62, 71] and its variants [68, 84]—as well in the literature for describing the non-equilibrium processes in the transition regime, nonetheless they are also beyond the scope of this thesis.

1.2.2 Gaseous mixtures

In practice, the gaseous mixtures are encountered more often than a single gas. Owing to different masses and different mean molecular velocities of different constituents in a gas-mixture, it is futile to consider a single velocity distribution function, i.e., the velocity distribution function of the whole mixture, for describing processes in gaseous mixtures. Therefore, the state of a gas-mixture comprising of N components is fully described by N velocity distribution functions (the velocity distribution function for each constituent in the mixture), which are governed by the N Boltzmann equations. The Boltzmann collision operators present in the Boltzmann equations for a gas-mixture are mathematically more intricate than those present in a single gas because the molecules of a constituent in the mixture collide with the molecules of the same constituent as well as with those of other constituents. Obviously, the direct solutions of the Boltzmann

equations or the DSMC solutions for gas-mixture flows are also computationally expensive in the transition regime.

Again, other alternatives for modeling flows of gaseous mixtures are offered by kinetic theory. Although, there are not as many kinetic models for gas-mixtures as for single gases, several authors have attempted for a BGK-like model for gas-mixtures, see e.g., [1, 14, 15, 32, 47, 64, 69, 90], however most of these models either fail to reproduce the correct transport coefficients or do not satisfy some fundamental properties. The recent works [14, 15] first consider the transport coefficients computed either by hydrodynamic limit of the Boltzmann equation or by experiments and then construct the BGK-like model by fitting these coefficients into the model, however both the works are restricted to obtain only correct Fick's and Newton's laws.

Both the Chapman–Enskog expansion method and the Grad's method of moments have also been developed for gaseous mixtures, see the textbook [23] for the former, and the references [128, 130] and the textbook [129] for the latter. Nonetheless, the use of higher order equations (beyond hydrodynamic level) resulting from the Chapman–Enskog expansion is not recommended due to aforementioned reasons in case of a single gas.

Moment equations for gaseous mixtures have been considered in the context of extended thermodynamics in [48] and have further been studied in [4, 5, 59]. However, typically, simplified models for the Boltzmann collision operators have been used and specific equations have only been given up to 13 moments for each constituent. Reference [128] can be regarded as pioneering work, which studies Grad's method of moments in a multi-component approach for gas-mixtures by considering 13 moments for each constituent. Reference [130] discusses the higher order Grad's moment equations too, however, it does not include—for example—the third rank tensors in the velocity distribution functions. Moreover, references [128, 130] consider the *production terms* or *Boltzmann collision integrals*—the terms resulting through the Boltzmann collision operator while deriving the moment equations—based on the *linearized* Boltzmann collision operators.

Consequently, the regularized moment method for gas-mixtures does not exist in the present literature, because the derivation of regularized moment equations requires the higher order moment equations of Grad (see [100, 102, 106]), which were not available in the literature until recently, see [45].

Despite the success of the Grad's method of moments and its variants—e.g., regularized moment method of Struchtrup and Torrilhon [106], globally hyperbolic regularization method of Cai et al. [17], etc.—in case of a single gas, the Grad's method of moments for gas-mixtures has received much less attention because—among other reasons—the proper boundary conditions associated with the Grad's moment equations for gas mixtures were also not available in the literature until recently (see [45]) and the computation of the full production terms for moment equations is overwhelmingly arduous, particularly in multi-temperature theory illustrated below.

The multi-temperature theory which considers different temperatures for different species in a gas-mixture is more authentic than the single temperature theory which assumes a common average temperature for the whole gas-mixture and in many physical situations—especially, in plasma physics—it becomes indispensable to use the former [83, 129]. Nevertheless, the latter is used more often than the former in the literature for simplicity, see e.g., [6, 23, 60, 73]. References

[4, 5, 48, 59, 128–130] also employ a single temperature theory, although the reference [48] and the textbook [129] consider the multi-temperature theory to explain its importance but switches promptly to a single temperature theory for simplicity.

1.3 Present work and organization of the thesis

1.3.1 Present work

The goal of the present thesis is to provide a framework of higher order Grad’s moment equations for studying the non-equilibrium processes in the context of gaseous mixture. This work contains the derivation of fully non-linear Grad’s $N \times 13$ -moment ($N \times G13$) equations and Grad’s $N \times 26$ -moment ($N \times G26$) equations for a gaseous mixture consisting of N monatomic-inert-ideal (simple) gases interacting with (a) Maxwell and (b) hard-sphere interaction potentials (the gas molecules interacting with Maxwell interaction potential are commonly referred to as Maxwell molecules and those interacting with hard-sphere interaction potential are commonly referred to as hard spheres in the literature), including the computation of explicit production terms for these equations. The present work also derives the complete set of boundary conditions—accompanying the aforementioned moment equations—based on Maxwell accommodation model. Further, the linear stability of the derived moment equations in case of binary gas-mixtures is verified and the linearized equations are exploited to study some of the benchmark problems for binary gas-mixtures in one and two dimensions. Additionally, the regularized moment equations are derived for binary gas-mixtures interacting with Maxwell interaction potential.

1.3.2 Organization of the thesis

Chapter 2

The chapter starts with the dynamics of a binary collision. Further, it introduces the phase densities and the Boltzmann equations for gaseous mixtures, and relates the physical quantities with the phase densities through the definition of moments. After this, the Boltzmann H -theorem for gas-mixtures is proved. Finally, the Grad’s method of moments is detailed and the $N \times G13$ and $N \times G26$ equations for N -component gaseous mixture are derived.

Chapter 3

This chapter demonstrates the methodology for computing the production terms associated with moment equations for gas-mixtures and presents the explicit expressions of the production terms for (a) Maxwell and (b) hard-sphere interaction potentials.

Chapter 4

The chapter addresses the issue of boundary conditions and extends the Maxwell accommodation model for single gases to gaseous mixtures in order to derive the complete set of boundary conditions complementing the moment equations for gaseous mixtures.

Chapter 5

In this chapter, the linear stability analysis is performed in order to verify that the $2\times G13$ and $2\times G26$ equations for binary gas-mixtures interacting with (a) Maxwell and (b) hard-sphere interaction potentials are stable with respect to linear wave perturbations.

Chapter 6

This chapter bears on the study of one-dimensional benchmark problem of heat transfer in binary gas-mixtures confined between two infinite parallel plates having different temperatures, and compares the results with those existing in the literature. Furthermore, another one-dimensional problem of a binary gas-mixtures with one component infinitely diluted is considered in this chapter, and for this problem, the analytical solutions are obtained and compared with the corresponding solutions obtained through the first order Chapman–Enskog expansion.

Chapter 7

The chapter discusses a numerical framework—for the linearized moment equations detailed in chapter 5—based on finite differences and applies it to solve a few one- and two-dimensional problems of binary gas-mixtures. The main focus of this chapter is on studying the convergence of the numerical method for different problems; in one dimension, the convergence is analyzed for the problems of chapter 6 whereas for the convergence analysis of two-dimensional problems, the two-dimensional benchmark problems of bottom-heated square cavity and lid-driven square cavity are considered.

Chapter 8

The chapter focuses on the detailed derivation of regularized moment equations for binary gas-mixtures interacting with Maxwell interaction potential via the order of magnitude method.

Chapter 9

The final conclusions and the outlook are presented in this chapter.

Chapter 2

Moment equations for gaseous mixtures

It is generally accepted that the description of a process in a gas through the infinite hierarchy of moment equations is equivalent to its description with the Boltzmann equation [102]. This chapter presents the derivation of moment equations for a mixture of monatomic-inert-ideal gases.

2.1 Boltzmann equations for mixture

2.1.1 Dynamics of binary collision

A binary collision between two molecules of masses m_α and m_β in a gaseous mixture leads to the following velocity transformation [60]:

$$\mathbf{c}'_\alpha = \mathbf{c}_\alpha - 2\mu_\beta \mathbf{k}_{\alpha\beta} (\mathbf{k}_{\alpha\beta} \cdot \mathbf{g}_{\alpha\beta}), \quad \mathbf{c}'_\beta = \mathbf{c}_\beta + 2\mu_\alpha \mathbf{k}_{\alpha\beta} (\mathbf{k}_{\alpha\beta} \cdot \mathbf{g}_{\alpha\beta}), \quad (2.1)$$

where $\mathbf{c}'_\alpha$ and $\mathbf{c}'_\beta$ are the velocities of the molecules α and β after the collision while $\mathbf{c}_\alpha$ and $\mathbf{c}_\beta$ are the velocities prior to the collision, $\mathbf{k}_{\alpha\beta}$ is the unit vector pointing from the center of α -molecule to that of β -molecule at the time of collision, $\mathbf{g}_{\alpha\beta} = \mathbf{c}_\alpha - \mathbf{c}_\beta$ is the relative velocity of α -molecule with respect to β -molecule, and $\mu_\alpha = m_\alpha/(m_\alpha + m_\beta)$ and $\mu_\beta = m_\beta/(m_\alpha + m_\beta)$ are the mass ratios of α and β molecules, respectively; the notations μ_α and μ_β for the mass ratios have been adopted from the textbook [28]. For more details on the dynamics of binary collision, the reader is referred to the textbook [60].

2.1.2 Boltzmann equations

The state of a gaseous mixture consisting of N monatomic-inert-ideal gases in the phase space is characterized by N velocity distribution functions of individual gases in the mixture, i.e., by $f_\alpha \equiv f_\alpha(\mathbf{r}, \mathbf{c}_\alpha, t)$ for $\alpha = 1, 2, \dots, N$. Here, $\mathbf{r} \equiv (x, y, z)^\top$, $\mathbf{c}_\alpha \equiv (c_x^{(\alpha)}, c_y^{(\alpha)}, c_z^{(\alpha)})^\top$ and t stand for position, instantaneous velocity of the α -constituent and time; moreover, we shall also use the notation x_i for a general component of the position vector $\mathbf{r}$. Each distribution function f_α is such that $f_\alpha d\mathbf{r} d\mathbf{c}_\alpha$ gives the number of molecules of the α -constituent at time t in an infinitesimal volume $d\mathbf{r}$ centred around position $\mathbf{r}$ whose velocities belong to an infinitesimal volume $d\mathbf{c}_\alpha$ in velocity space located around $\mathbf{c}_\alpha$. Thus, the number density of the α -constituent

is given by

$$n_\alpha \equiv n_\alpha(\mathbf{r}, t) = \int_{\mathbb{R}^3} f_\alpha d\mathbf{c}_\alpha. \quad (2.2)$$

In (2.2) and throughout this thesis, the integration over any velocity space stands for the volume integrals over all components of that velocity, e.g., $d\mathbf{c}_\alpha = dc_x^{(\alpha)} dc_y^{(\alpha)} dc_z^{(\alpha)}$, and the limits of integration for each component of the velocity extend over $\mathbb{R}$, unless otherwise stated.

The N velocity distribution functions in a N -component gas-mixture are governed by N Boltzmann equations

$$\frac{\partial f_\alpha}{\partial t} + c_i^{(\alpha)} \frac{\partial f_\alpha}{\partial x_i} + F_i^{(\alpha)} \frac{\partial f_\alpha}{\partial c_i^{(\alpha)}} = \sum_{\beta=1}^N \int_{\mathbb{R}^3} \int_0^{2\pi} \int_0^\infty (f'_\alpha f'_\beta - f_\alpha f_\beta) g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\beta, \quad \alpha = 1, 2, \dots, N. \quad (2.3)$$

In (2.3), $\mathbf{F}_\alpha \equiv (F_x^{(\alpha)}, F_y^{(\alpha)}, F_z^{(\alpha)})^\top$ is the external force per unit mass acting on the α -constituent, the phase densities with primes correspond to the phase densities with post-collisional velocities $(\mathbf{c}'_\alpha, \mathbf{c}'_\beta)$, e.g., $f'_\alpha \equiv f_\alpha(\mathbf{r}, \mathbf{c}'_\alpha, t)$, b is the collision parameter, the angle ϵ describes the orientation of the collision plane, and repeated indices (throughout the thesis except the indices n , t_i and t_j in chapter 4) imply Einstein summation convention. The right-hand side of the Boltzmann equation (2.3) accounts for the collisions among various molecules in the mixture and is termed as *Boltzmann collision operator* for the gas-mixture. The *equilibrium* state of the gas-mixture is defined in such a way that it renders the Boltzmann collision operator in the Boltzmann equation (2.3) to vanish for each α .

Henceforth, unless necessary, only one integration symbol without mentioning limits will be used for integrations over all variables in order to make the notations compact.

2.2 Moments of phase density

For a quantity, $\psi_\alpha \equiv \psi(\mathbf{r}, \mathbf{c}_\alpha, t)$, its average value $\langle \psi_\alpha \rangle$ is defined in terms of the distribution function f_α as

$$n_\alpha \langle \psi_\alpha \rangle = \int \psi_\alpha f_\alpha d\mathbf{c}_\alpha. \quad (2.4)$$

The quantity on the right-hand side of (2.4) is referred to as the *moment* of phase density with respect to ψ_α .

The average value of ψ_α for the whole mixture, $\langle \psi \rangle$, is given by

$$n \langle \psi \rangle = \sum_{\alpha=1}^N n_\alpha \langle \psi_\alpha \rangle = \sum_{\alpha=1}^N \int \psi_\alpha f_\alpha d\mathbf{c}_\alpha, \quad \text{where} \quad n = \sum_{\alpha=1}^N n_\alpha \quad (2.5)$$

is the number density of the whole gas-mixture and the quantity $n \langle \psi \rangle$ is referred to as the total quantity of the whole gas-mixture corresponding to $n_\alpha \langle \psi_\alpha \rangle$.

Some of the physical quantities for α -species, e.g., number density $n_\alpha(\mathbf{r}, t)$, mass density

$\rho_\alpha(\mathbf{r}, t)$, macroscopic velocity $\mathbf{v}_\alpha(\mathbf{r}, t)$, temperature $T_\alpha(\mathbf{r}, t)$, stress tensor $\boldsymbol{\sigma}_\alpha(\mathbf{r}, t)$ and heat flux $\mathbf{q}_\alpha(\mathbf{r}, t)$ of α -constituent are expressed in form of moments of phase density on choosing ψ_α as 1, m_α , $\mathbf{c}_\alpha$, $\frac{1}{2}m_\alpha C_\alpha^2$, $m_\alpha C_{\langle i}^{(\alpha)} C_{j \rangle}^{(\alpha)}$, $\frac{1}{2}m_\alpha C_\alpha^2 C_i^{(\alpha)}$ in (2.4):

$$\left. \begin{array}{ll} \text{number density} & n_\alpha = n_\alpha \langle 1 \rangle = \int f_\alpha d\mathbf{c}_\alpha, \\ \text{mass density} & \rho_\alpha = n_\alpha \langle m_\alpha \rangle = m_\alpha \int f_\alpha d\mathbf{c}_\alpha = m_\alpha n_\alpha, \\ \text{macroscopic velocity} & n_\alpha \mathbf{v}_\alpha = n_\alpha \langle \mathbf{c}_\alpha \rangle = \int \mathbf{c}_\alpha f_\alpha d\mathbf{c}_\alpha, \\ \text{temperature} & \frac{3}{2} \rho_\alpha \theta_\alpha = \frac{3}{2} k n_\alpha T_\alpha = \frac{1}{2} n_\alpha \langle m_\alpha C_\alpha^2 \rangle = \frac{1}{2} m_\alpha \int C_\alpha^2 f_\alpha d\mathbf{c}_\alpha, \\ \text{stress tensor} & \sigma_{ij}^{(\alpha)} = n_\alpha \langle m_\alpha C_{\langle i}^{(\alpha)} C_{j \rangle}^{(\alpha)} \rangle = m_\alpha \int C_{\langle i}^{(\alpha)} C_{j \rangle}^{(\alpha)} f_\alpha d\mathbf{c}_\alpha, \\ \text{heat flux} & q_i^{(\alpha)} = \frac{1}{2} n_\alpha \langle m_\alpha C_\alpha^2 C_i^{(\alpha)} \rangle = \frac{1}{2} m_\alpha \int C_\alpha^2 C_i^{(\alpha)} f_\alpha d\mathbf{c}_\alpha. \end{array} \right\} \quad (2.6)$$

In (2.6), $\theta_\alpha = k T_\alpha / m_\alpha$ is the temperature of the α -constituent in energy units with k being the Boltzmann constant, $\mathbf{C}_\alpha(\mathbf{r}, \mathbf{c}_\alpha, t) = \mathbf{c}_\alpha - \mathbf{v}(\mathbf{r}, t)$ is the peculiar velocity of an α -molecule with respect to the gas-mixture with $\mathbf{v}(\mathbf{r}, t)$ being the *hydrodynamic velocity* (or the *mass average velocity* [49] or the *mass-velocity* [23] or the *barycentric velocity* [48]) of the gas-mixture (defined below), and the angular brackets around the indices indicate the symmetric and trace-free tensor [102]. Denoting the total density, total pressure, total stress tensor and total heat flux for the whole gas-mixture by ρ , p , $\boldsymbol{\sigma}$ and $\mathbf{q}$, respectively, and average molecular velocity, average temperature for the whole gas-mixture by $\langle \mathbf{c} \rangle$ and T , respectively, (2.5) and (2.6) imply

$$\rho = \sum_{\alpha=1}^N \rho_\alpha, \quad n \langle \mathbf{c} \rangle = \sum_{\alpha=1}^N n_\alpha \mathbf{v}_\alpha, \quad p = k n T = \sum_{\alpha=1}^N k n_\alpha T_\alpha, \quad \sigma_{ij} = \sum_{\alpha=1}^N \sigma_{ij}^{(\alpha)}, \quad q_i = \sum_{\alpha=1}^N q_i^{(\alpha)}. \quad (2.7)$$

The hydrodynamic velocity $\mathbf{v}(\mathbf{r}, t)$ is defined as the ratio of total momentum density to total density:

$$\mathbf{v} = \frac{1}{\rho} \sum_{\alpha=1}^N \rho_\alpha \mathbf{v}_\alpha = \frac{1}{\rho} \sum_{\alpha=1}^N m_\alpha \int \mathbf{c}_\alpha f_\alpha d\mathbf{c}_\alpha, \quad (2.8)$$

In general, the hydrodynamic velocity $\mathbf{v}$ is different from the average molecular velocity $\langle \mathbf{c} \rangle$ as well as from the macroscopic velocity of each component $\mathbf{v}_\alpha$. In a gaseous mixture, this fact leads to a phenomenon called *diffusion* of one component with respect to another. The diffusion is characterized by the *diffusion velocity* of each component, which can be defined as either the difference between macroscopic velocity of the component $\mathbf{v}_\alpha$ and hydrodynamic velocity of the gas-mixture $\mathbf{v}$ or the difference between macroscopic velocity of the component $\mathbf{v}_\alpha$ and average molecular velocity of the gas-mixture $\langle \mathbf{c} \rangle$. The diffusion velocity of the α -constituent in the former case is $\mathbf{u}_\alpha = \mathbf{v}_\alpha - \mathbf{v}$ while that in the latter case is $\mathbf{U}_\alpha = \mathbf{v}_\alpha - \langle \mathbf{c} \rangle$.

Generally speaking, $\mathbf{u}_\alpha$ is appropriate for describing acceleration and friction driven processes whereas $\mathbf{U}_\alpha$ is sometimes more appropriate for describing some processes in slow moving gases [28]. Nevertheless, in this thesis, we shall adopt only the former ($\mathbf{u}_\alpha$) as a definition of the

diffusion velocity of the constituent α in a gaseous mixture.

Owing to relations (2.7)₁ and (2.8), the diffusion velocity $\mathbf{u}_\alpha$ satisfies

$$\sum_{\alpha=1}^N \rho_\alpha \mathbf{u}_\alpha = \mathbf{0}. \quad (2.9)$$

For any other value of ψ_α than those chosen above, the moments defined by (2.4) do not have physical meanings in general. Nevertheless, it is worth introducing the generic form of a trace-free moment for species of type α as

$$u_{i_1 \dots i_n}^{a(\alpha)} \equiv u_{i_1 \dots i_n}^{a(\alpha)}(\mathbf{r}, t) = m_\alpha \int C_\alpha^{2a} C_{i_1}^{(\alpha)} C_{i_2}^{(\alpha)} \dots C_{i_n}^{(\alpha)} f_\alpha d\mathbf{c}_\alpha \quad \text{with } a, n \in \mathbb{N}_0. \quad (2.10)$$

Clearly,

$$\rho_\alpha = u^{0(\alpha)}, \quad \rho_\alpha u_i^{(\alpha)} = u_i^{0(\alpha)}, \quad \rho_\alpha \theta_\alpha = \frac{1}{3} u^{1(\alpha)}, \quad \sigma_{ij}^{(\alpha)} = u_{ij}^{0(\alpha)} \quad \text{and} \quad q_i^{(\alpha)} = \frac{1}{2} u_i^{1(\alpha)}. \quad (2.11)$$

2.3 Boltzmann's H -theorem for gas-mixture

Consider a *uniform* (space independent) N -component simple gaseous mixture (i.e., the phase densities f_α of the constituents do not depend on $\mathbf{r}$) whose molecules are subject to *no external forces*, i.e., $\mathbf{F}_\alpha = \mathbf{0}$ for all α . The Boltzmann equation (2.3) for each α reduces to

$$\frac{\partial f_\alpha}{\partial t} = \sum_{\beta=1}^N \int (f'_\alpha f'_\beta - f_\alpha f_\beta) g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\beta. \quad (2.12)$$

The Boltzmann's H -theorem for gas-mixtures states that *in a uniform gas-mixture when no external forces act upon the molecules, the quantity*

$$H = \sum_{\alpha=1}^N \int f_\alpha \ln f_\alpha d\mathbf{c}_\alpha \quad (2.13)$$

is always a non-increasing function of time. The proof of the theorem is as follows.

The partial derivative of H with respect to t yields

$$\frac{\partial H}{\partial t} = \sum_{\alpha=1}^N \int (1 + \ln f_\alpha) \frac{\partial f_\alpha}{\partial t} d\mathbf{c}_\alpha.$$

Owing to (2.12), the above equation reads

$$\frac{\partial H}{\partial t} = \sum_{\alpha, \beta=1}^N \int (1 + \ln f_\alpha) (f'_\alpha f'_\beta - f_\alpha f_\beta) g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\alpha d\mathbf{c}_\beta.$$

Using the symmetry property of the collision integral [28], it further simplifies to

$$\begin{aligned}\frac{\partial H}{\partial t} &= \frac{1}{4} \sum_{\alpha, \beta=1}^N \int (\ln f_\alpha + \ln f_\beta - \ln f'_\alpha - \ln f'_\beta) (f'_\alpha f'_\beta - f_\alpha f_\beta) g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\alpha d\mathbf{c}_\beta \\ &= \frac{1}{4} \sum_{\alpha, \beta=1}^N \int \ln \left(\frac{f_\alpha f_\beta}{f'_\alpha f'_\beta} \right) (f'_\alpha f'_\beta - f_\alpha f_\beta) g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\alpha d\mathbf{c}_\beta.\end{aligned}\quad (2.14)$$

Since

$$\ln \left(\frac{f_\alpha f_\beta}{f'_\alpha f'_\beta} \right) \geq 0 \quad \text{iff} \quad f_\alpha f_\beta \geq f'_\alpha f'_\beta, \quad \text{and} \quad \ln \left(\frac{f_\alpha f_\beta}{f'_\alpha f'_\beta} \right) = 0 \quad \text{iff} \quad f_\alpha f_\beta = f'_\alpha f'_\beta,$$

it follows that

$$\frac{\partial H}{\partial t} \leq 0, \quad (2.15)$$

i.e., H is a non-increasing function of time. This completes the proof of the theorem.

The equality in (2.15) holds if $f_\alpha f_\beta = f'_\alpha f'_\beta$ or $\ln f_\alpha + \ln f_\beta = \ln f'_\alpha + \ln f'_\beta$ for all α, β . In other words, the equality in (2.15) holds if $\ln f_\alpha$ for all α are the summational invariants. Conversely, if $\ln f_\alpha$ for all α are the summational invariants, then (2.12) implies $\partial f_\alpha / \partial t = 0$ for each α and (2.14) implies $\partial H / \partial t = 0$. Now, in the equilibrium state, the Boltzmann collision operators for each α must vanish, i.e.,

$$\sum_{\beta=1}^N \int (f'_\alpha f'_\beta - f_\alpha f_\beta) g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\beta = 0 \quad \forall \quad \alpha. \quad (2.16)$$

It turns out that (2.16) admits one and only one solution which must be such that $\ln f_\alpha$ for each α is a summational invariant [28]. Further, since $\ln f_\alpha$ for each α is a summational invariant, it must be expressed as a linear combination of known summational invariants: mass, momentum and energy of the respective constituent, so that

$$\ln f_{\alpha|\text{eqb}} = m_\alpha \mathcal{A}_\alpha + m_\alpha \mathbf{c}_\alpha \cdot \mathbf{B}_\alpha + \frac{1}{2} m_\alpha c_\alpha^2 \mathcal{D}_\alpha, \quad (2.17)$$

where the unknown coefficients $\mathcal{A}_\alpha$, $\mathbf{B}_\alpha$ and $\mathcal{D}_\alpha$ are independent of $\mathbf{r}$ and t , since the equilibrium state corresponds to uniform steady state. These unknown coefficients are obtained by using the definitions of the hydrodynamic variables: n_α for all α , $\mathbf{v}$ and T . The details of the calculation are omitted here and they can be found in the textbooks [28, 60]. Finally, one obtains the equilibrium distribution functions as

$$f_{\alpha|\text{eqb}} = n_\alpha \left(\frac{m_\alpha}{2\pi kT} \right)^{3/2} \exp \left(-\frac{m_\alpha C_\alpha^2}{2kT} \right) \quad \text{for} \quad \alpha = 1, 2, \dots, N. \quad (2.18)$$

2.4 Moment equations

The governing equation for the moment (2.4) is obtained by multiplying the Boltzmann equation (2.3) with ψ_α and subsequently integrating over the velocity space $\mathbf{c}_\alpha$:

$$\int \psi_\alpha \left(\frac{\partial f_\alpha}{\partial t} + c_i^{(\alpha)} \frac{\partial f_\alpha}{\partial x_i} + F_i^{(\alpha)} \frac{\partial f_\alpha}{\partial c_i^{(\alpha)}} \right) d\mathbf{c}_\alpha = \sum_{\beta=1}^N \int \psi_\alpha (f'_\alpha f'_\beta - f_\alpha f_\beta) g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\alpha d\mathbf{c}_\beta.$$

Using the symmetry property of the Boltzmann collision operator, the above equation reads

$$\begin{aligned} \frac{D}{Dt} \int \psi_\alpha f_\alpha d\mathbf{c}_\alpha + \frac{\partial}{\partial x_i} \int \psi_\alpha C_i^{(\alpha)} f_\alpha d\mathbf{c}_\alpha + \frac{\partial v_i}{\partial x_i} \int \psi_\alpha f_\alpha d\mathbf{c}_\alpha - \int C_i^{(\alpha)} \frac{\partial \psi_\alpha}{\partial x_i} f_\alpha d\mathbf{c}_\alpha \\ - \int \left(\frac{D\psi_\alpha}{Dt} + F_i^{(\alpha)} \frac{\partial \psi_\alpha}{\partial c_i^{(\alpha)}} \right) f_\alpha d\mathbf{c}_\alpha = \sum_{\beta=1}^N \int (\psi'_\alpha - \psi_\alpha) f_\alpha f_\beta g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\alpha d\mathbf{c}_\beta, \end{aligned} \quad (2.19)$$

where $\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$ is the material derivative. We refer to (2.19) as the *transfer equation* and it is also the *moment equation* for the quantity $n_\alpha \langle \psi_\alpha \rangle$.

The moment equations for various moments are obtained by choosing various values of ψ_α in the transfer equation (2.19). However, the underlined term in the transfer equation (2.19)—no matter what the value of ψ_α is chosen—always render to produce higher order moments. Therefore, the moment equations form an infinite hierarchy of partial differential equations. However, in practice, only a finite number of moment equations are used.

The moment equations for physical quantities of the α -constituent ($\alpha = 1, 2, \dots, N$) are obtained by choosing ψ_α as m_α , $m_\alpha C_i^{(\alpha)}$, $\frac{1}{2} m_\alpha C_\alpha^2$, $m_\alpha C_{\langle i}^{(\alpha)} C_{j \rangle}^{(\alpha)}$, $\frac{1}{2} m_\alpha C_\alpha^2 C_i^{(\alpha)}$ in the transfer equation (2.19). They read

$$\frac{D\rho_\alpha}{Dt} + \frac{\partial(\rho_\alpha u_i^{(\alpha)})}{\partial x_i} + \rho_\alpha \frac{\partial v_i}{\partial x_i} = \mathcal{P}^{0(\alpha)}, \quad (2.20)$$

$$\frac{D(\rho_\alpha u_i^{(\alpha)})}{Dt} + \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{\partial(\rho_\alpha \theta_\alpha)}{\partial x_i} + \rho_\alpha u_i^{(\alpha)} \frac{\partial v_j}{\partial x_j} + \rho_\alpha u_j^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \rho_\alpha \left(\frac{Dv_i}{Dt} - F_i^{(\alpha)} \right) = \mathcal{P}_i^{0(\alpha)}, \quad (2.21)$$

$$\frac{3}{2} \frac{D(\rho_\alpha \theta_\alpha)}{Dt} + \frac{\partial q_i^{(\alpha)}}{\partial x_i} + \frac{5}{2} \rho_\alpha \theta_\alpha \frac{\partial v_i}{\partial x_i} + \sigma_{ij}^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \rho_\alpha u_i^{(\alpha)} \left(\frac{Dv_i}{Dt} - F_i^{(\alpha)} \right) = \frac{1}{2} \mathcal{P}^{1(\alpha)}, \quad (2.22)$$

$$\begin{aligned} \frac{D\sigma_{ij}^{(\alpha)}}{Dt} + \frac{\partial u_{ijk}^{0(\alpha)}}{\partial x_k} + \frac{4}{5} \frac{\partial q_{\langle i}^{(\alpha)}}{\partial x_{j \rangle}} + \sigma_{ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} + 2\sigma_{k\langle i}^{(\alpha)} \frac{\partial v_{j \rangle}}{\partial x_k} + 2\rho_\alpha \theta_\alpha \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \\ + 2\rho_\alpha u_{\langle i}^{(\alpha)} \left(\frac{Dv_{j \rangle}}{Dt} - F_{j \rangle}^{(\alpha)} \right) = \mathcal{P}_{ij}^{0(\alpha)}, \end{aligned} \quad (2.23)$$

$$\begin{aligned} \frac{Dq_i^{(\alpha)}}{Dt} + \frac{1}{2} \frac{\partial u_{ij}^{1(\alpha)}}{\partial x_j} + \frac{1}{6} \frac{\partial u^{2(\alpha)}}{\partial x_i} + u_{ijk}^{0(\alpha)} \frac{\partial v_j}{\partial x_k} + \frac{7}{5} q_i^{(\alpha)} \frac{\partial v_j}{\partial x_j} + \frac{7}{5} q_j^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \frac{2}{5} q_j^{(\alpha)} \frac{\partial v_j}{\partial x_i} \\ + \left(\sigma_{ij}^{(\alpha)} + \frac{5}{2} \rho_\alpha \theta_\alpha \delta_{ij} \right) \left(\frac{Dv_j}{Dt} - F_j^{(\alpha)} \right) = \frac{1}{2} \mathcal{P}_i^{1(\alpha)}, \end{aligned} \quad (2.24)$$

where

$$\mathcal{P}_{i_1 \dots i_n}^{a(\alpha)} = m_\alpha \sum_{\beta=1}^N \int \left\{ (C'_\alpha)^{2a} C'_{i_1}^{(\alpha)} \dots C'_{i_n}^{(\alpha)} - C_\alpha^{2a} C_{i_1}^{(\alpha)} \dots C_{i_n}^{(\alpha)} \right\} f_\alpha f_\beta g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\alpha d\mathbf{c}_\beta \quad (2.25)$$

are referred to as the *Boltzmann collision integrals* or the *production terms*. The evaluation of them will be treated in detail in chapter 3. Equations (2.20)–(2.24) may be referred to as the *partial* mass, momentum, energy, stress and heat flux balance equations, respectively.

The conservation laws—the mass, momentum and energy balance equations—for whole mixture can be obtained by summing each of (2.20)–(2.22) over α :

$$\left. \begin{aligned} \text{mass balance equation:} \quad & \frac{D\rho}{Dt} + \rho \frac{\partial v_i}{\partial x_i} = 0, \\ \text{momentum balance equation:} \quad & \rho \left(\frac{Dv_i}{Dt} - F_i \right) + \frac{\partial \sigma_{ij}}{\partial x_j} + \frac{\partial p}{\partial x_i} = 0, \\ \text{energy balance equation:} \quad & \frac{3}{2} k \frac{D(nT)}{Dt} + \frac{\partial q_i}{\partial x_i} + \frac{5}{2} p \frac{\partial v_i}{\partial x_i} + \sigma_{ij} \frac{\partial v_i}{\partial x_j} - \sum_{\alpha=1}^N \rho_\alpha u_i^{(\alpha)} F_i^{(\alpha)} = 0, \end{aligned} \right\} \quad (2.26)$$

where

$$\mathbf{F} = \frac{1}{\rho} \sum_{\alpha=1}^N \rho_\alpha \mathbf{F}_\alpha,$$

and conservation of mass, momentum and energy rendered the right-hand sides of the conservation laws vanish.

In three dimensions (3D), (2.20)–(2.24) represent $13N$ equations in $13N + 3$ variables— ρ_α , $u_i^{(\alpha)}$, θ_α , $\sigma_{ij}^{(\alpha)}$, $q_i^{(\alpha)}$ for $\alpha = 1, 2, \dots, N$, and v_i —along with the unknown higher order moments $u_{ijk}^{0(\alpha)}$, $u_{ij}^{1(\alpha)}$, $u^{2(\alpha)}$ and unknown production terms. However, owing to (2.9), equations (2.21) for $\alpha = 1, 2, \dots, N$ in 3D result only into $3N - 3$ independent equations. Therefore, in 3D (2.20), (2.22)–(2.24) for $\alpha = 1, 2, \dots, N$ and (2.21) for any $N - 1$ constituents along with (2.26)₂ form the system of so-called $13N$ moment equations for N -component gas-mixture, however, due to presence of unknown variables, the system of $13N$ moment equations is not yet closed. Alternatively, the definitions of total density and average temperature (2.7)_{1,3} make it possible to include total mass and energy balance equations (2.26)_{1,3} in system of $13N$ moment equations—in that case (2.20) and (2.22) for any $N - 1$ constituents can be used to get $13N$ independent equations again.

In order to close the system of moment equations (moment system), either the unknowns should be expressed in terms of the variables considered or the new governing equations for the unknown moments may be used. The problem with the latter approach is that the governing

equations for the unknown moments will contain even higher moments and this will go on, unless one uses the former approach. In the next sections, the closed set of $13N$ and $26N$ equations will be derived using both the approaches.

2.5 Grad's closure

For closing the moment system in case of a single gas, Grad [35] approximated the velocity distribution function with a finite linear combination of the n -dimensional Hermite polynomials [34]— $\mathcal{H}_{i_1 i_2 \dots i_n}^{(n)}(\mathbf{C})$ in dimensionless peculiar velocity $\mathbf{C}$ —and he evaluated the unknown coefficients in the expansion by satisfying the definitions of the moments considered with the approximated velocity distribution function, see [34, 35] for more details. Following Grad's strategy for a single gas, we also approximate the velocity distribution function for each component in a gas-mixture with a finite linear combination of the n -dimensional Hermite polynomials in dimensionless peculiar velocity of that component with respect to the whole mixture as

$$f_\alpha \approx f_M^{(\alpha)} \sum_{n=0}^N \frac{1}{n!} a_{i_1 i_2 \dots i_n}^{(\alpha)} \mathcal{H}_{i_1 i_2 \dots i_n}^{(n)} \quad \text{for } \alpha = 1, 2, \dots, N, \quad (2.27)$$

where

$$f_M^{(\alpha)} \equiv f_M^{(\alpha)}(\mathbf{r}, \mathbf{c}_\alpha, t) = n_\alpha \left(\frac{m_\alpha}{2\pi k T_\alpha} \right)^{3/2} \exp \left(-\frac{m_\alpha \mathbf{C}_\alpha^2}{2k T_\alpha} \right) \quad (2.28)$$

is the Maxwellian distribution function [129], $a_{i_1 i_2 \dots i_n}^{(\alpha)} = a_{i_1 i_2 \dots i_n}^{(\alpha)}(\mathbf{r}, t)$ are the unknown coefficients and $\mathcal{H}_{i_1 i_2 \dots i_n}^{(n)} \equiv \mathcal{H}_{i_1 i_2 \dots i_n}^{(n)}(\mathbf{C}_\alpha / \sqrt{\theta_\alpha})$ are the n -dimensional Hermite polynomials. It should be noted that $f_M^{(\alpha)}$ is a local Maxwellian but not the equilibrium distribution function $f_{\alpha|\text{eqb}}$, since n_α , T_α and $\mathbf{C}_\alpha$ in (2.28) may depend on $\mathbf{r}$ and t while they do not depend on $\mathbf{r}$ and t in (2.18) and, additionally, all the gases in the mixture have the common temperature T in equilibrium (cf. (2.18) and (2.28)). The unknown coefficients in (2.27) are evaluated by satisfying the definitions of moments considered with the approximated distribution function (2.27).

For the $13N$ moment theory, one expands the velocity distribution function for each component as

$$f_\alpha \approx f_{\alpha|\text{G13}} = f_M^{(\alpha)} \left(a^{(\alpha)} \mathcal{H}^{(0)} + a_i^{(\alpha)} \mathcal{H}_i^{(1)} + \frac{1}{2} a_{ij}^{(\alpha)} \mathcal{H}_{ij}^{(2)} + \frac{1}{6} a_{ijj}^{(\alpha)} \mathcal{H}_{ijj}^{(3)} \right)$$

and by satisfying the definitions of the physical quantities (2.6) with $f_{\alpha|\text{G13}}$, the unknown coefficients turn out to be

$$a^{(\alpha)} = 1, \quad a_i^{(\alpha)} = \frac{u_i^{(\alpha)}}{\sqrt{\theta_\alpha}}, \quad a_{ii}^{(\alpha)} = 0, \quad a_{\langle ij \rangle}^{(\alpha)} = \frac{\sigma_{ij}^{(\alpha)}}{\rho_\alpha \theta_\alpha}, \quad a_{ijj}^{(\alpha)} = \frac{6}{5} \frac{h_i^{(\alpha)}}{\rho_\alpha \theta_\alpha^{3/2}} \quad (2.29)$$

where

$$\mathbf{h}_\alpha = \mathbf{q}_\alpha - \frac{5}{2} \rho_\alpha \theta_\alpha \mathbf{u}_\alpha \quad (2.30)$$

is referred to as the *reduced partial heat flux* [130]. We refer to $f_{\alpha|G13}$ as Grad 13-moment (G13) distribution function for species α , and owing to (2.29), it reads

$$f_{\alpha|G13} = f_M^{(\alpha)} \left[1 + \frac{u_i^{(\alpha)} C_i^{(\alpha)}}{\theta_\alpha} + \frac{1}{2} \frac{\sigma_{ij}^{(\alpha)} C_i^{(\alpha)} C_j^{(\alpha)}}{\rho_\alpha \theta_\alpha^2} + \frac{1}{5} \frac{h_i^{(\alpha)} C_i^{(\alpha)}}{\rho_\alpha \theta_\alpha^2} \left(\frac{C_\alpha^2}{\theta_\alpha} - 5 \right) \right]. \quad (2.31)$$

2.6 Grad's $N \times 13$ -moment equations

In order to close the $13N$ moment equations of § 2.4, the unknown higher order moments— $u_{ijk}^{0(\alpha)}$, $u_{ij}^{1(\alpha)}$ and $u^{2(\alpha)}$ for $\alpha = 1, 2, \dots, N$ —are evaluated with the G13 distribution functions (2.31), this yields

$$u_{ijk|G13}^{0(\alpha)} = 0, \quad u_{ij|G13}^{1(\alpha)} = 7\theta_\alpha \sigma_{ij}^{(\alpha)} \quad \text{and} \quad u_{|G13}^{2(\alpha)} = 15\rho_\alpha \theta_\alpha^2 \quad \text{for} \quad \alpha = 1, 2, \dots, N. \quad (2.32)$$

Furthermore, the use of (2.31) for the velocity distribution functions of each constituent makes it possible to evaluate the production terms. Nevertheless, the evaluation procedure for a general interaction potential is not easy and it is detailed in chapter 3. Here, we shall just append the subscript “|G13” in the production terms to denote that they have been evaluated with the G13 distribution functions (2.31). The closed set of $13N$ moment equations obtained in this way are referred to as the Grad's $N \times 13$ -moment ($N \times G13$) equations. They read

$$\frac{D\rho_\alpha}{Dt} + \frac{\partial(\rho_\alpha u_i^{(\alpha)})}{\partial x_i} + \rho_\alpha \frac{\partial v_i}{\partial x_i} = \mathcal{P}_{|G13}^{0(\alpha)}, \quad (2.33)$$

$$\frac{D(\rho_\alpha u_i^{(\alpha)})}{Dt} + \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{\partial(\rho_\alpha \theta_\alpha)}{\partial x_i} + \rho_\alpha u_i^{(\alpha)} \frac{\partial v_j}{\partial x_j} + \rho_\alpha u_j^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \rho_\alpha \left(\frac{Dv_i}{Dt} - F_i^{(\alpha)} \right) = \mathcal{P}_{i|G13}^{0(\alpha)}, \quad (2.34)$$

$$\frac{3}{2} \frac{D(\rho_\alpha \theta_\alpha)}{Dt} + \frac{\partial q_i^{(\alpha)}}{\partial x_i} + \frac{5}{2} \rho_\alpha \theta_\alpha \frac{\partial v_i}{\partial x_i} + \sigma_{ij}^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \rho_\alpha u_i^{(\alpha)} \left(\frac{Dv_i}{Dt} - F_i^{(\alpha)} \right) = \frac{1}{2} \mathcal{P}_{|G13}^{1(\alpha)}, \quad (2.35)$$

$$\frac{D\sigma_{ij}^{(\alpha)}}{Dt} + \frac{4}{5} \frac{\partial q_{ij}^{(\alpha)}}{\partial x_j} + \sigma_{ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} + 2\sigma_{k(i}^{(\alpha)} \frac{\partial v_{j)}}{\partial x_k} + 2\rho_\alpha \theta_\alpha \frac{\partial v_{(i}}{\partial x_{j)}} + 2\rho_\alpha u_{(i}^{(\alpha)} \left(\frac{Dv_{j)}}{Dt} - F_{j)}^{(\alpha)} \right) = \mathcal{P}_{ij|G13}^{0(\alpha)}, \quad (2.36)$$

$$\begin{aligned} \frac{Dq_i^{(\alpha)}}{Dt} + \frac{7}{2} \theta_\alpha \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{7}{2} \sigma_{ij}^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_j} + \frac{5}{2} \frac{\partial(\rho_\alpha \theta_\alpha^2)}{\partial x_i} + \frac{7}{5} q_i^{(\alpha)} \frac{\partial v_j}{\partial x_j} + \frac{7}{5} q_j^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \frac{2}{5} q_j^{(\alpha)} \frac{\partial v_j}{\partial x_i} \\ + \left(\sigma_{ij}^{(\alpha)} + \frac{5}{2} \rho_\alpha \theta_\alpha \delta_{ij} \right) \left(\frac{Dv_j}{Dt} - F_j^{(\alpha)} \right) = \frac{1}{2} \mathcal{P}_{i|G13}^{1(\alpha)}, \end{aligned} \quad (2.37)$$

where (2.34) is considered for any $N - 1$ constituents along with (2.26)₂ while the rest of the equations are considered for all the constituents.

2.7 Grad's $N \times 26$ -moment equations

In order to incorporate more moments into the $13N$ moment system of § 2.4, one includes the equations for the unknown moments— $u_{ijk}^{0(\alpha)}$, $u_{ij}^{1(\alpha)}$ and $u^{2(\alpha)}$ ($\alpha = 1, 2, \dots, N$)—into the system instead of closing the system with G13 distribution functions. The equations for the unknown moments— $u_{ijk}^{0(\alpha)}$, $u_{ij}^{1(\alpha)}$ and $u^{2(\alpha)}$ —result by choosing ψ_α as $m_\alpha C_{\langle i}^{(\alpha)} C_j^{(\alpha)} C_k^{(\alpha)}$, $m_\alpha C_\alpha^2 C_{\langle i}^{(\alpha)} C_j^{(\alpha)}$, and $m_\alpha C_\alpha^4$ in the transfer equation (2.19):

$$\begin{aligned} \frac{Du_{ijk}^{0(\alpha)}}{Dt} + u_{ijk}^{0(\alpha)} \frac{\partial v_l}{\partial x_l} + \frac{\partial u_{ijkl}^{0(\alpha)}}{\partial x_l} + \frac{3}{7} \frac{\partial u_{\langle ij}^{1(\alpha)}}{\partial x_k} + 3u_{l\langle ij}^{0(\alpha)} \frac{\partial v_k}{\partial x_l} + \frac{12}{5} q_{\langle i}^{(\alpha)} \frac{\partial v_k}{\partial x_j} \\ + 3\sigma_{\langle ij}^{(\alpha)} \left(\frac{Dv_k}{Dt} - F_k^{(\alpha)} \right) = \mathcal{P}_{ijk}^{0(\alpha)}, \end{aligned} \quad (2.38)$$

$$\begin{aligned} \frac{Du_{ij}^{1(\alpha)}}{Dt} + u_{ij}^{1(\alpha)} \frac{\partial v_k}{\partial x_k} + \frac{\partial u_{ijk}^{1(\alpha)}}{\partial x_k} + \frac{2}{5} \frac{\partial u_{\langle i}^{2(\alpha)}}{\partial x_j} + 2u_{ijkl}^{0(\alpha)} \frac{\partial v_l}{\partial x_l} + \frac{6}{7} u_{\langle ij}^{1(\alpha)} \frac{\partial v_k}{\partial x_k} + \frac{4}{5} u_{k\langle i}^{1(\alpha)} \frac{\partial v_k}{\partial x_j} \\ + 2u_{k\langle i}^{1(\alpha)} \frac{\partial v_j}{\partial x_k} + \frac{14}{15} u^{2(\alpha)} \frac{\partial v_{\langle i}}{\partial x_j} + 2u_{ijk}^{0(\alpha)} \left(\frac{Dv_k}{Dt} - F_k^{(\alpha)} \right) + \frac{28}{5} q_{\langle i}^{(\alpha)} \left(\frac{Dv_j}{Dt} - F_j^{(\alpha)} \right) = \mathcal{P}_{ij}^{1(\alpha)}, \end{aligned} \quad (2.39)$$

$$\frac{Du^{2(\alpha)}}{Dt} + \frac{7}{3} u^{2(\alpha)} \frac{\partial v_i}{\partial x_i} + \frac{\partial u_i^{2(\alpha)}}{\partial x_i} + 4u_{ij}^{1(\alpha)} \frac{\partial v_i}{\partial x_j} + 8q_i^{(\alpha)} \left(\frac{Dv_i}{Dt} - F_i^{(\alpha)} \right) = \mathcal{P}^{2(\alpha)}. \quad (2.40)$$

Inclusion of (2.38)–(2.40) into the $13N$ moment system of § 2.4 leads to the system of $26N$ moment equations in 3D. Nevertheless, the system of $26N$ moment equations is not closed because the higher order moments— $u_{ijkl}^{0(\alpha)}$, $u_{ijk}^{1(\alpha)}$, $u_i^{2(\alpha)}$ —and the production terms are not known.

Often, it is more convenient to write the moment equations in terms of the new variables

$$\left. \begin{aligned} m_{ijk}^{(\alpha)} &= u_{ijk}^{0(\alpha)} - u_{ijk|G13}^{0(\alpha)} = u_{ijk}^{0(\alpha)}, \\ R_{ij}^{(\alpha)} &= u_{ij}^{1(\alpha)} - u_{ij|G13}^{1(\alpha)} = u_{ij}^{1(\alpha)} - 7\theta_\alpha \sigma_{ij}^{(\alpha)}, \\ \Delta_\alpha &= u^{2(\alpha)} - u_{|G13}^{2(\alpha)} = u^{2(\alpha)} - 15\rho_\alpha \theta_\alpha^2. \end{aligned} \right\} \quad (2.41)$$

In terms of the new variables (2.41), the governing equations for stresses and heat fluxes (eqs. (2.23) and (2.24)) change to

$$\begin{aligned} \frac{D\sigma_{ij}^{(\alpha)}}{Dt} + \frac{\partial m_{ijk}^{(\alpha)}}{\partial x_k} + \frac{4}{5} \frac{\partial q_{\langle i}^{(\alpha)}}{\partial x_j} + \sigma_{ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} + 2\sigma_{k\langle i}^{(\alpha)} \frac{\partial v_j}{\partial x_k} + 2\rho_\alpha \theta_\alpha \frac{\partial v_{\langle i}}{\partial x_j} \\ + 2\rho_\alpha u_{\langle i}^{(\alpha)} \left(\frac{Dv_j}{Dt} - F_j^{(\alpha)} \right) = \mathcal{P}_{ij}^{0(\alpha)}, \end{aligned} \quad (2.42)$$

$$\begin{aligned} \frac{Dq_i^{(\alpha)}}{Dt} + \frac{1}{2} \frac{\partial R_{ij}^{(\alpha)}}{\partial x_j} + \frac{7}{2} \theta_\alpha \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{7}{2} \sigma_{ij}^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_j} + \frac{1}{6} \frac{\partial \Delta_\alpha}{\partial x_i} + \frac{5}{2} \frac{\partial (\rho_\alpha \theta_\alpha^2)}{\partial x_i} + m_{ijk}^{(\alpha)} \frac{\partial v_j}{\partial x_k} \\ + \frac{7}{5} q_i^{(\alpha)} \frac{\partial v_j}{\partial x_j} + \frac{7}{5} q_j^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \frac{2}{5} q_j^{(\alpha)} \frac{\partial v_j}{\partial x_i} + \left(\sigma_{ij}^{(\alpha)} + \frac{5}{2} \rho_\alpha \theta_\alpha \delta_{ij} \right) \left(\frac{Dv_j}{Dt} - F_j^{(\alpha)} \right) = \frac{1}{2} \mathcal{P}_i^{1(\alpha)}. \end{aligned} \quad (2.43)$$

The governing equations for the new variables (2.41) result from (2.38)–(2.42) and they read

$$\begin{aligned} \frac{Dm_{ijk}^{(\alpha)}}{Dt} + m_{ijk}^{(\alpha)} \frac{\partial v_l}{\partial x_l} + \frac{\partial u_{ijkl}^{0(\alpha)}}{\partial x_l} + \frac{3}{7} \frac{\partial R_{ij}^{(\alpha)}}{\partial x_k} + 3\theta_\alpha \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_k} + 3\sigma_{ij}^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_k} + 3m_{l[ij}^{(\alpha)} \frac{\partial v_k]}{\partial x_l} \\ + \frac{12}{5} q_{[i}^{(\alpha)} \frac{\partial v_k]}{\partial x_j} + 3\sigma_{ij}^{(\alpha)} \left(\frac{Dv_k}{Dt} - F_k^{(\alpha)} \right) = \mathcal{P}_{ijk}^{0(\alpha)}, \end{aligned} \quad (2.44)$$

$$\begin{aligned} \frac{DR_{ij}^{(\alpha)}}{Dt} + R_{ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} + \frac{\partial u_{ijk}^{1(\alpha)}}{\partial x_k} + \frac{2}{5} \frac{\partial u_{ij}^{2(\alpha)}}{\partial x_j} + 2u_{ijkl}^{0(\alpha)} \frac{\partial v_k}{\partial x_l} - \frac{28}{5} \theta_\alpha \frac{\partial q_{[i}^{(\alpha)}}{\partial x_j]} + 4\theta_\alpha \sigma_{k[i}^{(\alpha)} \frac{\partial v_k]}{\partial x_j} + 4\theta_\alpha \sigma_{k[i}^{(\alpha)} \frac{\partial v_j]}{\partial x_k} \\ - \frac{8}{3} \theta_\alpha \sigma_{ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} - \frac{14}{3} \frac{1}{\rho_\alpha} \sigma_{ij}^{(\alpha)} \frac{\partial q_k^{(\alpha)}}{\partial x_k} - \frac{14}{3} \frac{1}{\rho_\alpha} \sigma_{ij}^{(\alpha)} \sigma_{kl}^{(\alpha)} \frac{\partial v_k}{\partial x_l} + 7\theta_\alpha \sigma_{ij}^{(\alpha)} \frac{\partial u_k^{(\alpha)}}{\partial x_k} + 7 \frac{1}{\rho_\alpha} \theta_\alpha u_k^{(\alpha)} \sigma_{ij}^{(\alpha)} \frac{\partial \rho_\alpha}{\partial x_k} \\ - 7\theta_\alpha \frac{\partial m_{ijk}^{(\alpha)}}{\partial x_k} + \frac{6}{7} R_{ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} + \frac{4}{5} R_{k[i}^{(\alpha)} \frac{\partial v_k]}{\partial x_j} + 2R_{k[i}^{(\alpha)} \frac{\partial v_j]}{\partial x_k} + \frac{14}{15} \Delta_\alpha \frac{\partial v_{[i}}{\partial x_j]} + 2m_{ijk}^{(\alpha)} \left(\frac{Dv_k}{Dt} - F_k^{(\alpha)} \right) \\ + \frac{28}{5} \left(q_{[i}^{(\alpha)} - \frac{5}{2} \rho_\alpha \theta_\alpha u_{[i}^{(\alpha)} \right) \left(\frac{Dv_j]}{Dt} - F_j^{(\alpha)} \right) - \frac{14}{3} \sigma_{ij}^{(\alpha)} u_k^{(\alpha)} \left(\frac{Dv_k}{Dt} - F_k^{(\alpha)} \right) \\ = \mathcal{P}_{ij}^{1(\alpha)} - 7\theta_\alpha \mathcal{P}_{ij}^{0(\alpha)} - \frac{7}{3} \sigma_{ij}^{(\alpha)} \frac{1}{\rho_\alpha} \mathcal{P}^{1(\alpha)} + 7 \frac{1}{\rho_\alpha} \theta_\alpha \sigma_{ij}^{(\alpha)} \mathcal{P}^{0(\alpha)}, \end{aligned} \quad (2.45)$$

$$\begin{aligned} \frac{D\Delta_\alpha}{Dt} + \frac{7}{3} \Delta_\alpha \frac{\partial v_i}{\partial x_i} + \frac{\partial u_i^{2(\alpha)}}{\partial x_i} + 8\theta_\alpha \sigma_{ij}^{(\alpha)} \frac{\partial v_i}{\partial x_j} - 20\theta_\alpha \frac{\partial q_i^{(\alpha)}}{\partial x_i} + 15\rho_\alpha \theta_\alpha^2 \frac{\partial u_i^{(\alpha)}}{\partial x_i} + 15\theta_\alpha^2 u_i^{(\alpha)} \frac{\partial \rho_\alpha}{\partial x_i} \\ + 4R_{ij}^{(\alpha)} \frac{\partial v_i}{\partial x_j} + 8 \left(q_i^{(\alpha)} - \frac{5}{2} \rho_\alpha \theta_\alpha u_i^{(\alpha)} \right) \left(\frac{Dv_i}{Dt} - F_i^{(\alpha)} \right) = \mathcal{P}^{2(\alpha)} - 10\theta_\alpha \mathcal{P}^{1(\alpha)}. \end{aligned} \quad (2.46)$$

Equations (2.20)–(2.22), and (2.42)–(2.46) along with (2.26)₂ form the system of $26N$ moment equations, where (2.21) needs to be considered for any $N - 1$ constituents while the other equations need to be considered for all the constituents.

The system of $26N$ moment equations obtained above is closed by approximating the velocity distribution function for each constituent with Grad 26-moment (G26) distribution function

$$\begin{aligned} f_{\alpha|G26} = f_M^{(\alpha)} \left[1 + \frac{u_i^{(\alpha)} C_i^{(\alpha)}}{\theta_\alpha} + \frac{1}{2} \frac{\sigma_{ij}^{(\alpha)} C_i^{(\alpha)} C_j^{(\alpha)}}{\rho_\alpha \theta_\alpha^2} + \frac{1}{5} \frac{h_i^{(\alpha)} C_i^{(\alpha)}}{\rho_\alpha \theta_\alpha^2} \left(\frac{C_\alpha^2}{\theta_\alpha} - 5 \right) + \frac{1}{6} \frac{m_{ijk}^{(\alpha)} C_i^{(\alpha)} C_j^{(\alpha)} C_k^{(\alpha)}}{\rho_\alpha \theta_\alpha^3} \right. \\ \left. + \frac{1}{28} \frac{R_{ij}^{(\alpha)} C_i^{(\alpha)} C_j^{(\alpha)}}{\rho_\alpha \theta_\alpha^3} \left(\frac{C_\alpha^2}{\theta_\alpha} - 7 \right) + \frac{1}{8} \frac{\Delta_\alpha}{\rho_\alpha \theta_\alpha^2} \left(1 - \frac{2}{3} \frac{C_\alpha^2}{\theta_\alpha} + \frac{1}{15} \frac{C_\alpha^4}{\theta_\alpha^2} \right) \right]. \end{aligned} \quad (2.47)$$

With the G26 distribution functions (2.47), the unknown higher order moments and the production terms are expressed in terms of the $26N$ moments considered; the unknown higher order moments become

$$u_{ijkl|G26}^{0(\alpha)} = 0, \quad u_{ijk|G26}^{1(\alpha)} = 9\theta_\alpha m_{ijk}^{(\alpha)}, \quad u_{i|G26}^{2(\alpha)} = 28\theta_\alpha q_i^{(\alpha)} - 35\rho_\alpha \theta_\alpha^2 u_i^{(\alpha)} \quad \text{for } \alpha = 1, 2, \dots, N \quad (2.48)$$

and, again, the evaluation of the production terms is detailed in chapter 3—however, here, we shall just append the subscript “|G26” in the production terms to denote that they have been

evaluated with the G26 distribution functions (2.47). The closed set of $26N$ moment equations obtained in this way are referred to as the Grad's $N \times 26$ -moment ($N \times \text{G26}$) equations. They read

$$\frac{D\rho_\alpha}{Dt} + \frac{\partial(\rho_\alpha u_i^{(\alpha)})}{\partial x_i} + \rho_\alpha \frac{\partial v_i}{\partial x_i} = \mathcal{P}_{|\text{G26}}^{0(\alpha)}, \quad (2.49)$$

$$\frac{D(\rho_\alpha u_i^{(\alpha)})}{Dt} + \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{\partial(\rho_\alpha \theta_\alpha)}{\partial x_i} + \rho_\alpha u_i^{(\alpha)} \frac{\partial v_j}{\partial x_j} + \rho_\alpha u_j^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \rho_\alpha \left(\frac{Dv_i}{Dt} - F_i^{(\alpha)} \right) = \mathcal{P}_{i|\text{G26}}^{0(\alpha)}, \quad (2.50)$$

$$\frac{3}{2} \frac{D(\rho_\alpha \theta_\alpha)}{Dt} + \frac{\partial q_i^{(\alpha)}}{\partial x_i} + \frac{5}{2} \rho_\alpha \theta_\alpha \frac{\partial v_i}{\partial x_i} + \sigma_{ij}^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \rho_\alpha u_i^{(\alpha)} \left(\frac{Dv_i}{Dt} - F_i^{(\alpha)} \right) = \frac{1}{2} \mathcal{P}_{|\text{G26}}^{1(\alpha)}, \quad (2.51)$$

$$\begin{aligned} \frac{D\sigma_{ij}^{(\alpha)}}{Dt} + \frac{\partial m_{ijk}^{(\alpha)}}{\partial x_k} + \frac{4}{5} \frac{\partial q_{\langle i}^{(\alpha)}}{\partial x_{j\rangle}} + \sigma_{ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} + 2\sigma_{k\langle i}^{(\alpha)} \frac{\partial v_{j\rangle}}{\partial x_k} + 2\rho_\alpha \theta_\alpha \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \\ + 2\rho_\alpha u_{\langle i}^{(\alpha)} \left(\frac{Dv_{j\rangle}}{Dt} - F_{j\rangle}^{(\alpha)} \right) = \mathcal{P}_{ij|\text{G26}}^{0(\alpha)}, \end{aligned} \quad (2.52)$$

$$\begin{aligned} \frac{Dq_i^{(\alpha)}}{Dt} + \frac{1}{2} \frac{\partial R_{ij}^{(\alpha)}}{\partial x_j} + \frac{7}{2} \theta_\alpha \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{7}{2} \sigma_{ij}^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_j} + \frac{1}{6} \frac{\partial \Delta_\alpha}{\partial x_i} + \frac{5}{2} \frac{\partial(\rho_\alpha \theta_\alpha^2)}{\partial x_i} + m_{ijk}^{(\alpha)} \frac{\partial v_j}{\partial x_k} \\ + \frac{7}{5} q_i^{(\alpha)} \frac{\partial v_j}{\partial x_j} + \frac{7}{5} q_j^{(\alpha)} \frac{\partial v_i}{\partial x_j} + \frac{2}{5} q_j^{(\alpha)} \frac{\partial v_j}{\partial x_i} + \left(\sigma_{ij}^{(\alpha)} + \frac{5}{2} \rho_\alpha \theta_\alpha \delta_{ij} \right) \left(\frac{Dv_j}{Dt} - F_j^{(\alpha)} \right) = \frac{1}{2} \mathcal{P}_{i|\text{G26}}^{1(\alpha)}, \end{aligned} \quad (2.53)$$

$$\begin{aligned} \frac{Dm_{ijk}^{(\alpha)}}{Dt} + m_{ijk}^{(\alpha)} \frac{\partial v_l}{\partial x_l} + \frac{3}{7} \frac{\partial R_{ij}^{(\alpha)}}{\partial x_k} + 3\theta_\alpha \frac{\partial \sigma_{\langle ij}^{(\alpha)}}{\partial x_{k\rangle}} + 3\sigma_{\langle ij}^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_{k\rangle}} + 3m_{l\langle ij}^{(\alpha)} \frac{\partial v_k}{\partial x_l} + \frac{12}{5} q_{\langle i}^{(\alpha)} \frac{\partial v_k}{\partial x_{j\rangle}} \\ + 3\sigma_{\langle ij}^{(\alpha)} \left(\frac{Dv_k}{Dt} - F_{k\rangle}^{(\alpha)} \right) = \mathcal{P}_{ijk|\text{G26}}^{0(\alpha)}, \end{aligned} \quad (2.54)$$

$$\begin{aligned} \frac{DR_{ij}^{(\alpha)}}{Dt} + R_{ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} + 2\theta_\alpha \frac{\partial m_{ijk}^{(\alpha)}}{\partial x_k} + 9m_{ijk}^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_k} + \frac{28}{5} \theta_\alpha \frac{\partial q_{\langle i}^{(\alpha)}}{\partial x_{j\rangle}} + \frac{56}{5} q_{\langle i}^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_{j\rangle}} - 14\rho_\alpha \theta_\alpha^2 \frac{\partial u_{\langle i}^{(\alpha)}}{\partial x_{j\rangle}} \\ - 14\theta_\alpha^2 u_{\langle i}^{(\alpha)} \frac{\partial \rho_\alpha}{\partial x_{j\rangle}} - 28\rho_\alpha \theta_\alpha u_{\langle i}^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_{j\rangle}} + 4\theta_\alpha \sigma_{k\langle i}^{(\alpha)} \frac{\partial v_k}{\partial x_{j\rangle}} + 4\theta_\alpha \sigma_{k\langle i}^{(\alpha)} \frac{\partial v_{j\rangle}}{\partial x_k} - \frac{8}{3} \theta_\alpha \sigma_{ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} \\ - \frac{14}{3} \frac{1}{\rho_\alpha} \sigma_{ij}^{(\alpha)} \frac{\partial q_k^{(\alpha)}}{\partial x_k} - \frac{14}{3} \frac{1}{\rho_\alpha} \sigma_{ij}^{(\alpha)} \sigma_{kl}^{(\alpha)} \frac{\partial v_k}{\partial x_l} + 7\theta_\alpha \sigma_{ij}^{(\alpha)} \frac{\partial u_k^{(\alpha)}}{\partial x_k} + 7 \frac{1}{\rho_\alpha} \theta_\alpha u_k^{(\alpha)} \sigma_{ij}^{(\alpha)} \frac{\partial \rho_\alpha}{\partial x_k} \\ + \frac{6}{7} R_{\langle ij}^{(\alpha)} \frac{\partial v_k}{\partial x_k} + \frac{4}{5} R_{k\langle i}^{(\alpha)} \frac{\partial v_k}{\partial x_{j\rangle}} + 2R_{k\langle i}^{(\alpha)} \frac{\partial v_{j\rangle}}{\partial x_k} + \frac{14}{15} \Delta_\alpha \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + 2m_{ijk}^{(\alpha)} \left(\frac{Dv_k}{Dt} - F_k^{(\alpha)} \right) \\ + \frac{28}{5} \left(q_{\langle i}^{(\alpha)} - \frac{5}{2} \rho_\alpha \theta_\alpha u_{\langle i}^{(\alpha)} \right) \left(\frac{Dv_{j\rangle}}{Dt} - F_{j\rangle}^{(\alpha)} \right) - \frac{14}{3} \sigma_{ij}^{(\alpha)} u_k^{(\alpha)} \left(\frac{Dv_k}{Dt} - F_k^{(\alpha)} \right) \\ = \mathcal{P}_{ij|\text{G26}}^{1(\alpha)} - 7\theta_\alpha \mathcal{P}_{ij|\text{G26}}^{0(\alpha)} - \frac{7}{3} \sigma_{ij}^{(\alpha)} \frac{1}{\rho_\alpha} \mathcal{P}_{|\text{G26}}^{1(\alpha)} + 7 \frac{1}{\rho_\alpha} \theta_\alpha \sigma_{ij}^{(\alpha)} \mathcal{P}_{|\text{G26}}^{0(\alpha)}, \end{aligned} \quad (2.55)$$

$$\begin{aligned}
& \frac{D\Delta_\alpha}{Dt} + \frac{7}{3}\Delta_\alpha \frac{\partial v_i}{\partial x_i} + 8\theta_\alpha \sigma_{ij}^{(\alpha)} \frac{\partial v_i}{\partial x_j} + 8\theta_\alpha \frac{\partial q_i^{(\alpha)}}{\partial x_i} + 28q_i^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_i} - 20\rho_\alpha \theta_\alpha^2 \frac{\partial u_i^{(\alpha)}}{\partial x_i} - 20\theta_\alpha^2 u_i^{(\alpha)} \frac{\partial \rho_\alpha}{\partial x_i} \\
& - 70\rho_\alpha \theta_\alpha u_i^{(\alpha)} \frac{\partial \theta_\alpha}{\partial x_i} + 4R_{ij}^{(\alpha)} \frac{\partial v_i}{\partial x_j} + 8 \left(q_i^{(\alpha)} - \frac{5}{2}\rho_\alpha \theta_\alpha u_i^{(\alpha)} \right) \left(\frac{Dv_i}{Dt} - F_i^{(\alpha)} \right) = \mathcal{P}_{|G26}^{2(\alpha)} - 10\theta_\alpha \mathcal{P}_{|G26}^{1(\alpha)}.
\end{aligned} \tag{2.56}$$

Equations (2.49)–(2.56) along with (2.26)₂ in 3D represent the $N \times G26$ equations, where (2.50) needs to be considered for any $N - 1$ constituents while the other equations need to be considered for all the constituents.

Chapter 3

Boltzmann collision integrals

The procedure for computing the production terms for a gaseous mixture is not very different from that for a single gas and the procedure for the latter can be found in many textbooks, e.g., [60, 102]. Nevertheless, computing the full non-linear production terms—even for a single gas—is not easy due to the presence of enormous number of terms at intermediate steps during the procedure.

In this chapter, we present the procedure for evaluating the general production terms (2.25) for gaseous mixtures by assuming that the distribution functions for all the constituents in the mixture are approximated with (a) G13 distribution functions and (b) G26 distribution functions. We have implemented the procedure in the computer algebra software MATHEMATICA[®]. The findings have been published in [44] and the source code for the computation is available at [41]. Using this source code the fully non-linear production terms for a single gas, a granular gas or a gaseous mixture can be computed—in principle, for any interaction potential and for any number of moments. However, due to their cumbersome form, we restrict ourselves to the production terms for 13- and 26-moment case and present them for the α -constituent ($\alpha = 1, 2, \dots, N$) in a gaseous mixture comprising of N simple gases interacting with (a) Maxwell (b) hard-sphere interaction potentials.

3.1 Procedure

The goal is to compute the production term (2.25), which can be written as

$$\mathcal{P}_{i_1 \dots i_n}^{a(\alpha)} = \sum_{\beta=1}^N P_{\langle i_1 \dots i_n \rangle}^{a(\alpha\beta)}, \quad (3.1)$$

where

$$P_{\langle i_1 \dots i_n \rangle}^{a(\alpha\beta)} = m_\alpha \int \left\{ (C'_\alpha)^{2a} C'_{\langle i_1}^{(\alpha)} \dots C'_{i_n \rangle}^{(\alpha)} - C_\alpha^{2a} C_{\langle i_1}^{(\alpha)} \dots C_{i_n \rangle}^{(\alpha)} \right\} f_\alpha f_\beta g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\alpha d\mathbf{c}_\beta. \quad (3.2)$$

However, since the squared velocities in (3.2) can easily be expressed in index notation using Einstein summation convention, for instance $C_\alpha^2 = C_{i_0}^{(\alpha)} C_{i_0}^{(\alpha)}$, and the indices in each term of (3.2) can be adjusted accordingly, we shall first compute

$$P_{i_1 \dots i_n}^{0(\alpha\beta)} = m_\alpha \int \left(C_{i_1}^{(\alpha)} \dots C_{i_n}^{(\alpha)} - C_{i_1}^{(\alpha)} \dots C_{i_n}^{(\alpha)} \right) f_\alpha f_\beta g_{\alpha\beta} b db d\epsilon d\mathbf{c}_\alpha d\mathbf{c}_\beta \quad (3.3)$$

instead of computing (3.1) directly. In the end, we take the trace of each term in the result and that will give the contribution from the collisions of the α -gas molecules with the β -gas molecules. Finally, the result is summed over β to include the contribution from each type of

collision and that would be the required production term.

3.1.1 General idea

Similar to a single gas, the general idea behind how to compute (3.3) is to reduce the integrals over velocity spaces in (3.3) into two integrals, which can be separated. When a common temperature for all the gases in the mixture as well as for the whole mixture is assumed (viz., in the single temperature theory), the transformation of the velocities $\mathbf{c}_\alpha$ and $\mathbf{c}_\beta$ to the relative velocity and the velocity of the center of mass converts the integrals over the velocity spaces $\mathbf{c}_\alpha$ and $\mathbf{c}_\beta$ in (3.3) into two separate integrals—one over the relative velocity and the other over the center of mass velocity, see e.g. [23, 28, 60]. Unfortunately, the same trick does not work if different temperatures for different constituents in the mixture are considered (viz., in the multi-temperature theory). Indeed, the two separate integrals in this case are obtained by transforming the velocities $\mathbf{c}_\alpha$ and $\mathbf{c}_\beta$ into the relative velocity $\mathbf{g}_{\alpha\beta} = \mathbf{c}_\alpha - \mathbf{c}_\beta = \mathbf{C}_\alpha - \mathbf{C}_\beta$ and another velocity $\mathbf{h}_{\alpha\beta} = (\theta_\beta \mathbf{C}_\alpha + \theta_\alpha \mathbf{C}_\beta)/\vartheta$, where ϑ can be anything having the dimensions of temperature in energy units. The two transformations are related via the relation $d\mathbf{c}_\alpha d\mathbf{c}_\beta = d\mathbf{C}_\alpha d\mathbf{C}_\beta = (\vartheta/(2\theta))^3 d\mathbf{g}_{\alpha\beta} d\mathbf{h}_{\alpha\beta}$, where $\theta = (\theta_\alpha + \theta_\beta)/2$. This transformation leads to

$$\frac{C_\alpha^2}{\theta_\alpha} + \frac{C_\beta^2}{\theta_\beta} = \frac{1}{2\theta} \left(g_{\alpha\beta}^2 + \frac{\vartheta^2}{\theta_\alpha \theta_\beta} h_{\alpha\beta}^2 \right). \quad (3.4)$$

Zhdanov [129] chooses ϑ as 2θ so that the Jacobian of the transformation is unity. However, following [42], here we choose ϑ as $2\sqrt{\theta_\alpha \theta_\beta}$. Although, the Jacobian of the transformation is not unity in this case, but if one scales the velocities $\mathbf{c}_\gamma$ and $\mathbf{C}_\gamma$ with $\sqrt{\theta_\gamma}$ ($\gamma \in \{\alpha, \beta\}$), and $\mathbf{g}_{\alpha\beta}$ and $\mathbf{h}_{\alpha\beta}$ with $\sqrt{\theta}$, the Jacobian with respect to scaled velocities turns to unity. Since, we shall be dealing with the dimensionless velocities, the latter definition of ϑ is more adequate for our description. Therefore, hereafter, we shall use

$$\mathbf{h}_{\alpha\beta} = \frac{1}{2} \left(\sqrt{\frac{\theta_\beta}{\theta_\alpha}} \mathbf{C}_\alpha + \sqrt{\frac{\theta_\alpha}{\theta_\beta}} \mathbf{C}_\beta \right) \quad \text{so that} \quad \frac{C_\alpha^2}{2\theta_\alpha} + \frac{C_\beta^2}{2\theta_\beta} = \frac{1}{\theta} \left(\frac{g_{\alpha\beta}^2}{4} + h_{\alpha\beta}^2 \right). \quad (3.5)$$

3.1.2 Full tensorial expression

Let us first replace the post-collisional velocities in (3.3) with pre-collisional velocities by using relation (2.1)₁ in different form $C_i'^{(\alpha)} = C_i^{(\alpha)} - 2\mu_\beta k_i^{(\alpha\beta)} g_{\alpha\beta} \cos \Theta_{\alpha\beta}$, where $\Theta_{\alpha\beta}$ is the angle between contact vector $\mathbf{k}_{\alpha\beta}$ and the relative velocity $\mathbf{g}_{\alpha\beta}$. For better readability, we drop the superscript “ $(\alpha\beta)$ ” and the subscript “ $\alpha\beta$ ” from the contact vector and the transformed velocities. The product of post-collisional velocities in (3.3) turns into

$$C_{i_1}'^{(\alpha)} \cdots C_{i_n}'^{(\alpha)} = \sum_{j=0}^n (-2\mu_\beta)^j \binom{n}{j} k_{i_1} k_{i_2} \cdots k_{i_j} C_{i_{j+1}}^{(\alpha)} \cdots C_{i_{n-1}}^{(\alpha)} C_{i_n}^{(\alpha)} g^j \cos^j \Theta_{\alpha\beta}, \quad (3.6)$$

where the round brackets around the indices denote the symmetric part of the corresponding tensor [102]. Substituting (3.6) into (3.3), one obtains

$$P_{i_1 \dots i_n}^{0(\alpha\beta)} = m_\alpha \sum_{j=1}^n (-2\mu_\beta)^j \binom{n}{j} \int I_{(i_1 \dots i_j} C_{i_{j+1}}^{(\alpha)} \dots C_{i_n}^{(\alpha)} g^j f_\alpha f_\beta d\mathbf{c}_\alpha d\mathbf{c}_\beta, \quad (3.7)$$

where

$$I_{i_1 \dots i_n} = \int k_{i_1} \dots k_{i_n} \cos^n \Theta_{\alpha\beta} g b db d\epsilon \quad (3.8)$$

is termed as the *scattering vector integral*. The structure of the integrand in (3.8) suggests that $I_{i_1 \dots i_n}$ will have the form

$$I_{i_1 \dots i_n} = \sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} a_j^{(n)} \delta_{(i_1 i_2} \dots \delta_{i_{2j-1} i_{2j}} \frac{g_{i_{2j+1}}}{g} \dots \frac{g_{i_n}}{g}, \quad (3.9)$$

where the coefficients $a_j^{(n)} \equiv a_j^{(n)}(g)$ are unknowns and depend only on the relative speed g . The computation of the coefficients $a_j^{(n)}$ is detailed in § 3.1.2.1. The use of (3.9), eventually, unveils the tensorial structure of $P_{i_1 \dots i_n}^{0(\alpha\beta)}$. We have

$$\begin{aligned} P_{i_1 \dots i_n}^{0(\alpha\beta)} &= m_\alpha \sum_{j=1}^n \sum_{l=0}^{\lfloor \frac{j}{2} \rfloor} (-2\mu_\beta)^j \binom{n}{j} \delta_{(i_1 i_2} \dots \delta_{i_{2l-1} i_{2l}} \\ &\quad \times \int a_l^{(j)}(g) g^{2l} g_{i_{2l+1}} \dots g_{i_j} C_{i_{j+1}}^{(\alpha)} \dots C_{i_n}^{(\alpha)} f_\alpha f_\beta d\mathbf{c}_\alpha d\mathbf{c}_\beta, \end{aligned} \quad (3.10)$$

where all the collision aspects are hidden in the coefficients $a_l^{(j)}(g)$. Expression (3.10) is entered as the starting point in MATHEMATICA[®] program.

For general interaction potentials, specific forms of the distribution functions f_α and f_β must be provided in order to compute $P_{i_1 \dots i_n}^{0(\alpha\beta)}$ further. Here, we approximate both the distribution functions f_α and f_β with (a) G13 distribution functions (2.31) and (b) G26 distribution functions (2.47).

3.1.2.1 Computation of the coefficients $a_j^{(n)}$

The unknown coefficients $a_j^{(n)}$ follow by appropriately contracting the two forms of $I_{i_1 \dots i_n}$ in (3.8) and (3.9) with combinations of g_i/g and with combinations of Kronecker deltas δ_{ij} successively, and this leads to scalar relations that provide a linear system for the coefficients depending on the scalar integrals

$$I^{(n)} = \int \cos^{2n} \Theta_{\alpha\beta} g b db d\epsilon = 2\pi \int \cos^{2n} \Theta_{\alpha\beta} g b db, \quad \text{where } n \in \mathbb{N}. \quad (3.11)$$

From (3.8) and (3.9), one has

$$I_i = \int k_i \cos \Theta_{\alpha\beta} g b db d\epsilon = a_0^{(1)} \frac{g_i}{g}.$$

Contracting the above equation with g_i/g and using the relation $k_i g_i = g \cos \Theta_{\alpha\beta}$, it, readily, follows

$$a_0^{(1)} = I^{(1)}. \quad (3.12)$$

Again, from (3.8) and (3.9), one has

$$I_{ij} = \int k_i k_j \cos^2 \Theta_{\alpha\beta} g b db d\epsilon = a_0^{(2)} \frac{g_i g_j}{g^2} + a_1^{(2)} \delta_{ij}.$$

Contracting the above equation with $(g_i g_j)/g^2$ and with δ_{ij} successively, one obtains

$$I^{(2)} = a_0^{(2)} + a_1^{(2)} \quad \text{and} \quad I^{(1)} = a_0^{(2)} + 3a_1^{(2)},$$

and, thus

$$a_0^{(2)} = \frac{1}{2} (3I^{(2)} - I^{(1)}) \quad \text{and} \quad a_1^{(2)} = \frac{1}{2} (I^{(1)} - I^{(2)}). \quad (3.13)$$

The next integrals are treated analogously and one, eventually, finds

$$a_0^{(3)} = \frac{1}{2} (5I^{(3)} - 3I^{(2)}) \quad \text{and} \quad a_1^{(3)} = \frac{3}{2} (I^{(2)} - I^{(3)}), \quad (3.14)$$

$$\begin{aligned} a_0^{(4)} &= \frac{1}{8} (35I^{(4)} - 30I^{(3)} + 3I^{(2)}), \quad a_1^{(4)} = -\frac{3}{4} (5I^{(4)} - 6I^{(3)} + I^{(2)}) \\ \text{and} \quad a_2^{(4)} &= \frac{3}{8} (I^{(4)} - 2I^{(3)} + I^{(2)}), \end{aligned} \quad (3.15)$$

and so on.

By changing the angle $\Theta_{\alpha\beta}$ to the scattering angle $\chi_{\alpha\beta} = \pi - 2\Theta_{\alpha\beta}$ and exploiting the identity

$$(1-x)^n = \sum_{j=1}^n (-1)^{j-1} \binom{n}{j} (1-x^j),$$

the integrals $I^{(n)}$ in (3.11) can be expressed in another form, which is more close to standard *Omega* integrals [60]

$$\Omega_{\alpha\beta}^{(l,r)} = \int_0^\infty \int_0^\infty e^{-\gamma_{\alpha\beta}^2} \gamma_{\alpha\beta}^{2r+3} (1 - \cos^l \chi_{\alpha\beta}) b db d\gamma_{\alpha\beta}, \quad (3.16)$$

where $\chi_{\alpha\beta} = \pi - 2\Theta_{\alpha\beta}$ is the scattering angle. In terms of the scattering angle, $I^{(n)}$ becomes

$$I^{(n)} = 2\pi \int \left(\frac{1 - \cos \chi_{\alpha\beta}}{2} \right)^n g b db = \frac{\pi}{2^{n-1}} \sum_{j=1}^n (-1)^{j-1} \binom{n}{j} \int (1 - \cos^j \chi_{\alpha\beta}) g b db. \quad (3.17)$$

3.1.3 Integration over velocity spaces

To perform the remaining integrals in (3.10), the velocities $\mathbf{c}_\alpha$ and $\mathbf{c}_\beta$ are transformed to $\mathbf{g}$ and $\mathbf{h}$ using (3.5). With the G13 or G26 distribution functions for f_α and f_β , and using relation (3.5)₂, one obtains two separate integrals—one over $\mathbf{g}$ and other over $\mathbf{h}$. The precise expression of the integrals are involved as the transformation of velocities acts on velocity components $C_i^{(\alpha)}$'s as well as on both the distribution functions f_α and f_β approximated with G13 or G26 distribution functions. However, any single integration over $\mathbf{h}$ results into a combination of Kronecker deltas, since it has the form

$$\int h^{2n} h_{i_1} \cdots h_{i_p} \exp\left(-\frac{h^2}{\theta}\right) d\mathbf{h} \quad \text{with} \quad n, p \in \mathbb{N}_0. \quad (3.18)$$

The integral in (3.18) vanishes if p is an odd integer. For even p , the integration is performed by transforming $\mathbf{h}$ into spherical coordinate system. It follows

$$\begin{aligned} \int h^{2n} h_{i_1} \cdots h_{i_p} \exp\left(-\frac{h^2}{\theta}\right) d\mathbf{h} &= \int_0^\infty h^{2n+p+2} \exp\left(-\frac{h^2}{\theta}\right) dh \cdot \int_0^{2\pi} \int_0^\pi \nu_{i_1} \cdots \nu_{i_p} \sin \Theta d\Theta d\varphi \\ &= \frac{1}{2} \theta^{\frac{2n+p+3}{2}} \Gamma\left(\frac{2n+p+3}{2}\right) \cdot \frac{4\pi}{p+1} \delta_{(i_1 i_2 \delta_{i_3 i_4} \cdots \delta_{i_{p-1} i_p})}, \end{aligned} \quad (3.19)$$

where $\nu_i = h_i/h = \{\sin \Theta \cos \varphi, \sin \Theta \sin \varphi, \cos \Theta\}_i$ are components of the direction vector.

The remaining integral in $P_{i_1 \cdots i_n}^{0(\alpha\beta)}$ is the integration over $\mathbf{g}$. This integral is also performed by transforming $\mathbf{g}$ into spherical coordinate system. The vectorial part in the integral, i.e., the integrals over polar angle and azimuthal angle, are evaluated in terms of Kronecker deltas as above. The remaining scalar part, i.e., the integral over g , cannot be fully performed as the integrand contains the unknowns $I^{(n)}$, which have appeared through the unknown coefficients $a_l^{(j)}(g)$, see § 3.1.2.1. Nevertheless, by changing the variable g to $2\sqrt{\theta} \gamma_{\alpha\beta}$, where $\gamma_{\alpha\beta}$ is dimensionless relative speed of α -gas molecules with respect to β -gas molecules, the integral over g can be expressed in terms of the Omega integrals (3.16). As soon as one specifies the interaction potential, the Omega integrals are known and integral over g can also be fully performed.

3.1.4 Dimensionless scaling

In MATHEMATICA[®] program, the dimensionless quantities are used. The quantities in (3.3) have been scaled as follows.

$$\hat{g}_i = \frac{g_i}{\sqrt{\theta}}, \quad \hat{h}_i = \frac{h_i}{\sqrt{\theta}}, \quad \hat{C}_i'^{(\gamma)} = \frac{C_i'^{(\gamma)}}{\sqrt{\theta_\gamma}}, \quad \hat{C}_i^{(\gamma)} = \frac{C_i^{(\gamma)}}{\sqrt{\theta_\gamma}}, \quad \hat{f}_\gamma(\hat{\mathbf{C}}_\gamma) = \frac{\theta_\gamma^{3/2}}{n_\gamma} f_\gamma(\mathbf{C}_\gamma), \quad \gamma \in \{\alpha, \beta\}.$$

Additionally, a reference differential cross section B_0 is chosen to define $\hat{b} d\hat{b} = b db/B_0$. In terms of the dimensionless variables defined above, expression (3.3) reads

$$\frac{P_{i_1 \cdots i_n}^{0(\alpha\beta)}}{\rho_\alpha \theta_\alpha^{n/2} Z} = \int \left(\hat{C}_{i_1}'^{(\alpha)} \cdots \hat{C}_{i_n}'^{(\alpha)} - \hat{C}_{i_1}^{(\alpha)} \cdots \hat{C}_{i_n}^{(\alpha)} \right) \hat{f}_\alpha(\hat{\mathbf{C}}_\alpha) \hat{f}_\beta(\hat{\mathbf{C}}_\beta) \hat{g} \hat{b} d\hat{b} d\epsilon d\hat{\mathbf{C}}_\alpha d\hat{\mathbf{C}}_\beta$$

with collision frequency $Z = n_\beta B_0 \sqrt{\theta}$. The dimensionless distribution functions in the above equation are replaced with corresponding dimensionless G13 or G26 distribution functions ($\gamma \in \{\alpha, \beta\}$):

$$\hat{f}_{\gamma|G13} = \left(\frac{1}{2\pi}\right)^{3/2} \exp\left(-\frac{\hat{C}_\gamma^2}{2}\right) \left[1 + \frac{u_i^{(\gamma)}}{\sqrt{\theta_\gamma}} \hat{C}_i^{(\gamma)} + \frac{1}{2} \frac{\sigma_{ij}^{(\gamma)}}{\rho_\gamma \theta_\gamma} \hat{C}_i^{(\gamma)} \hat{C}_j^{(\gamma)} + \frac{1}{5} \frac{h_i^{(\gamma)}}{\rho_\gamma \theta_\gamma^{3/2}} \hat{C}_i^{(\gamma)} (\hat{C}_\gamma^2 - 5)\right]$$

or

$$\begin{aligned} \hat{f}_{\gamma|G26} = & \left(\frac{1}{2\pi}\right)^{3/2} \exp\left(-\frac{\hat{C}_\gamma^2}{2}\right) \left[1 + \frac{u_i^{(\gamma)}}{\sqrt{\theta_\gamma}} \hat{C}_i^{(\gamma)} + \frac{1}{2} \frac{\sigma_{ij}^{(\gamma)}}{\rho_\gamma \theta_\gamma} \hat{C}_i^{(\gamma)} \hat{C}_j^{(\gamma)} + \frac{1}{5} \frac{h_i^{(\gamma)}}{\rho_\gamma \theta_\gamma^{3/2}} \hat{C}_i^{(\gamma)} (\hat{C}_\gamma^2 - 5)\right. \\ & \left. + \frac{1}{6} \frac{m_{ijk}^{(\gamma)}}{\rho_\gamma \theta_\gamma^{3/2}} \hat{C}_i^{(\gamma)} \hat{C}_j^{(\gamma)} \hat{C}_k^{(\gamma)} + \frac{1}{28} \frac{R_{ij}^{(\gamma)}}{\rho_\gamma \theta_\gamma^2} \hat{C}_i^{(\gamma)} \hat{C}_j^{(\gamma)} (\hat{C}_\gamma^2 - 7) + \frac{1}{8} \frac{\Delta_\gamma}{\rho_\gamma \theta_\gamma^2} \left(1 - \frac{2}{3} \hat{C}_\gamma^2 + \frac{1}{15} \hat{C}_\gamma^4\right)\right]. \end{aligned}$$

It should be noted that in the MATHEMATICA[®] program we have not used the dimensionless moments in the distribution functions for convenience; nevertheless, one can also use the dimensionless moments scaled with appropriate powers of ρ_γ and θ_γ without any problem. Moreover, the dimensionless quantities are not explicitly marked in the MATHEMATICA[®] program in order to simplify the notations.

3.2 Production terms

Implementing the procedure of §3.1 in MATHEMATICA[®] program, we compute the production terms associated with $N \times G13$ equations and $N \times G26$ equations for any interaction potential. Nevertheless, due to their cumbersome forms, we present them only for (a) Maxwell and (b) hard-sphere interaction potentials. In the following, we present the production terms for the α -constituent ($\alpha = 1, 2, \dots, N$) associated with systems of $N \times G13$ and $N \times G26$ equations. In case of hard-sphere interaction potential, we shall also use the following abbreviation for brevity.

$$\Delta\hat{\theta} = \frac{\mu_\alpha \theta_\alpha - \mu_\beta \theta_\beta}{\theta} = \frac{1}{\theta} \frac{k(T_\alpha - T_\beta)}{m_\alpha + m_\beta}. \quad (3.20)$$

It is worth pointing out that the production terms below are written in such a way that all the linear terms appear first followed by the non-linear terms. Moreover, the linear and non-linear terms which on replacing β with α vanish are written before the corresponding linear and non-linear terms which on replacing β with α do not vanish. With such an arrangement of terms, one can readily obtain the production terms for a single gas α by ignoring the summation and replacing β with α .

3.2.1 Production terms in $N \times G13$ system

3.2.1.1 Maxwell interaction potential

$$\mathcal{P}_{|G13}^{0(\alpha)} = 0, \quad (3.21)$$

$$\mathcal{P}_{i|G13}^{0(\alpha)} = -\frac{4}{3}a_1\rho_\alpha \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left(u_i^{(\alpha)} - u_i^{(\beta)} \right), \quad (3.22)$$

$$\frac{1}{2}\mathcal{P}_{i|G13}^{1(\alpha)} = -4a_1 \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[\mu_\alpha k n_\alpha (T_\alpha - T_\beta) - \frac{1}{3}(\mu_\alpha - \mu_\beta) \rho_\alpha u_i^{(\alpha)} u_i^{(\beta)} \right], \quad (3.23)$$

$$\begin{aligned} \mathcal{P}_{ij|G13}^{0(\alpha)} = & -2 \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[\sigma_{ij}^{(\alpha)} + \frac{1}{3}(4a_1 - 3)(\mu_\alpha - \mu_\beta) \sigma_{ij}^{(\alpha)} + \frac{1}{3}(4a_1 - 3) \mu_\beta \left(\sigma_{ij}^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} \sigma_{ij}^{(\beta)} \right) \right. \\ & \left. - \frac{2}{3} \left\{ 3\mu_\beta + 2a_1(\mu_\alpha - \mu_\beta) \right\} \rho_\alpha u_i^{(\alpha)} u_j^{(\beta)} \right], \end{aligned} \quad (3.24)$$

$$\begin{aligned} \frac{1}{2}\mathcal{P}_{i|G13}^{1(\alpha)} = & -\frac{2}{3} \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[2h_i^{(\alpha)} + 2(3a_1 - 1)(\mu_\alpha - \mu_\beta) h_i^{(\alpha)} + 10a_1 \mu_\beta \theta \rho_\alpha \left(u_i^{(\alpha)} - u_i^{(\beta)} \right) \right. \\ & + 4(2a_1 - 1) \mu_\beta^2 \left(h_i^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} \right) + 2\mu_\alpha \mu_\beta \left(u_j^{(\beta)} \sigma_{ij}^{(\alpha)} + \frac{\rho_\alpha}{\rho_\beta} u_j^{(\alpha)} \sigma_{ij}^{(\beta)} \right) \\ & - (\mu_\alpha - \mu_\beta) \left\{ \left(3\mu_\beta + 2a_1(\mu_\alpha - \mu_\beta) \right) u_j^{(\beta)} \sigma_{ij}^{(\alpha)} + (4a_1 - 1) \mu_\beta \frac{\rho_\alpha}{\rho_\beta} u_j^{(\alpha)} \sigma_{ij}^{(\beta)} \right\} \\ & \left. + 5\rho_\alpha \left\{ 2a_1 u_i^{(\alpha)} + \left(2\mu_\beta + a_1(\mu_\alpha - 3\mu_\beta) \right) \left(u_i^{(\alpha)} - u_i^{(\beta)} \right) \right\} \frac{k(T_\alpha - T_\beta)}{m_\alpha + m_\beta} \right]. \end{aligned} \quad (3.25)$$

3.2.1.2 Hard-sphere interaction potential

$$\mathcal{P}_{i|G13}^{0(\alpha)} = 0, \quad (3.26)$$

$$\begin{aligned} \mathcal{P}_{i|G13}^{0(\alpha)} = & - \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[\frac{5}{3} \rho_\alpha \left(u_i^{(\alpha)} - u_i^{(\beta)} \right) + \frac{1}{6\theta} \left(h_i^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} \right) \right. \\ & \left. - \frac{1}{6\theta} \left(\sigma_{ij}^{(\alpha)} u_j^{(\beta)} - \frac{\rho_\alpha}{\rho_\beta} \sigma_{ij}^{(\beta)} u_j^{(\alpha)} \right) + \frac{1}{60} \frac{1}{\rho_\beta \theta^2} \left(\sigma_{ij}^{(\alpha)} h_j^{(\beta)} - \sigma_{ij}^{(\beta)} h_j^{(\alpha)} \right) \right], \end{aligned} \quad (3.27)$$

$$\begin{aligned} \frac{1}{2}\mathcal{P}_{i|G13}^{1(\alpha)} = & - \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[5\rho_\alpha \theta \Delta \hat{\theta} - \frac{1}{3} \frac{1}{\theta} \mu_\beta \left(h_i^{(\alpha)} u_i^{(\beta)} - \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} u_i^{(\alpha)} \right) \right. \\ & - \frac{1}{3} (\mu_\alpha - \mu_\beta) \frac{1}{\rho_\beta} \left(5\rho_\alpha \rho_\beta u_i^{(\alpha)} u_i^{(\beta)} - \frac{1}{2} \frac{1}{\theta} \sigma_{ij}^{(\alpha)} \sigma_{ij}^{(\beta)} - \frac{3}{20} \frac{1}{\theta^2} h_i^{(\alpha)} h_i^{(\beta)} + \frac{3}{2} \frac{1}{\theta} \rho_\beta h_i^{(\alpha)} u_i^{(\beta)} \right. \\ & \left. + \frac{1}{2} \frac{1}{\theta} \rho_\alpha h_i^{(\beta)} u_i^{(\alpha)} \right) - \frac{1}{2} \Delta \hat{\theta} \left\{ \frac{5}{3} \rho_\alpha u_i^{(\alpha)} u_i^{(\beta)} + \frac{1}{12} \frac{1}{\rho_\beta \theta} \sigma_{ij}^{(\alpha)} \sigma_{ij}^{(\beta)} + \frac{1}{20} \frac{1}{\rho_\beta \theta^2} h_i^{(\alpha)} h_i^{(\beta)} \right. \\ & \left. \left. - \frac{1}{6} \frac{1}{\theta} \left(h_i^{(\alpha)} u_i^{(\beta)} + \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} u_i^{(\alpha)} \right) \right\} \right], \end{aligned} \quad (3.28)$$

$$\begin{aligned}
\mathcal{P}_{ij|G13}^{0(\alpha)} = & - \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_{\beta} \left[4\mu_{\beta} \left\{ \sigma_{ij}^{(\alpha)} + \frac{1}{3} \left(\sigma_{ij}^{(\alpha)} - \frac{\rho_{\alpha}}{\rho_{\beta}} \sigma_{ij}^{(\beta)} \right) \right\} + \frac{10}{3} (\mu_{\alpha} - \mu_{\beta}) \sigma_{ij}^{(\alpha)} \right. \\
& - \mu_{\beta} \frac{1}{\rho_{\beta}} \left(4\rho_{\alpha} \rho_{\beta} u_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} - \frac{2}{7} \frac{1}{\theta} \sigma_{k\langle i}^{(\alpha)} \sigma_{j\rangle k}^{(\beta)} - \frac{1}{25} \frac{1}{\theta^2} h_{\langle i}^{(\alpha)} h_{j\rangle}^{(\beta)} + \frac{2}{3} \frac{1}{\theta} \rho_{\beta} h_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} \right. \\
& + \left. \frac{2}{15} \frac{1}{\theta} \rho_{\alpha} h_{\langle i}^{(\beta)} u_{j\rangle}^{(\alpha)} \right) - (\mu_{\alpha} - \mu_{\beta}) \frac{1}{\rho_{\beta}} \left(\frac{10}{3} \rho_{\alpha} \rho_{\beta} u_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} - \frac{1}{3} \frac{1}{\theta} \sigma_{k\langle i}^{(\alpha)} \sigma_{j\rangle k}^{(\beta)} - \frac{3}{50} \frac{1}{\theta^2} h_{\langle i}^{(\alpha)} h_{j\rangle}^{(\beta)} \right. \\
& + \left. \frac{3}{5} \frac{1}{\theta} \rho_{\beta} h_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} + \frac{1}{3} \frac{1}{\theta} \rho_{\alpha} h_{\langle i}^{(\beta)} u_{j\rangle}^{(\alpha)} \right) + \frac{1}{3} \Delta\hat{\theta} \left\{ \sigma_{ij}^{(\alpha)} + \frac{\rho_{\alpha}}{\rho_{\beta}} \sigma_{ij}^{(\beta)} - 2\rho_{\alpha} u_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} \right. \\
& \left. \left. - \frac{1}{7} \frac{1}{\rho_{\beta} \theta} \sigma_{k\langle i}^{(\alpha)} \sigma_{j\rangle k}^{(\beta)} - \frac{3}{50} \frac{1}{\rho_{\beta} \theta^2} h_{\langle i}^{(\alpha)} h_{j\rangle}^{(\beta)} + \frac{1}{5} \frac{1}{\theta} \left(h_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} + \frac{\rho_{\alpha}}{\rho_{\beta}} h_{\langle i}^{(\beta)} u_{j\rangle}^{(\alpha)} \right) \right\} \right], \quad (3.29)
\end{aligned}$$

$$\begin{aligned}
\frac{1}{2} \mathcal{P}_{i|G13}^{1(\alpha)} = & - \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_{\beta} \left[\frac{8}{3} \mu_{\beta} h_i^{(\alpha)} + 5(\mu_{\alpha} - \mu_{\beta}) h_i^{(\alpha)} + \frac{1}{6} \mu_{\beta} (5 + 27\mu_{\beta}) \left(h_i^{(\alpha)} - \frac{\rho_{\alpha}}{\rho_{\beta}} h_i^{(\beta)} \right) \right. \\
& + \frac{5}{3} \mu_{\beta} (5 + \mu_{\beta}) \rho_{\alpha} \theta \left(u_i^{(\alpha)} - u_i^{(\beta)} \right) + \frac{1}{4} \mu_{\beta}^2 \frac{1}{\rho_{\beta}} \left(-\frac{10}{3} \rho_{\beta} \sigma_{ij}^{(\alpha)} u_j^{(\beta)} + 14\rho_{\alpha} \sigma_{ij}^{(\beta)} u_j^{(\alpha)} \right. \\
& + \left. \frac{13}{5} \frac{1}{\theta} \sigma_{ij}^{(\alpha)} h_j^{(\beta)} + \frac{3}{5} \frac{1}{\theta} \sigma_{ij}^{(\beta)} h_j^{(\alpha)} \right) - \frac{1}{4} (\mu_{\alpha} - \mu_{\beta}) \frac{1}{\rho_{\beta}} \left(\frac{2}{3} (10 - 11\mu_{\beta}) \rho_{\beta} \sigma_{ij}^{(\alpha)} u_j^{(\beta)} \right. \\
& + 2\mu_{\beta} \rho_{\alpha} \sigma_{ij}^{(\beta)} u_j^{(\alpha)} + \frac{1}{15} (10 - 57\mu_{\beta}) \frac{1}{\theta} \sigma_{ij}^{(\alpha)} h_j^{(\beta)} - \frac{1}{5} (6 - 11\mu_{\beta}) \frac{1}{\theta} \sigma_{ij}^{(\beta)} h_j^{(\alpha)} \Big) \\
& + \frac{1}{4} \Delta\hat{\theta} \left\{ \left(9 - 8\mu_{\beta} - \frac{1}{2} \Delta\hat{\theta} \right) h_i^{(\alpha)} - \frac{1}{3} \left(5 - 24\mu_{\beta} - \frac{3}{2} \Delta\hat{\theta} \right) \frac{\rho_{\alpha}}{\rho_{\beta}} h_i^{(\beta)} \right. \\
& + 10 \left(5 - 4\mu_{\beta} + \frac{1}{2} \Delta\hat{\theta} \right) \rho_{\alpha} \theta u_i^{(\alpha)} - \frac{10}{3} \left(5 - 12\mu_{\beta} + \frac{3}{2} \Delta\hat{\theta} \right) \rho_{\alpha} \theta u_i^{(\beta)} \\
& - \frac{1}{3} \left(23 - 24\mu_{\beta} - \frac{3}{2} \Delta\hat{\theta} \right) \sigma_{ij}^{(\alpha)} u_j^{(\beta)} + \left(3 - 8\mu_{\beta} - \frac{1}{2} \Delta\hat{\theta} \right) \frac{\rho_{\alpha}}{\rho_{\beta}} \sigma_{ij}^{(\beta)} u_j^{(\alpha)} \\
& \left. \left. + \frac{1}{30} \left(23 - 36\mu_{\beta} - \frac{9}{2} \Delta\hat{\theta} \right) \frac{1}{\rho_{\beta} \theta} \sigma_{ij}^{(\alpha)} h_j^{(\beta)} - \frac{1}{10} \left(7 - 12\mu_{\beta} - \frac{3}{2} \Delta\hat{\theta} \right) \frac{1}{\rho_{\beta} \theta} \sigma_{ij}^{(\beta)} h_j^{(\alpha)} \right\} \right]. \quad (3.30)
\end{aligned}$$

3.2.2 Production terms in $N \times G26$ system

3.2.2.1 Maxwell interaction potential

$$\mathcal{P}_{i|G26}^{0(\alpha)} = 0, \quad (3.31)$$

$$\mathcal{P}_{i|G26}^{0(\alpha)} = -\frac{4}{3} a_1 \rho_{\alpha} \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_{\beta} \left(u_i^{(\alpha)} - u_i^{(\beta)} \right), \quad (3.32)$$

$$\frac{1}{2} \mathcal{P}_{i|G26}^{1(\alpha)} = -4a_1 \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_{\beta} \left[\mu_{\alpha} k n_{\alpha} (T_{\alpha} - T_{\beta}) - \frac{1}{3} (\mu_{\alpha} - \mu_{\beta}) \rho_{\alpha} u_i^{(\alpha)} u_i^{(\beta)} \right], \quad (3.33)$$

$$\begin{aligned} \mathcal{P}_{ij|G26}^{0(\alpha)} = & -2 \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_{\beta} \left[\sigma_{ij}^{(\alpha)} + \frac{1}{3}(4a_1 - 3)(\mu_{\alpha} - \mu_{\beta})\sigma_{ij}^{(\alpha)} + \frac{1}{3}(4a_1 - 3)\mu_{\beta} \left(\sigma_{ij}^{(\alpha)} - \frac{\rho_{\alpha}}{\rho_{\beta}}\sigma_{ij}^{(\beta)} \right) \right. \\ & \left. - \frac{2}{3} \left\{ 3\mu_{\beta} + 2a_1(\mu_{\alpha} - \mu_{\beta}) \right\} \rho_{\alpha} u_{\langle i}^{(\alpha)} u_{j \rangle}^{(\beta)} \right], \end{aligned} \quad (3.34)$$

$$\begin{aligned} \frac{1}{2} \mathcal{P}_{i|G26}^{1(\alpha)} = & -\frac{2}{3} \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_{\beta} \left[2h_i^{(\alpha)} + 2(3a_1 - 1)(\mu_{\alpha} - \mu_{\beta})h_i^{(\alpha)} + 10a_1\mu_{\beta}\theta\rho_{\alpha} \left(u_i^{(\alpha)} - u_i^{(\beta)} \right) \right. \\ & + 4(2a_1 - 1)\mu_{\beta}^2 \left(h_i^{(\alpha)} - \frac{\rho_{\alpha}}{\rho_{\beta}}h_i^{(\beta)} \right) + 2\mu_{\alpha}\mu_{\beta} \left(u_j^{(\beta)}\sigma_{ij}^{(\alpha)} + \frac{\rho_{\alpha}}{\rho_{\beta}}u_j^{(\alpha)}\sigma_{ij}^{(\beta)} \right) \\ & - (\mu_{\alpha} - \mu_{\beta}) \left\{ \left(3\mu_{\beta} + 2a_1(\mu_{\alpha} - \mu_{\beta}) \right) u_j^{(\beta)}\sigma_{ij}^{(\alpha)} + (4a_1 - 1)\mu_{\beta} \frac{\rho_{\alpha}}{\rho_{\beta}}u_j^{(\alpha)}\sigma_{ij}^{(\beta)} \right\} \\ & \left. + 5\rho_{\alpha} \left\{ 2a_1u_i^{(\alpha)} + \left(2\mu_{\beta} + a_1(\mu_{\alpha} - 3\mu_{\beta}) \right) \left(u_i^{(\alpha)} - u_i^{(\beta)} \right) \right\} \frac{k(T_{\alpha} - T_{\beta})}{m_{\alpha} + m_{\beta}} \right], \end{aligned} \quad (3.35)$$

$$\begin{aligned} \mathcal{P}_{ijk|G26}^{0(\alpha)} = & -\sum_{\beta=1}^N \nu_{\alpha\beta} \mu_{\beta} \left[3m_{ijk}^{(\alpha)} + (4a_1 - 3)(\mu_{\alpha} - \mu_{\beta})m_{ijk}^{(\alpha)} \right. \\ & + \frac{2}{3}(5a_3 + 3a_1 - 9)\mu_{\beta}^2 \left(m_{ijk}^{(\alpha)} - \frac{\rho_{\alpha}}{\rho_{\beta}}m_{ijk}^{(\beta)} \right) - 6\mu_{\alpha}\mu_{\beta} \left(u_{\langle i}^{(\beta)}\sigma_{jk \rangle}^{(\alpha)} + \frac{\rho_{\alpha}}{\rho_{\beta}}u_{\langle i}^{(\alpha)}\sigma_{jk \rangle}^{(\beta)} \right) \\ & - 2(\mu_{\alpha} - \mu_{\beta}) \left\{ \left(2a_1 - (5a_3 - a_1 - 3)\mu_{\beta} \right) u_{\langle i}^{(\beta)}\sigma_{jk \rangle}^{(\alpha)} + (5a_3 - a_1 - 6)\mu_{\beta} \frac{\rho_{\alpha}}{\rho_{\beta}}u_{\langle i}^{(\alpha)}\sigma_{jk \rangle}^{(\beta)} \right\} \\ & \left. - 10(a_3 - a_1)\mu_{\alpha}\mu_{\beta} \left(u_{\langle i}^{(\beta)}\sigma_{jk \rangle}^{(\alpha)} - \frac{\rho_{\alpha}}{\rho_{\beta}}u_{\langle i}^{(\alpha)}\sigma_{jk \rangle}^{(\beta)} \right) \right], \end{aligned} \quad (3.36)$$

$$\begin{aligned} \mathcal{P}_{ij|G26}^{1(\alpha)} = & -\sum_{\beta=1}^N \nu_{\alpha\beta} \mu_{\beta} \left[\frac{7}{3}R_{ij}^{(\alpha)} + 14\theta\sigma_{ij}^{(\alpha)} - \frac{14}{3}(\mu_{\alpha} - \mu_{\beta}) \left(3 - 2(4a_1 - 3)\mu_{\beta} \right) \theta\sigma_{ij}^{(\alpha)} \right. \\ & + \frac{1}{3}(\mu_{\alpha} - \mu_{\beta}) \left\{ (16a_1 - 7)\mu_{\alpha}^2 + (16a_1 - 6)\mu_{\alpha}\mu_{\beta} + (12a_3 + 20a_1 - 27)\mu_{\beta}^2 \right\} R_{ij}^{(\alpha)} \\ & + \frac{28}{3}(4a_1 - 3)\mu_{\beta}^2\theta \left(\sigma_{ij}^{(\alpha)} - \frac{\rho_{\alpha}}{\rho_{\beta}}\sigma_{ij}^{(\beta)} \right) + \frac{4}{3}(3a_3 + 5a_1 - 7)\mu_{\beta}^3 \left(R_{ij}^{(\alpha)} - \frac{\rho_{\alpha}}{\rho_{\beta}}R_{ij}^{(\beta)} \right) \\ & - 56\mu_{\beta}^2\rho_{\alpha}\theta u_{\langle i}^{(\alpha)}u_{j \rangle}^{(\beta)} + \frac{32}{3}\mu_{\beta}^3 \frac{1}{\rho_{\beta}}\sigma_{k\langle i}^{(\alpha)}\sigma_{j \rangle k}^{(\beta)} - \frac{112}{5}\mu_{\alpha}\mu_{\beta}^2 \left(u_{\langle i}^{(\beta)}h_{j \rangle}^{(\alpha)} + \frac{\rho_{\alpha}}{\rho_{\beta}}u_{\langle i}^{(\alpha)}h_{j \rangle}^{(\beta)} \right) \\ & + \frac{16}{3}\mu_{\alpha}\mu_{\beta}^2 \left(u_k^{(\beta)}m_{ijk}^{(\alpha)} + \frac{\rho_{\alpha}}{\rho_{\beta}}u_k^{(\alpha)}m_{ijk}^{(\beta)} \right) - \frac{112}{3}a_1\mu_{\beta}(\mu_{\alpha} - \mu_{\beta})\theta\rho_{\alpha}u_{\langle i}^{(\alpha)}u_{j \rangle}^{(\beta)} \\ & - \frac{8}{3}\mu_{\beta}(\mu_{\alpha} - \mu_{\beta}) \left\{ (4a_1 - 3)\mu_{\alpha} - (3a_3 + a_1 - 2)\mu_{\beta} \right\} \frac{1}{\rho_{\beta}}\sigma_{k\langle i}^{(\alpha)}\sigma_{j \rangle k}^{(\beta)} \\ & - \frac{112}{15}(3a_3 + a_1 - 5)\mu_{\beta}^2(\mu_{\alpha} - \mu_{\beta}) \frac{\rho_{\alpha}}{\rho_{\beta}}u_{\langle i}^{(\alpha)}h_{j \rangle}^{(\beta)} \\ & - \frac{56}{15}(\mu_{\alpha} - \mu_{\beta}) \left\{ 2a_1\mu_{\alpha}^2 - (4a_1 - 7)\mu_{\alpha}\mu_{\beta} + (2a_1 - 3)\mu_{\beta}^2 \right\} u_{\langle i}^{(\beta)}h_{j \rangle}^{(\alpha)} \\ & - \frac{4}{3}(a_3 + 7a_1 - 5)\mu_{\beta}^2(\mu_{\alpha} - \mu_{\beta}) \frac{\rho_{\alpha}}{\rho_{\beta}}u_k^{(\alpha)}m_{ijk}^{(\beta)} \\ & \left. - \frac{4}{3}(\mu_{\alpha} - \mu_{\beta}) \left\{ 2a_1\mu_{\alpha}^2 - (4a_1 - 2)\mu_{\alpha}\mu_{\beta} + (5a_3 - 3a_1 - 3)\mu_{\beta}^2 \right\} u_k^{(\beta)}m_{ijk}^{(\alpha)} \right] \end{aligned}$$

$$\begin{aligned}
& -\frac{28}{3} \left(4a_1\mu_\alpha^2 - (4a_1 - 7)\mu_\alpha\mu_\beta + (6a_3 + 2a_1 - 7)\mu_\beta^2 \right) \frac{k(T_\alpha - T_\beta)}{m_\alpha + m_\beta} \sigma_{ij}^{(\alpha)} \\
& + \frac{14}{3} \mu_\beta \left((4a_1 - 3)\mu_\alpha - (6a_3 + 6a_1 - 11)\mu_\beta \right) \frac{k(T_\alpha - T_\beta)}{m_\alpha + m_\beta} \left(\sigma_{ij}^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} \sigma_{ij}^{(\beta)} \right) \\
& - \frac{28}{3} \left(2a_1\mu_\alpha^2 - (8a_1 - 7)\mu_\alpha\mu_\beta + (6a_3 - 7)\mu_\beta^2 \right) \frac{k(T_\alpha - T_\beta)}{m_\alpha + m_\beta} \rho_\alpha u_{\langle i}^{(\alpha)} u_{j \rangle}^{(\beta)} \\
& - \frac{112}{5} (a_3 - a_1) \mu_\alpha \mu_\beta^2 \left(u_{\langle i}^{(\beta)} h_{j \rangle}^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} u_{\langle i}^{(\alpha)} h_{j \rangle}^{(\beta)} \right) \\
& + \frac{16}{3} (a_3 - a_1) \mu_\alpha \mu_\beta^2 \left(u_k^{(\beta)} m_{ijk}^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} u_k^{(\alpha)} m_{ijk}^{(\beta)} \right) \Big], \tag{3.37}
\end{aligned}$$

$$\begin{aligned}
\mathcal{P}_{|G26}^{2(\alpha)} = & -\frac{4}{3} \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[\Delta_\alpha + (\mu_\alpha - \mu_\beta) \left\{ (4a_1 - 1)\mu_\alpha^2 + 4a_1\mu_\alpha\mu_\beta + (8a_1 - 3)\mu_\beta^2 \right\} \Delta_\alpha \right. \\
& + 4(2a_1 - 1)\mu_\beta^3 \left(\Delta_\alpha - \frac{\rho_\alpha}{\rho_\beta} \Delta_\beta \right) + 120a_1\mu_\beta\rho_\alpha\theta \frac{k(T_\alpha - T_\beta)}{m_\alpha + m_\beta} + 8\mu_\alpha\mu_\beta^2 \frac{1}{\rho_\beta} \sigma_{ij}^{(\alpha)} \sigma_{ij}^{(\beta)} \\
& + 60 \left\{ \mu_\beta + a_1(\mu_\alpha - \mu_\beta) \right\} \rho_\alpha \left\{ \frac{k(T_\alpha - T_\beta)}{m_\alpha + m_\beta} \right\}^2 - 2\mu_\beta(4a_1 - 3)(\mu_\alpha - \mu_\beta)^2 \frac{1}{\rho_\beta} \sigma_{ij}^{(\alpha)} \sigma_{ij}^{(\beta)} \\
& - 20(\mu_\alpha - \mu_\beta) \left\{ 2a_1\mu_\beta\theta - \left(2(a_1 - 1)\mu_\beta - a_1(\mu_\alpha - \mu_\beta) \right) \frac{k(T_\alpha - T_\beta)}{m_\alpha + m_\beta} \right\} \rho_\alpha u_i^{(\alpha)} u_i^{(\beta)} \\
& \left. - 8(\mu_\alpha - \mu_\beta) \left\{ 2(2a_1 - 1)\mu_\beta^2 \frac{\rho_\alpha}{\rho_\beta} u_i^{(\alpha)} h_i^{(\beta)} + \left(2\mu_\alpha\mu_\beta + a_1(\mu_\alpha - \mu_\beta)^2 \right) u_i^{(\beta)} h_i^{(\alpha)} \right\} \right]. \tag{3.38}
\end{aligned}$$

3.2.2.2 Hard-sphere interaction potential

$$\mathcal{P}_{|G26}^{0(\alpha)} = 0, \tag{3.39}$$

$$\begin{aligned}
\mathcal{P}_{|G26}^{0(\alpha)} = & -\sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[\frac{5}{3} \rho_\alpha \left(u_i^{(\alpha)} - u_i^{(\beta)} \right) + \frac{1}{6\theta} \left(h_i^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} \right) \right. \\
& - \frac{1}{6\theta} \left(\sigma_{ij}^{(\alpha)} u_j^{(\beta)} - \frac{\rho_\alpha}{\rho_\beta} \sigma_{ij}^{(\beta)} u_j^{(\alpha)} \right) + \frac{1}{168\theta^2} \left(R_{ij}^{(\alpha)} u_j^{(\beta)} - \frac{\rho_\alpha}{\rho_\beta} R_{ij}^{(\beta)} u_j^{(\alpha)} \right) \\
& + \frac{1}{288\theta^2} \left(\Delta_\alpha u_i^{(\beta)} - \frac{\rho_\alpha}{\rho_\beta} \Delta_\beta u_i^{(\alpha)} \right) + \frac{1}{60} \frac{1}{\rho_\beta \theta^2} \left(\sigma_{ij}^{(\alpha)} h_j^{(\beta)} - \sigma_{ij}^{(\beta)} h_j^{(\alpha)} \right) \\
& - \frac{1}{560} \frac{1}{\rho_\beta \theta^3} \left(R_{ij}^{(\alpha)} h_j^{(\beta)} - R_{ij}^{(\beta)} h_j^{(\alpha)} \right) - \frac{1}{960} \frac{1}{\rho_\beta \theta^3} \left(\Delta_\alpha h_i^{(\beta)} - \Delta_\beta h_i^{(\alpha)} \right) \\
& \left. - \frac{1}{168} \frac{1}{\rho_\beta \theta^2} \left(m_{ijk}^{(\alpha)} \sigma_{jk}^{(\beta)} - m_{ijk}^{(\beta)} \sigma_{jk}^{(\alpha)} \right) + \frac{1}{1568} \frac{1}{\rho_\beta \theta^3} \left(m_{ijk}^{(\alpha)} R_{jk}^{(\beta)} - m_{ijk}^{(\beta)} R_{jk}^{(\alpha)} \right) \right], \tag{3.40}
\end{aligned}$$

$$\begin{aligned}
\frac{1}{2} \mathcal{P}_{|G26}^{1(\alpha)} = & -\sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[5\rho_\alpha\theta\Delta\hat{\theta} + \frac{1}{12}\frac{1}{\theta}(\mu_\alpha - \mu_\beta)\Delta_\alpha + \frac{1}{12}\frac{1}{\theta}\mu_\beta \left(\Delta_\alpha - \frac{\rho_\alpha}{\rho_\beta} \Delta_\beta \right) \right. \\
& \left. - \frac{1}{3}\frac{1}{\theta}\mu_\beta \left(h_i^{(\alpha)} u_i^{(\beta)} - \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} u_i^{(\alpha)} \right) + \frac{1}{168} \frac{1}{\rho_\beta \theta^2} \mu_\beta \left(\sigma_{ij}^{(\alpha)} R_{ij}^{(\beta)} - \sigma_{ij}^{(\beta)} R_{ij}^{(\alpha)} \right) \right]
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3}(\mu_\alpha - \mu_\beta) \frac{1}{\rho_\beta} \left(5\rho_\alpha \rho_\beta u_i^{(\alpha)} u_i^{(\beta)} - \frac{1}{2} \frac{1}{\theta} \sigma_{ij}^{(\alpha)} \sigma_{ij}^{(\beta)} - \frac{3}{20} \frac{1}{\theta^2} h_i^{(\alpha)} h_i^{(\beta)} - \frac{1}{56} \frac{1}{\theta^2} m_{ijk}^{(\alpha)} m_{ijk}^{(\beta)} \right. \\
& - \frac{3}{784} \frac{1}{\theta^3} R_{ij}^{(\alpha)} R_{ij}^{(\beta)} - \frac{1}{640} \frac{1}{\theta^3} \Delta_\alpha \Delta_\beta + \frac{3}{2} \frac{1}{\theta} \rho_\beta h_i^{(\alpha)} u_i^{(\beta)} + \frac{1}{2} \frac{1}{\theta} \rho_\alpha h_i^{(\beta)} u_i^{(\alpha)} + \frac{1}{56} \frac{1}{\theta^2} \sigma_{ij}^{(\alpha)} R_{ij}^{(\beta)} \\
& + \frac{1}{28} \frac{1}{\theta^2} \sigma_{ij}^{(\beta)} R_{ij}^{(\alpha)} \left. \right) - \frac{1}{2} \Delta \hat{\theta} \left\{ \frac{1}{48} \frac{1}{\theta} \left(\Delta_\alpha + \frac{\rho_\alpha}{\rho_\beta} \Delta_\beta \right) + \frac{5}{3} \rho_\alpha u_i^{(\alpha)} u_i^{(\beta)} + \frac{1}{12} \frac{1}{\rho_\beta \theta} \sigma_{ij}^{(\alpha)} \sigma_{ij}^{(\beta)} \right. \\
& + \frac{1}{20} \frac{1}{\rho_\beta \theta^2} h_i^{(\alpha)} h_i^{(\beta)} + \frac{1}{168} \frac{1}{\rho_\beta \theta^2} m_{ijk}^{(\alpha)} m_{ijk}^{(\beta)} + \frac{5}{3136} \frac{1}{\rho_\beta \theta^3} R_{ij}^{(\alpha)} R_{ij}^{(\beta)} + \frac{1}{1536} \frac{1}{\rho_\beta \theta^3} \Delta_\alpha \Delta_\beta \\
& \left. - \frac{1}{6} \frac{1}{\theta} \left(h_i^{(\alpha)} u_i^{(\beta)} + \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} u_i^{(\alpha)} \right) - \frac{1}{112} \frac{1}{\rho_\beta \theta^2} \left(\sigma_{ij}^{(\alpha)} R_{ij}^{(\beta)} + \sigma_{ij}^{(\beta)} R_{ij}^{(\alpha)} \right) \right\}, \quad (3.41)
\end{aligned}$$

$$\begin{aligned}
\mathcal{P}_{ij|G26}^{0(\alpha)} = & - \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[4\mu_\beta \left\{ \sigma_{ij}^{(\alpha)} + \frac{1}{28\theta} R_{ij}^{(\alpha)} + \frac{1}{3} \left(\sigma_{ij}^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} \sigma_{ij}^{(\beta)} \right) + \frac{1}{42\theta} \left(R_{ij}^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} R_{ij}^{(\beta)} \right) \right\} \right. \\
& + \frac{1}{6} (\mu_\alpha - \mu_\beta) \left(20\sigma_{ij}^{(\alpha)} + \frac{1}{\theta} R_{ij}^{(\alpha)} \right) \\
& - \mu_\beta \frac{1}{\rho_\beta} \left(\frac{1}{180} \frac{1}{\theta^2} \sigma_{ij}^{(\alpha)} \Delta_\beta + \frac{1}{360} \frac{1}{\theta^2} \sigma_{ij}^{(\beta)} \Delta_\alpha - \frac{1}{1120} \frac{1}{\theta^3} R_{ij}^{(\alpha)} \Delta_\beta + 4\rho_\alpha \rho_\beta u_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} \right. \\
& - \frac{2}{7} \frac{1}{\theta} \sigma_{k\langle i}^{(\alpha)} \sigma_{j\rangle k}^{(\beta)} - \frac{1}{25} \frac{1}{\theta^2} h_{\langle i}^{(\alpha)} h_{j\rangle}^{(\beta)} - \frac{1}{126} \frac{1}{\theta^2} m_{kl\langle i}^{(\alpha)} m_{j\rangle kl}^{(\beta)} - \frac{3}{2744} \frac{1}{\theta^3} R_{k\langle i}^{(\alpha)} R_{j\rangle k}^{(\beta)} \\
& + \frac{2}{3} \frac{1}{\theta} \rho_\beta h_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} + \frac{2}{15} \frac{1}{\theta} \rho_\alpha h_{\langle i}^{(\beta)} u_{j\rangle}^{(\alpha)} + \frac{10}{21} \frac{1}{\theta} \rho_\beta m_{ijk}^{(\alpha)} u_k^{(\beta)} - \frac{4}{21} \frac{1}{\theta} \rho_\alpha m_{ijk}^{(\beta)} u_k^{(\alpha)} \\
& - \frac{4}{105} \frac{1}{\theta^2} m_{ijk}^{(\alpha)} h_k^{(\beta)} + \frac{1}{105} \frac{1}{\theta^2} m_{ijk}^{(\beta)} h_k^{(\alpha)} + \frac{1}{294} \frac{1}{\theta^2} \sigma_{k\langle i}^{(\alpha)} R_{j\rangle k}^{(\beta)} + \frac{5}{294} \frac{1}{\theta^2} \sigma_{k\langle i}^{(\beta)} R_{j\rangle k}^{(\alpha)} \left. \right) \\
& - (\mu_\alpha - \mu_\beta) \frac{1}{\rho_\beta} \left(\frac{1}{144} \frac{1}{\theta^2} \sigma_{ij}^{(\alpha)} \Delta_\beta + \frac{1}{180} \frac{1}{\theta^2} \sigma_{ij}^{(\beta)} \Delta_\alpha - \frac{1}{960} \frac{1}{\theta^3} R_{ij}^{(\alpha)} \Delta_\beta - \frac{1}{1680} \frac{1}{\theta^3} R_{ij}^{(\beta)} \Delta_\alpha \right. \\
& + \frac{10}{3} \rho_\alpha \rho_\beta u_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} - \frac{1}{3} \frac{1}{\theta} \sigma_{k\langle i}^{(\alpha)} \sigma_{j\rangle k}^{(\beta)} - \frac{3}{50} \frac{1}{\theta^2} h_{\langle i}^{(\alpha)} h_{j\rangle}^{(\beta)} - \frac{1}{84} \frac{1}{\theta^2} m_{kl\langle i}^{(\alpha)} m_{j\rangle kl}^{(\beta)} \\
& - \frac{11}{5488} \frac{1}{\theta^3} R_{k\langle i}^{(\alpha)} R_{j\rangle k}^{(\beta)} + \frac{3}{5} \frac{1}{\theta} \rho_\beta h_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} + \frac{1}{3} \frac{1}{\theta} \rho_\alpha h_{\langle i}^{(\beta)} u_{j\rangle}^{(\alpha)} + \frac{1}{3} \frac{1}{\theta} \rho_\beta m_{ijk}^{(\alpha)} u_k^{(\beta)} \\
& - \frac{1}{30} \frac{1}{\theta^2} m_{ijk}^{(\alpha)} h_k^{(\beta)} - \frac{1}{105} \frac{1}{\theta^2} m_{ijk}^{(\beta)} h_k^{(\alpha)} + \frac{1}{84} \frac{1}{\theta^2} \sigma_{k\langle i}^{(\alpha)} R_{j\rangle k}^{(\beta)} + \frac{11}{588} \frac{1}{\theta^2} \sigma_{k\langle i}^{(\beta)} R_{j\rangle k}^{(\alpha)} \left. \right) \\
& + \frac{1}{3} \Delta \hat{\theta} \left\{ \sigma_{ij}^{(\alpha)} + \frac{\rho_\alpha}{\rho_\beta} \sigma_{ij}^{(\beta)} - \frac{1}{28} \frac{1}{\theta} \left(R_{ij}^{(\alpha)} + \frac{\rho_\alpha}{\rho_\beta} R_{ij}^{(\beta)} \right) + \frac{1}{160} \frac{1}{\rho_\beta \theta^2} \left(\sigma_{ij}^{(\alpha)} \Delta_\beta + \sigma_{ij}^{(\beta)} \Delta_\alpha \right) \right. \\
& - \frac{1}{896} \frac{1}{\rho_\beta \theta^3} \left(R_{ij}^{(\alpha)} \Delta_\beta + R_{ij}^{(\beta)} \Delta_\alpha \right) - 2\rho_\alpha u_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} - \frac{1}{7} \frac{1}{\rho_\beta \theta} \sigma_{k\langle i}^{(\alpha)} \sigma_{j\rangle k}^{(\beta)} \\
& - \frac{3}{50} \frac{1}{\rho_\beta \theta^2} h_{\langle i}^{(\alpha)} h_{j\rangle}^{(\beta)} - \frac{1}{84} \frac{1}{\rho_\beta \theta^2} m_{kl\langle i}^{(\alpha)} m_{j\rangle kl}^{(\beta)} - \frac{15}{5488} \frac{1}{\rho_\beta \theta^3} R_{k\langle i}^{(\alpha)} R_{j\rangle k}^{(\beta)} \\
& + \frac{1}{5} \frac{1}{\theta} \left(h_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} + \frac{\rho_\alpha}{\rho_\beta} h_{\langle i}^{(\beta)} u_{j\rangle}^{(\alpha)} \right) + \frac{1}{14} \frac{1}{\theta} \left(m_{ijk}^{(\alpha)} u_k^{(\beta)} + \frac{\rho_\alpha}{\rho_\beta} m_{ijk}^{(\beta)} u_k^{(\alpha)} \right) \\
& \left. - \frac{3}{140} \frac{1}{\rho_\beta \theta^2} \left(m_{ijk}^{(\alpha)} h_k^{(\beta)} + m_{ijk}^{(\beta)} h_k^{(\alpha)} \right) + \frac{3}{196} \frac{1}{\rho_\beta \theta^2} \left(\sigma_{k\langle i}^{(\alpha)} R_{j\rangle k}^{(\beta)} + \sigma_{k\langle i}^{(\beta)} R_{j\rangle k}^{(\alpha)} \right) \right\}, \quad (3.42)
\end{aligned}$$

$$\frac{1}{2} \mathcal{P}_{i|G26}^{1(\alpha)} = - \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[\frac{8}{3} \mu_\beta h_i^{(\alpha)} + 5(\mu_\alpha - \mu_\beta) h_i^{(\alpha)} + \frac{1}{6} \mu_\beta (5 + 27\mu_\beta) \left(h_i^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} \right) \right]$$

$$\begin{aligned}
& + \frac{5}{3} \mu_\beta (5 + \mu_\beta) \rho_\alpha \theta \left(u_i^{(\alpha)} - u_i^{(\beta)} \right) + \frac{1}{4} \mu_\beta^2 \frac{1}{\rho_\beta} \left(\frac{3}{80} \frac{1}{\theta^2} h_i^{(\alpha)} \Delta_\beta + \frac{1}{144} \frac{1}{\theta^2} h_i^{(\beta)} \Delta_\alpha \right. \\
& - \frac{5}{24} \frac{1}{\theta} \rho_\alpha u_i^{(\alpha)} \Delta_\beta - \frac{49}{72} \frac{1}{\theta} \rho_\beta u_i^{(\beta)} \Delta_\alpha - \frac{10}{3} \rho_\beta \sigma_{ij}^{(\alpha)} u_j^{(\beta)} + 14 \rho_\alpha \sigma_{ij}^{(\beta)} u_j^{(\alpha)} - \frac{7}{6} \frac{1}{\theta} \rho_\beta R_{ij}^{(\alpha)} u_j^{(\beta)} \\
& + \frac{11}{14} \frac{1}{\theta} \rho_\alpha R_{ij}^{(\beta)} u_j^{(\alpha)} + \frac{13}{5} \frac{1}{\theta} \sigma_{ij}^{(\alpha)} h_j^{(\beta)} + \frac{3}{5} \frac{1}{\theta} \sigma_{ij}^{(\beta)} h_j^{(\alpha)} - \frac{19}{420} \frac{1}{\theta^2} R_{ij}^{(\alpha)} h_j^{(\beta)} + \frac{1}{140} \frac{1}{\theta^2} R_{ij}^{(\beta)} h_j^{(\alpha)} \\
& - \frac{31}{42} \frac{1}{\theta} m_{ijk}^{(\alpha)} \sigma_{jk}^{(\beta)} - \frac{1}{42} \frac{1}{\theta} m_{ijk}^{(\beta)} \sigma_{jk}^{(\alpha)} + \frac{83}{1176} \frac{1}{\theta^2} m_{ijk}^{(\alpha)} R_{jk}^{(\beta)} - \frac{19}{1176} \frac{1}{\theta^2} m_{ijk}^{(\beta)} R_{jk}^{(\alpha)} \Big) \\
& - \frac{1}{4} (\mu_\alpha - \mu_\beta) \frac{1}{\rho_\beta} \left(\frac{1}{240} (10 - 29\mu_\beta) \frac{1}{\theta^2} h_i^{(\alpha)} \Delta_\beta - \frac{1}{720} (44 - 71\mu_\beta) \frac{1}{\theta^2} h_i^{(\beta)} \Delta_\alpha \right. \\
& + \frac{5}{8} \mu_\beta \frac{1}{\theta} \rho_\alpha u_i^{(\alpha)} \Delta_\beta + \frac{1}{72} (44 - 13\mu_\beta) \frac{1}{\theta} \rho_\beta u_i^{(\beta)} \Delta_\alpha + \frac{2}{3} (10 - 11\mu_\beta) \rho_\beta \sigma_{ij}^{(\alpha)} u_j^{(\beta)} \\
& + 2\mu_\beta \rho_\alpha \sigma_{ij}^{(\beta)} u_j^{(\alpha)} + \frac{1}{42} (56 - 13\mu_\beta) \frac{1}{\theta} \rho_\beta R_{ij}^{(\alpha)} u_j^{(\beta)} + \frac{1}{2} \mu_\beta \frac{1}{\theta} \rho_\alpha R_{ij}^{(\beta)} u_j^{(\alpha)} \\
& + \frac{1}{15} (10 - 57\mu_\beta) \frac{1}{\theta} \sigma_{ij}^{(\alpha)} h_j^{(\beta)} - \frac{1}{5} (6 - 11\mu_\beta) \frac{1}{\theta} \sigma_{ij}^{(\beta)} h_j^{(\alpha)} - \frac{1}{420} (56 - 83\mu_\beta) \frac{1}{\theta^2} R_{ij}^{(\alpha)} h_j^{(\beta)} \\
& + \frac{1}{140} (6 - 25\mu_\beta) \frac{1}{\theta^2} R_{ij}^{(\beta)} h_j^{(\alpha)} - \frac{1}{42} (28 - 53\mu_\beta) \frac{1}{\theta} m_{ijk}^{(\alpha)} \sigma_{jk}^{(\beta)} - \frac{37}{42} \mu_\beta \frac{1}{\theta} m_{ijk}^{(\beta)} \sigma_{jk}^{(\alpha)} \\
& + \frac{1}{1176} (28 - 115\mu_\beta) \frac{1}{\theta^2} m_{ijk}^{(\alpha)} R_{jk}^{(\beta)} - \frac{1}{1176} (26 - 83\mu_\beta) \frac{1}{\theta^2} m_{ijk}^{(\beta)} R_{jk}^{(\alpha)} \Big) \\
& + \frac{1}{4} \Delta \hat{\theta} \left\{ \left(9 - 8\mu_\beta - \frac{1}{2} \Delta \hat{\theta} \right) h_i^{(\alpha)} - \frac{1}{3} \left(5 - 24\mu_\beta - \frac{3}{2} \Delta \hat{\theta} \right) \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} \right. \\
& + 10 \left(5 - 4\mu_\beta + \frac{1}{2} \Delta \hat{\theta} \right) \rho_\alpha \theta u_i^{(\alpha)} - \frac{10}{3} \left(5 - 12\mu_\beta + \frac{3}{2} \Delta \hat{\theta} \right) \rho_\alpha \theta u_i^{(\beta)} \\
& + \frac{1}{160} \left(9 - 16\mu_\beta - \frac{5}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} h_i^{(\alpha)} \Delta_\beta - \frac{1}{480} \left(29 - 48\mu_\beta - \frac{15}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} h_i^{(\beta)} \Delta_\alpha \\
& - \frac{1}{48} \left(5 - 12\mu_\beta - \frac{3}{2} \Delta \hat{\theta} \right) \frac{1}{\theta} \frac{\rho_\alpha}{\rho_\beta} u_i^{(\alpha)} \Delta_\beta + \frac{1}{144} \left(29 - 36\mu_\beta - \frac{9}{2} \Delta \hat{\theta} \right) \frac{1}{\theta} u_i^{(\beta)} \Delta_\alpha \\
& - \frac{1}{3} \left(23 - 24\mu_\beta - \frac{3}{2} \Delta \hat{\theta} \right) \sigma_{ij}^{(\alpha)} u_j^{(\beta)} + \left(3 - 8\mu_\beta - \frac{1}{2} \Delta \hat{\theta} \right) \frac{\rho_\alpha}{\rho_\beta} \sigma_{ij}^{(\beta)} u_j^{(\alpha)} \\
& + \frac{1}{84} \left(35 - 36\mu_\beta - \frac{9}{2} \Delta \hat{\theta} \right) \frac{1}{\theta} R_{ij}^{(\alpha)} u_j^{(\beta)} - \frac{3}{28} \left(1 - 4\mu_\beta - \frac{1}{2} \Delta \hat{\theta} \right) \frac{1}{\theta} \frac{\rho_\alpha}{\rho_\beta} R_{ij}^{(\beta)} u_j^{(\alpha)} \\
& + \frac{1}{30} \left(23 - 36\mu_\beta - \frac{9}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta} \sigma_{ij}^{(\alpha)} h_j^{(\beta)} - \frac{1}{10} \left(7 - 12\mu_\beta - \frac{3}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta} \sigma_{ij}^{(\beta)} h_j^{(\alpha)} \\
& - \frac{1}{280} \left(35 - 48\mu_\beta - \frac{15}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} R_{ij}^{(\alpha)} h_j^{(\beta)} + \frac{3}{280} \left(7 - 16\mu_\beta - \frac{5}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} R_{ij}^{(\beta)} h_j^{(\alpha)} \\
& - \frac{1}{84} \left(31 - 36\mu_\beta - \frac{9}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta} m_{ijk}^{(\alpha)} \sigma_{jk}^{(\beta)} + \frac{1}{84} \left(13 - 36\mu_\beta - \frac{9}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta} m_{ijk}^{(\beta)} \sigma_{jk}^{(\alpha)} \\
& + \frac{1}{784} \left(31 - 48\mu_\beta - \frac{15}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} m_{ijk}^{(\alpha)} R_{jk}^{(\beta)} \\
& \left. - \frac{1}{784} \left(25 - 48\mu_\beta - \frac{15}{2} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} m_{ijk}^{(\beta)} R_{jk}^{(\alpha)} \right\}, \tag{3.43}
\end{aligned}$$

$$\mathcal{P}_{ijk|G26}^{0(\alpha)} = - \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[12 \mu_\beta^2 \left\{ m_{ijk}^{(\alpha)} + \frac{3}{28} \left(m_{ijk}^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} m_{ijk}^{(\beta)} \right) \right\} + (\mu_\alpha - \mu_\beta) (5 + 6\mu_\beta) m_{ijk}^{(\alpha)} \right]$$

$$\begin{aligned}
& -\mu_\beta^2 \frac{1}{\rho_\beta} \left(\frac{1}{160} \frac{1}{\theta^2} m_{ijk}^{(\alpha)} \Delta_\beta + \frac{1}{224} \frac{1}{\theta^2} m_{ijk}^{(\beta)} \Delta_\alpha + \frac{55}{7} \rho_\beta \sigma_{ij}^{(\alpha)} u_k^{(\beta)} + \frac{29}{7} \rho_\alpha \sigma_{ij}^{(\beta)} u_k^{(\alpha)} \right. \\
& - \frac{9}{70} \frac{1}{\theta} \sigma_{ij}^{(\alpha)} h_k^{(\beta)} + \frac{3}{10} \frac{1}{\theta} \sigma_{ij}^{(\beta)} h_k^{(\alpha)} + \frac{17}{28} \frac{1}{\theta} \rho_\beta R_{ij}^{(\alpha)} u_k^{(\beta)} + \frac{37}{196} \frac{1}{\theta} \rho_\alpha R_{ij}^{(\beta)} u_k^{(\alpha)} \\
& - \frac{31}{1960} \frac{1}{\theta^2} R_{ij}^{(\alpha)} h_k^{(\beta)} - \frac{53}{1960} \frac{1}{\theta^2} R_{ij}^{(\beta)} h_k^{(\alpha)} - \frac{23}{42} \frac{1}{\theta} \sigma_{l(i}^{(\alpha)} m_{jk)l}^{(\beta)} - \frac{13}{42} \frac{1}{\theta} \sigma_{l(i}^{(\beta)} m_{jk)l}^{(\alpha)} \\
& \left. + \frac{23}{1176} \frac{1}{\theta^2} R_{l(i}^{(\alpha)} m_{jk)l}^{(\beta)} - \frac{11}{1176} \frac{1}{\theta^2} R_{l(i}^{(\beta)} m_{jk)l}^{(\alpha)} \right) \\
& - (\mu_\alpha - \mu_\beta) \frac{1}{\rho_\beta} \left(\frac{1}{480} (5 - 2\mu_\beta) \frac{1}{\theta^2} m_{ijk}^{(\alpha)} \Delta_\beta - \frac{1}{420} (1 - 4\mu_\beta) \frac{1}{\theta^2} m_{ijk}^{(\beta)} \Delta_\alpha \right. \\
& + (5 + 2\mu_\beta) \rho_\beta \sigma_{ij}^{(\alpha)} u_k^{(\beta)} + 4\mu_\beta \rho_\alpha \sigma_{ij}^{(\beta)} u_k^{(\alpha)} + \frac{1}{10} (5 - 6\mu_\beta) \frac{1}{\theta} \sigma_{ij}^{(\alpha)} h_k^{(\beta)} \\
& - \frac{2}{35} (7 - 12\mu_\beta) \frac{1}{\theta} \sigma_{ij}^{(\beta)} h_k^{(\alpha)} + \frac{1}{196} (91 + 22\mu_\beta) \frac{1}{\theta} \rho_\beta R_{ij}^{(\alpha)} u_k^{(\beta)} + \frac{2}{7} \mu_\beta \frac{1}{\theta} \rho_\alpha R_{ij}^{(\beta)} u_k^{(\alpha)} \\
& - \frac{1}{1960} (91 - 58\mu_\beta) \frac{1}{\theta^2} R_{ij}^{(\alpha)} h_k^{(\beta)} + \frac{1}{490} (7 - 25\mu_\beta) \frac{1}{\theta^2} R_{ij}^{(\beta)} h_k^{(\alpha)} \\
& - \frac{4}{7} \mu_\beta \frac{1}{\theta} \sigma_{l(i}^{(\alpha)} m_{jk)l}^{(\beta)} - \frac{1}{14} (7 - 2\mu_\beta) \frac{1}{\theta} \sigma_{l(i}^{(\beta)} m_{jk)l}^{(\alpha)} \\
& - \frac{1}{98} (1 - 3\mu_\beta) \frac{1}{\theta^2} R_{l(i}^{(\alpha)} m_{jk)l}^{(\beta)} + \frac{1}{392} (7 - 10\mu_\beta) \frac{1}{\theta^2} R_{l(i}^{(\beta)} m_{jk)l}^{(\alpha)} \Big) \\
& + \frac{1}{7} \Delta \hat{\theta} \left\{ \left(7 - 4\mu_\beta - \frac{1}{4} \Delta \hat{\theta} \right) m_{ijk}^{(\alpha)} + 4 \left(\mu_\beta + \frac{1}{16} \Delta \hat{\theta} \right) \frac{\rho_\alpha}{\rho_\beta} m_{ijk}^{(\beta)} \right. \\
& + \frac{1}{160} \left(7 - 8\mu_\beta - \frac{5}{4} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} m_{ijk}^{(\alpha)} \Delta_\beta - \frac{1}{40} \left(1 - 2\mu_\beta - \frac{5}{16} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} m_{ijk}^{(\beta)} \Delta_\alpha \\
& - 2 \left(7 - 6\mu_\beta - \frac{3}{8} \Delta \hat{\theta} \right) \sigma_{ij}^{(\alpha)} u_k^{(\beta)} + \left(7 - 12\mu_\beta - \frac{3}{4} \Delta \hat{\theta} \right) \frac{\rho_\alpha}{\rho_\beta} \sigma_{ij}^{(\beta)} u_k^{(\alpha)} \\
& + \frac{1}{5} \left(7 - 9\mu_\beta - \frac{9}{8} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta} \sigma_{ij}^{(\alpha)} h_k^{(\beta)} - \frac{1}{10} \left(13 - 18\mu_\beta - \frac{9}{4} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta} \sigma_{ij}^{(\beta)} h_k^{(\alpha)} \\
& + \frac{1}{14} \left(10 - 9\mu_\beta - \frac{9}{8} \Delta \hat{\theta} \right) \frac{1}{\theta} R_{ij}^{(\alpha)} u_k^{(\beta)} - \frac{1}{28} \left(7 - 18\mu_\beta - \frac{9}{4} \Delta \hat{\theta} \right) \frac{1}{\theta} \frac{\rho_\alpha}{\rho_\beta} R_{ij}^{(\beta)} u_k^{(\alpha)} \\
& - \frac{3}{70} \left(5 - 6\mu_\beta - \frac{15}{16} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} R_{ij}^{(\alpha)} h_k^{(\beta)} + \frac{3}{280} \left(13 - 24\mu_\beta - \frac{15}{4} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} R_{ij}^{(\beta)} h_k^{(\alpha)} \\
& + \frac{1}{2} \left(1 - 2\mu_\beta - \frac{1}{4} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta} \sigma_{l(i}^{(\alpha)} m_{jk)l}^{(\beta)} - \left(\mu_\alpha - \frac{1}{8} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta} \sigma_{l(i}^{(\beta)} m_{jk)l}^{(\alpha)} \\
& \left. - \frac{1}{56} \left(5 - 8\mu_\beta - \frac{5}{4} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} R_{l(i}^{(\alpha)} m_{jk)l}^{(\beta)} + \frac{1}{28} \left(3 - 4\mu_\beta - \frac{5}{8} \Delta \hat{\theta} \right) \frac{1}{\rho_\beta \theta^2} R_{l(i}^{(\beta)} m_{jk)l}^{(\alpha)} \right\} \Big], \tag{3.44}
\end{aligned}$$

$$\begin{aligned}
\mathcal{P}_{ij|G26}^{1(\alpha)} = & -\frac{1}{3} \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[\frac{2}{7} \mu_\beta^3 \left\{ 247 R_{ij}^{(\alpha)} + 1260 \theta \sigma_{ij}^{(\alpha)} + 88 \left(R_{ij}^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} R_{ij}^{(\beta)} \right) \right. \right. \\
& + 448 \theta \left(\sigma_{ij}^{(\alpha)} - \frac{\rho_\alpha}{\rho_\beta} \sigma_{ij}^{(\beta)} \right) \Big\} + (\mu_\alpha - \mu_\beta) \left(\frac{1}{7} (140 + 63\mu_\beta + 395\mu_\beta^2) R_{ij}^{(\alpha)} \right. \\
& - 4\mu_\beta^2 \frac{\rho_\alpha}{\rho_\beta} R_{ij}^{(\beta)} + 28\mu_\beta (5 + 9\mu_\beta) \theta \sigma_{ij}^{(\alpha)} - 56\mu_\beta^2 \frac{\rho_\alpha}{\rho_\beta} \theta \sigma_{ij}^{(\beta)} \Big) \\
& \left. + \mu_\beta^3 \frac{1}{\rho_\beta} \left(\frac{7}{240} \frac{1}{\theta^2} R_{ij}^{(\alpha)} \Delta_\beta + \frac{1}{105} \frac{1}{\theta^2} R_{ij}^{(\beta)} \Delta_\alpha + \frac{7}{60} \frac{1}{\theta} \sigma_{ij}^{(\alpha)} \Delta_\beta - \frac{2}{15} \frac{1}{\theta} \sigma_{ij}^{(\beta)} \Delta_\alpha \right) \right]
\end{aligned}$$

$$\begin{aligned}
& -360\rho_\alpha\rho_\beta\theta u_{\langle i}^{(\alpha)}u_{j\rangle}^{(\beta)} + \frac{428}{7}\sigma_{k\langle i}^{(\alpha)}\sigma_{j\rangle k}^{(\beta)} - \frac{94}{25}\frac{1}{\theta}h_{\langle i}^{(\alpha)}h_{j\rangle}^{(\beta)} - \frac{29}{21}\frac{1}{\theta}m_{kl\langle i}^{(\alpha)}m_{j\rangle kl}^{(\beta)} \\
& - \frac{19}{1372}\frac{1}{\theta^2}R_{k\langle i}^{(\alpha)}R_{j\rangle k}^{(\beta)} - \frac{748}{5}\rho_\beta h_{\langle i}^{(\alpha)}u_{j\rangle}^{(\beta)} - \frac{332}{5}\rho_\alpha h_{\langle i}^{(\beta)}u_{j\rangle}^{(\alpha)} - 32\rho_\beta m_{ijk}^{(\alpha)}u_k^{(\beta)} \\
& + \frac{244}{7}\rho_\alpha m_{ijk}^{(\beta)}u_k^{(\alpha)} + \frac{208}{35}\frac{1}{\theta}m_{ijk}^{(\alpha)}h_k^{(\beta)} + \frac{58}{35}\frac{1}{\theta}m_{ijk}^{(\beta)}h_k^{(\alpha)} + \frac{167}{49}\frac{1}{\theta}\sigma_{k\langle i}^{(\alpha)}R_{j\rangle k}^{(\beta)} + \frac{47}{49}\frac{1}{\theta}\sigma_{k\langle i}^{(\beta)}R_{j\rangle k}^{(\alpha)} \\
& - \frac{(\mu_\alpha - \mu_\beta)}{\rho_\beta} \left(\frac{1}{96}(4 - 19\mu_\beta + 13\mu_\beta^2)\frac{1}{\theta^2}R_{ij}^{(\alpha)}\Delta_\beta + \frac{1}{840}(14 - 107\mu_\beta + 122\mu_\beta^2)\frac{1}{\theta^2}R_{ij}^{(\beta)}\Delta_\alpha \right. \\
& + \frac{7}{120}\mu_\beta(25 - 31\mu_\beta)\frac{1}{\theta}\sigma_{ij}^{(\alpha)}\Delta_\beta - \frac{1}{60}(28 - 110\mu_\beta + 101\mu_\beta^2)\frac{1}{\theta}\sigma_{ij}^{(\beta)}\Delta_\alpha \\
& + 28\mu_\beta(5 + 7\mu_\beta)\rho_\alpha\rho_\beta\theta u_{\langle i}^{(\alpha)}u_{j\rangle}^{(\beta)} + \frac{2}{7}\mu_\beta(7 - 227\mu_\beta)\sigma_{k\langle i}^{(\alpha)}\sigma_{j\rangle k}^{(\beta)} \\
& + \frac{1}{25}(70 - 371\mu_\beta + 467\mu_\beta^2)\frac{1}{\theta}h_{\langle i}^{(\alpha)}h_{j\rangle}^{(\beta)} - \frac{1}{42}\mu_\beta(117 - 169\mu_\beta)\frac{1}{\theta}m_{kl\langle i}^{(\alpha)}m_{j\rangle kl}^{(\beta)} \\
& + \frac{1}{2744}(154 - 1051\mu_\beta + 1027\mu_\beta^2)\frac{1}{\theta^2}R_{k\langle i}^{(\alpha)}R_{j\rangle k}^{(\beta)} + \frac{2}{5}(70 - 21\mu_\beta + 307\mu_\beta^2)\rho_\beta h_{\langle i}^{(\alpha)}u_{j\rangle}^{(\beta)} \\
& + \frac{14}{5}\mu_\beta(5 + 29\mu_\beta)\rho_\alpha h_{\langle i}^{(\beta)}u_{j\rangle}^{(\alpha)} + \frac{2}{7}(35 - 63\mu_\beta + 116\mu_\beta^2)\rho_\beta m_{ijk}^{(\alpha)}u_k^{(\beta)} - \frac{2}{7}\mu_\beta^2\rho_\alpha m_{ijk}^{(\beta)}u_k^{(\alpha)} \\
& + \frac{1}{35}(35 - 343\mu_\beta + 106\mu_\beta^2)\frac{1}{\theta}m_{ijk}^{(\alpha)}h_k^{(\beta)} - \frac{1}{35}\mu_\beta(118 - 181\mu_\beta)\frac{1}{\theta}m_{ijk}^{(\beta)}h_k^{(\alpha)} \\
& + \frac{1}{98}\mu_\beta(161 - 587\mu_\beta)\frac{1}{\theta}\sigma_{k\langle i}^{(\alpha)}R_{j\rangle k}^{(\beta)} - \frac{1}{98}(154 - 521\mu_\beta + 467\mu_\beta^2)\frac{1}{\theta}\sigma_{k\langle i}^{(\beta)}R_{j\rangle k}^{(\alpha)} \\
& + \Delta\hat{\theta} \left\{ \frac{1}{14} \left(182 - 299\mu_\beta + 150\mu_\beta^2 - 2(10 - 9\mu_\beta)\Delta\hat{\theta} + \frac{3}{2}(\Delta\hat{\theta})^2 \right) R_{ij}^{(\alpha)} \right. \\
& - \frac{5}{14} \left(\mu_\beta(7 - 30\mu_\beta) + \frac{1}{10}(7 - 36\mu_\beta)\Delta\hat{\theta} - \frac{3}{10}(\Delta\hat{\theta})^2 \right) \frac{\rho_\alpha}{\rho_\beta} R_{ij}^{(\beta)} \\
& + 2 \left(70 - 91\mu_\beta + 54\mu_\beta^2 + 2(7 - 6\mu_\beta)\Delta\hat{\theta} - \frac{1}{2}(\Delta\hat{\theta})^2 \right) \theta \sigma_{ij}^{(\alpha)} \\
& - 2 \left(\mu_\beta(7 - 54\mu_\beta) - \frac{1}{2}(7 - 24\mu_\beta)\Delta\hat{\theta} + \frac{1}{2}(\Delta\hat{\theta})^2 \right) \frac{\rho_\alpha}{\rho_\beta} \theta \sigma_{ij}^{(\beta)} \\
& + \frac{1}{2240} \left(182 - 619\mu_\beta + 486\mu_\beta^2 - 50(2 - 3\mu_\beta)\Delta\hat{\theta} + \frac{35}{2}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta^2} R_{ij}^{(\alpha)} \Delta_\beta \\
& + \frac{1}{2240} \left(104 - 475\mu_\beta + 486\mu_\beta^2 - \frac{5}{2}(31 - 60\mu_\beta)\Delta\hat{\theta} + \frac{35}{2}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta^2} R_{ij}^{(\beta)} \Delta_\alpha \\
& - \frac{7}{240} \left(10 - 45\mu_\beta + 42\mu_\beta^2 - \frac{6}{7}(7 - 12\mu_\beta)\Delta\hat{\theta} + \frac{15}{14}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} \sigma_{ij}^{(\alpha)} \Delta_\beta \\
& - \frac{1}{240} \left(104 - 351\mu_\beta + 294\mu_\beta^2 - \frac{3}{2}(31 - 48\mu_\beta)\Delta\hat{\theta} + \frac{15}{2}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} \sigma_{ij}^{(\beta)} \Delta_\alpha \\
& - 2 \left(35 - 98\mu_\beta + 108\mu_\beta^2 + \frac{1}{2}(35 - 48\mu_\beta)\Delta\hat{\theta} - (\Delta\hat{\theta})^2 \right) \rho_\alpha \theta u_{\langle i}^{(\alpha)}u_{j\rangle}^{(\beta)} \\
& + \frac{1}{7} \left(77 - 334\mu_\beta + 300\mu_\beta^2 - \frac{1}{2}(47 - 72\mu_\beta)\Delta\hat{\theta} + 3(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta} \sigma_{k\langle i}^{(\alpha)}\sigma_{j\rangle k}^{(\beta)} \\
& + \frac{1}{50} \left(175 - 666\mu_\beta + 588\mu_\beta^2 - \frac{3}{2}(59 - 96\mu_\beta)\Delta\hat{\theta} + 15(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} h_{\langle i}^{(\alpha)}h_{j\rangle}^{(\beta)} \\
& + \frac{1}{84} \left(45 - 222\mu_\beta + 196\mu_\beta^2 - \frac{1}{2}(59 - 96\mu_\beta)\Delta\hat{\theta} + 5(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} m_{kl\langle i}^{(\alpha)}m_{j\rangle kl}^{(\beta)} \\
& + \frac{3}{5488} \left(265 - 1094\mu_\beta + 972\mu_\beta^2 - \frac{5}{2}(71 - 120\mu_\beta)\Delta\hat{\theta} + 35(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta^2} R_{k\langle i}^{(\alpha)}R_{j\rangle k}^{(\beta)}
\end{aligned}$$

$$\begin{aligned}
& - \left(35 - 86\mu_\beta + 60\mu_\beta^2 - \frac{1}{10}(59 - 72\mu_\beta)\Delta\hat{\theta} + \frac{3}{5}(\Delta\hat{\theta})^2 \right) h_{\langle i}^{(\alpha)} u_{j\rangle}^{(\beta)} \\
& - \frac{1}{5} \left(35 - 238\mu_\beta + 300\mu_\beta^2 - \frac{1}{2}(35 - 72\mu_\beta)\Delta\hat{\theta} + 3(\Delta\hat{\theta})^2 \right) \frac{\rho_\alpha}{\rho_\beta} h_{\langle i}^{(\beta)} u_{j\rangle}^{(\alpha)} \\
& - \frac{5}{7} \left(28 - 55\mu_\beta + 30\mu_\beta^2 - \frac{1}{10}(37 - 36\mu_\beta)\Delta\hat{\theta} + \frac{3}{10}(\Delta\hat{\theta})^2 \right) m_{ijk}^{(\alpha)} u_k^{(\beta)} \\
& + \frac{1}{7} \left(\mu_\beta(59 - 150\mu_\beta) + (5 - 18\mu_\beta)\Delta\hat{\theta} - \frac{3}{2}(\Delta\hat{\theta})^2 \right) \frac{\rho_\alpha}{\rho_\beta} m_{ijk}^{(\beta)} u_k^{(\alpha)} \\
& + \frac{1}{70} \left(140 - 423\mu_\beta + 294\mu_\beta^2 - \frac{3}{2}(37 - 48\mu_\beta)\Delta\hat{\theta} + \frac{15}{2}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} m_{ijk}^{(\alpha)} h_k^{(\beta)} \\
& + \frac{1}{70} \left(40 - 243\mu_\beta + 294\mu_\beta^2 - 3(11 - 24\mu_\beta)\Delta\hat{\theta} + \frac{15}{2}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} m_{ijk}^{(\beta)} h_k^{(\alpha)} \\
& - \frac{1}{196} \left(77 - 522\mu_\beta + 588\mu_\beta^2 - \frac{3}{2}(47 - 96\mu_\beta)\Delta\hat{\theta} + 15(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} \sigma_{k\langle i}^{(\alpha)} R_{j\rangle k}^{(\beta)} \\
& - \frac{1}{196} \left(265 - 810\mu_\beta + 588\mu_\beta^2 - \frac{3}{2}(71 - 96\mu_\beta)\Delta\hat{\theta} + 15(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} \sigma_{k\langle i}^{(\beta)} R_{j\rangle k}^{(\alpha)} \Bigg\}, \tag{3.45}
\end{aligned}$$

$$\begin{aligned}
\mathcal{P}_{|G26}^{2(\alpha)} = & - \sum_{\beta=1}^N \nu_{\alpha\beta} \mu_\beta \left[\frac{32}{3} \mu_\beta^3 \Delta_\alpha + \frac{2}{3} (\mu_\alpha - \mu_\beta) (10 + 3\mu_\beta + 23\mu_\beta^2) \Delta_\alpha \right. \\
& + \frac{10}{3} \mu_\beta^2 (1 + 3\mu_\beta) \left(\Delta_\alpha - \frac{\rho_\alpha}{\rho_\beta} \Delta_\beta \right) + 40\mu_\beta (5 + \mu_\beta) \rho_\alpha \theta^2 \Delta\hat{\theta} \\
& + \frac{32}{3} \mu_\beta^3 \frac{1}{\rho_\beta} \left(\sigma_{ij}^{(\alpha)} \sigma_{ij}^{(\beta)} + \frac{2}{5} \frac{1}{\theta} h_i^{(\alpha)} h_i^{(\beta)} - \frac{1}{14} \frac{1}{\theta} m_{ijk}^{(\alpha)} m_{ijk}^{(\beta)} + \frac{1}{784} \frac{1}{\theta^2} R_{ij}^{(\alpha)} R_{ij}^{(\beta)} \right. \\
& + \frac{1}{480} \frac{1}{\theta^2} \Delta_\alpha \Delta_\beta - \frac{13}{4} \rho_\beta h_i^{(\alpha)} u_i^{(\beta)} + \frac{13}{4} \rho_\alpha h_i^{(\beta)} u_i^{(\alpha)} + \frac{23}{224} \frac{1}{\theta} \sigma_{ij}^{(\alpha)} R_{ij}^{(\beta)} - \frac{1}{32} \frac{1}{\theta} \sigma_{ij}^{(\beta)} R_{ij}^{(\alpha)} \Bigg) \\
& - \frac{1}{3} (\mu_\alpha - \mu_\beta) \frac{1}{\rho_\beta} \left(40\mu_\beta (5 + \mu_\beta) \rho_\alpha \rho_\beta \theta u_i^{(\alpha)} u_i^{(\beta)} - 4\mu_\beta (1 + 19\mu_\beta) \sigma_{ij}^{(\alpha)} \sigma_{ij}^{(\beta)} \right. \\
& + \frac{2}{5} (10 - 83\mu_\beta + 89\mu_\beta^2) \frac{1}{\theta} h_i^{(\alpha)} h_i^{(\beta)} - \frac{1}{7} \mu_\beta (21 - 43\mu_\beta) \frac{1}{\theta} m_{ijk}^{(\alpha)} m_{ijk}^{(\beta)} \\
& + \frac{1}{98} (7 - 58\mu_\beta + 61\mu_\beta^2) \frac{1}{\theta^2} R_{ij}^{(\alpha)} R_{ij}^{(\beta)} + \frac{1}{240} (10 - 61\mu_\beta + 55\mu_\beta^2) \frac{1}{\theta^2} \Delta_\alpha \Delta_\beta \\
& + 4(10 - 9\mu_\beta + 43\mu_\beta^2) \rho_\beta h_i^{(\alpha)} u_i^{(\beta)} + 4\mu_\beta (5 + 17\mu_\beta) \rho_\alpha h_i^{(\beta)} u_i^{(\alpha)} \\
& + \frac{1}{7} \mu_\beta (13 - 64\mu_\beta) \frac{1}{\theta} \sigma_{ij}^{(\alpha)} R_{ij}^{(\beta)} - \frac{1}{7} (14 - 58\mu_\beta + 49\mu_\beta^2) \frac{1}{\theta} \sigma_{ij}^{(\beta)} R_{ij}^{(\alpha)} \Bigg) \\
& + \Delta\hat{\theta} \left\{ 20 \left(5 - 6\mu_\beta + \frac{1}{2} \Delta\hat{\theta} \right) \Delta\hat{\theta} \rho_\alpha \theta^2 \right. \\
& + \frac{1}{12} \left(64 - 121\mu_\beta + 75\mu_\beta^2 - \frac{1}{2} (17 - 18\mu_\beta) \Delta\hat{\theta} + \frac{3}{4} (\Delta\hat{\theta})^2 \right) \Delta_\alpha \\
& - \frac{25}{12} \left(\mu_\beta (1 - 3\mu_\beta) + \frac{1}{50} (5 - 18\mu_\beta) \Delta\hat{\theta} - \frac{3}{100} (\Delta\hat{\theta})^2 \right) \frac{\rho_\alpha}{\rho_\beta} \Delta_\beta \\
& - \frac{20}{3} \left(5 - 17\mu_\beta + 27\mu_\beta^2 + 2(2 - 3\mu_\beta) \Delta\hat{\theta} - \frac{1}{4} (\Delta\hat{\theta})^2 \right) \rho_\alpha \theta u_i^{(\alpha)} u_i^{(\beta)} \\
& + \frac{1}{3} \left(14 - 73\mu_\beta + 75\mu_\beta^2 - \frac{1}{2} (11 - 18\mu_\beta) \Delta\hat{\theta} + \frac{3}{4} (\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta} \sigma_{ij}^{(\alpha)} \sigma_{ij}^{(\beta)} \Bigg\}
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{15} \left(37 - 153\mu_\beta + 147\mu_\beta^2 - 3(7 - 12\mu_\beta)\Delta\hat{\theta} + \frac{15}{4}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} h_i^{(\alpha)} h_i^{(\beta)} \\
& + \frac{1}{42} \left(9 - 51\mu_\beta + 49\mu_\beta^2 - (7 - 12\mu_\beta)\Delta\hat{\theta} + \frac{5}{4}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} m_{ijk}^{(\alpha)} m_{ijk}^{(\beta)} \\
& + \frac{1}{784} \left(58 - 257\mu_\beta + 243\mu_\beta^2 - \frac{5}{2}(17 - 30\mu_\beta)\Delta\hat{\theta} + \frac{35}{4}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta^2} R_{ij}^{(\alpha)} R_{ij}^{(\beta)} \\
& + \frac{1}{1920} \left(64 - 257\mu_\beta + 243\mu_\beta^2 - \frac{5}{2}(17 - 30\mu_\beta)\Delta\hat{\theta} + \frac{35}{4}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta^2} \Delta_\alpha \Delta_\beta \\
& - \frac{2}{3} \left(37 - 97\mu_\beta + 75\mu_\beta^2 - (7 - 9\mu_\beta)\Delta\hat{\theta} + \frac{3}{4}(\Delta\hat{\theta})^2 \right) h_i^{(\alpha)} u_i^{(\beta)} \\
& - \frac{2}{3} \left(5 - 49\mu_\beta + 75\mu_\beta^2 - (4 - 9\mu_\beta)\Delta\hat{\theta} + \frac{3}{4}(\Delta\hat{\theta})^2 \right) \frac{\rho_\alpha}{\rho_\beta} h_i^{(\beta)} u_i^{(\alpha)} \\
& - \frac{1}{84} \left(14 - 117\mu_\beta + 147\mu_\beta^2 - \frac{3}{2}(11 - 24\mu_\beta)\Delta\hat{\theta} + \frac{15}{4}(\Delta\hat{\theta})^2 \right) \frac{1}{\rho_\beta\theta} \sigma_{ij}^{(\alpha)} R_{ij}^{(\beta)} \\
& - \frac{1}{84} \left\{ 58 - 189\mu_\beta + 147\mu_\beta^2 - \frac{3}{2}(17 - 24\mu_\beta)\Delta\hat{\theta} + \frac{15}{4}(\Delta\hat{\theta})^2 \right\} \frac{1}{\rho_\beta\theta} \sigma_{ij}^{(\beta)} R_{ij}^{(\alpha)} \Bigg]. \quad (3.46)
\end{aligned}$$

3.2.3 Collision frequencies and coefficients a_i 's in the production terms

The collision frequencies appearing in the production terms are defined as

$$\nu_{ij} = \frac{16}{5} \sqrt{\pi} n_j \Omega_{ij}^{(2,2)} \sqrt{\frac{\theta_i + \theta_j}{2}}, \quad i, j \in \{\alpha, \beta\} \quad (3.47)$$

with $\Omega_{ij}^{(2,2)} = \Omega_{ji}^{(2,2)}$. It should be noted that the collision frequencies are such that the total number of collisions between the α - and β -gas molecules remains balanced, i.e., $n_\alpha \nu_{\alpha\beta} = n_\beta \nu_{\beta\alpha}$ [27, 124]. In case of hard spheres, $\Omega_{ij}^{(2,2)}$ are given by

$$\Omega_{ij}^{(2,2)} = \left(\frac{d_i + d_j}{2} \right)^2, \quad i, j \in \{\alpha, \beta\} \quad (3.48)$$

where d_α and d_β are the diameters of the α - and β -gas molecules, respectively.

The constants a_i are defined as $a_i = A_i/A_2$ [60] with

$$A_i = \sqrt{2} \int_0^{\pi/4} \frac{1 - (-1)^i \cos^i(2\zeta)}{\sin^2(2\phi)} d\phi; \quad \zeta = \sqrt{\cos(2\phi)} \int_0^{\pi/2} \frac{d\psi}{\sqrt{1 - \sin^2\phi \sin^2\psi}}. \quad (3.49)$$

The numerical values of first few constants are $a_1 = 0.9673 \approx 29/30$, $a_2 = 1$, $a_3 = 1.3416 \approx 51/38$.

Chapter 4

Boundary conditions

In order to solve the boundary value problems with moment equations derived in chapter 2, the moment equations must be supplemented with the boundary conditions, which describe the interaction between gas molecules and the solid wall (boundary). Since the moment equations are derived from the Boltzmann equation by considering the appropriate moments of the velocity distribution function, the boundary conditions associated with the moment equations can be expected to follow by taking the appropriate moments of the velocity distribution function in its boundary condition. Nevertheless, since the gas molecules interact with the solid wall in a very complicated way that depends on the microscopic surface structure of the wall as well as on the interaction potential between the gas molecules and the wall and, usually, it is not possible to accurately describe this interaction [20, 102], the topic of boundary conditions is debatable.

Often, simplified wall-gas interaction models—which assume smooth wall—are used in the literature. The most common and one of the simplest model is the Maxwell accommodation model [66]. It considers a (constant) single accommodation coefficient, which is a physical quantity characterizing the behaviour of gas molecules in their collision with the solid wall. The other well-known model for the gas-surface interaction is the Cercignani-Lampis model [21], which considers two accommodation coefficients. Recently, Struchtrup [104] proposed a modification of the Maxwell accommodation model that considers velocity dependent accommodation coefficients. However, the latter two models are yet to be exploited in the context of moment equations.

The work of Gu and Emerson [38] may be regarded as the pioneering work which constructs the boundary conditions for the R13 equations based on the Maxwell accommodation model. Reference [118] advances the topic of boundary conditions by overcoming the inconsistencies in [38]. Reference [39] further applies the Maxwell accommodation model to derive the boundary conditions for the regularized 26-moment (R26) equations. Our paper [45] extends the Maxwell accommodation model to gaseous mixtures in order to derive the boundary conditions for $N \times G26$ equations.

In this chapter, the Maxwell accommodation model for a single gas is extended to gaseous mixtures in order to derive the boundary conditions for $N \times G13$ and $N \times G26$ equations.

4.1 Boundary conditions for a single gas

4.1.1 Maxwell accommodation model

Maxwell [66] speculated that the gas molecules colliding with the solid wall can be rebounded after the collision in two ways, namely *specular reflection* and *diffuse reflection*. In a specular reflection, the tangential component of the velocity of a molecule hitting the wall does not

change while the normal component of that merely changes its sign and, therefore, no energy is transferred during the process. On the contrary, in a diffuse reflection, the molecules hitting the wall accommodate at the wall and return to the gas—after interaction—with the properties (e.g., temperature and velocity) of the wall.

Maxwell accommodation model states that a fraction χ of the gas molecules hitting the wall is diffusively reflected while the remaining fraction $(1 - \chi)$ of those undergoes specular reflection. It, further, annexes that the diffusively reflected molecules enter the gas with the distribution function of the thermalized gas molecules at the wall, f_w , which is a Maxwellian and given by

$$f_w(\mathbf{C}_w) = \frac{\rho_w}{m} \left(\frac{1}{2\pi\theta_w} \right)^{3/2} \exp \left(-\frac{C_w^2}{2\theta_w} \right), \quad \text{where} \quad \theta_w = \frac{kT_w}{m} \quad \text{and} \quad \mathbf{C}_w = \mathbf{c} - \mathbf{v}_w. \quad (4.1)$$

The symbol χ in Maxwell accommodation model is the accommodation coefficient which has to be given or measured. In principle, the accommodation coefficient χ depends on the velocity of the molecules [102, 104], however—for simplicity—it is assumed constant in Maxwell accommodation model. In (4.1), m is the mass of the gas molecule; $\mathbf{c}$ is the instantaneous velocity of the molecule; ρ_w is the density of the thermalized molecules at the wall (also referred to as wall density occasionally) and it is determined by ensuring that there is no accumulation of the molecules at the wall; T_w and $\mathbf{v}_w$ are the temperature and the velocity of the wall, respectively; and $\mathbf{C}_w$ is the velocity of the molecule in the reference frame of the wall. Let us introduce the unit normal $\mathbf{n}$ on the wall pointing into the gas so that $\mathbf{n} \cdot \mathbf{C}_w < 0$ for the molecules hitting the wall while $\mathbf{n} \cdot \mathbf{C}_w > 0$ for the molecules rebounding from the wall. Typically, the velocity of the gas $\mathbf{v}$ is different from the wall velocity $\mathbf{v}_w$, so that the gas has a non-vanishing slip velocity $\mathbf{V} = \mathbf{v} - \mathbf{v}_w$. Furthermore, we assume that gas cannot penetrate the wall; consequently, the normal component of the slip velocity vanishes, i.e., $\mathbf{n} \cdot \mathbf{V} = 0$. Thus, the slip velocity of the gas is parallel to the wall.

According to Maxwell's accommodation model, the velocity distribution function in the infinitesimal neighbourhood of the wall is given by

$$f_{\text{nw}}(\mathbf{c}) = \begin{cases} \chi f_w(\mathbf{C}_w) + (1 - \chi)f^*(\mathbf{c}), & \mathbf{n} \cdot \mathbf{C}_w > 0 \\ f(\mathbf{c}), & \mathbf{n} \cdot \mathbf{C}_w \leq 0 \end{cases} \quad (4.2)$$

where f is the distribution function of molecules hitting the wall, f^* is the distribution function of specularly reflected molecules from the wall, and the subscript 'nw' is used to denote 'near wall'. The distribution function f^* follows from f analogously by reversing the sign of normal component of velocity, c_n .

4.1.2 Boundary conditions

The boundary condition for the velocity distribution function is determined by the fact that it should be continuous near the wall. In other words, the distribution function of the gas, f , should be equal to the distribution function of the gas in the infinitesimal neighbourhood of the wall, f_{nw} , given by (4.2). Therefore, the boundary condition for any function $\psi \equiv \psi(\mathbf{r}, \mathbf{c}, t)$ is obtained by assuming that the moment of the velocity distribution function with respect to ψ

should be continuous near the wall, i.e.,

$$\int \psi f(\mathbf{c}) d\mathbf{c} = \int \psi f_{\text{nw}}(\mathbf{c}) d\mathbf{c}. \quad (4.3)$$

Thus, by choosing the value of ψ same as that considered while deriving the moment equation for $\int \psi f(\mathbf{c}) d\mathbf{c}$, the boundary condition associated with the moment equation can be obtained. Nevertheless, by choosing the value of ψ same as that considered while deriving the corresponding moment equation, condition (4.3) provides more boundary conditions than required. However, by considering the special case of no accommodation ($\chi = 0$), Grad [35] concluded that only those moments which are of odd degree in C_n —where $C_n = \mathbf{n} \cdot \mathbf{C}$ is the normal component of the peculiar velocity of the gas, $\mathbf{C} = \mathbf{c} - \mathbf{v}$ —need to be considered for deriving the meaningful boundary conditions. Therefore, without loss of generality, let us assume that ψ is of odd degree in C_n .

It is easy to understand the derivation of boundary conditions for the case when the normal on the wall coincides with one of the axis in Cartesian coordinate system. Let the normal from the wall (into the gas) be pointing towards positive x -axis and ψ be of odd degree in C_x . The boundary condition (4.3) in the light of (4.2) reads

$$\begin{aligned} \int \psi(C_x) f(C_x) d\mathbf{c} &= \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{-\infty}^0 \psi(C_x) f(C_x) dC_x dC_y dC_z \\ &\quad + \int_{\mathbb{R}} \int_{\mathbb{R}} \int_0^{\infty} \psi(C_x) [\chi f_w(C_x) + (1 - \chi) f(-C_x)] dC_x dC_y dC_z, \end{aligned} \quad (4.4)$$

where we have used the relations $\mathbf{C}_w = \mathbf{C} + \mathbf{V}$ and $V_x = 0$ in f_w and explicitly mentioned only the normal component of the velocity (C_x) in the arguments of the functions, though all the functions may still depend on position, time and other components of the velocities $\mathbf{C}$ and/or $\mathbf{V}$. Additionally, the relation $d\mathbf{c} = d\mathbf{C}$ has also been used on the right-hand side. Since, ψ is of odd degree in C_x , (4.4) further simplifies to

$$\int \psi(C_x) f(C_x) d\mathbf{c} = \chi \int_{\mathbb{R}} \int_{\mathbb{R}} \left(\int_0^{\infty} \psi(C_x) f_w(C_x) dC_x + \underbrace{\int_{-\infty}^0 \psi(C_x) f(C_x) dC_x}_{\text{underlined}} \right) dC_y dC_z. \quad (4.5)$$

The underlined integral in (4.5) can be further reduced by decomposing the velocity distribution function into even and odd functions in C_x , i.e., $f(C_x) = f^{(\text{even})}(C_x) + f^{(\text{odd})}(C_x)$. It should be noted that this decomposition is possible, at least, for Grad-type distribution functions

considered in this thesis. One can write the underlined term in (4.5) as follows.

$$\begin{aligned}
\int_{-\infty}^0 \psi(C_x) f(C_x) dC_x &= \int_{-\infty}^0 \psi(C_x) f^{(\text{odd})}(C_x) dC_x + \int_{-\infty}^0 \psi(C_x) f^{(\text{even})}(C_x) dC_x \\
&= \frac{1}{2} \int_{-\infty}^{\infty} \psi(C_x) f^{(\text{odd})}(C_x) dC_x - \int_0^{\infty} \psi(C_x) f^{(\text{even})}(C_x) dC_x \\
&= \frac{1}{2} \int_{-\infty}^{\infty} \psi(C_x) f(C_x) dC_x - \int_0^{\infty} \psi(C_x) f^{(\text{even})}(C_x) dC_x, \tag{4.6}
\end{aligned}$$

where the fact that ψ is an odd function in C_x has been exploited at every step. Also, in the last step we could drop the superscript on f and could integrate the complete f owing to the fact that $\psi(C_x) \times f^{(\text{even})}(C_x)$ is an odd function in C_x and, therefore, the integral of it over $\mathbb{R}$ vanishes. Insertion of (4.6) into (4.5) yields

$$\int \psi(C_x) f(C_x) d\mathbf{c} = \frac{2\chi}{2-\chi} \int_{\mathbb{R}} \int_{\mathbb{R}} \left(\int_0^{\infty} \psi(C_x) f_w(C_x) dC_x - \int_0^{\infty} \psi(C_x) f^{(\text{even})}(C_x) dC_x \right) dC_y dC_z. \tag{4.7}$$

Since the integral over f_w could depend on the other components of velocities $\mathbf{C}$ and $\mathbf{V}$, it is easier, indeed, to evaluate the integral containing f_w by transforming the variable from $\mathbf{C}$ to $\mathbf{C}_w$ using the relation $\mathbf{C} = \mathbf{C}_w - \mathbf{V}$ in boundary condition (4.7). With this transformation, the boundary condition can be written as

$$\begin{aligned}
\int \psi(C_x) f(C_x) d\mathbf{c} &= \frac{2\chi}{2-\chi} \left[\int_{\mathbb{R}} \int_{\mathbb{R}} \int_0^{\infty} \psi(C_{w,x}) f_w(C_{w,x}) dC_{w,x} dC_{w,y} dC_{w,z} \right. \\
&\quad \left. - \int_{\mathbb{R}} \int_{\mathbb{R}} \int_0^{\infty} \psi(C_x) f^{(\text{even})}(C_x) dC_x dC_y dC_z \right], \tag{4.8}
\end{aligned}$$

where $C_{w,i}$ for $i \in \{x, y, z\}$ are the components of $\mathbf{C}_w$, and, again, only the normal components of the velocities are explicitly mentioned in the arguments of the functions.

The boundary condition for a general normal direction $\mathbf{n}$ can be derived analogously. It reads

$$\begin{aligned}
\int_{\mathbb{R}^3} \psi(C_n) f(C_n) dC_n dC_{t_1} dC_{t_2} &= \frac{2\chi}{2-\chi} \left[\int_{\mathbb{R}} \int_{\mathbb{R}} \int_0^{\infty} \psi(C_{w,n}) f_w(C_{w,n}) dC_{w,n} dC_{w,t_1} dC_{w,t_2} \right. \\
&\quad \left. - \int_{\mathbb{R}} \int_{\mathbb{R}} \int_0^{\infty} \psi(C_n) f^{(\text{even})}(C_n) dC_n dC_{t_1} dC_{t_2} \right], \tag{4.9}
\end{aligned}$$

where $\mathbf{t}_1$ and $\mathbf{t}_2$ are the two orthonormal directions in the plane of the wall and, again, only the normal components of the velocities are explicitly mentioned in the arguments of the functions.

The boundary conditions associated with Grad's moment equations are derived by replacing

f in (4.9) by the Grad distribution function and choosing the appropriate values for ψ similar to those chosen while deriving the Grad's moment equations (but only those which are of odd degree in C_n). Moreover, the full- and half-space integrals in (4.7) can be performed by employing the procedure detailed in the appendix of the textbook [102].

An extra condition is, often, required along with the boundary conditions constructed by Maxwell accommodation model for solving the boundary value problems in a given domain. This extra condition results from physics by the fact that the mass of the gas in a given domain Γ must be equal to a given value M_0 because gas molecules cannot permeate through the boundary of the domain, i.e.,

$$\int_{\Gamma} \rho dV = M_0, \quad (4.10)$$

where dV is infinitesimal control volume in the domain Γ .

4.2 Boundary conditions for gaseous mixtures

4.2.1 Maxwell accommodation model

We extend the Maxwell accommodation model to gaseous mixtures in a natural way by considering the Maxwell accommodation model for each component in the mixture separately like in case of a single gas. In other words, we say that according to Maxwell accommodation model for gaseous mixture, a fraction χ_α of the α -gas molecules ($\alpha = 1, 2, \dots, N$) hitting the wall is diffusively reflected while the remaining fraction $(1 - \chi_\alpha)$ of those undergoes specular reflection. Moreover, the diffusively reflected α -gas molecules rebound from the wall with the distribution function of the thermalized α -gas molecules on the wall, $f_w^{(\alpha)}$, which is given by

$$f_w^{(\alpha)}(\mathbf{C}_w^{(\alpha)}) = \frac{\rho_w^{(\alpha)}}{m_\alpha} \left(\frac{1}{2\pi\theta_w^{(\alpha)}} \right)^{3/2} \exp \left(-\frac{(\mathbf{C}_w^{(\alpha)})^2}{2\theta_w^{(\alpha)}} \right), \quad (4.11)$$

where $\rho_w^{(\alpha)}$ is the density of the thermalized α -gas molecules at the wall and is determined by ensuring that there is no accumulation of the α -gas molecules at the wall; $\theta_w^{(\alpha)} = kT_w/m_\alpha$ with T_w being the temperature of the wall; $\mathbf{C}_w^{(\alpha)} = \mathbf{c}_\alpha - \mathbf{v}_w$ is the velocity of the α -gas molecule in the reference frame of the wall, with $\mathbf{v}_w$ being the velocity of the wall. The symbol χ_α is the accommodation coefficient for the α -constituent and, similar to a single gas case, it may also depend on the velocity of the α -gas molecules, however—for simplicity—we assume that the accommodation coefficients for all components in the mixture are constants (but not necessarily same for all the constituents).

Thus, according to Maxwell accommodation model for gaseous mixture, the velocity distribution function of the α -constituent ($\alpha = 1, 2, \dots, N$) in an infinitesimal neighbourhood of the

wall is given by

$$f_{\text{nw}}^{(\alpha)}(\mathbf{c}_\alpha) = \begin{cases} \chi_\alpha f_w^{(\alpha)}(\mathbf{C}_w^{(\alpha)}) + (1 - \chi_\alpha) f_\alpha^*(\mathbf{c}_\alpha), & \mathbf{n} \cdot \mathbf{C}_w^{(\alpha)} > 0 \\ f_\alpha(\mathbf{c}_\alpha), & \mathbf{n} \cdot \mathbf{C}_w^{(\alpha)} \leq 0 \end{cases} \quad (4.12)$$

where $\mathbf{n}$ is, again, the unit normal on the wall pointing into the gas and f_α^* is the distribution function of the specularly reflected α -gas molecules which is obtained by just reversing the sign of the normal component of $\mathbf{c}_\alpha$ in f_α . The slip velocity of the mixture, $\mathbf{V} = \mathbf{v} - \mathbf{v}_w$ is parallel to the wall, i.e., its normal component—again—vanishes by assuming that none of the gases in the mixture can permeate through the wall. It is emphasized here that $\mathbf{v}$ is the hydrodynamic velocity of the mixture.

4.2.2 Boundary conditions

As none of the gas molecules can seep through the wall, the normal components of the diffusion velocities of the gases in the mixture also vanish at the wall. This leads to boundary conditions

$$u_n^{(\alpha)}|_{\text{wall}} = 0 \quad \text{for } \alpha = 1, 2, \dots, N. \quad (4.13)$$

The other boundary condition for any function $\psi_\alpha \equiv \psi_\alpha(\mathbf{r}, \mathbf{c}_\alpha, t)$ is constructed—in a similar way as for a single gas—by the fact that the moment of the velocity distribution function of α -constituent with respect to ψ_α should be continuous near the wall, i.e.,

$$\int \psi_\alpha f_\alpha(\mathbf{c}_\alpha) d\mathbf{c}_\alpha = \int \psi_\alpha f_{\text{nw}}^{(\alpha)}(\mathbf{c}_\alpha) d\mathbf{c}_\alpha. \quad (4.14)$$

Boundary condition (4.14) for any moment, again, yields more boundary conditions than required and the correct number of boundary conditions for a constituent α is obtained by borrowing Grad's strategy for a single gas. We say that only those moments which are of odd degree in $C_n^{(\alpha)} (= \mathbf{n} \cdot \mathbf{C}_\alpha)$ are needed for computing the required boundary conditions associated with the moment equations for the α -constituent.

Similar to a single gas case, by assuming—without loss of generality—that ψ_α is of odd degree in $C_n^{(\alpha)}$, boundary condition (4.14) simplifies to

$$\begin{aligned} & \int_{\mathbb{R}^3} \psi_\alpha(C_n^{(\alpha)}) f_\alpha(C_n^{(\alpha)}) dC_n^{(\alpha)} dC_{t_1}^{(\alpha)} dC_{t_2}^{(\alpha)} \\ &= \frac{2\chi_\alpha}{2 - \chi_\alpha} \left[\int_{\mathbb{R}} \int_{\mathbb{R}} \int_0^\infty \psi_\alpha(C_{w,n}^{(\alpha)}) f_w^{(\alpha)}(C_{w,n}^{(\alpha)}) dC_{w,n}^{(\alpha)} dC_{w,t_1}^{(\alpha)} dC_{w,t_2}^{(\alpha)} \right. \\ & \quad \left. - \int_{\mathbb{R}} \int_{\mathbb{R}} \int_0^\infty \psi_\alpha(C_n^{(\alpha)}) f_\alpha^{\text{(even)}}(C_n^{(\alpha)}) dC_n^{(\alpha)} dC_{t_1}^{(\alpha)} dC_{t_2}^{(\alpha)} \right], \end{aligned} \quad (4.15)$$

where $\mathbf{t}_1$ and $\mathbf{t}_2$ are, again, the two orthonormal directions in the plane of the wall and only the normal components of the velocities are explicitly mentioned in the arguments of the functions.

The integrals in (4.15) can also be computed by replacing the distribution function for the α -constituent in (4.15) by Grad distribution function for the α -constituent, and using the procedure detailed in the appendix of the textbook [102] for evaluating the full- and half-space integrals.

The required extra conditions in case of gaseous mixture, again, result from physics by the fact that the mass of the α -constituent ($\alpha = 1, 2, \dots, N$) in a given domain Γ must be equal to a given value $M_0^{(\alpha)}$ because the gas molecules cannot permeate through the boundary of the domain, i.e.,

$$\int_{\Gamma} \rho_{\alpha} dV = M_0^{(\alpha)} \quad \text{for } \alpha = 1, 2, \dots, N \quad (4.16)$$

where dV is infinitesimal control volume in the domain Γ .

We have implemented the evaluation strategy of the boundary conditions too in the computer algebra software MATHEMATICA[®] in order to compute the boundary conditions associated with moment equations for a single gas (not presented here) as well as for a gaseous mixture.

4.2.2.1 Boundary conditions for $N \times \text{G13}$ equations

In addition to boundary conditions (4.13) and (4.16), the other boundary conditions associated with $N \times \text{G13}$ equations are derived by replacing the distribution function of the α -constituent ($\alpha = 1, 2, \dots, N$) in (4.15) with the G13 distribution function for α -constituent (2.31). Moreover, Grad's strategy restricts the choices for ψ_{α} to

$$\psi_{\alpha} = m_{\alpha} \left\{ C_n^{(\alpha)}, C_n^{(\alpha)} C_{t_i}^{(\alpha)}, \frac{1}{2} C_{\alpha}^2 C_n^{(\alpha)} \right\}, \quad \text{where } i \in \{1, 2\}.$$

For the first choice, i.e., $\psi_{\alpha} = m_{\alpha} C_n^{(\alpha)}$, boundary condition (4.15) in view of (4.13) provides the definition of $\rho_w^{(\alpha)}$:

$$\rho_w^{(\alpha)} \equiv m_{\alpha} n_w^{(\alpha)} := \frac{P_{\alpha}}{\sqrt{\theta_w^{(\alpha)}} \sqrt{\theta_{\alpha}}}, \quad \text{where } P_{\alpha} = \rho_{\alpha} \theta_{\alpha} + \frac{1}{2} \sigma_{nn}^{(\alpha)}. \quad (4.17)$$

The other choices of ψ_{α} yield the boundary conditions corresponding to stress and heat flux of the α -constituent. These boundary conditions read ($i \in \{1, 2\}$)

$$\sigma_{nt_i}^{(\alpha)} = -\frac{\chi_{\alpha}}{2 - \chi_{\alpha}} \sqrt{\frac{2}{\pi \theta_{\alpha}}} \left[P_{\alpha} V_{t_i} + \frac{1}{2} \rho_{\alpha} \theta_{\alpha} u_{t_i}^{(\alpha)} + \frac{1}{5} q_{t_i}^{(\alpha)} \right], \quad (4.18)$$

$$q_n^{(\alpha)} = -\frac{\chi_{\alpha}}{2 - \chi_{\alpha}} \sqrt{\frac{2}{\pi \theta_{\alpha}}} \left[2 P_{\alpha} (\theta_{\alpha} - \theta_w^{(\alpha)}) + \frac{1}{2} \theta_{\alpha} \sigma_{nn}^{(\alpha)} - \frac{1}{2} P_{\alpha} V^2 \right]. \quad (4.19)$$

Obviously, (4.17)–(4.19) are valid only at the wall. Equations (4.13), (4.16), (4.18) and (4.19) for $\alpha = 1, 2, \dots, N$ form the complete set of non-linear boundary conditions for the $N \times \text{G13}$ equations derived in chapter 2.

4.2.2.2 Boundary conditions for $N \times \text{G26}$ equations

In addition to boundary conditions (4.13) and (4.16), the other boundary conditions associated with $N \times \text{G26}$ equations are derived by replacing the distribution function of the α -constituent ($\alpha = 1, 2, \dots, N$) in (4.15) with the G26 distribution function for α -constituent (2.47). Moreover, Grad's strategy restricts the choices for ψ_α to

$$\psi_\alpha = m_\alpha \left\{ C_n^{(\alpha)}, C_n^{(\alpha)} C_{t_i}^{(\alpha)}, \frac{1}{2} C_\alpha^2 C_n^{(\alpha)}, C_n^{(\alpha)} C_n^{(\alpha)} C_n^{(\alpha)}, C_n^{(\alpha)} C_{t_i}^{(\alpha)} C_{t_j}^{(\alpha)}, C_\alpha^2 C_n^{(\alpha)} C_{t_i}^{(\alpha)} \right\},$$

where $i, j \in \{1, 2\}$. Again, for the first choice, i.e., $\psi_\alpha = m_\alpha C_n^{(\alpha)}$, boundary condition (4.15) in view of (4.13) provides the definition of $\rho_w^{(\alpha)}$:

$$\rho_w^{(\alpha)} \equiv m_\alpha n_w^{(\alpha)} := \frac{P_\alpha}{\sqrt{\theta_w^{(\alpha)}} \sqrt{\theta_\alpha}}, \quad \text{where} \quad P_\alpha = \rho_\alpha \theta_\alpha + \frac{1}{2} \sigma_{nn}^{(\alpha)} - \frac{1}{28} \frac{R_{nn}^{(\alpha)}}{\theta_\alpha} - \frac{1}{120} \frac{\Delta_\alpha}{\theta_\alpha}. \quad (4.20)$$

The other choices of ψ_α yield the following boundary conditions ($i, j \in \{1, 2\}$)

$$\sigma_{nt_i}^{(\alpha)} = -\frac{\chi_\alpha}{2 - \chi_\alpha} \sqrt{\frac{2}{\pi \theta_\alpha}} \left[P_\alpha V_{t_i} + \frac{1}{2} \rho_\alpha \theta_\alpha u_{t_i}^{(\alpha)} + \frac{1}{5} q_{t_i}^{(\alpha)} + \frac{1}{2} m_{nnt_i}^{(\alpha)} \right], \quad (4.21)$$

$$q_n^{(\alpha)} = -\frac{\chi_\alpha}{2 - \chi_\alpha} \sqrt{\frac{2}{\pi \theta_\alpha}} \left[2P_\alpha (\theta_\alpha - \theta_w^{(\alpha)}) + \frac{1}{2} \theta_\alpha \sigma_{nn}^{(\alpha)} + \frac{5}{28} R_{nn}^{(\alpha)} + \frac{1}{15} \Delta_\alpha - \frac{1}{2} P_\alpha V^2 \right], \quad (4.22)$$

$$m_{nnn}^{(\alpha)} = \frac{\chi_\alpha}{2 - \chi_\alpha} \sqrt{\frac{2}{\pi \theta_\alpha}} \left[\frac{2}{5} P_\alpha (\theta_\alpha - \theta_w^{(\alpha)}) - \frac{7}{5} \theta_\alpha \sigma_{nn}^{(\alpha)} - \frac{1}{14} R_{nn}^{(\alpha)} + \frac{1}{75} \Delta_\alpha - \frac{3}{5} P_\alpha V^2 \right], \quad (4.23)$$

$$m_{nt_i t_i}^{(\alpha)} = -\frac{\chi_\alpha}{2 - \chi_\alpha} \sqrt{\frac{2}{\pi \theta_\alpha}} \left[\frac{1}{5} P_\alpha (\theta_\alpha - \theta_w^{(\alpha)}) - \frac{1}{5} \theta_\alpha \sigma_{nn}^{(\alpha)} + \theta_\alpha \sigma_{t_i t_i}^{(\alpha)} + \frac{1}{14} R_{t_i t_i}^{(\alpha)} + \frac{1}{150} \Delta_\alpha + \frac{1}{5} P_\alpha V^2 - P_\alpha V_{t_i}^2 \right], \quad (4.24)$$

$$m_{nt_1 t_2}^{(\alpha)} = -\frac{\chi_\alpha}{2 - \chi_\alpha} \sqrt{\frac{2}{\pi \theta_\alpha}} \left[\theta_\alpha \sigma_{t_1 t_2}^{(\alpha)} + \frac{1}{14} R_{t_1 t_2}^{(\alpha)} - P_\alpha V_{t_1} V_{t_2} \right], \quad (4.25)$$

$$R_{nt_i}^{(\alpha)} = \frac{\chi_\alpha}{2 - \chi_\alpha} \sqrt{\frac{2}{\pi \theta_\alpha}} \left[6P_\alpha (\theta_\alpha - \theta_w^{(\alpha)}) V_{t_i} + P_\alpha \theta_\alpha V_{t_i} + \frac{13}{2} \rho_\alpha \theta_\alpha^2 u_{t_i}^{(\alpha)} - \frac{11}{5} \theta_\alpha q_{t_i}^{(\alpha)} - \frac{1}{2} \theta_\alpha m_{nnt_i}^{(\alpha)} - P_\alpha V^2 V_{t_i} \right]. \quad (4.26)$$

Obviously, (4.20)–(4.26) are also valid only at the wall. Equations (4.13), (4.16), and (4.21)–(4.26) for $\alpha = 1, 2, \dots, N$ form the complete set of non-linear boundary conditions for the $N \times \text{G26}$ equations derived in chapter 2.

Chapter 5

Linear stability analysis

It is extremely important for the validity of a model that the solutions from the model are stable to small perturbations [26, 120]. For a single gas case, Bobylev [10] concluded that the Burnett and other higher order equations resulting from the Chapman–Enskog expansion of the Boltzmann equation are linearly unstable whereas the Grad’s moment equations are linearly stable. It entails to scrutinize the validity of the Grad’s moment equations for gaseous mixtures derived in chapter 2.

This chapter and the following chapters of this thesis focus on binary gas-mixtures of simple gases. In this chapter, the linear stability analysis is performed on the Grad’s 2×13 -moment ($2 \times G13$) and Grad’s 2×26 -moment ($2 \times G26$) equations for binary gas-mixtures in order to examine their stability. Moreover, the linear stability is scrutinized for two types of gas molecules: (a) Maxwell molecules and (b) hard spheres.

5.1 Linearized moment equations for binary gas-mixtures

Consider a binary gas-mixture comprised of two gases α and β without any external forces acting on them. For linear stability analysis, we linearise the $2 \times G26$ equations for the mixture by perturbing the field variables around their respective ground states, i.e.,

$$\left. \begin{aligned} v_i &= \varepsilon \tilde{v}_i, & n_\gamma &= n_\gamma^\circ + \varepsilon \tilde{n}_\gamma, & T_\gamma &= T_\circ + \varepsilon \tilde{T}_\gamma, & u_i^{(\gamma)} &= \varepsilon \tilde{u}_i^{(\gamma)}, & \sigma_{ij}^{(\gamma)} &= \varepsilon \tilde{\sigma}_{ij}^{(\gamma)}, \\ q_i^{(\gamma)} &= \varepsilon \tilde{q}_i^{(\gamma)}, & m_{ijk}^{(\gamma)} &= \varepsilon \tilde{m}_{ijk}^{(\gamma)}, & R_{ij}^{(\gamma)} &= \varepsilon \tilde{R}_{ij}^{(\gamma)}, & \Delta_\gamma &= \varepsilon \tilde{\Delta}_\gamma, & \text{for } \gamma &\in \{\alpha, \beta\}. \end{aligned} \right\} \quad (5.1)$$

In (5.1), ε is a small parameter, n_γ° is the ground state value of number density of the γ -constituent ($\gamma \in \{\alpha, \beta\}$), $T_\circ$ is the ground state value of temperature of the mixture, the ground state values of the other field variables are zeros, and the quantities with tilde are the corresponding perturbations in the field variables from their ground state values. Note that the temperature difference $T_\alpha - T_\beta = \varepsilon (\tilde{T}_\alpha - \tilde{T}_\beta)$ is also a small quantity. Moreover, in order to write the $2 \times G13$ and $2 \times G26$ equations in more efficacious form, we express them in dimensionless form using the scaling ($\gamma \in \{\alpha, \beta\}$)

$$\left. \begin{aligned} \hat{v}_i &= \frac{\tilde{v}_i}{v_\circ}, & \hat{n}_\gamma &= \frac{\tilde{n}_\gamma}{n_\gamma^\circ}, & \hat{T}_\gamma &= \frac{\tilde{T}_\gamma}{T_\circ}, & \hat{u}_i^{(\gamma)} &= \frac{\tilde{u}_i^{(\gamma)}}{(\theta_\gamma^\circ)^{1/2}}, & \hat{\sigma}_{ij}^{(\gamma)} &= \frac{\tilde{\sigma}_{ij}^{(\gamma)}}{\rho_\gamma^\circ \theta_\gamma^\circ}, \\ \hat{q}_i^{(\gamma)} &= \frac{\tilde{q}_i^{(\gamma)}}{\rho_\gamma^\circ (\theta_\gamma^\circ)^{3/2}}, & \hat{m}_{ijk}^{(\gamma)} &= \frac{\tilde{m}_{ijk}^{(\gamma)}}{\rho_\gamma^\circ (\theta_\gamma^\circ)^{3/2}}, & \hat{R}_{ij}^{(\gamma)} &= \frac{\tilde{R}_{ij}^{(\gamma)}}{\rho_\gamma^\circ (\theta_\gamma^\circ)^2}, & \hat{\Delta}_\gamma &= \frac{\tilde{\Delta}_\gamma}{\rho_\gamma^\circ (\theta_\gamma^\circ)^2}, \end{aligned} \right\} \quad (5.2)$$

where $\rho_\gamma^\circ = m_\gamma n_\gamma^\circ$, $\theta_\gamma^\circ = kT_\circ/m_\gamma$, $v_\circ$ is a velocity scale and hats over the quantities denote the dimensionless perturbations in field variables from their respective ground states. Furthermore, the space and time are scaled by scaling: $\hat{x}_i = x_i/L$ and $\hat{t} = t(v_\circ/L)$. The velocity scale $v_\circ$,

hereafter wherever required in this thesis, is taken as $v_o = \sqrt{kT_o/m}$ —where $m = x_\alpha^\circ m_\alpha + x_\beta^\circ m_\beta$ is the mean molecular mass of the mixture, and $x_\alpha^\circ = n_\alpha^\circ/n_o$ and $x_\beta^\circ = n_\beta^\circ/n_o$ are the mole fractions of the gases α and β , respectively, in the ground state with $n_o = n_\alpha^\circ + n_\beta^\circ$ being the total number density in the ground state—so that in the limiting cases of $x_\alpha^\circ = 0$ or $x_\beta^\circ = 0$, the linear-dimensionless system of moment equations (see below) for the non-vanishing component in the binary gas-mixture reduces to the corresponding system of Grad moment equations for the single gas β or α , respectively.

5.1.1 Dimensionless equations

5.1.1.1 $2 \times \text{G26}$ equations

The linear-dimensionless G26 equations for the α -constituent in a binary gas-mixture consisting of α and β gases read

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \left(\frac{\partial \hat{n}_\alpha}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} \right) + \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} = 0, \quad (5.3)$$

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{t}} + \frac{v_o^2}{\theta_\alpha^\circ} \frac{\partial \hat{v}_i}{\partial \hat{t}} + \frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{x}_j} + \frac{\partial \hat{T}_\alpha}{\partial \hat{x}_i} + \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} = -\frac{1}{\text{Kn} \Omega} x_\beta^\circ \left[\delta_1 \hat{u}_i^{(\alpha)} + \delta_2 \hat{q}_i^{(\alpha)} - \delta_3 \hat{u}_i^{(\beta)} - \delta_4 \hat{q}_i^{(\beta)} \right], \quad (5.4)$$

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \left(\frac{3}{2} \frac{\partial \hat{T}_\alpha}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} \right) - \frac{3}{2} \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} + \frac{\partial \hat{q}_i^{(\alpha)}}{\partial \hat{x}_i} = -\frac{1}{\text{Kn} \Omega} x_\beta^\circ \left[\delta_5 (\hat{T}_\alpha - \hat{T}_\beta) + \delta_6 \hat{\Delta}_\alpha - \delta_7 \hat{\Delta}_\beta \right], \quad (5.5)$$

$$\begin{aligned} & \frac{v_o}{\sqrt{\theta_\alpha^\circ}} \left(\frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{t}} + 2 \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right) + \frac{\partial \hat{m}_{ijk}^{(\alpha)}}{\partial \hat{x}_k} + \frac{4}{5} \frac{\partial \hat{q}_{\langle i}}{\partial \hat{x}_{j \rangle}} \\ &= -\frac{1}{\text{Kn} \Omega} \left[x_\alpha^\circ \Omega_\alpha \left(\hat{\sigma}_{ij}^{(\alpha)} + \delta_8 \hat{R}_{ij}^{(\alpha)} \right) + x_\beta^\circ \left(\delta_9 \hat{\sigma}_{ij}^{(\alpha)} + \delta_{10} \hat{R}_{ij}^{(\alpha)} - \delta_{11} \hat{\sigma}_{ij}^{(\beta)} - \delta_{12} \hat{R}_{ij}^{(\beta)} \right) \right], \end{aligned} \quad (5.6)$$

$$\begin{aligned} & \frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{q}_i^{(\alpha)}}{\partial \hat{t}} + \frac{5}{2} \frac{v_o^2}{\theta_\alpha^\circ} \frac{\partial \hat{v}_i}{\partial \hat{t}} + \frac{1}{2} \frac{\partial \hat{R}_{ij}^{(\alpha)}}{\partial \hat{x}_j} + \frac{7}{2} \frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{x}_j} + \frac{1}{6} \frac{\partial \hat{\Delta}_\alpha}{\partial \hat{x}_i} + 5 \frac{\partial \hat{T}_\alpha}{\partial \hat{x}_i} + \frac{5}{2} \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} \\ &= -\frac{1}{\text{Kn} \Omega} \left[\frac{2}{3} x_\alpha^\circ \Omega_\alpha \left(\hat{q}_i^{(\alpha)} - \frac{5}{2} \hat{u}_i^{(\alpha)} \right) + x_\beta^\circ \left(\delta_{13} \hat{q}_i^{(\alpha)} - \delta_{14} \hat{u}_i^{(\alpha)} - \delta_{15} \hat{q}_i^{(\beta)} - \delta_{16} \hat{u}_i^{(\beta)} \right) \right], \end{aligned} \quad (5.7)$$

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{m}_{ijk}^{(\alpha)}}{\partial \hat{t}} + \frac{3}{7} \frac{\partial \hat{R}_{ij}^{(\alpha)}}{\partial \hat{x}_k} + 3 \frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{x}_k} = -\frac{1}{\text{Kn} \Omega} \left[\frac{3}{2} x_\alpha^\circ \Omega_\alpha \hat{m}_{ijk}^{(\alpha)} + x_\beta^\circ \left(\delta_{17} \hat{m}_{ijk}^{(\alpha)} - \delta_{18} \hat{m}_{ijk}^{(\beta)} \right) \right], \quad (5.8)$$

$$\begin{aligned} & \frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{R}_{ij}^{(\alpha)}}{\partial \hat{t}} + 2 \frac{\partial \hat{m}_{ijk}^{(\alpha)}}{\partial \hat{x}_k} + \frac{28}{5} \frac{\partial \hat{q}_{\langle i}}{\partial \hat{x}_{j \rangle}} - 14 \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_j} \\ &= -\frac{1}{\text{Kn} \Omega} \left[x_\alpha^\circ \Omega_\alpha \left(\delta_{19} \hat{R}_{ij}^{(\alpha)} + \delta_{20} \hat{\sigma}_{ij}^{(\alpha)} \right) + x_\beta^\circ \left(\delta_{21} \hat{R}_{ij}^{(\alpha)} + \delta_{22} \hat{\sigma}_{ij}^{(\alpha)} - \delta_{23} \hat{R}_{ij}^{(\beta)} - \delta_{24} \hat{\sigma}_{ij}^{(\beta)} \right) \right], \end{aligned} \quad (5.9)$$

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{\Delta}_\alpha}{\partial \hat{t}} + 8 \frac{\partial \hat{q}_i^{(\alpha)}}{\partial \hat{x}_i} - 20 \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} = - \frac{1}{\text{Kn} \Omega} \left[\frac{2}{3} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{\Delta}_\alpha + \mathbf{x}_\beta^\circ \left\{ \delta_{25} \hat{\Delta}_\alpha - \delta_{26} \hat{\Delta}_\beta + \delta_{27} (\hat{T}_\alpha - \hat{T}_\beta) \right\} \right]. \quad (5.10)$$

In (5.3)–(5.10),

$$\text{Kn} = \frac{\ell}{L} \quad \text{with} \quad \ell = \frac{5}{16\sqrt{\pi} n_o \left(\mathbf{x}_\alpha^\circ \Omega_{\alpha\alpha}^{(2,2)} + \mathbf{x}_\beta^\circ \Omega_{\beta\beta}^{(2,2)} \right)} \quad (5.11)$$

is the Knudsen number and L is a macroscopic length scale pertaining to the problem under consideration;

$$\Omega_\alpha = \frac{\Omega_{\alpha\alpha}^{(2,2)}}{\Omega_{\alpha\beta}^{(2,2)}} \quad \text{and} \quad \Omega_\beta = \frac{\Omega_{\beta\beta}^{(2,2)}}{\Omega_{\alpha\beta}^{(2,2)}} \quad (5.12)$$

are the ratios directly related to collisional cross sections; $\Omega = \mathbf{x}_\alpha^\circ \Omega_\alpha + \mathbf{x}_\beta^\circ \Omega_\beta$; and the coefficients $\delta_8, \delta_{19}, \delta_{20}$ are constants while the other δ_i 's depend only on the mass ratios of the constituents. The coefficients δ_i 's for Maxwell interaction potential are given by

$$\left. \begin{aligned} \delta_1 &= \frac{2\sqrt{2}}{3} a_1 \sqrt{\mu_\beta}, & \delta_2 &= 0, & \delta_3 &= \frac{2\sqrt{2}}{3} a_1 \sqrt{\mu_\alpha}, \\ \delta_4 &= 0, & \delta_5 &= 2\sqrt{2} a_1 \mu_\alpha \sqrt{\mu_\beta}, & \delta_6 &= 0, \\ \delta_7 &= 0, & \delta_8 &= 0, & \delta_9 &= \frac{\sqrt{2}}{3} (4a_1 \mu_\alpha + 3\mu_\beta) \sqrt{\mu_\beta}, \\ \delta_{10} &= 0, & \delta_{11} &= \frac{\sqrt{2}}{3} (4a_1 - 3) \mu_\alpha \sqrt{\mu_\beta}, & \delta_{12} &= 0, \\ \delta_{13} &= \frac{2\sqrt{2}}{3} (3a_1 \mu_\alpha^2 + 2\mu_\alpha \mu_\beta + a_1 \mu_\beta^2) \sqrt{\mu_\beta}, \\ \delta_{14} &= \frac{10\sqrt{2}}{3} \{ \mu_\beta + a_1 (\mu_\alpha - \mu_\beta) \} \mu_\alpha \sqrt{\mu_\beta}, \\ \delta_{15} &= \frac{4\sqrt{2}}{3} (2a_1 - 1) \mu_\alpha \mu_\beta \sqrt{\mu_\alpha}, \\ \delta_{16} &= \frac{5\sqrt{2}}{3} \{ a_1 - 2(2a_1 - 1) \mu_\alpha \mu_\beta \} \sqrt{\mu_\alpha}, \\ \delta_{17} &= \frac{\sqrt{2}}{3} \{ 6a_1 \mu_\alpha^2 + 9\mu_\alpha \mu_\beta + (5a_3 - 3a_1) \mu_\beta^2 \} \sqrt{\mu_\beta}, \\ \delta_{18} &= \frac{\sqrt{2}}{3} (5a_3 + 3a_1 - 9) \mu_\alpha \mu_\beta \sqrt{\mu_\alpha}, & \delta_{19} &= \frac{7}{6}, & \delta_{20} &= 0, \\ \delta_{21} &= \frac{\sqrt{2}}{3} \left[3\mu_\beta + 2\mu_\alpha \{ 4a_1 \mu_\alpha^2 + 4\mu_\alpha \mu_\beta + (3a_3 + a_1 - 3) \mu_\beta^2 \} \right] \sqrt{\mu_\beta}, \\ \delta_{22} &= 0, & \delta_{23} &= \frac{2\sqrt{2}}{3} (3a_3 + 5a_1 - 7) \mu_\alpha^2 \mu_\beta \sqrt{\mu_\beta}, \\ \delta_{24} &= 0, & \delta_{25} &= \frac{8\sqrt{2}}{3} \mu_\alpha (a_1 \mu_\alpha^2 + \mu_\alpha \mu_\beta + a_1 \mu_\beta^2) \sqrt{\mu_\beta}, \\ \delta_{26} &= \frac{8\sqrt{2}}{3} (2a_1 - 1) \mu_\alpha^2 \mu_\beta \sqrt{\mu_\beta}, & \delta_{27} &= 0, \end{aligned} \right\} \quad (5.13)$$

while those for hard-sphere interaction potential are given by

$$\left. \begin{aligned} \delta_1 &= \frac{5}{6\sqrt{2}}(1 + \mu_\alpha)\sqrt{\mu_\beta}, & \delta_2 &= \frac{1}{3\sqrt{2}}\mu_\beta\sqrt{\mu_\beta}, & \delta_3 &= \frac{5}{6\sqrt{2}}(1 + \mu_\beta)\sqrt{\mu_\alpha}, \\ \delta_4 &= \frac{1}{3\sqrt{2}}\mu_\alpha\sqrt{\mu_\alpha}, & \delta_5 &= \frac{5}{\sqrt{2}}\mu_\alpha\sqrt{\mu_\beta}, & \delta_6 &= \frac{1}{6\sqrt{2}}\mu_\alpha\mu_\beta\sqrt{\mu_\beta}, & \delta_7 &= \frac{1}{6\sqrt{2}}\mu_\alpha^2\sqrt{\mu_\beta}, \\ \delta_8 &= \frac{1}{28}, & \delta_9 &= \frac{\sqrt{2}}{3}(3 + 2\mu_\alpha)\sqrt{\mu_\beta}, & \delta_{10} &= \frac{1}{21\sqrt{2}}(3 + 4\mu_\alpha)\mu_\beta\sqrt{\mu_\beta}, \\ \delta_{11} &= \frac{2\sqrt{2}}{3}\mu_\alpha\sqrt{\mu_\beta}, & \delta_{12} &= \frac{2\sqrt{2}}{21}\mu_\alpha^2\sqrt{\mu_\beta}, & \delta_{13} &= \frac{1}{2\sqrt{2}}(6 - 5\mu_\alpha + 9\mu_\alpha^2)\sqrt{\mu_\beta}, \\ \delta_{14} &= \frac{5}{12\sqrt{2}}(6 - 13\mu_\alpha + 27\mu_\alpha^2)\sqrt{\mu_\beta}, & \delta_{15} &= \frac{1}{6\sqrt{2}}(5 + 27\mu_\beta)\mu_\alpha\sqrt{\mu_\alpha}, \\ \delta_{16} &= \frac{5}{12\sqrt{2}}(12 - 34\mu_\alpha + 27\mu_\alpha^2)\sqrt{\mu_\alpha}, & \delta_{17} &= \frac{1}{7\sqrt{2}}(16 + 10\mu_\alpha + 9\mu_\alpha^2)\sqrt{\mu_\beta}, \\ \delta_{18} &= \frac{9}{7\sqrt{2}}\mu_\alpha\mu_\beta\sqrt{\mu_\alpha}, & \delta_{19} &= \frac{205}{168}, & \delta_{20} &= \frac{1}{2}, \\ \delta_{21} &= \frac{1}{21\sqrt{2}}(51 + 32\mu_\alpha - 63\mu_\alpha^2 + 120\mu_\alpha^3)\sqrt{\mu_\beta}, \\ \delta_{22} &= \frac{\sqrt{2}}{3}(3 + 4\mu_\alpha)\mu_\beta\sqrt{\mu_\beta}, & \delta_{23} &= \frac{20\sqrt{2}}{7}\mu_\alpha^2\mu_\beta\sqrt{\mu_\beta}, \\ \delta_{24} &= \frac{4\sqrt{2}}{3}\mu_\alpha\mu_\beta\sqrt{\mu_\beta}, & \delta_{25} &= \frac{\sqrt{2}}{3}\mu_\alpha(13 - 18\mu_\alpha + 15\mu_\alpha^2)\sqrt{\mu_\beta}, \\ \delta_{26} &= 5\sqrt{2}\mu_\alpha^2\mu_\beta\sqrt{\mu_\beta}, & \delta_{27} &= 10\sqrt{2}\mu_\alpha\mu_\beta\sqrt{\mu_\beta}. \end{aligned} \right\} \quad (5.14)$$

While writing the coefficients δ_i 's, the relation $\mu_\alpha + \mu_\beta = 1$ has been exploited. It should be noted that $\Omega_{ij}^{(2,2)}$'s for hard-sphere interaction potential are given by (3.48).

The G26 equations for the β -constituent follow by interchanging α and β in (5.3)–(5.10) and also in (5.13) and (5.14). Note that the G26 equations for the α -constituent, (5.3)–(5.10), as well as the similar equations for the β -constituent contain the dimensionless hydrodynamic velocity $\hat{\mathbf{v}}$ whose governing equation is the dimensionless momentum balance equation for the mixture

$$\mathbf{x}_\alpha^\circ \left(\frac{v_\alpha^2}{\theta_\alpha^\circ} \frac{\partial \hat{v}_i}{\partial \hat{t}} + \frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{x}_j} + \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} + \frac{\partial \hat{T}_\alpha}{\partial \hat{x}_i} \right) + \mathbf{x}_\beta^\circ \left(\frac{v_\beta^2}{\theta_\beta^\circ} \frac{\partial \hat{v}_i}{\partial \hat{t}} + \frac{\partial \hat{\sigma}_{ij}^{(\beta)}}{\partial \hat{x}_j} + \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} + \frac{\partial \hat{T}_\beta}{\partial \hat{x}_i} \right) = 0. \quad (5.15)$$

Therefore, (5.3)–(5.10) and the similar equations for the β -constituent along with (5.15) form the system of dimensionless $2 \times \text{G26}$ equations for a binary gas-mixture comprising of α and β gases, where one needs to consider only one of the two balance equations for the diffusion velocities in the light of relation $\rho_\alpha \mathbf{u}_\alpha + \rho_\beta \mathbf{u}_\beta = \mathbf{0}$ for binary gas-mixture.

5.1.1.2 $2 \times \text{G13}$ equations

In the system of $2 \times \text{G13}$ equations for a binary gas-mixture comprising of α and β gases, the G13 equations for the α -constituent are equations (5.3)–(5.7) upon setting the higher moments— $\hat{m}_{ijk}^{(\alpha)}$, $\hat{R}_{ij}^{(\alpha)}$ and $\hat{\Delta}_\alpha$ —to zero in them, and the G13 equations for the β -constituent follow by interchanging α and β in the G13 equations for the α -constituent. Again, owing to aforementioned reason, the dimensionless total momentum balance equation (5.15) is included in the

system of $2 \times G13$ equations while one of the two balance equations for the diffusion velocities is discarded.

5.1.2 Moment equations in one dimension

In the next section, we shall analyze the behaviour of linear waves anticipated by $2 \times G13$ and $2 \times G26$ equations for both Maxwell and hard-sphere interaction potentials. To this end, we consider the systems of dimensionless moment equations in one-dimensional setting.

5.1.2.1 $2 \times G26$ equations

The one-dimensional G26 equations for the α -constituent in a binary gas-mixture comprising of α and β gases read

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \left(\frac{\partial \hat{n}_\alpha}{\partial \hat{t}} + \frac{\partial \hat{v}_x}{\partial \hat{x}} \right) + \frac{\partial \hat{u}_x^{(\alpha)}}{\partial \hat{x}} = 0, \quad (5.16)$$

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{u}_x^{(\alpha)}}{\partial \hat{t}} + \frac{v_o^2}{\theta_\alpha^\circ} \frac{\partial \hat{v}_x}{\partial \hat{t}} + \frac{\partial \hat{\sigma}_{xx}^{(\alpha)}}{\partial \hat{x}} + \frac{\partial \hat{T}_\alpha}{\partial \hat{x}} + \frac{\partial \hat{n}_\alpha}{\partial \hat{x}} = -\frac{1}{\text{Kn} \Omega} x_\beta^\circ \left(\delta_1 \hat{u}_x^{(\alpha)} + \delta_2 \hat{q}_x^{(\alpha)} - \delta_3 \hat{u}_x^{(\beta)} - \delta_4 \hat{q}_x^{(\beta)} \right), \quad (5.17)$$

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \left(\frac{3}{2} \frac{\partial \hat{T}_\alpha}{\partial \hat{t}} + \frac{\partial \hat{v}_x}{\partial \hat{x}} \right) - \frac{3}{2} \frac{\partial \hat{u}_x^{(\alpha)}}{\partial \hat{x}} + \frac{\partial \hat{q}_x^{(\alpha)}}{\partial \hat{x}} = -\frac{1}{\text{Kn} \Omega} x_\beta^\circ \left[\delta_5 (\hat{T}_\alpha - \hat{T}_\beta) + \delta_6 \hat{\Delta}_\alpha - \delta_7 \hat{\Delta}_\beta \right], \quad (5.18)$$

$$\begin{aligned} & \frac{v_o}{\sqrt{\theta_\alpha^\circ}} \left(\frac{\partial \hat{\sigma}_{xx}^{(\alpha)}}{\partial \hat{t}} + \frac{4}{3} \frac{\partial \hat{v}_x}{\partial \hat{x}} \right) + \frac{\partial \hat{m}_{xxx}^{(\alpha)}}{\partial \hat{x}} + \frac{8}{15} \frac{\partial \hat{q}_x^{(\alpha)}}{\partial \hat{x}} \\ &= -\frac{1}{\text{Kn} \Omega} \left[x_\alpha^\circ \Omega_\alpha \left(\hat{\sigma}_{xx}^{(\alpha)} + \delta_8 \hat{R}_{xx}^{(\alpha)} \right) + x_\beta^\circ \left(\delta_9 \hat{\sigma}_{xx}^{(\alpha)} + \delta_{10} \hat{R}_{xx}^{(\alpha)} - \delta_{11} \hat{\sigma}_{xx}^{(\beta)} - \delta_{12} \hat{R}_{xx}^{(\beta)} \right) \right], \end{aligned} \quad (5.19)$$

$$\begin{aligned} & \frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{q}_x^{(\alpha)}}{\partial \hat{t}} + \frac{5}{2} \frac{v_o^2}{\theta_\alpha^\circ} \frac{\partial \hat{v}_x}{\partial \hat{t}} + \frac{1}{2} \frac{\partial \hat{R}_{xx}^{(\alpha)}}{\partial \hat{x}} + \frac{7}{2} \frac{\partial \hat{\sigma}_{xx}^{(\alpha)}}{\partial \hat{x}} + \frac{1}{6} \frac{\partial \hat{\Delta}_\alpha}{\partial \hat{x}} + 5 \frac{\partial \hat{T}_\alpha}{\partial \hat{x}} + \frac{5}{2} \frac{\partial \hat{n}_\alpha}{\partial \hat{x}} \\ &= -\frac{1}{\text{Kn} \Omega} \left[\frac{2}{3} x_\alpha^\circ \Omega_\alpha \left(\hat{q}_x^{(\alpha)} - \frac{5}{2} \hat{u}_x^{(\alpha)} \right) + x_\beta^\circ \left(\delta_{13} \hat{q}_x^{(\alpha)} - \delta_{14} \hat{u}_x^{(\alpha)} - \delta_{15} \hat{q}_x^{(\beta)} - \delta_{16} \hat{u}_x^{(\beta)} \right) \right], \end{aligned} \quad (5.20)$$

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{m}_{xxx}^{(\alpha)}}{\partial \hat{t}} + \frac{9}{35} \frac{\partial \hat{R}_{xx}^{(\alpha)}}{\partial \hat{x}} + \frac{9}{5} \frac{\partial \hat{\sigma}_{xx}^{(\alpha)}}{\partial \hat{x}} = -\frac{1}{\text{Kn} \Omega} \left[\frac{3}{2} x_\alpha^\circ \Omega_\alpha \hat{m}_{xxx}^{(\alpha)} + x_\beta^\circ \left(\delta_{17} \hat{m}_{xxx}^{(\alpha)} - \delta_{18} \hat{m}_{xxx}^{(\beta)} \right) \right], \quad (5.21)$$

$$\begin{aligned} & \frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{R}_{xx}^{(\alpha)}}{\partial \hat{t}} + 2 \frac{\partial \hat{m}_{xxx}^{(\alpha)}}{\partial \hat{x}} + \frac{56}{15} \frac{\partial \hat{q}_x^{(\alpha)}}{\partial \hat{x}} - \frac{28}{3} \frac{\partial \hat{u}_x^{(\alpha)}}{\partial \hat{x}} \\ &= -\frac{1}{\text{Kn} \Omega} \left[x_\alpha^\circ \Omega_\alpha \left(\delta_{19} \hat{R}_{xx}^{(\alpha)} + \delta_{20} \hat{\sigma}_{xx}^{(\alpha)} \right) + x_\beta^\circ \left(\delta_{21} \hat{R}_{xx}^{(\alpha)} + \delta_{22} \hat{\sigma}_{xx}^{(\alpha)} - \delta_{23} \hat{R}_{xx}^{(\beta)} - \delta_{24} \hat{\sigma}_{xx}^{(\beta)} \right) \right], \end{aligned} \quad (5.22)$$

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} \frac{\partial \hat{\Delta}_\alpha}{\partial \hat{t}} + 8 \frac{\partial \hat{q}_x^{(\alpha)}}{\partial \hat{x}} - 20 \frac{\partial \hat{u}_x^{(\alpha)}}{\partial \hat{x}} = -\frac{1}{\text{Kn} \Omega} \left[\frac{2}{3} x_\alpha^\circ \Omega_\alpha \hat{\Delta}_\alpha + x_\beta^\circ \left\{ \delta_{25} \hat{\Delta}_\alpha - \delta_{26} \hat{\Delta}_\beta + \delta_{27} (\hat{T}_\alpha - \hat{T}_\beta) \right\} \right]. \quad (5.23)$$

The one-dimensional G26 equations for the β -constituent follow by interchanging α and β in (5.16)–(5.23), and the dimensionless momentum balance equation for the mixture in one dimension (1D) reads

$$x_\alpha^\circ \left(\frac{v_o^2}{\theta_\alpha^\circ} \frac{\partial \hat{v}_x}{\partial \hat{t}} + \frac{\partial \hat{\sigma}_{xx}^{(\alpha)}}{\partial \hat{x}} + \frac{\partial \hat{n}_\alpha}{\partial \hat{x}} + \frac{\partial \hat{T}_\alpha}{\partial \hat{x}} \right) + x_\beta^\circ \left(\frac{v_o^2}{\theta_\beta^\circ} \frac{\partial \hat{v}_x}{\partial \hat{t}} + \frac{\partial \hat{\sigma}_{xx}^{(\beta)}}{\partial \hat{x}} + \frac{\partial \hat{n}_\beta}{\partial \hat{x}} + \frac{\partial \hat{T}_\beta}{\partial \hat{x}} \right) = 0. \quad (5.24)$$

Therefore, the system of linear one-dimensional 2×G26 equations consists of equations (5.16)–(5.23), similar equations for the β -constituent and equation (5.24), where we shall discard the equation for diffusion velocity of the β -constituent and eliminate the diffusion velocity of the β -constituent in other equations by the diffusion velocity of the α -constituent.

5.1.2.2 2×G13 equations

The system of linear one-dimensional 2×G13 equations for a binary gas-mixture comprising of α and β gases contains equations (5.16)–(5.20) upon setting $\hat{m}_{xxx}^{(\alpha)}$, $\hat{R}_{xx}^{(\alpha)}$ and $\hat{\Delta}_\alpha$ to zero, similar equations for the β -constituent which follow by interchanging α and β in the equations for the α -constituent and equation (5.24), where we shall again discard the equation for diffusion velocity of the β -constituent and eliminate the diffusion velocity of the β -constituent in other equations by the diffusion velocity of the α -constituent.

5.2 Dispersion relations

For the linear stability analysis of a system, the plane wave solution of the form

$$\mathbf{U} = \mathbf{U}_0 \exp \{i(\kappa x - \omega t)\}$$

is assumed. Here, i is the imaginary unit, κ is the wavenumber, ω is the complex frequency, $\mathbf{U}$ contains all the field variables in the system with $\mathbf{U}_0$ containing their respective complex amplitudes. The imaginary part of the frequency ω evinces a disturbance which grows with time (unstable) or decays with time (stable), depending on whether the imaginary part of ω is positive or negative, respectively.

Let the length scale be the inverse of the wavenumber κ and scale for the frequency ω be κv_o so that the dimensionless position is $\hat{x} = \kappa x$ and the dimensionless frequency is $\hat{\omega} = \omega / (\kappa v_o)$. For

the above one-dimensional systems of moment equations, we assume the plane wave solutions

$$\hat{\mathbf{U}} = \hat{\mathbf{U}}_0 \exp \{i(\hat{x} - \hat{\omega}t)\}, \quad (5.25)$$

where the vector $\hat{\mathbf{U}}$ for the 2×G13 equations in 1D is

$$\hat{\mathbf{U}} = \{\hat{n}_\alpha, \hat{u}_x^{(\alpha)}, \hat{T}_\alpha, \hat{\sigma}_{xx}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{n}_\beta, \hat{T}_\beta, \hat{\sigma}_{xx}^{(\beta)}, \hat{q}_x^{(\beta)}, \hat{v}_x\}^\top \quad (5.26)$$

and that for the 2×G26 equations in 1D is

$$\hat{\mathbf{U}} = \{\hat{n}_\alpha, \hat{u}_x^{(\alpha)}, \hat{T}_\alpha, \hat{\sigma}_{xx}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{m}_{xxx}^{(\alpha)}, \hat{R}_{xx}^{(\alpha)}, \hat{\Delta}_\alpha, \hat{n}_\beta, \hat{T}_\beta, \hat{\sigma}_{xx}^{(\beta)}, \hat{q}_x^{(\beta)}, \hat{m}_{xxx}^{(\beta)}, \hat{R}_{xx}^{(\beta)}, \hat{\Delta}_\beta, \hat{v}_x\}^\top, \quad (5.27)$$

and $\hat{\mathbf{U}}_0$ contains the complex amplitudes of the corresponding field variables in the respective systems. In this case, the Knudsen number appearing in the moment equations above is $\text{Kn} = \ell \kappa$, which now takes the role of dimensionless wavenumber. Each system of moment equations can be written as

$$\mathcal{A}(\hat{\omega}, \text{Kn}, \mathbf{x}_\alpha^\circ, \mu_\alpha, \Omega_\alpha, \Omega_\beta) \hat{\mathbf{U}} = \mathbf{0}. \quad (5.28)$$

For the non-trivial solution $\hat{\mathbf{U}}$ of (5.28), the determinant of matrix $\mathcal{A}(\hat{\omega}, \text{Kn}, \mathbf{x}_\alpha^\circ, \mu_\alpha, \Omega_\alpha, \Omega_\beta)$ must vanish, i.e., $\det\{\mathcal{A}(\hat{\omega}, \text{Kn}, \mathbf{x}_\alpha^\circ, \mu_\alpha, \Omega_\alpha, \Omega_\beta)\} = 0$, which provides the so-called dispersion relation between ω and κ (between $\hat{\omega}$ and Kn here).

For spatial disturbances, the wavenumber κ is real and the frequency ω is complex. The corresponding wave has phase velocity $v_{\text{ph}} = \text{Re}(\omega)/\kappa$ and damping $\varsigma = \text{Im}(\omega)$. For stability, the damping must be non-positive, i.e., $\varsigma \leq 0$.

5.3 Results

In order to analyze the linear stability of the 2×G13 and 2×G26 equations, we consider three binary gas-mixtures of noble gases: neon-argon (Ne–Ar), helium-argon (He–Ar) and helium-xenon (He–Xe) with mole fractions of the lighter gases in each mixture as 0.25, 0.50 and 0.75 as our examples. The mixtures considered are in order of small-to-large mass differences. The molecular masses of the gases in these mixtures are $m_{\text{He}} = 4.0026$, $m_{\text{Ne}} = 20.1791$, $m_{\text{Ar}} = 39.948$, $m_{\text{Xe}} = 131.293$ in atomic units. The parameters Ω_α and Ω_β for these mixtures in case of hard-sphere interaction potential are computed by calculating the diameters through the exact formula for viscosity of a single gas given in [86, 97] and the experimental data on the viscosities of the single gases at temperature 300 K given in [56]. However, the computation of parameters Ω_α and Ω_β in case of Maxwell interaction potential is not so straightforward, since one needs explicit viscosity formulas for a single gas as well as for a gas-mixture which may be obtained through the rigorous Chapman–Enskog expansion to first order on the respective Boltzmann equations or on the respective moment equations. Here, in case of Maxwell interaction potential, we compute the viscosity formulas for single gases and binary gas-mixtures by performing Chapman–Enskog expansion on respective Grad’s moment equations, see chapter 8, and use the experimental data on the viscosities of the single gases and binary gas-mixtures at temperature 300 K given in [56].

Interaction potential	Mixture	Mole fraction (x_α°)	Ω_α	Ω_β
Maxwell	Ne–Ar	$x_{\text{Ne}}^\circ = 0.25$	0.7155	1.4154
		$x_{\text{Ne}}^\circ = 0.50$	0.7158	1.4162
		$x_{\text{Ne}}^\circ = 0.75$	0.7153	1.4151
	He–Ar	$x_{\text{He}}^\circ = 0.25$	0.5825	1.6154
		$x_{\text{He}}^\circ = 0.50$	0.5808	1.6106
		$x_{\text{He}}^\circ = 0.75$	0.5772	1.6007
	He–Xe	$x_{\text{He}}^\circ = 0.25$	0.4439	2.1997
		$x_{\text{He}}^\circ = 0.50$	0.4407	2.1842
		$x_{\text{He}}^\circ = 0.75$	0.4355	2.1582
Hard-sphere	Ne–Ar		0.6907	1.3664
	He–Ar		0.5631	1.5615
	He–Xe		0.3843	1.9046

Table 5.1: Parameters Ω_α and Ω_β for different binary gas-mixtures.

Nevertheless, since only a limited viscosity data from experiments is available in the literature (available only for the mole fractions 0.25, 0.5 and 0.75 in [56]), the parameters Ω_α and Ω_β for Maxwell molecules could be computed only for mole fractions 0.25, 0.5 and 0.75. The parameters Ω_α and Ω_β for both the interaction potentials are illustrated in table 5.1. It can be seen from the table that the relative difference in the values of both Ω_α and Ω_β for Maxwell interaction potential in comparison to their corresponding values for hard-sphere interaction potential is within 4% for Ne–Ar and He–Ar mixtures while approximately 15% for He–Xe mixture which has the largest mass difference among the considered binary mixtures.

5.3.1 General remarks about eigenmodes

The $2 \times G13$ equations for Maxwell molecules as well as for hard spheres contain 10 eigenmodes which result from the eigenvalues of the matrix $\mathcal{A}(\hat{\omega}, \text{Kn}, x_\alpha^\circ, \mu_\alpha, \Omega_\alpha, \Omega_\beta)$ that has dimension 10×10 for $2 \times G13$ equations (cf. (5.26)), while the $2 \times G26$ equations for Maxwell molecules as well as for hard spheres contain 16 eigenmodes because the matrix $\mathcal{A}(\hat{\omega}, \text{Kn}, x_\alpha^\circ, \mu_\alpha, \Omega_\alpha, \Omega_\beta)$ has dimension 16×16 for $2 \times G26$ equations (cf. (5.27)). The eigenmodes for all type of Grad's moment systems considered are plotted in figures 5.1–5.4.

Figures 5.1–5.4 illustrate the eigenmodes in the considered binary gas-mixtures computed with the systems of $2 \times G13$ equations for Maxwell molecules, $2 \times G26$ equations for Maxwell molecules, $2 \times G13$ equations for hard spheres and $2 \times G26$ equations for hard spheres, respectively, in $(\hat{v}_{\text{ph}}, \hat{\varsigma})$ plane, where $\hat{v}_{\text{ph}} = v_{\text{ph}}/v_o$ is the dimensionless phase velocity and $\hat{\varsigma} = \varsigma \ell / v_o$ is the dimensionless damping. The top, middle and bottom rows in each of figures 5.1–5.4 depict the

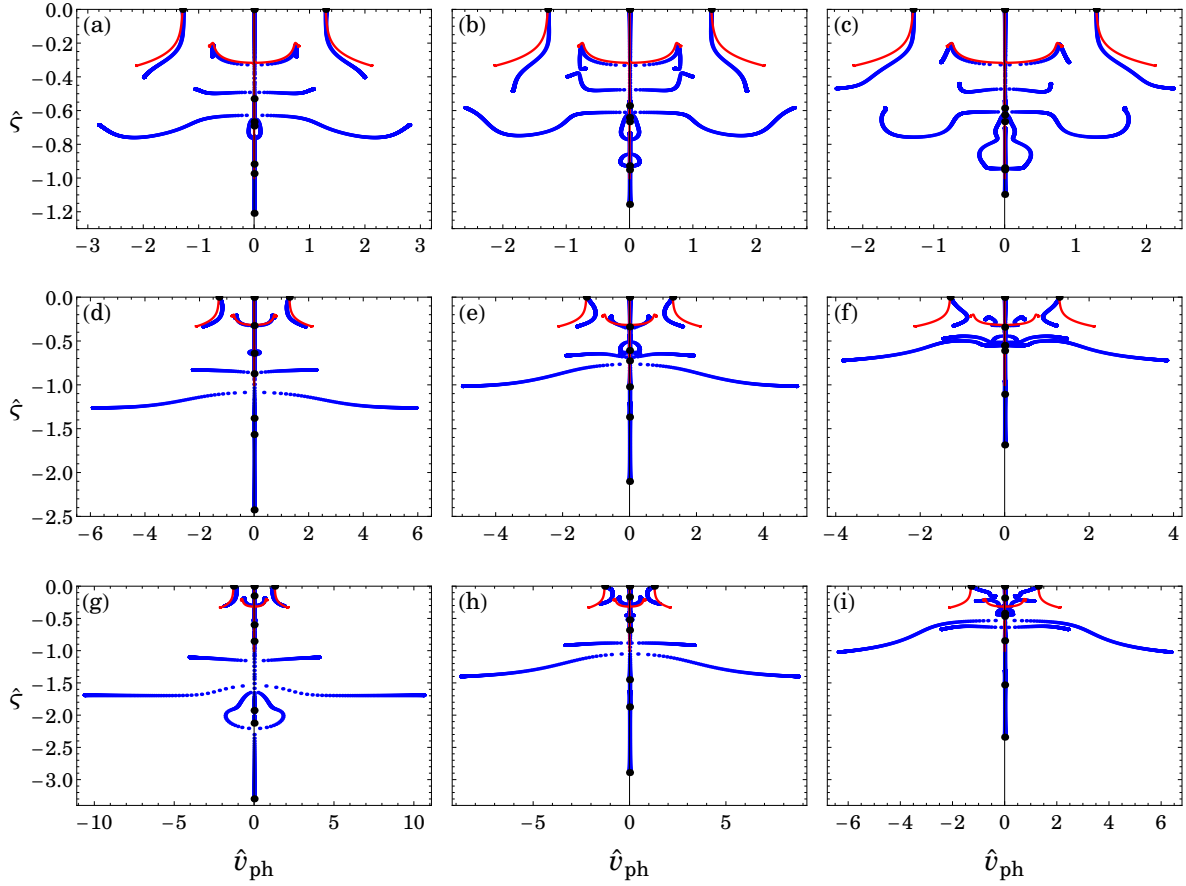


Figure 5.1: Eigenmodes for mixtures of Ne–Ar (top row), He–Ar (middle row) and He–Xe (bottom row) computed with $2\times\text{G13}$ equations for Maxwell molecules, and those for a single gas computed with G13 equations for Maxwell molecules. The red and blue curves represent the single gas and binary gas-mixture modes, respectively. The black dots depict the starting point of the binary gas-mixture modes at $\text{Kn} = \kappa = 0$. (a) Ne–Ar ($x_{\text{Ne}}^{\circ} = 0.25$), (b) Ne–Ar ($x_{\text{Ne}}^{\circ} = 0.50$), (c) Ne–Ar ($x_{\text{Ne}}^{\circ} = 0.75$), (d) He–Ar ($x_{\text{He}}^{\circ} = 0.25$), (e) He–Ar ($x_{\text{He}}^{\circ} = 0.50$), (f) He–Ar ($x_{\text{He}}^{\circ} = 0.75$), (g) He–Xe ($x_{\text{He}}^{\circ} = 0.25$), (h) He–Xe ($x_{\text{He}}^{\circ} = 0.50$), (i) He–Xe ($x_{\text{He}}^{\circ} = 0.75$).

modes for the mixtures of Ne–Ar, He–Ar and He–Xe, respectively, whereas the left, middle and right columns in each of figures 5.1–5.4 show the modes when the mole fractions of lighter gases in the mixtures are 0.25, 0.50 and 0.75, respectively. For all the plots in figures 5.1–5.4, the Knudsen number (Kn) varies from 0 to 5 along the curves and the black dots represent the starting points of the eigenmodes of binary gas-mixtures at $\text{Kn} = \kappa = 0$. The blue curves in each plot of figures 5.1–5.4 delineate the eigenmodes for mixtures while the red curves display those for a single gas; the (red) curves for a single gas are included only for comparison. In the limiting case when a component in the mixture is negligible, the eigenmodes for the other component in the mixture coincide with those for a single gas. Notice that for the $2\times\text{G26}$ systems (figures 5.2 and 5.4), there are two single gas modes (red curves) having non-zero phase velocities and non-zero damping in each sub-figure of figures 5.2 and 5.4; however, the single gas modes (red curves) having non-zero phase velocities and non-zero damping are not present in the figures for $2\times\text{G13}$ systems (figures 5.1 and 5.3). In the limiting cases when a component in the mixture is negligible, the starting points of two mixture modes (black dots) from the

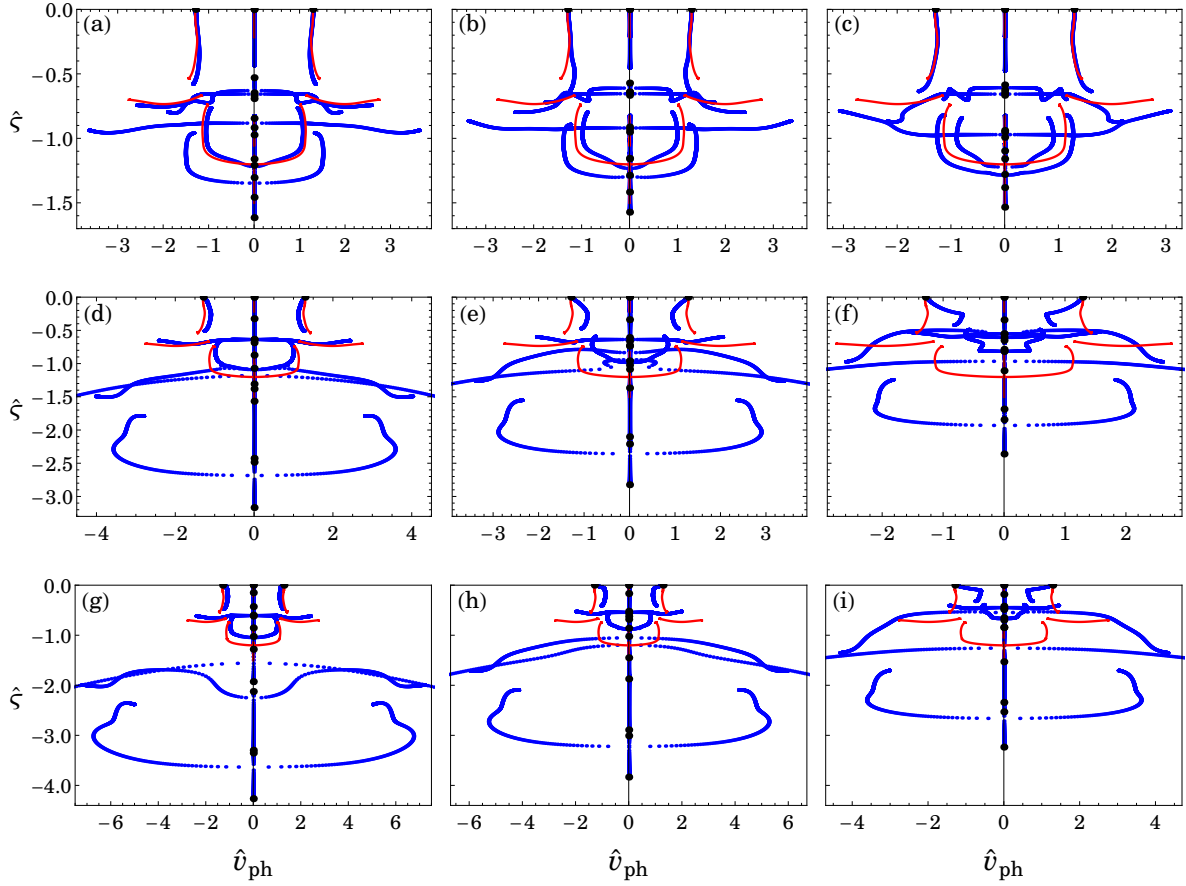


Figure 5.2: Eigenmodes for mixtures of Ne–Ar (top row), He–Ar (middle row) and He–Xe (bottom row) computed with $2\times\text{G26}$ equations for Maxwell molecules, and those for a single gas computed with G26 equations for Maxwell molecules. The red and blue curves represent the single gas and binary gas-mixture modes, respectively. The black dots depict the starting point of the binary gas-mixture modes at $\text{Kn} = \kappa = 0$. (a) Ne–Ar ($x_{\text{Ne}}^\circ = 0.25$), (b) Ne–Ar ($x_{\text{Ne}}^\circ = 0.50$), (c) Ne–Ar ($x_{\text{Ne}}^\circ = 0.75$), (d) He–Ar ($x_{\text{He}}^\circ = 0.25$), (e) He–Ar ($x_{\text{He}}^\circ = 0.50$), (f) He–Ar ($x_{\text{He}}^\circ = 0.75$), (g) He–Xe ($x_{\text{He}}^\circ = 0.25$), (h) He–Xe ($x_{\text{He}}^\circ = 0.50$), (i) He–Xe ($x_{\text{He}}^\circ = 0.75$).

$2\times\text{G26}$ systems begin approaching the starting points of aforementioned single gas modes when the mole fraction of either component in the mixture starts approaching 0 or 1, and the two mixture modes merge with the corresponding single gas modes when the mole fraction of either component in the mixture is very close to 0 or 1.

In each plot of figures 5.1–5.4, two sound modes—the modes starting with zero damping—commence with non-zero velocities and one with zero velocity at $\text{Kn} = \kappa = 0$. The other modes in each plots of figures 5.1–5.4 are pure diffusion modes—the modes beginning with zero velocity—having negative damping; some of these modes in each plot bifurcate into damped propagating waves for larger value of the Knudsen number, Kn .

As the mass ratios of the lighter gases in the gas-mixtures of Ne–Ar, He–Ar and He–Xe are $\mu_{\text{Ne}} = 0.3356$, $\mu_{\text{He}} = 0.0911$ and $\mu_{\text{He}} = 0.0296$, respectively, we observe that the damping increases with the increase in mass ratio of the lighter gas in the mixture for any mole fraction and any Grad’s moment system considered. Moreover, for any mixture damping also increases with increase in the mole fraction of the lighter gas in the mixture for any Grad’s moment

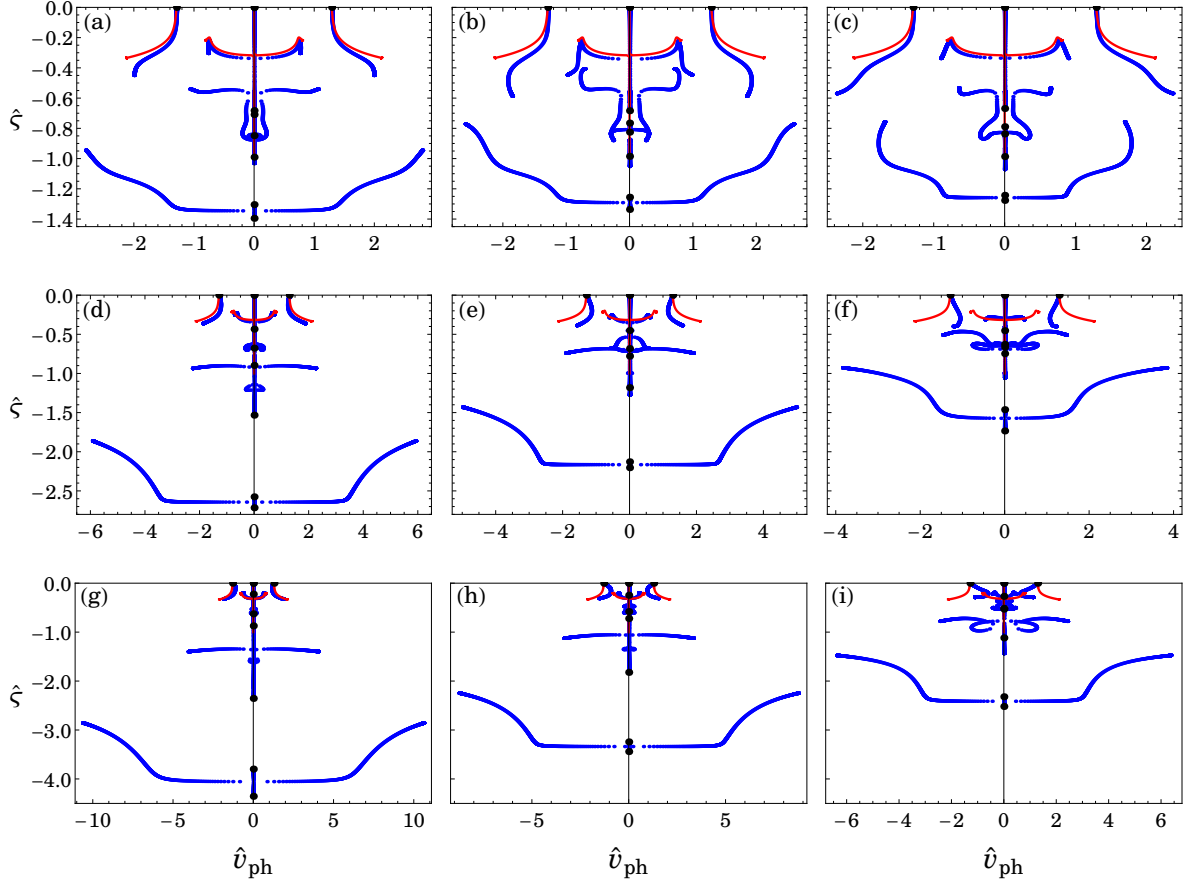


Figure 5.3: Eigenmodes for mixtures of Ne–Ar (top row), He–Ar (middle row) and He–Xe (bottom row) computed with $2\times G13$ equations for hard spheres, and those for a single gas computed with $G13$ equations for hard spheres. The red and blue curves represent the single gas and binary gas-mixture modes, respectively. The black dots depict the starting point of the binary gas-mixture modes at $\text{Kn} = \kappa = 0$. (a) Ne–Ar ($x_{\text{Ne}}^o = 0.25$), (b) Ne–Ar ($x_{\text{Ne}}^o = 0.50$), (c) Ne–Ar ($x_{\text{Ne}}^o = 0.75$), (d) He–Ar ($x_{\text{He}}^o = 0.25$), (e) He–Ar ($x_{\text{He}}^o = 0.50$), (f) He–Ar ($x_{\text{He}}^o = 0.75$), (g) He–Xe ($x_{\text{He}}^o = 0.25$), (h) He–Xe ($x_{\text{He}}^o = 0.50$), (i) He–Xe ($x_{\text{He}}^o = 0.75$).

system considered. It is apparent from figures 5.1–5.4 that the propagating waves from all the four Grad’s moment systems considered travel faster on decreasing the mass ratio of the lighter gas in the mixture for any mole fraction in general while they usually travel slower with increasing the mole fraction of the lighter gas in a binary gas-mixture. Also, the starting values of diffusion modes (the values at black dots) for Maxwell molecules are slightly bigger than those for hard spheres both in case of $2\times G13$ systems (cf. figures 5.1 and 5.3) as well as in case of $2\times G26$ systems (cf. figures 5.2 and 5.4).

5.3.2 Concluding remarks

We have examined the value of damping $\hat{\zeta}$ for several different permissible values of the parameters Kn , x_α^o , μ_α , Ω_α , Ω_β , and found that the damping $\hat{\zeta}$ remains always non-positive, which is visible in figures 5.1–5.4 as well for the binary gas-mixtures considered. Thus, we conclude, *empirically*, that the $2\times G13$ equations and $2\times G26$ equations for binary gas-mixture are linearly

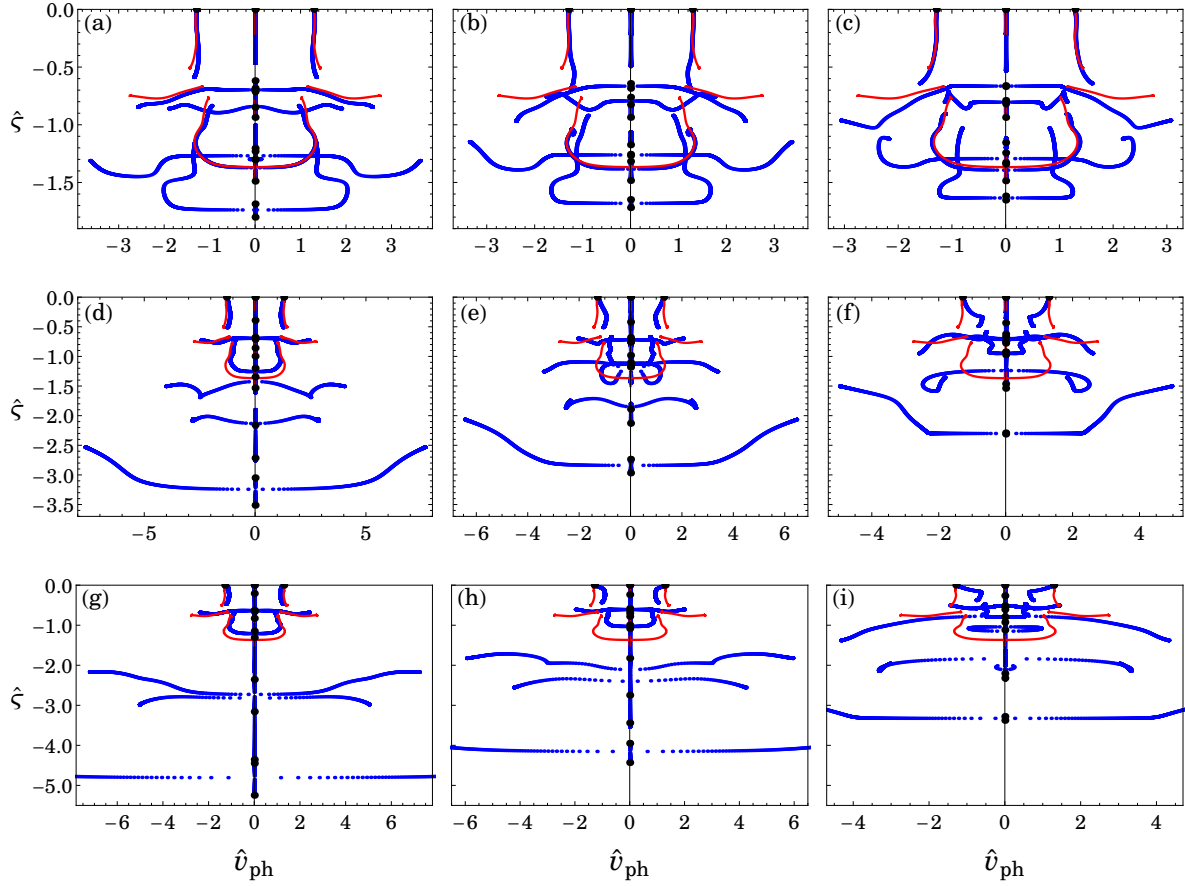


Figure 5.4: Eigenmodes for mixtures of Ne–Ar (top row), He–Ar (middle row) and He–Xe (bottom row) computed with $2\times\text{G26}$ equations for hard spheres, and those for a single gas computed with G26 equations for hard spheres. The red and blue curves represent the single gas and binary gas-mixture modes, respectively. The black dots depict the starting point of the binary gas-mixture modes at $\text{Kn} = \kappa = 0$. (a) Ne–Ar ($x_{\text{Ne}}^{\circ} = 0.25$), (b) Ne–Ar ($x_{\text{Ne}}^{\circ} = 0.50$), (c) Ne–Ar ($x_{\text{Ne}}^{\circ} = 0.75$), (d) He–Ar ($x_{\text{He}}^{\circ} = 0.25$), (e) He–Ar ($x_{\text{He}}^{\circ} = 0.50$), (f) He–Ar ($x_{\text{He}}^{\circ} = 0.75$), (g) He–Xe ($x_{\text{He}}^{\circ} = 0.25$), (h) He–Xe ($x_{\text{He}}^{\circ} = 0.50$), (i) He–Xe ($x_{\text{He}}^{\circ} = 0.75$).

stable, at least for Maxwell and hard-sphere interaction potentials.

Chapter 6

Heat transfer in one dimension

Heat transfer in a gas confined between two infinite parallel plates having different temperatures is a classical problem in rarefied gas dynamics, since the steady heat flux is one of the simplest example of non-equilibrium through which different methods and approaches can be examined and compared. The problem has been well studied by many researchers in the context of single gases, see e.g., [7, 29, 37, 61, 74, 75, 88] and the references cited in [74, 75, 98]. However, the same problem has certainly been less studied in the context of gaseous mixtures and there exists very few papers in the literature on this problem in the context of gaseous mixtures [4, 30, 31, 45, 58, 78, 87, 97, 126]. To the best of author's knowledge, the first paper on heat transfer between parallel plates in the context of binary gas-mixtures goes back to 1970s [126]. More recently, Kosuge et al. [58] have investigated the non-linear heat transfer based on the numerical solution of the Boltzmann equations. Reference [30] studies the problem using the linearized McCormack kinetic model [67] of the Boltzmann equations. Reference [87] also reports the results based on McCormack kinetic model, but uses two interaction potentials, namely, hard-sphere interaction potential and the so-called realistic potential. References [31, 78] study the problem on the basis of linearized Boltzmann equations for binary gas-mixtures with hard-sphere interaction potential. Reference [4] studies the problem via linearized extended thermodynamics with 13 moments for each constituent in a binary gas-mixture. Reference [97] reports the results based on the DSMC method with an implementation of *ab initio* potential. We have studied the same problem with Grad's 26-moment equations for each component in a binary gas-mixtures with Maxwell molecules in [45].

In this chapter, we shall investigate the heat transfer problem of binary gas-mixtures confined between two infinite parallel plates having different temperatures with the $2 \times G13$ and $2 \times G26$ equations, both for Maxwell and hard-sphere interaction potentials. Moreover, we shall also study the one-dimensional steady state flow of the infinitely diluted component in a binary gas-mixture. The infinitely diluted component in the mixture is like a contaminant, whose motion may not be described by particle based methods, e.g., DSMC method, due to insufficient number of molecules. Interestingly, for this problem, the system of equations for the non-diluted component decouples from that for the diluted one as the former behaves like a single gas and, consequently, this problem possesses the analytical solution too.

6.1 Heat transfer between parallel plates

6.1.1 Problem description

Let us consider a binary gas-mixture of gases α and β confined between two infinite parallel plates placed at $x = \pm L/2$ and let the temperature of the left plate (at $x = -L/2$) and that of

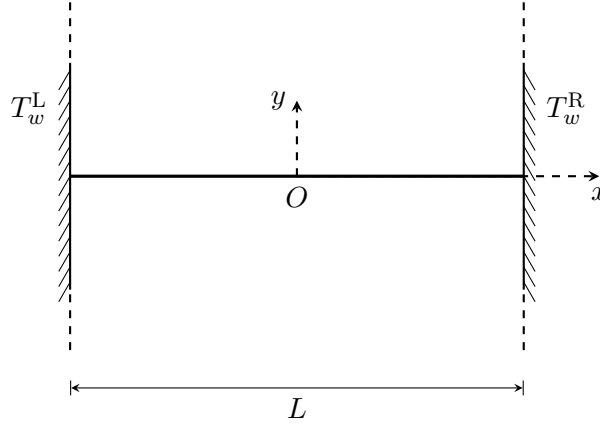


Figure 6.1: Schematic for the heat transfer problem in a binary gas-mixture confined between infinite parallel plates having different temperatures; y -axis is included just for illustration purposes.

the right plate (at $x = L/2$) be $T_w^L = T_o + \varepsilon \Delta \tilde{T}_w/2$ and $T_w^R = T_o - \varepsilon \Delta \tilde{T}_w/2$, respectively. The schematic of the problem is shown in figure 6.1. Owing to the temperature difference between the plates, the heat transfer takes place in the normal direction to the plates, i.e., in the x -direction, and therefore, the y -axis in figure 6.1 is just for illustration purposes. The temperature difference between the plates $\varepsilon \Delta \tilde{T}_w$ is taken very small in comparison to T_o so that the linearized equations and linearized boundary conditions are sufficient for the description of the process; notice the smallness parameter ε as a multiplier in the temperature difference, this parameter is same as that used in the linearization (cf. (5.1)). The scales used for non-dimensionalization are same as those in (5.2). Moreover, it should be noted that in contrast to the length scale adopted while studying the linear stability in the previous chapter, the length scale for the present problem is L , the gap between the plates.

6.1.2 Method of solution

The goal is to study the heat transfer in steady and rest state for the aforementioned problem. To this end, the systems of linear-dimensionless $2 \times G13$ and $2 \times G26$ equations in 1D are obtained by substituting $\partial(\cdot)/\partial \hat{t} = 0$ and $\hat{v}_x = 0$ in the moment equations detailed in § 5.1.2; also, recall that the velocity scale v_o is given by $v_o = \sqrt{kT_o/m}$ with $m = x_\alpha^o m_\alpha + x_\beta^o m_\beta$ being the mean molecular mass of the mixture. The relevant boundary conditions for the above one-dimensional problem are (4.13), (4.16), (4.18), (4.19) in case of $2 \times G13$ equations, and (4.13), (4.16), (4.21)–(4.23) in case of $2 \times G26$ equations—all for both the species.

Boundary conditions (4.18) as well as (4.21) for the problem under consideration just imply that the slip velocity vanishes, i.e, $\mathbf{V} = \mathbf{0}$, and the other boundary conditions—for the problem under consideration—in linear-dimensionless form are as follows. Boundary conditions (4.13) and (4.16) read

$$\int_{-1/2}^{1/2} \hat{n}_\alpha d\hat{x} = 0, \quad \int_{-1/2}^{1/2} \hat{n}_\beta d\hat{x} = 0, \quad (6.1)$$

$$\hat{u}_x^{(\alpha)} \left(-\frac{1}{2} \right) = \hat{u}_x^{(\alpha)} \left(\frac{1}{2} \right) = \hat{u}_x^{(\beta)} \left(-\frac{1}{2} \right) = \hat{u}_x^{(\beta)} \left(\frac{1}{2} \right) = 0. \quad (6.2)$$

The remaining boundary condition associated with 2×G13 equations, (4.19), reads ($\gamma \in \{\alpha, \beta\}$)

$$\hat{q}_x^{(\gamma)} = -\mathbf{n}_x \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[2 \left(\hat{T}_\gamma - \mathbf{n}_x \frac{\Delta \hat{T}_w}{2} \right) + \frac{1}{2} \hat{\sigma}_{xx}^{(\gamma)} \right], \quad (6.3)$$

while the remaining boundary conditions associated with 2×G26 equations, (4.22) and (4.23), read ($\gamma \in \{\alpha, \beta\}$)

$$\hat{q}_x^{(\gamma)} = -\mathbf{n}_x \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[2 \left(\hat{T}_\gamma - \mathbf{n}_x \frac{\Delta \hat{T}_w}{2} \right) + \frac{1}{2} \hat{\sigma}_{xx}^{(\gamma)} + \frac{5}{28} \hat{R}_{xx}^{(\gamma)} + \frac{1}{15} \hat{\Delta}_\gamma \right], \quad (6.4)$$

$$\hat{m}_{xxx}^{(\gamma)} = \mathbf{n}_x \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[\frac{2}{5} \left(\hat{T}_\gamma - \mathbf{n}_x \frac{\Delta \hat{T}_w}{2} \right) - \frac{7}{5} \hat{\sigma}_{xx}^{(\gamma)} - \frac{1}{14} \hat{R}_{xx}^{(\gamma)} + \frac{1}{75} \hat{\Delta}_\gamma \right], \quad (6.5)$$

where

$$\mathbf{n}_x = \begin{cases} 1 & \text{for left plate} \\ -1 & \text{for right plate} \end{cases} \quad \text{and} \quad \Delta \hat{T}_w = \frac{\Delta \tilde{T}_w}{T_o}.$$

It is worth reminding that the conditions (6.2)–(6.5) are valid only at the left and right walls, i.e., at $\hat{x} = \pm 1/2$.

The above-mentioned systems of moment equations for the problem along with the above-mentioned boundary conditions are solved numerically using the finite difference method, for which the (dimensionless) gap between the plates is discretized into 101 equispaced points (or into 100 intervals of equal size) and the method gives solution within less than a couple of seconds for both the interaction potentials. We skip the details of the numerical method here and they can be found in § 7.1 where we shall also study its convergence. Nevertheless, it may be perceived from chapter 7 that for numerical solutions, the moment equations are slightly modified by adding few small terms in some equations so that boundary conditions (6.1) are not needed, although they are automatically implemented with an error which is of the same order as the order of error from the numerical method.

6.1.3 Results

Following [87], we shall compute the dimensionless total heat flux between the plates $\hat{q}_x$, given by,

$$\hat{q}_x = \frac{q_x}{\sqrt{2} n_o k T_o v_o \Delta \hat{T}_w} = \sqrt{\frac{\mu_\alpha x_\alpha^\circ + \mu_\beta x_\beta^\circ}{2}} \left(\frac{x_\alpha^\circ}{\sqrt{\mu_\alpha}} \hat{q}_x^{(\alpha)} + \frac{x_\beta^\circ}{\sqrt{\mu_\beta}} \hat{q}_x^{(\beta)} \right) \frac{1}{\Delta \hat{T}_w} \quad (6.6)$$

for three noble gas mixtures: Ne–Ar, He–Ar and He–Xe through the 2×G13 and 2×G26 equations, both for Maxwell and hard-sphere interaction potentials, and compare the results with those for the same problem in [87] obtained via a direct discretization of the Boltzmann equa-

tions with an implementation of the so-called realistic interaction potential. It should be noted that the total heat flux in (6.6) is scaled with $\sqrt{2}n_o kT_o v_o \Delta\hat{T}_w$ only for comparing the results with [87], albeit later in chapter 8, we shall use the scaling $n_o kT_o v_o$ for non-dimensionlization of the total heat flux. The ideas behind using such a scaling here for the non-dimensionlization of the total heat flux are that the velocity scale in the present thesis is taken as $v_o = \sqrt{kT_o/m}$ while that in [87] is taken as $(\sqrt{2}v_o)$, and the extra factor $\Delta\hat{T}_w$ in the scaling of the total heat flux renders the dimensionless total heat flux independent of $\Delta\hat{T}_w$.

Further, the diffuse scattering boundary conditions considered in [87] correspond to the boundary conditions with accommodation coefficients $\chi_\alpha = \chi_\beta = 1$ derived in the present thesis. It should also be noticed that the rarefaction parameter $\delta = LkT_o n_o / (\sqrt{2}\eta v_o)$ used in [87] relates to the Knudsen number (5.11)₁ by $\text{Kn} = 1/(\sqrt{2}\delta)$, which leads to an expression for the viscosity of a binary gas-mixture

$$\eta = \frac{5}{16\sqrt{\pi}} \frac{\sqrt{kT_o m}}{\left(x_\alpha^\circ \Omega_{\alpha\alpha}^{(2,2)} + x_\beta^\circ \Omega_{\beta\beta}^{(2,2)}\right)}. \quad (6.7)$$

This expression gives reasonable agreement with viscosities of binary gas-mixtures obtained through experimental data at 300 K given in [56]. Nevertheless, a viscosity formula for binary gas-mixtures can also be obtained through a rigorous Chapman–Enskog expansion on the moment equations, see chapter 8.

Once again, the mixtures considered are in order of small-to-large mass differences and the molecular masses of the gases in these mixtures are $m_{\text{He}} = 4.0026$, $m_{\text{Ne}} = 20.1791$, $m_{\text{Ar}} = 39.948$, $m_{\text{Xe}} = 131.293$ in atomic units. However, since only a limited viscosity data from experiments is available in the literature (available only for the mole fractions 0.25, 0.5 and 0.75 in [56]), for the problem under consideration and henceforth wherever required, the ratios of collisional cross sections (5.12) in case of Maxwell molecules are approximated with those in case of hard spheres. In other words, for both Maxwell as well as hard-sphere interaction potentials, we shall use only the values corresponding to hard-sphere interaction potential in table 5.1 for Ω_α and Ω_β .

Figures 6.2 and 6.3 illustrate the variation of the total heat flux with change in mole fraction of the lighter gas in each mixture for $\text{Kn} = 0.0707$ ($\delta = 10$) and $\text{Kn} = 0.7071$ ($\delta = 1$), respectively. The small circles in figures 6.2 and 6.3 denote the data from [87] obtained by a direct discretization of the Boltzmann equations and using the realistic potential. The red, blue and green colors (for small circles as well as for the lines) in each figure correspond to results for Ne–Ar, He–Ar and He–Xe mixtures, respectively. Moreover, in both figures 6.2 and 6.3, the top and bottom rows depict the solutions for Maxwell and hard-sphere interaction potentials, respectively, whereas the left and right columns show the solutions from 2×G13 equations and 2×G26 equations, respectively.

From figures 6.2 and 6.3, the following points are deduced.

- (i) The total heat flux of the mixture increases with increasing rarefaction. All types of Grad’s moment system under consideration for both Maxwell and hard-sphere interaction potentials confirm this. A detailed quantitative comparison of the total heat fluxes, even for high Knudsen numbers, in case of 2×G26 equations with Maxwell molecules can be

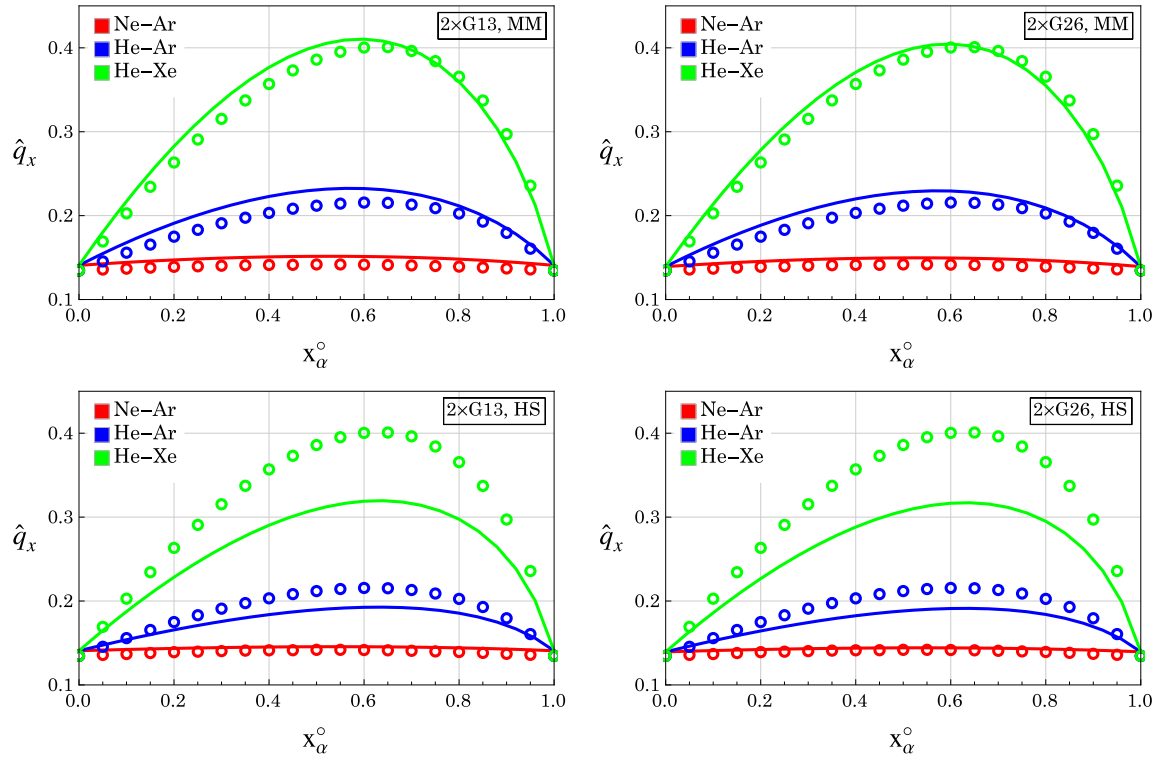


Figure 6.2: Dimensionless total heat flux $\hat{q}_x$ plotted over the mole fraction of the lighter gases x_α^o in the mixtures of Ne–Ar, He–Ar and He–Xe for $\text{Kn} = 0.0707$. The circles denote the data from [87] obtained using realistic potential. The top and bottom rows of the figure depict the solutions for Maxwell and hard-sphere interaction potentials, respectively, whereas the left and right columns show the solutions through $2\times\text{G13}$ equations and $2\times\text{G26}$ equations, respectively.

found in [45]. It should also be noticed that although both the Grad’s moment systems ($2\times\text{G13}$ as well as $2\times\text{G26}$) for Maxwell interaction potential overestimate the actual results in general, the results from them are not very far from those of [87].

- (ii) In general, the results obtained through $2\times\text{G26}$ equations—in comparison with those obtained through $2\times\text{G13}$ equations—are more close to the results of [87].
- (iii) In case of Maxwell interaction potential (top row in each figure), the results are more close to those from [87] when the mixture is less rarefied, i.e., for the smaller Knudsen number ($\text{Kn} = 0.0707$). This means that as rarefaction increases, the results starts deviating more from the actual ones. Consequently, it might be necessary to include more and more moments into the system with increasing rarefaction.
- (iv) On the contrary, the results in case of hard-sphere interaction potential (bottom row in each figure) match very well with those from [87] when the mixture is more rarefied (figure 6.3) whereas when the mixture is less rarefied the results from the moment equations underestimate the actual results significantly, although the qualitative behaviour of the former remains very similar to the latter. It is also clear from the bottom row of figure 6.2 that the significant difference in results from moment equations and those from [87] is for He–Xe mixture, which is case of large mass differences; for small mass differences (Ne–Ar), the two results match quite well when the rarefaction is small ($\text{Kn} = 0.0707$).

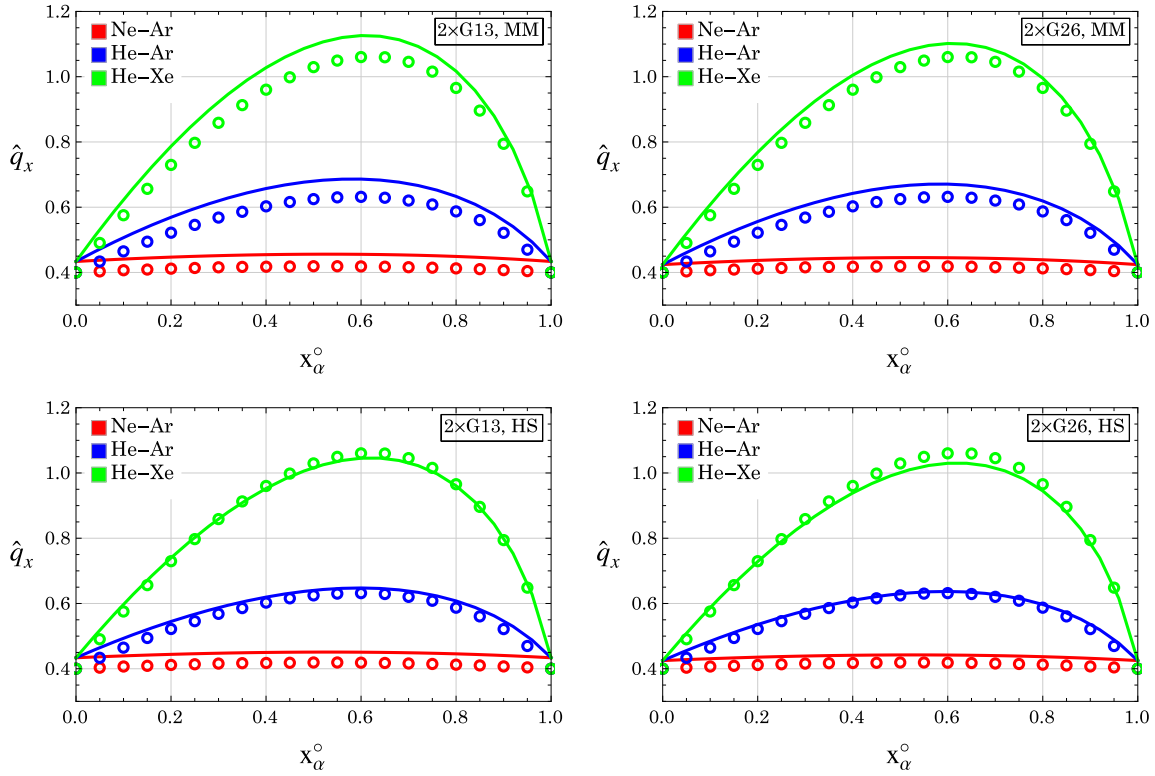


Figure 6.3: Dimensionless total heat flux $\hat{q}_x$ plotted over the mole fraction of the lighter gases x_α^o in the mixtures of Ne–Ar, He–Ar and He–Xe for $\text{Kn} = 0.7071$. The circles denote the data from [87] obtained using realistic potential. The top and bottom rows of the figure depict the solutions for Maxwell and hard-sphere interaction potentials, respectively, whereas the left and right columns show the solutions through $2\times\text{G13}$ equations and $2\times\text{G26}$ equations, respectively.

In other words, for small rarefaction and hard-sphere interaction potential (bottom row of figure 6.2), the deviation in results from the moment equations and the actual results increases with increasing mass differences in the mixture. In fact, the authors of [87] have also pointed out that in the hydrodynamic/slip-flow regime, i.e., when $\text{Kn} \lesssim 0.0707$, the total heat flux computed with hard-sphere interaction potential can deviate up to 15% from that computed with realistic potential whereas in the transition regime, i.e., when $\text{Kn} \gtrsim 0.7071$, the difference in heat flux computed with hard-sphere interaction potential and that computed with realistic potential remains less than 5%.

- (v) Similar to [87], the results from all types of moment equations under consideration also confirm that the maximum heat flux is observed when the mole fraction of the lighter gas in the mixture is around 0.62.

Clearly, the results from the moment systems under consideration agree with those of [87], at least qualitatively, including the results for hard-sphere interaction potential at $\text{Kn} = 0.0707$ (bottom row of figure 6.2). Still, possible reasons for the deviations in the results are the use of an interaction potentials based on Maxwell molecules and hard spheres which influence the form of the productions terms in the moment system, and the use of a simplified expression for the mean free path (5.11)₂ implying the viscosity formula (6.7). It may also be inferred from figures 6.2 and 6.3 as well as from the above discussion that as an alternative to the realistic

potential, the Maxwell interaction potential could be a preferable choice over the hard-sphere interaction potential in the hydrodynamic/slip-flow regime while the hard-sphere interaction potential could be a preferable choice over the Maxwell interaction potential in the transition regime. Thus, the moment equations for gas-mixtures derived in the present thesis provide an enticing and reliable framework as an alternative to the computationally expensive method.

6.2 One-dimensional flow of the infinitely diluted component in a binary gas-mixture

6.2.1 Problem description

We again consider a mixture of two gases α and β —in which the component α is infinitely diluted (i.e., $n_\alpha^\circ \approx 0$)—confined in a one-dimensional channel of length L , and let the temperatures of the left wall (at $x = -L/2$) and that of right wall (at $x = L/2$) of the channel be $T_w^L = T_o + \varepsilon \Delta \tilde{T}_w/2$ and $T_w^R = T_o - \varepsilon \Delta \tilde{T}_w/2$, respectively, see figure 6.4. Thus, the set-up is very similar to the previous problem, however, now the β -component in the mixture behaves like a single gas while the α -component acts as a contaminant. We are interested in studying the flow of the contaminant, i.e., of the α -constituent, in the background of the β -component. The problem is interesting because firstly it possesses the analytical solution—thanks to the decoupling of equations for the β -constituent from those for the α -constituent, secondly the flow of the infinitely diluted (α)-component may not be traced by particle based methods, such as DSMC method, due to insufficient number of particles, and thirdly it can be taken as motivation to set up experiments where one would like to collect the contaminant.

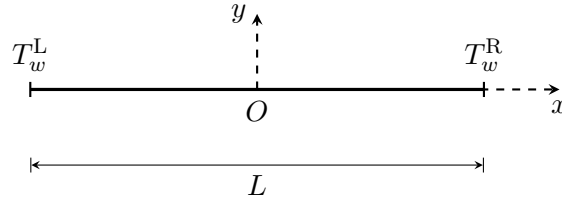


Figure 6.4: Schematic of a one-dimensional channel with the walls having different temperatures; y -axis is included just for illustration purposes.

6.2.2 Method of solution

We are interested in solving the problem analytically. To this end, the systems of linear-dimensionless $2 \times G13$ and $2 \times G26$ equations in 1D are obtained by substituting $d(\cdot)/d\hat{t} = 0$, $\hat{v}_x = 0$, $x_\alpha^\circ = 0$ and $x_\beta^\circ = 1$ in the moment equations detailed in § 5.1.2; moreover, for the problem under consideration, the velocity scale v_o becomes $v_o = \sqrt{kT_o/m_\beta}$, $\Omega = \Omega_\beta$, and the Knudsen number Kn becomes the Knudsen number for the single gas β (cf. (5.11)). The required boundary conditions are exactly same as those in § 6.1.2, and the momentum balance equation of the mixture for the problem under consideration is exactly same as the balance equation for diffusion velocity of the β -constituent. Moreover, for the problem under consideration, both the

2×G13 and 2×G26 systems simplify a lot; the equations for the α -constituent in 2×G26 system read

$$\frac{d\hat{u}_x^{(\alpha)}}{d\hat{x}} = 0, \quad (6.8)$$

$$\frac{d\hat{\sigma}_{xx}^{(\alpha)}}{d\hat{x}} + \frac{d\hat{T}_\alpha}{d\hat{x}} + \frac{d\hat{n}_\alpha}{d\hat{x}} = -\frac{1}{\text{Kn}\Omega_\beta} \left(\delta_2 \hat{q}_x^{(\alpha)} - \delta_4 \hat{q}_x^{(\beta)} \right), \quad (6.9)$$

$$\frac{d\hat{q}_x^{(\alpha)}}{d\hat{x}} = -\frac{1}{\text{Kn}\Omega_\beta} \left[\delta_5 (\hat{T}_\alpha - \hat{T}_\beta) + \delta_6 \hat{\Delta}_\alpha - \delta_7 \hat{\Delta}_\beta \right], \quad (6.10)$$

$$\frac{d\hat{m}_{xxx}^{(\alpha)}}{d\hat{x}} + \frac{8}{15} \frac{d\hat{q}_x^{(\alpha)}}{d\hat{x}} = -\frac{1}{\text{Kn}\Omega_\beta} \left(\delta_9 \hat{\sigma}_{xx}^{(\alpha)} + \delta_{10} \hat{R}_{xx}^{(\alpha)} - \delta_{11} \hat{\sigma}_{xx}^{(\beta)} - \delta_{12} \hat{R}_{xx}^{(\beta)} \right), \quad (6.11)$$

$$\frac{1}{2} \frac{d\hat{R}_{xx}^{(\alpha)}}{d\hat{x}} + \frac{7}{2} \frac{d\hat{\sigma}_{xx}^{(\alpha)}}{d\hat{x}} + \frac{1}{6} \frac{d\hat{\Delta}_\alpha}{d\hat{x}} + 5 \frac{d\hat{T}_\alpha}{d\hat{x}} + \frac{5}{2} \frac{d\hat{n}_\alpha}{d\hat{x}} = -\frac{1}{\text{Kn}\Omega_\beta} \left(\delta_{13} \hat{q}_x^{(\alpha)} - \delta_{15} \hat{q}_x^{(\beta)} \right), \quad (6.12)$$

$$\frac{9}{35} \frac{d\hat{R}_{xx}^{(\alpha)}}{d\hat{x}} + \frac{9}{5} \frac{d\hat{\sigma}_{xx}^{(\alpha)}}{d\hat{x}} = -\frac{1}{\text{Kn}\Omega_\beta} \left(\delta_{17} \hat{m}_{xxx}^{(\alpha)} - \delta_{18} \hat{m}_{xxx}^{(\beta)} \right), \quad (6.13)$$

$$2 \frac{d\hat{m}_{xxx}^{(\alpha)}}{d\hat{x}} + \frac{56}{15} \frac{d\hat{q}_x^{(\alpha)}}{d\hat{x}} = -\frac{1}{\text{Kn}\Omega_\beta} \left(\delta_{21} \hat{R}_{xx}^{(\alpha)} + \delta_{22} \hat{\sigma}_{xx}^{(\alpha)} - \delta_{23} \hat{R}_{xx}^{(\beta)} - \delta_{24} \hat{\sigma}_{xx}^{(\beta)} \right), \quad (6.14)$$

$$8 \frac{d\hat{q}_x^{(\alpha)}}{d\hat{x}} = -\frac{1}{\text{Kn}\Omega_\beta} \left[\delta_{25} \hat{\Delta}_\alpha - \delta_{26} \hat{\Delta}_\beta + \delta_{27} (\hat{T}_\alpha - \hat{T}_\beta) \right]. \quad (6.15)$$

and the equations for the β -constituent in 2×G26 system read

$$\frac{d\hat{u}_x^{(\beta)}}{d\hat{x}} = 0, \quad (6.16)$$

$$\frac{d\hat{\sigma}_{xx}^{(\beta)}}{d\hat{x}} + \frac{d\hat{T}_\beta}{d\hat{x}} + \frac{d\hat{n}_\beta}{d\hat{x}} = 0, \quad (6.17)$$

$$\frac{d\hat{q}_x^{(\beta)}}{d\hat{x}} = 0, \quad (6.18)$$

$$\frac{d\hat{m}_{xxx}^{(\beta)}}{d\hat{x}} + \frac{8}{15} \frac{d\hat{q}_x^{(\beta)}}{d\hat{x}} = -\frac{1}{\text{Kn}} \left(\hat{\sigma}_{xx}^{(\beta)} + \delta_8 \hat{R}_{xx}^{(\beta)} \right), \quad (6.19)$$

$$\frac{1}{2} \frac{d\hat{R}_{xx}^{(\beta)}}{d\hat{x}} + \frac{7}{2} \frac{d\hat{\sigma}_{xx}^{(\beta)}}{d\hat{x}} + \frac{1}{6} \frac{d\hat{\Delta}_\beta}{d\hat{x}} + 5 \frac{d\hat{T}_\beta}{d\hat{x}} + \frac{5}{2} \frac{d\hat{n}_\beta}{d\hat{x}} = -\frac{2}{3} \frac{1}{\text{Kn}} \hat{q}_x^{(\beta)}, \quad (6.20)$$

$$\frac{9}{35} \frac{d\hat{R}_{xx}^{(\beta)}}{d\hat{x}} + \frac{9}{5} \frac{d\hat{\sigma}_{xx}^{(\beta)}}{d\hat{x}} = -\frac{3}{2} \frac{1}{\text{Kn}} \hat{m}_{xxx}^{(\beta)}, \quad (6.21)$$

$$2 \frac{d\hat{m}_{xxx}^{(\beta)}}{d\hat{x}} + \frac{56}{15} \frac{d\hat{q}_x^{(\beta)}}{d\hat{x}} = -\frac{1}{\text{Kn}} \left(\delta_{19} \hat{R}_{xx}^{(\beta)} + \delta_{20} \hat{\sigma}_{xx}^{(\beta)} \right), \quad (6.22)$$

$$8 \frac{d\hat{q}_x^{(\beta)}}{d\hat{x}} = -\frac{2}{3} \frac{1}{\text{Kn}} \hat{\Delta}_\beta. \quad (6.23)$$

While writing (6.8)–(6.23), we have also used the results $\hat{u}_x^{(\alpha)} = \hat{u}_x^{(\beta)} = 0$, which follow from (6.8) and (6.16) on using boundary conditions (6.2), in order to simplify other equations. It should also be noted that (6.16)–(6.23) are the one-dimensional linear-dimensionless G26 equations in steady and rest state for a single gas, where the mass balance equation (6.16) is identically satisfied. Again, $2 \times \text{G13}$ equations for the present problem are (6.8)–(6.12) and (6.16)–(6.20) upon setting $\hat{m}_{xxx}^{(\alpha)}$, $\hat{R}_{xx}^{(\alpha)}$, $\hat{\Delta}_\alpha$, $\hat{m}_{xxx}^{(\beta)}$, $\hat{R}_{xx}^{(\beta)}$ and $\hat{\Delta}_\beta$ to zero.

6.2.2.1 Analytical solution

The equations for the β -constituent (eqs. (6.16)–(6.23)) are decoupled from those for the α -constituent. Therefore, one can easily solve them to obtain the solution for the background (the β -constituent):

$$\hat{n}_\beta = \mathbf{c}_1 - \hat{T}_\beta, \quad \hat{u}_x^{(\beta)} = 0, \quad \hat{T}_\beta = -\frac{4}{15} \frac{1}{\text{Kn}} \mathbf{c}_2 x + \mathbf{c}_3, \quad \hat{\sigma}_{xx}^{(\beta)} = 0, \quad \hat{q}_x^{(\beta)} = \mathbf{c}_2 \quad (6.24)$$

in case of $2 \times \text{G13}$ equations, and

$$\left. \begin{aligned} \hat{n}_\beta &= \mathbf{c}_4 - \hat{T}_\beta - \hat{\sigma}_{xx}^{(\beta)}, \quad \hat{u}_x^{(\beta)} = 0, \quad \hat{T}_\beta = -\frac{4}{15} \frac{1}{\text{Kn}} \mathbf{c}_5 x + \mathbf{c}_6 - \frac{(2+a)}{5} \hat{\sigma}_{xx}^{(\beta)}, \\ \hat{\sigma}_{xx}^{(\beta)} &= \mathbf{c}_7 e^{\frac{1}{\text{Kn}} b x} + \mathbf{c}_8 e^{-\frac{1}{\text{Kn}} b x}, \quad \hat{q}_x^{(\beta)} = \mathbf{c}_5, \quad \hat{m}_{xxx}^{(\beta)} = \frac{1}{b} \left(\mathbf{c}_7 e^{\frac{1}{\text{Kn}} b x} - \mathbf{c}_8 e^{-\frac{1}{\text{Kn}} b x} \right), \\ \hat{R}_{xx}^{(\beta)} &= a \hat{\sigma}_{xx}^{(\beta)}, \quad \hat{\Delta}_\beta = 0 \end{aligned} \right\} \quad (6.25)$$

in case of $2 \times \text{G26}$ equations. The constants a and b are given by

$$a = \frac{2 - \gamma_{20}}{\gamma_{19} - 2\gamma_8}, \quad b = \sqrt{\frac{35}{6} \left(\frac{\gamma_{19} - \gamma_8 \gamma_{20}}{2 - 14\gamma_8 + 7\gamma_{19} - \gamma_{20}} \right)}; \quad (6.26)$$

the integration constants $\mathbf{c}_1, \mathbf{c}_2$ and $\mathbf{c}_3$ —which follow from boundary conditions (6.1)₂ and (6.3) at both the walls for the β -constituent—turn out to be

$$\mathbf{c}_1 = \mathbf{c}_3 = 0 \quad \text{and} \quad \mathbf{c}_2 = \frac{\left(\frac{\chi_\beta}{2 - \chi_\beta} \right) \sqrt{\frac{2}{\pi}} \Delta \hat{T}_w}{1 + \frac{4}{15} \frac{1}{\text{Kn}} \left(\frac{\chi_\beta}{2 - \chi_\beta} \right) \sqrt{\frac{2}{\pi}}}; \quad (6.27)$$

and the integration constants $\mathbf{c}_4, \mathbf{c}_5, \dots, \mathbf{c}_8$ follow from boundary conditions (6.1)₂ and (6.4), (6.5) at both the walls for the β -constituent, however, except $\mathbf{c}_6$ which is zero, the values of other integration constants are too cumbersome to write here.

The above solutions for the β -constituent are inserted into the respective systems of equations for the α -constituent (eqs. (6.9)–(6.12) upon setting $\hat{m}_{xxx}^{(\alpha)}, \hat{R}_{xx}^{(\alpha)}, \hat{\Delta}_\alpha, \hat{m}_{xxx}^{(\beta)}, \hat{R}_{xx}^{(\beta)}$ and $\hat{\Delta}_\beta$ to zero in case of 2×G13 equations, and eqs. (6.9)–(6.15) in case of 2×G26 equations; notice that (6.8) is omitted here while considering the system of equations for the α -constituent because (6.8) along with boundary condition (6.2) merely implies that $\hat{u}_x^{(\alpha)} = 0$), which now turn into inhomogeneous systems of first order ordinary differential equations of the form $\tilde{A} \frac{d\tilde{U}}{dx} = \tilde{B}\tilde{U} + \tilde{g}(\hat{x})$ with $\tilde{A}$ and $\tilde{B}$ being constant matrices, $\tilde{g}(\hat{x})$ being the vector containing solutions from the β -system, and $\tilde{U}$ being the vector containing unknowns— $\tilde{U} = \{\hat{n}_\alpha, \hat{T}_\alpha, \hat{\sigma}_{xx}^{(\alpha)}, \hat{q}_x^{(\alpha)}\}^\top$ in case of 2×G13 equations while $\tilde{U} = \{\hat{n}_\alpha, \hat{T}_\alpha, \hat{\sigma}_{xx}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{m}_{xxx}^{(\alpha)}, \hat{R}_{xx}^{(\alpha)}, \hat{\Delta}_\alpha\}^\top$ in case of 2×G26 equations. Nevertheless, for both 2×G13 and 2×G26 cases, the matrix $\tilde{A}$ is not invertible since the dimension of null space of $\tilde{A}$ is non-zero (1 in case of 2×G13 equations and 2 in case of 2×G26 equations). The null space of matrix $(\tilde{A})^\top$ is now used to express some of the unknowns in terms of others. The null space of $(\tilde{A})^\top$ is $\{0, -\frac{8}{15}, 1, 0\}^\top$ in case of 2×G13 equations and $\{0, -8, 0, 0, 0, 0, 1\}^\top, \{0, -\frac{8}{3}, -2, 0, 0, 1, 0\}^\top$ in case of 2×G26 equations, which leads to

$$\hat{\sigma}_{xx}^{(\alpha)} = \frac{8}{15} \frac{\delta_5}{\delta_9} (\hat{T}_\alpha - \hat{T}_\beta) + \frac{\delta_{11}}{\delta_9} \hat{\sigma}_{xx}^{(\beta)} \quad (6.28)$$

in case of 2×G13 equations, and

$$\left. \begin{aligned} \hat{\Delta}_\alpha &= \left(\frac{\delta_{27} - 8\delta_5}{8\delta_6 - \delta_{25}} \right) (\hat{T}_\alpha - \hat{T}_\beta), \\ \hat{R}_{xx}^{(\alpha)} &= \frac{1}{(\delta_{21} - 2\delta_{10})} \left[\frac{8}{3} \left(\frac{\delta_6 \delta_{27} - \delta_5 \delta_{25}}{8\delta_6 - \delta_{25}} \right) (\hat{T}_\alpha - \hat{T}_\beta) \right. \\ &\quad \left. + (2\delta_9 - \delta_{22}) \hat{\sigma}_{xx}^{(\alpha)} + \{(\delta_{24} - 2\delta_{11}) + a(\delta_{23} - 2\delta_{12})\} \hat{\sigma}_{xx}^{(\beta)} \right] \end{aligned} \right\} \quad (6.29)$$

in case of 2×G26 equations. Therefore, equation (6.11) in case of 2×G13 equations and equations (6.14) and (6.15) in case of 2×G26 equations are omitted from the respective systems of equations for the α -constituent, and solution (6.28) in case of 2×G13 equations and solution (6.29) in case of 2×G26 equations is substituted into the remaining equations for α -constituent. In this way, the remaining equations for the α -constituent again turn into inhomogeneous systems of first order ordinary differential equations of the form $A \frac{d\bar{U}}{dx} = B\bar{U} + \mathbf{g}(\hat{x})$ with A and B being constant matrices, $\mathbf{g}(\hat{x})$ being the vector containing solutions from the β -system, and $\bar{U}$ being the vector containing unknowns— $\bar{U} = \{\hat{n}_\alpha, \hat{T}_\alpha, \hat{q}_x^{(\alpha)}\}^\top$ in case of 2×G13 equations while $\bar{U} = \{\hat{n}_\alpha, \hat{T}_\alpha, \hat{\sigma}_{xx}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{m}_{xxx}^{(\alpha)}\}^\top$ in case of 2×G26 equations, but the matrix A is invertible this time for both the cases of 2×G13 and 2×G26 equations as well as for both Maxwell and hard-sphere interaction potentials.

The general solution of system $A \frac{d\bar{U}}{dx} = B\bar{U} + \mathbf{g}(\hat{x})$ is the solution of corresponding homogeneous problem, $A \frac{d\bar{U}}{dx} = B\bar{U}$, plus a particular solution of $A \frac{d\bar{U}}{dx} = B\bar{U} + \mathbf{g}(\hat{x})$. The solution of homogeneous problem, $A \frac{d\bar{U}}{dx} = B\bar{U}$, is obtained by computing the eigenvalues and eigenvectors of the matrix $A^{-1}B$ and a particular solution of $A \frac{d\bar{U}}{dx} = B\bar{U} + \mathbf{g}(\hat{x})$ can be computed by the

variation of parameters method. In the final solution of $A \frac{d\bar{U}}{dx} = B\bar{U} + \mathbf{g}(\hat{x})$, the integration constants—three in cases of 2×G13 equations and five in case of 2×G26 equations—are computed using remaining three boundary conditions (6.1)₁ and (6.3) at both the walls in case of 2×G13 equations and remaining five boundary conditions (6.1)₁, (6.4) and (6.5) at both the walls in case of 2×G26 equations.

6.2.2.2 First order Chapman–Enskog solution

In order to perform a comparative study of the analytical solution obtained via moment equations with standard hydrodynamic laws, we perform a Chapman–Enskog (CE) like expansion on the moment equations. To first order, the expansion leads to Fick, Navier–Stokes and Fourier laws, see chapter 8 for more details, and we shall refer to these solutions as first order CE solution. We expand the non-conserved quantities (Ψ) in a given moment system in powers of the Knudsen number (Kn) as

$$\Psi = \Psi_{|0} + \text{Kn} \Psi_{|1} + \text{Kn}^2 \Psi_{|2} + \dots,$$

where, for the moment systems of § 6.2.2,

$$\Psi \in \{\hat{u}_x^{(\alpha)}, \hat{T}_\alpha - \hat{T}_\beta, \hat{\sigma}_{xx}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{\sigma}_{xx}^{(\beta)}, \hat{q}_x^{(\beta)}\}$$

in case of 2×G13 equations while

$$\Psi \in \{\hat{u}_x^{(\alpha)}, \hat{T}_\alpha - \hat{T}_\beta, \hat{\sigma}_{xx}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{m}_{xxx}^{(\alpha)}, \hat{R}_{xx}^{(\alpha)}, \hat{\Delta}_\alpha, \hat{\sigma}_{xx}^{(\beta)}, \hat{q}_x^{(\beta)}, \hat{m}_{xxx}^{(\beta)}, \hat{R}_{xx}^{(\beta)}, \hat{\Delta}_\beta\}$$

in case of 2×G26 equations, and the quantities $\Psi_{|0}, \Psi_{|1}, \Psi_{|2}, \dots$ are of order $\mathcal{O}(\text{Kn}^0)$. Notice that we have not included $\hat{u}_x^{(\beta)}$ in the list of non-conserved quantities, since we have already concluded that it vanishes for the problem under consideration (the gas β behaves like a single gas). The value of quantity Ψ truncated to Kn^1 , i.e., $\Psi = \Psi_{|0} + \text{Kn} \Psi_{|1}$ is the first order solution for Ψ , which we are interested in.

We insert these expansions into the balance equations (in different moment systems) of non-conserved quantities and compute $\Psi_{|0}$ and $\Psi_{|1}$ for all the quantities by comparing the coefficients of Kn^{-1} and Kn^0 on both sides of the equations, respectively. It readily follows that $\Psi_{|0} = 0$ for all the non-conserved quantities. The quantities $\Psi_{|1}$ along with the remaining equations in their respective moment systems and boundary conditions yield the first order CE solution:

$$\left. \begin{aligned} \hat{n}_\alpha(\hat{x}) &= \left[1 - \frac{5}{2} \left(\frac{\delta_2 + \frac{3}{2} \frac{(\delta_{15}\delta_2 - \delta_{13}\delta_4)}{\Omega_\beta}}{\delta_{13} - \frac{5}{2}\delta_2} \right) \right] \Delta \hat{T}_w \hat{x}, & \hat{n}_\beta(\hat{x}) &= \Delta \hat{T}_w \hat{x}, \\ \hat{u}_x^{(\alpha)}(\hat{x}) = \hat{u}_x^{(\beta)}(\hat{x}) &= 0, & \hat{T}_\alpha(\hat{x}) = \hat{T}_\beta(\hat{x}) &= -\Delta \hat{T}_w \hat{x}, & \hat{\sigma}_{xx}^{(\alpha)}(\hat{x}) = \hat{\sigma}_{xx}^{(\beta)}(\hat{x}) &= 0, \\ \hat{q}_x^{(\alpha)}(\hat{x}) &= \frac{5}{2} \text{Kn} \left[\frac{\Omega_\beta + \frac{3}{2} (\delta_{15} - \frac{5}{2}\delta_4)}{\delta_{13} - \frac{5}{2}\delta_2} \right] \Delta \hat{T}_w, & \hat{q}_x^{(\beta)}(\hat{x}) &= \frac{15}{4} \text{Kn} \Delta \hat{T}_w \end{aligned} \right\} \quad (6.30)$$

for both the 2×G13 and 2×G26 systems and, additionally, for 2×G26 system, $\hat{m}_{xxx}^{(\alpha)}(\hat{x}) = \hat{m}_{xxx}^{(\beta)}(\hat{x}) = \hat{R}_{xx}^{(\alpha)}(\hat{x}) = \hat{R}_{xx}^{(\beta)}(\hat{x}) = \hat{\Delta}_\alpha(\hat{x}) = \hat{\Delta}_\beta(\hat{x}) = 0$. It can also be noted that for Maxwell

interaction potential, the number densities of both the constituents from first order CE solution are equal and are negative of their temperatures, i.e., $\hat{n}_\alpha = \hat{n}_\beta = -\hat{T}_\alpha = -\hat{T}_\beta = \Delta\hat{T}_w \hat{x}$, since $\delta_2 = \delta_4 = 0$ and $\delta_{13} \neq 0$ for Maxwell interaction potential.

6.2.3 Results

We again consider the three binary mixtures of noble gases: Ne–Ar, He–Ar and He–Xe as our examples. However, as the general behaviours of the macroscopic quantities are somewhat similar in all the mixtures, here, we present the results only for Ne–Ar mixture with Ne being the infinitely diluted component, and Ne–Ar mixture with Ar being the infinitely diluted component and the similar results for He–Ar and He–Xe mixture are presented in appendix A. Furthermore, even though the amount of the infinitely diluted component in a mixture is so small that its own temperature, normal stress and heat flux do not influence the properties of the mixture significantly, yet we shall also discuss the temperature, normal stress and heat flux of the diluted component in addition to its number density.

Figures 6.5–6.8 illustrate the variations of the number density, temperature, normal stress and heat flux, respectively, of the infinitely diluted component in the Ne–Ar mixture with Ne being the diluted component in the right half of the channel. The results are shown only in the right half of the channel owing to the symmetry of the problem. The values of other parameters for figures 6.5–6.8 are $\Delta\hat{T}_w = 0.5$, $\chi_\alpha = 1$ and $\chi_\beta = 0.1$. In all figures 6.5–6.8, the top and bottom rows show the plots for the $2\times G13$ and $2\times G26$ equations, respectively, whereas the left and right columns depict them for Maxwell and hard-sphere interaction potentials, respectively. Furthermore, in each figure, the continuous and dashed lines denote the analytical and first order CE solutions, respectively. As can be seen from (6.30) that except the heat fluxes of the constituents, no other quantity depends on the Knudsen number in first order CE solution, therefore all the dashed lines (for different Knudsen numbers) in figures 6.5–6.7 are overlapped. In general, the results for Maxwell and hard-sphere interaction potentials are qualitatively similar for both the $2\times G13$ and $2\times G26$ systems for any physical quantity (compare the plots in the left and right columns of each figure). However, the first order CE solutions are not even close to the analytical solutions for any case.

Number density: Figure 6.5 displays the variation of the number density of the infinitely diluted component (Ne) in the right half of the channel. All the plots in the figure elucidate that the molecules of the infinitely diluted gas tend to stay near the colder side of the channel. Nevertheless, the quantitative values of the number densities from the $2\times G13$ systems are much bigger than those from the $2\times G26$ systems for both Maxwell and hard-sphere interaction potentials (compare the plots in the top and bottom rows). Moreover, the quantitative values of the number densities for Maxwell interaction potential are also higher than those for hard-sphere interaction potential. The values of number densities from any moment system under consideration are much smaller than those from first order CE solution, which do not even depend on the Knudsen number. When increasing the Knudsen number, the number density increases until its profile becomes almost a straight line and then it starts decreasing with increasing Knudsen number. Indeed, this happens due to the Knudsen layers which are present for all the quantities but visible near the walls only for small Knudsen numbers (red and blue curves) because

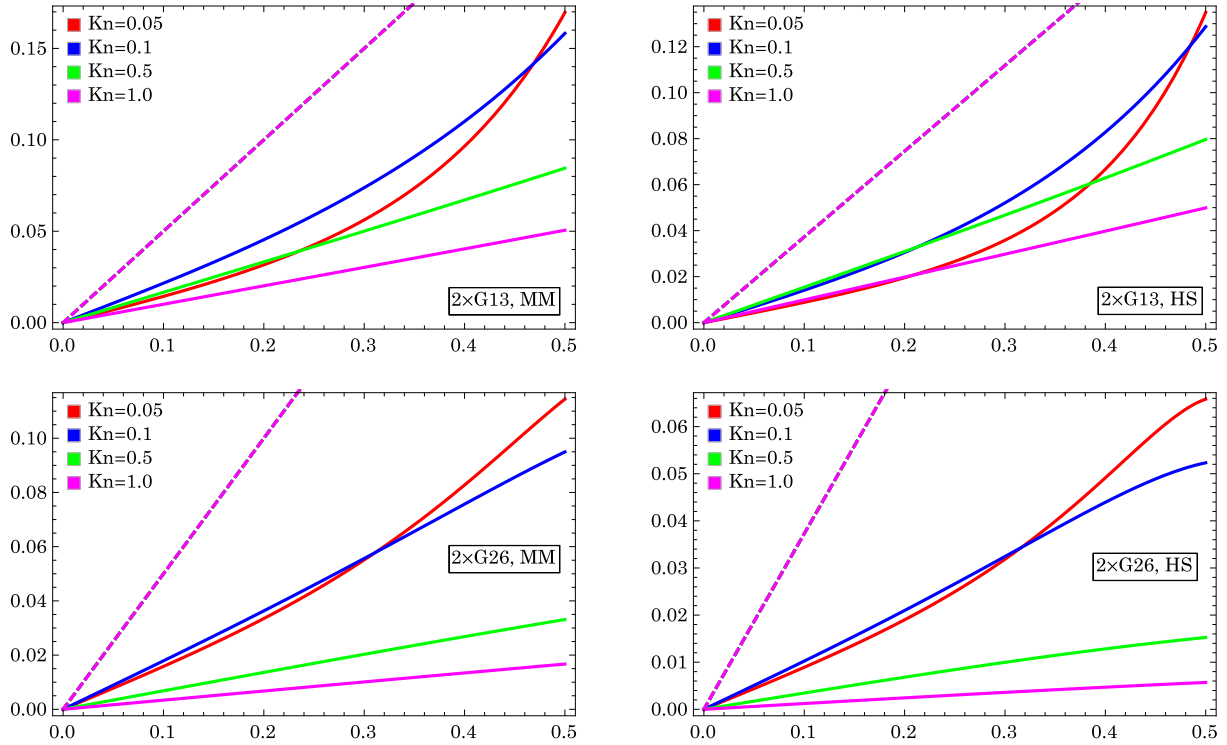


Figure 6.5: Number density of the infinitely diluted (lighter) component in Ne–Ar mixture, $\hat{n}_{\text{Ne}}(\hat{x})$, plotted in right half of the channel for different Knudsen numbers and for different moment systems. The top and bottom rows show the plots for the $2\times\text{G13}$ and $2\times\text{G26}$ equations, respectively, while the left and right columns depict the plots for Maxwell and hard-sphere interaction potentials, respectively. The continuous and dashed lines (overlapped here) denote the analytical and first order CE solutions, respectively. The values of other parameters are $\Delta\hat{T}_w = 0.5$, $\chi_\alpha = 1$ and $\chi_\beta = 0.1$.

they starts covering more and more region of the channel with increasing Knudsen number. The Knudsen layers are relatively more visible when the heavier component in the mixture is infinitely diluted (see figures corresponding to mixtures with heavier component being infinitely diluted in appendix A). For the mixtures with high mass differences and lighter component being diluted, the number density profile is almost a straight line already at $\text{Kn} = 0.05$, and therefore it continuously decreases with increasing Knudsen number (compare figures 6.5, A.5 and A.13).

Temperature: Figure 6.6 exhibits the variation of the temperature of the infinitely diluted component (Ne) in the right half of the channel. The quantitative values of the temperature for a given Knudsen number are approximately same for all types of moment systems under consideration. Nevertheless, its values from the $2\times\text{G13}$ systems are slightly higher than those from the corresponding $2\times\text{G26}$ systems. In contrast to number density, the temperature slightly decreases until its profile becomes almost a straight line and then it starts increasing with increasing Knudsen number. The values of temperatures from any moment system under consideration are much higher than those from the first order CE solution, which also do not depend on the Knudsen number. For the mixtures with high mass differences and lighter component being diluted, the temperature profile too is almost a straight line already at $\text{Kn} = 0.05$, and therefore it continuously increases with increasing Knudsen number (compare figures 6.6, A.6 and A.14). Apparently, the temperature profiles are opposite of the corresponding number density profiles,

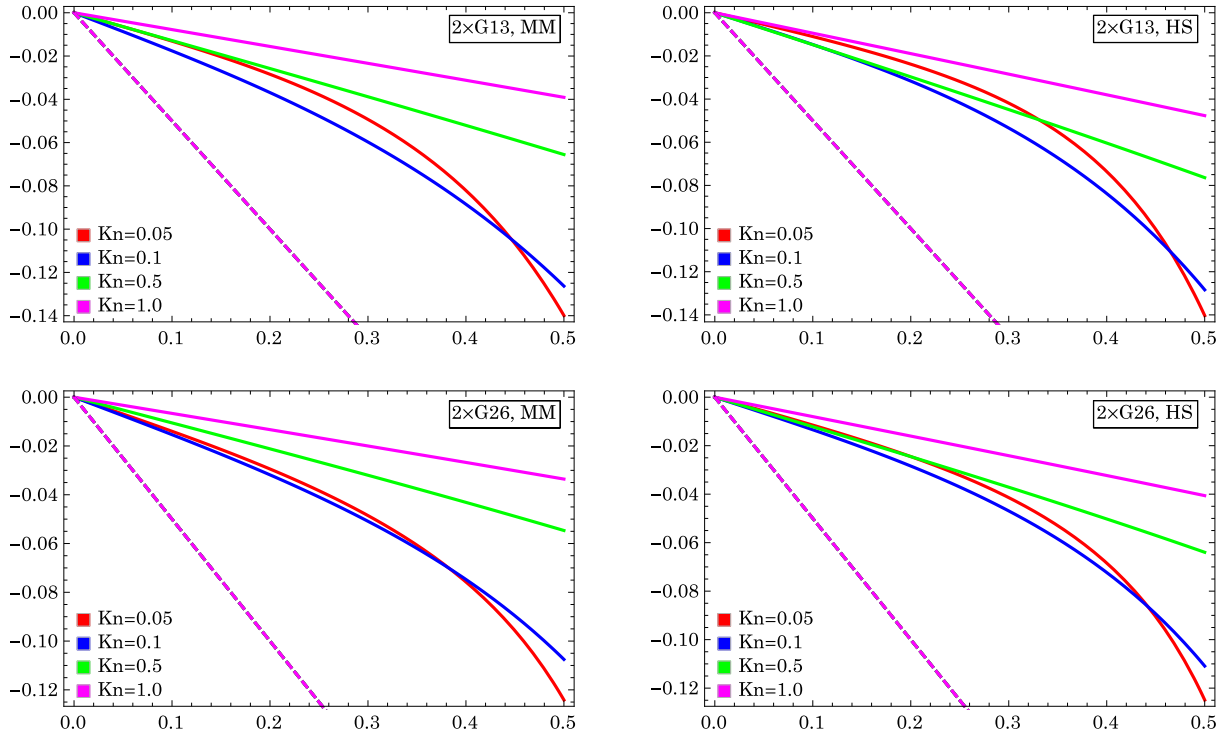


Figure 6.6: Temperature of the infinitely diluted (lighter) component in Ne–Ar mixture, $\hat{T}_{\text{Ne}}(\hat{x})$, plotted in right half of the channel for different Knudsen numbers and for different moment systems. The top and bottom rows show the plots for the $2\times\text{G13}$ and $2\times\text{G26}$ equations, respectively, while the left and right columns depict the plots for Maxwell and hard-sphere interaction potentials, respectively. The continuous and dashed lines (overlapped here) denote the analytical and first order CE solutions, respectively. The values of other parameters are same as those in figure 6.5.

at least qualitatively, in general.

Normal stress: Figure 6.7 illustrates the variation of the normal stress of the infinitely diluted component (Ne) in the right half of the channel. First of all, from all the plots in the figure, it can be deduced that all the moment systems yield the non-zero normal stresses (of the diluted component)—although they are small—for all Knudsen numbers in contrast to the first order CE solution which always produces zero normal stress. Interestingly, on one hand, the normal stresses are qualitatively similar for Maxwell and hard-sphere interaction potentials (compare the plots on the left and right columns); on the other hand, the normal stresses obtained with the $2\times\text{G13}$ systems are quite different from those obtained with the $2\times\text{G26}$ systems (compare the plots on the top and bottom rows). The $2\times\text{G26}$ systems (bottom row) depict both positive and negative values for the normal stresses whereas the $2\times\text{G13}$ systems (top row) delineate only the negative values for the same; in particular, for large Knudsen numbers (green and pink curves), the $2\times\text{G13}$ systems yield negative normal stresses while $2\times\text{G26}$ systems yield positive normal stresses. This is due to the coupling of the balance equation for stress with the higher order moments in the $2\times\text{G26}$ systems, which apparently induces the secondary Knudsen layers. The Knudsen layers can be better understood from the figures corresponding to normal stress of the diluted component in the mixtures with heavier components being diluted (figures A.3, A.11 and A.19). For small Knudsen number (red curves in these figures), the stress from $2\times\text{G13}$

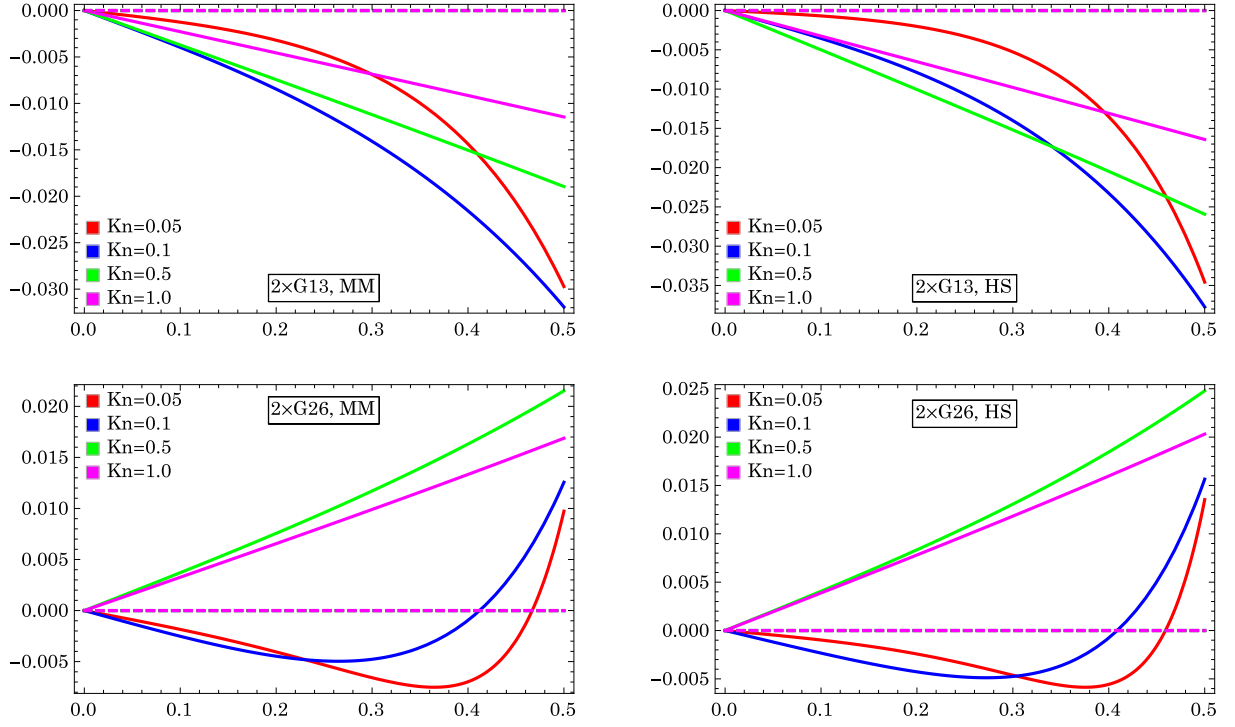


Figure 6.7: Normal stress of the infinitely diluted (lighter) component in Ne–Ar mixture, $\hat{\sigma}_{xx}^{(\text{Ne})}(\hat{x})$, plotted in right half of the channel for different Knudsen numbers and for different moment systems. The top and bottom rows show the plots for the $2\times\text{G13}$ and $2\times\text{G26}$ equations, respectively, while the left and right columns depict the plots for Maxwell and hard-sphere interaction potentials, respectively. The continuous and dashed lines (overlapped here) denote the analytical and first order CE solutions, respectively. The values of other parameters are same as those in figure 6.5.

system is almost zero in the middle of the channel and decreases when moving towards the right wall; however, the stress from $2\times\text{G26}$ system is also almost zero in the middle of the channel, nevertheless, while moving towards the right wall, it first decreases but starts increasing afterwards due to secondary Knudsen layer. The normal stresses of the diluted components in He–Ar and He–Xe mixtures with lighter (or heavier) component being diluted are qualitatively similar to that in Ne–Ar mixtures with Ne (or Ar) being diluted (compare figures 6.7, A.7 and A.15, and figures A.3, A.11 and A.19). Nevertheless, for all the moment systems, the absolute value of the normal stress of the diluted component decreases with increasing mass ratio when the lighter component in each mixture is diluted whereas the same is not true when the heavier component in each mixture is diluted.

Heat flux: Figure 6.8 shows the variation of the heat flux of the infinitely diluted component (Ne) in the right half of the channel. From (6.30), the heat flux from the first order CE solution is constant but depends on the Knudsen number. The values of heat flux from the first order CE solution for Knudsen numbers 0.5 and 1 are 1.16 and 2.32 in case of Maxwell interaction potential while 1.017 and 2.034 in case of hard-sphere interaction potential, and therefore they do not appear in the plots. The plot ranges are shown in this way for clarity. For a given Knudsen number, the value of heat flux from any moment system is much smaller than that from the first order CE solution. In contrast to heat flux from the first order CE solution, the heat flux

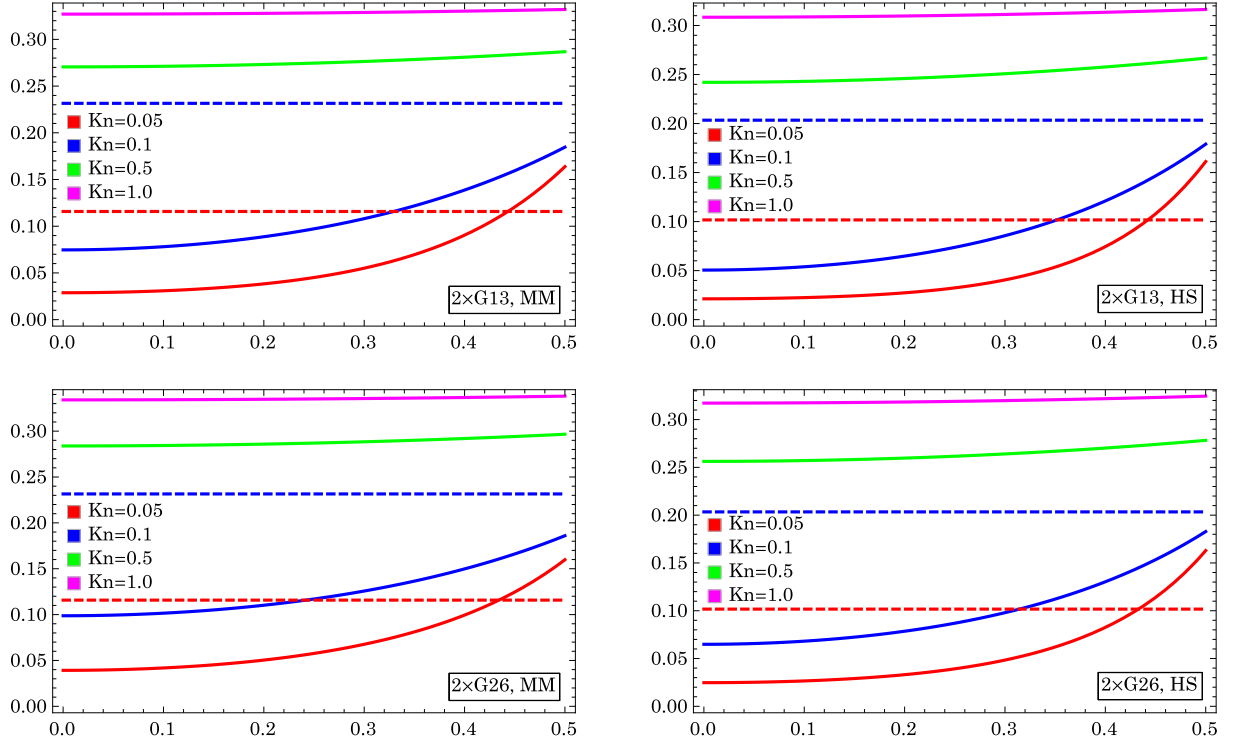


Figure 6.8: Heat flux of the infinitely diluted (lighter) component in Ne–Ar mixture, $\hat{q}_x^{(\text{Ne})}(\hat{x})$, plotted in right half of the channel for different Knudsen numbers and for different moment systems. The top and bottom rows show the plots for the $2\times\text{G13}$ and $2\times\text{G26}$ equations, respectively, while the left and right columns depict the plots for Maxwell and hard-sphere interaction potentials, respectively. The continuous and dashed lines denote the analytical and first order CE solutions, respectively. The values of other parameters are same as those in figure 6.5. The green and pink dashed lines lie outside the range of plots.

from any moment system has a non-constant profile for all Knudsen numbers (when zoomed in for high Knudsen number). It may be argued that the heat flux from any moment system under consideration is also constant in the bulk of channel but not near the walls, where it is non-constant due to Knudsen layers. Similar to the first order CE solution, the heat flux from any moment system also increases with increasing Knudsen number. Again, the values of heat flux from the moment systems with Maxwell interaction potential are slightly higher than those from the corresponding moment systems with hard-sphere interaction potential (compare the plots on the left and right columns). Similarly, for both Maxwell and hard-sphere interaction potentials, the heat flux from the $2\times\text{G26}$ system is slightly higher than that from the corresponding $2\times\text{G13}$ system (compare the plots on the top and bottom rows). The heat flux profiles for He–Ar and He–Xe mixtures are qualitatively (as well as quantitatively to some extent) similar to those for Ne–Ar mixture (compare figures 6.8, A.8 and A.16, and figures A.4, A.12 and A.20).

As we have seen, the first order CE solution has very limited scope, for example, it can not take care for the accommodation coefficients. On the contrary, many possibilities are still there with the moment systems; one can analyze the same properties with different moment systems by varying different parameters, for instance, with $\chi_\beta = 1$ and all other parameters same as above the heat flux profile is inverted. However, these are beyond the scope of the present thesis and will be considered elsewhere.

Chapter 7

Numerical method for moment equations

For most practical problems, the associated differential equations do not possess analytical solution in general. Therefore, it often becomes imperative to solve the problem numerically, and thus numerical simulation is undoubtedly a valuable tool to solve practical problems.

In this chapter, we shall employ the finite difference method—which is the simplest numerical method for solving the differential equations—in order to solve the (linear) Grad’s moment equations for binary gas-mixtures detailed in chapter 5. Particularly, we shall focus on the convergence of the numerical method for different problems in one and two dimensions.

7.1 Flow of infinitely diluted component in a binary gas-mixture

The problem is described in § 6.2.1 and we have seen that it was possible to solve the problem analytically. In this section, we shall solve the same problem numerically and analyze the convergence of numerical method towards the analytical solution. To this end, we again consider the system of one-dimensional linear-dimensionless $2 \times G13$ and $2 \times G26$ equations detailed in § 5.1.2 in steady and rest state, i.e., by substituting $\partial(\cdot)/\partial \hat{t} = 0$, $\hat{v}_x = 0$, but without inserting the particular values of x_α° and x_β° so that the equations and the numerical method would also be applicable to the problem of § 6.1.1 as well as to any other one-dimensional problems of binary gas-mixtures in which none of the component is necessarily diluted. In the end, one can substitute $x_\alpha^\circ = 0$ and $x_\beta^\circ = 1$ or vice-versa in the results in order to obtain the numerical solution for the present problem under consideration.

From the mass balance equations of both the constituents (eq. (5.16) and similar equation for the β -constituent) and the boundary conditions for the diffusion velocities (6.2), it readily follows that the diffusion velocities of both the constituents vanish, i.e., $\hat{u}_x^{(\alpha)} = \hat{u}_x^{(\beta)} = 0$, for one-dimensional problems in steady and rest state. Therefore, the relation $\rho_\alpha \mathbf{u}_\alpha + \rho_\beta \mathbf{u}_\beta = \mathbf{0}$ is automatically satisfied for these problems and, moreover, it is not necessary to include the momentum balance equation of the mixture into the system since $\hat{v}_x = 0$ (in all other equations) due to rest state. Therefore, for the numerical solution, we shall omit the momentum balance equation of the mixture and include the balance equation for diffusion velocity of the β -constituent instead, in order to maintain the symmetry. Furthermore, owing to the numerical stabilization, small terms $\epsilon_1 \hat{n}_\alpha$ and $\epsilon_2 \hat{T}_\alpha$ are added on the left-hand sides of mass and energy balance equations for the α -constituent (eqs. (5.16) and (5.18) in steady and rest state), respectively, and $\epsilon_1 \hat{n}_\beta$ and $\epsilon_2 \hat{T}_\beta$ are added on the left-hand sides of mass and energy balance equations for the β -constituent, analogously. Here, all ϵ_i ’s are constants whose values can be chosen in such a way that the accuracy of the solution is maintained, we shall come back to the discussion

on values of ϵ_i 's after describing the numerical method. Owing to the addition of these small terms, boundary conditions (6.1) are not required for the numerical solution.

The resulting $2 \times G13$ and $2 \times G26$ systems of moment equations can be written as

$$P \frac{d\mathbf{U}}{d\hat{x}} + Q \mathbf{U} = \mathbf{0}, \quad (7.1)$$

where P and Q are constant matrices and $\mathbf{U}$ is the vector containing all the unknowns

$$\mathbf{U} = \{\hat{n}_\alpha, \hat{u}_x^{(\alpha)}, \hat{T}_\alpha, \hat{\sigma}_{xx}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{n}_\beta, \hat{u}_x^{(\beta)}, \hat{T}_\beta, \hat{\sigma}_{xx}^{(\beta)}, \hat{q}_x^{(\beta)}\}^\top$$

in case of $2 \times G13$ equations while

$$\mathbf{U} = \{\hat{n}_\alpha, \hat{u}_x^{(\alpha)}, \hat{T}_\alpha, \hat{\sigma}_{xx}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{m}_{xxx}^{(\alpha)}, \hat{R}_{xx}^{(\alpha)}, \hat{\Delta}_\alpha, \hat{n}_\beta, \hat{u}_x^{(\beta)}, \hat{T}_\beta, \hat{\sigma}_{xx}^{(\beta)}, \hat{q}_x^{(\beta)}, \hat{m}_{xxx}^{(\beta)}, \hat{R}_{xx}^{(\beta)}, \hat{\Delta}_\beta\}^\top$$

in case of $2 \times G26$ equations. We now discretize the dimensionless channel width (dimensionless gap between the plates in the other one-dimensional problem), which is 1, into N_i identical intervals of size $\Delta x = 1/N_i$ using $(N_i + 1)$ equispaced nodes $x_j = -\frac{1}{2} + j \Delta x$ where $j = 0, 1, \dots, N_i$; clearly, $x_0 = -\frac{1}{2}$ and $x_{N_i} = \frac{1}{2}$. With this discretization, (7.1) at each node x_j for $j \in \{0, 1, \dots, N_i\}$ takes the form

$$P \mathbf{U}'_j + Q \mathbf{U}_j = \mathbf{0}, \quad (7.2)$$

where $\mathbf{U}_j = \mathbf{U}(x_j)$ and $\mathbf{U}'_j$ is the numerical approximation for the derivative in (7.1) at point x_j . At the interior nodes (i.e., at $x_1, x_2, \dots, x_{N_i-1}$), the derivative is approximated with the central difference scheme whereas at the left and right corners (i.e., at nodes x_0 and x_{N_i}), it is approximated with the forward and backward difference schemes, respectively. In other words, the derivative in (7.1) is approximated with

$$\mathbf{U}'_j = \begin{cases} \frac{U_{j+1} - U_j}{\Delta x} & \text{for } j = 0, \\ \frac{U_{j+1} - U_{j-1}}{2 \Delta x} & \text{for } j \in \{1, 2, \dots, N_i - 1\}, \\ \frac{U_j - U_{j-1}}{\Delta x} & \text{for } j = N_i. \end{cases} \quad (7.3)$$

Furthermore, at the left and right corners (i.e., at nodes x_0 and x_{N_i} , respectively), one needs to incorporate the remaining boundary conditions—(6.2) and (6.3) in case of $2 \times G13$ equations, and (6.2), (6.4) and (6.5) in case of $2 \times G26$ equations. For this, in case of $2 \times G13$ equations, we replace the moment equations for variables $\hat{u}_x^{(\alpha)}$, $\hat{u}_x^{(\beta)}$, $\hat{q}_x^{(\alpha)}$ and $\hat{q}_x^{(\beta)}$ in (7.2) for $j = 0, N_i$ with the corresponding boundary conditions (in discretized form) for these quantities at the left and right walls. Similarly, in case of $2 \times G26$ equations, we replace the equations for variables $\hat{u}_x^{(\alpha)}$, $\hat{u}_x^{(\beta)}$, $\hat{q}_x^{(\alpha)}$, $\hat{q}_x^{(\beta)}$, $\hat{m}_{xxx}^{(\alpha)}$ and $\hat{m}_{xxx}^{(\beta)}$ in (7.2) for $j = 0, N_i$ with the corresponding boundary conditions (in discretized form) for these quantities at the left and right walls. Combining all the discrete vectors $\mathbf{U}_j$'s into a vector $\mathbf{X} = \{\mathbf{U}_0, \mathbf{U}_1, \dots, \mathbf{U}_{N_i}\}^\top$, the full system of discretized moment equations can be written in form of $\mathcal{A} \mathbf{X} = \mathbf{b}$ where $\mathcal{A}$ is a constant matrix while $\mathbf{b}$ is a known constant vector. Nevertheless, matrix $\mathcal{A}$ still contains the constants ϵ_i 's. Since, the central difference scheme gives second order convergence (which will be verified below), i.e., the

error in numerical results will be of order $\mathcal{O}(\Delta x^2)$, the constants ϵ_i 's are taken proportional to Δx^2 with each proportionality constant having a suitable value such that the error due to extra added terms and the error due to the numerical scheme will be of same order, and thus overall accuracy of the results will not be affected because of additional terms; we have taken $\epsilon_1 = \epsilon_2 = c\Delta x^2$, with $c < 1$. The algebraic system $\mathcal{A}\mathbf{X} = \mathbf{b}$, can then be solved for $\mathbf{X}$ using any standard iterative method, such as Gauss–Seidel method, for solving a linear system of equations.

Order of convergence: The error in numerical solution is computed in L^∞ -norm (the maximum norm) which for a field variable ϱ is given by

$$\|\text{err}(\varrho)\|_\infty = \max_j |\varrho^{(\text{ex})}(x_j) - \varrho_j^{(\text{num})}|, \quad (7.4)$$

where $\varrho^{(\text{ex})}(x_j)$ and $\varrho_j^{(\text{num})}$ are the exact and numerical solutions, respectively, for the quantity ϱ at node j .

We have computed the error in numerical solution in L^∞ -norm for all the field variables in several binary gas-mixtures with different permissible values of the parameters and found second order convergence, i.e., the error in numerical solution is of order $\mathcal{O}(\Delta x^2)$, in all the cases. As an example, we show the convergence results for the mixture of He–Xe—which has the largest mass ratio among Ne–Ar, He–Ar and He–Xe mixtures—in figure 7.1, which illustrates the $\log_{10}$ - $\log_{10}$ plots of the error in numerical solution of the number densities of the lighter (left column) and heavier (right column) components in the mixture over number of intervals in discretization $N_i = 20, 50, 100, 200, 500, 1000$ for Knudsen numbers $\text{Kn} = 0.05, 0.1, 0.5, 1$ and different moment systems considered: (top row) $2 \times \text{G13}$ equations with Maxwell interaction potential, (second row from top) $2 \times \text{G13}$ equations with hard-sphere interaction potential, (third row from top) $2 \times \text{G26}$ equations with Maxwell interaction potential, and (bottom row) $2 \times \text{G26}$ equations with hard-sphere interaction potential. The values of other parameters for figure 7.1 are $\Delta \hat{T}_w = 0.5$, $\chi_\alpha = \chi_\beta = 1$. The black line in each sub-figure of figure 7.1 has slope -2 and is included only for comparison.

7.2 Flow of a binary gas-mixture in one-dimension

Here, we consider the similar problem as above but none of the component in the mixture is necessarily diluted. The numerical method for the problem is exactly same as explained above, however, the exact solution is not easy to obtain this time. In numerical studies, when the exact solution is not available, it is prevalent to use a reference numerical solution obtained with very refined grid for studying the convergence of a numerical method. Therefore, for the present problem, we study the convergence of the numerical method through the reference numerical solution obtained by discretizing the dimensionless channel width into 2001 equispaced nodes (or 2000 intervals of equal size). Again, we compute the error in numerical solution in L^∞ -norm which for a field variable ϱ is now given by

$$\|\text{err}(\varrho)\|_\infty = \max_j |\varrho_j^{(\text{ref})} - \varrho_j^{(\text{num})}|, \quad (7.5)$$

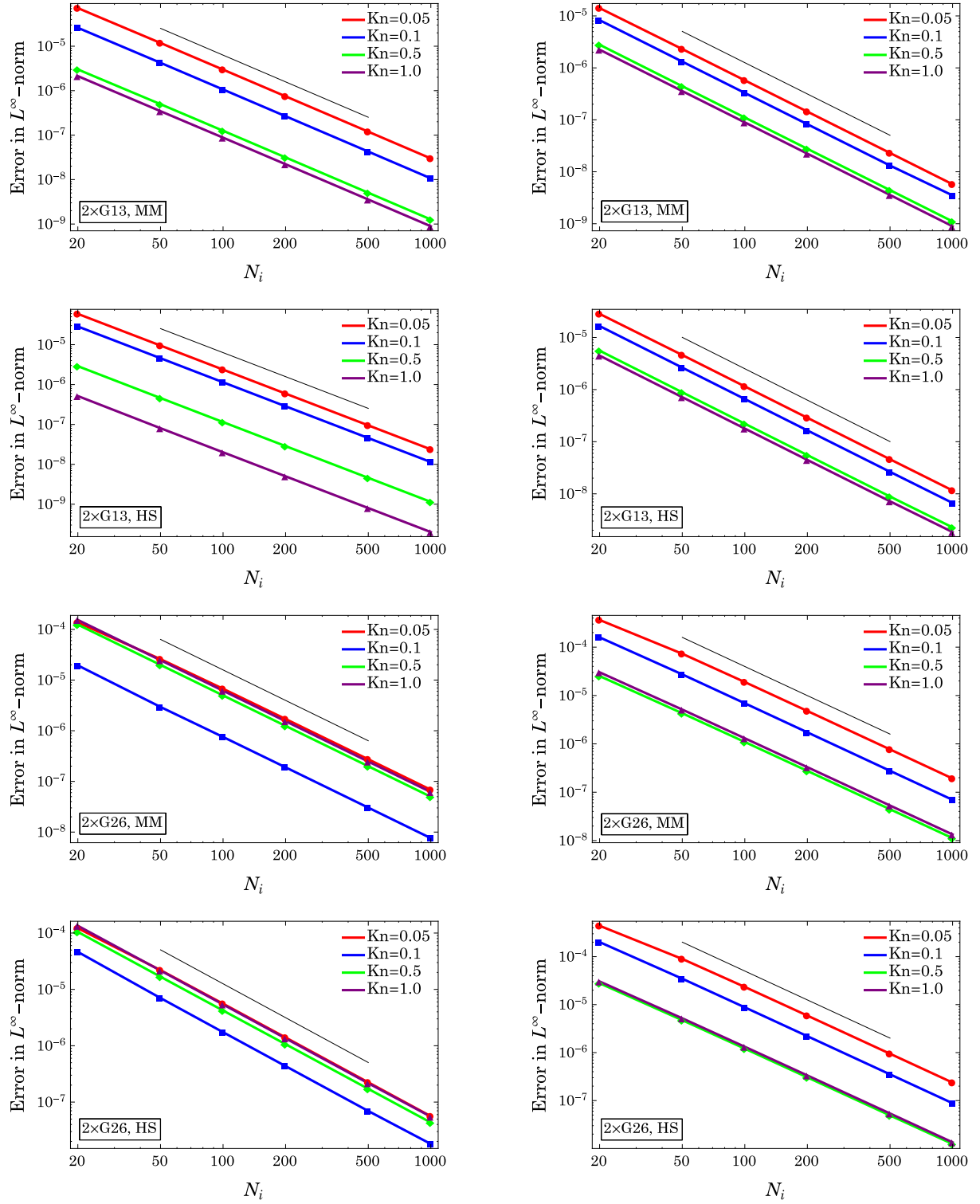


Figure 7.1: Convergence of the numerical method for number densities of the lighter (left column) and heavier (right column) components in He-Xe mixture with $x_{\text{He}}^{\circ} \approx 0$ for different moment systems: (top row) 2×G13 equations with Maxwell interaction potential, (second row from top) 2×G13 equations with hard-sphere interaction potential, (third row from top) 2×G26 equations with Maxwell interaction potential, and (bottom row) 2×G26 equations with hard-sphere interaction potential. The black line has slope -2 and is included only for comparison. The other parameters are $\Delta \hat{T}_w = 0.5$ and $\chi_{\alpha} = \chi_{\beta} = 1$.

where $\varrho_j^{(\text{ref})}$ and $\varrho_j^{(\text{num})}$ are the reference solution and the numerical solution, respectively, for the quantity ϱ at node j .

We have again computed the error in numerical solution in L^∞ -norm for all the field variables in several binary gas-mixtures with different permissible values of the parameters and, again, found second order convergence in all the cases. As an example, we show the convergence results anew for the He–Xe mixture with mole fraction of the lighter component in the mixture as $x_{\text{He}}^\circ = 0.75$ —in figure 7.2, which illustrates the $\log_{10}$ - $\log_{10}$ plots of the error in numerical solution of number densities of the lighter (left column) and heavier (right column) components in the mixture over number of intervals in discretization $N_i = 20, 50, 100, 200, 500$ for Knudsen numbers $\text{Kn} = 0.05, 0.1, 0.5, 1$ and different moment systems considered: (top row) $2 \times \text{G13}$ equations with Maxwell interaction potential, (second row from top) $2 \times \text{G13}$ equations with hard-sphere interaction potential, (third row from top) $2 \times \text{G26}$ equations with Maxwell interaction potential, and (bottom row) $2 \times \text{G26}$ equations with hard-sphere interaction potential. The values of other parameters for figure 7.2 are also $\Delta \hat{T}_w = 0.5$, $\chi_\alpha = \chi_\beta = 1$. The black line in each sub-figure of figure 7.2 has slope -2 and is included only for comparison.

7.3 Flow of a binary gas-mixture in a bottom-heated square cavity

In micro-devices, it is quite common to have a hot plate surrounded by several other cold plates maintained at ambient temperature, and to close and package this system in vacuum. Rarefied (or non-rarefied) gases are usually present in the package and the heat transfer takes place from hot to cold plates [16, 81, 93, 94]. Here, we consider the heat transfer in a binary gas-mixture confined in a square cavity whose bottom wall is heated while all other walls at a cold temperature and present the results on numerical convergence. The preliminary results for the same problem are demonstrated in chapter 9.

7.3.1 Problem description

We consider a binary mixture of gases α and β in steady state confined in a square cavity of side length L . Let the bottom of the cavity be hot in comparison to its other sides; let the temperature of the bottom of the cavity be $T_H = T_\circ + \varepsilon \tilde{T}_H$ while the temperatures of its all other sides be $T_C = T_\circ$; and let all the walls of the cavity are stationary (i.e., $\mathbf{v}_w = \mathbf{0}$ for all the walls). The schematic of the problem is shown in figure 7.3. The temperature difference between the hot wall and any cold wall of the cavity $T_H - T_C = \varepsilon \tilde{T}_H$ is again taken very small in comparison to $T_\circ$ so that the linearized equations and linearized boundary conditions are sufficient for the description of the process; notice again that the smallness parameter ε as a multiplier in the temperature difference is same as that used in the linearization (cf. (5.1)). The third dimension z of the cavity is assumed very long so that heat transfer takes place essentially in two dimensions (x and y), and thus z -axis in figure 7.3 is just for illustration purposes. The scales used for non-dimensionalization are same as those in (5.2); additionally, the length scale for the present problem is L , the side length of the square cavity, and the velocity and temperature of the walls are scaled with $v_\circ$ and $T_\circ$, respectively.

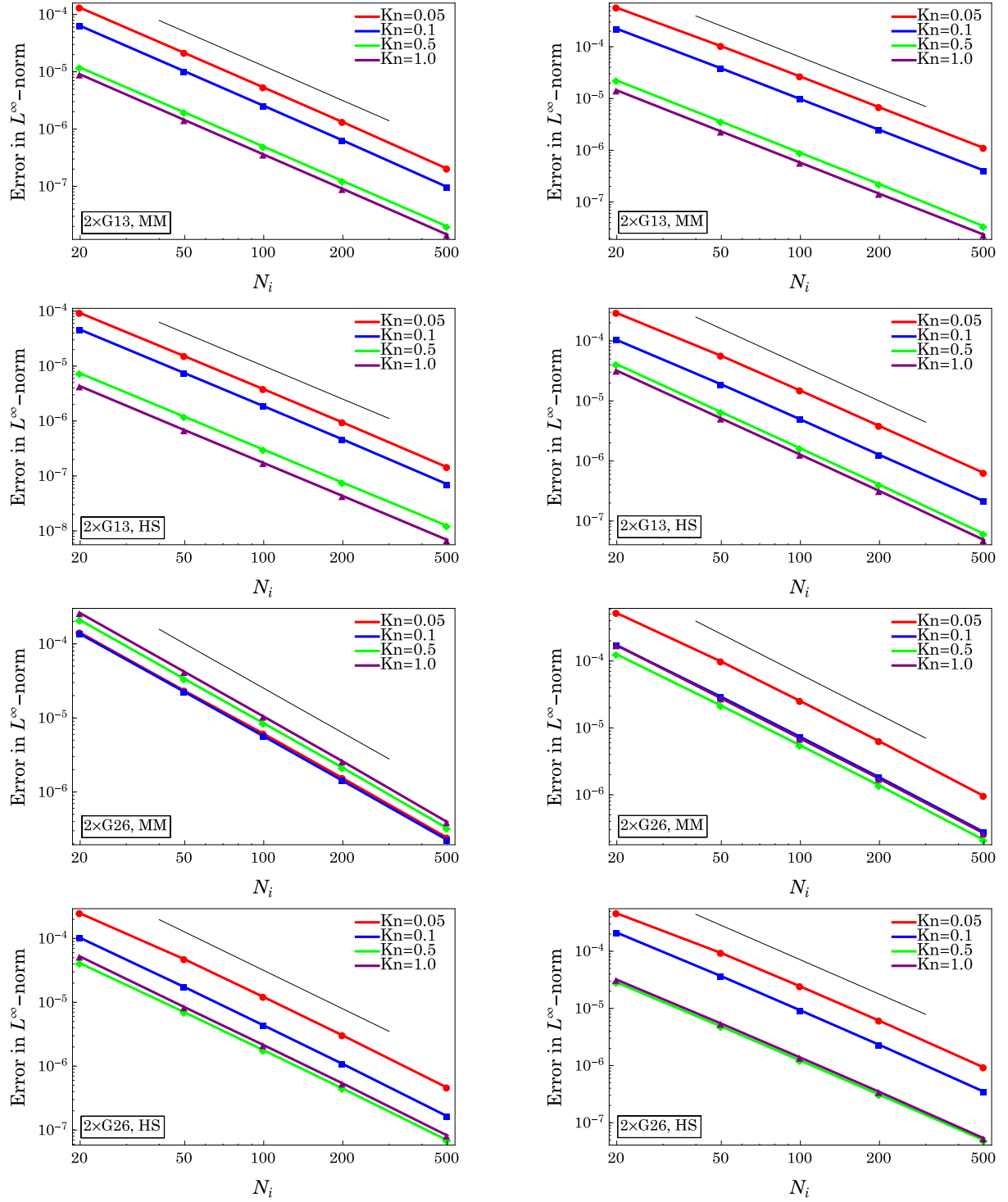


Figure 7.2: Convergence of the numerical method for number densities of the lighter (left column) and heavier (right column) components in He-Xe mixture with $x_{\text{He}}^o = 0.75$ for different moment systems: (top row) $2 \times \text{G13}$ equations with Maxwell interaction potential, (second row from top) $2 \times \text{G13}$ equations with hard-sphere interaction potential, (third row from top) $2 \times \text{G26}$ equations with Maxwell interaction potential, and (bottom row) $2 \times \text{G26}$ equations with hard-sphere interaction potential. The black line has slope -2 and is included only for comparison. The other parameters are same as those for figure 7.1.

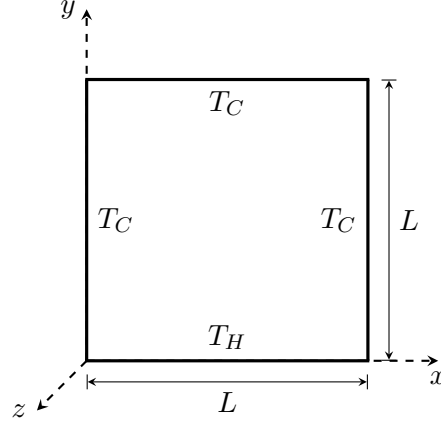


Figure 7.3: Schematic of a two-dimensional bottom heated square cavity; z -axis is included just for illustration purposes.

7.3.2 Relevant moment equations and boundary conditions

The steady state two-dimensional $2 \times G13$ and $2 \times G26$ equations in linear-dimensionless form follow from the three-dimensional equations of § 5.1.1 in a straightforward way on substituting $\partial(\cdot)/\partial \hat{t} = 0$ and using the relations

$$\frac{\partial \hat{\psi}_{\langle i}}{\partial \hat{x}_{j \rangle}} = \begin{cases} \frac{2}{3} \frac{\partial \hat{\psi}_x}{\partial \hat{x}} - \frac{1}{3} \frac{\partial \hat{\psi}_y}{\partial \hat{y}} & \text{for } i = j = x, \\ \frac{1}{2} \frac{\partial \hat{\psi}_y}{\partial \hat{x}} + \frac{1}{2} \frac{\partial \hat{\psi}_x}{\partial \hat{y}} & \text{for } i \neq j \text{ and } i, j \in \{x, y\}, \\ -\frac{1}{3} \frac{\partial \hat{\psi}_x}{\partial \hat{x}} + \frac{2}{3} \frac{\partial \hat{\psi}_y}{\partial \hat{y}} & \text{for } i = j = y \end{cases}$$

and

$$\frac{\partial \hat{\psi}_{\langle ij}}{\partial \hat{x}_{k \rangle}} = \begin{cases} \frac{3}{5} \frac{\partial \hat{\psi}_{xx}}{\partial \hat{x}} - \frac{2}{5} \frac{\partial \hat{\psi}_{xy}}{\partial \hat{y}} & \text{for } i = j = x, \\ \frac{1}{3} \frac{\partial \hat{\psi}_{xx}}{\partial \hat{y}} + \frac{8}{15} \frac{\partial \hat{\psi}_{xy}}{\partial \hat{x}} - \frac{2}{15} \frac{\partial \hat{\psi}_{yy}}{\partial \hat{y}} & \text{for } i = j = x \text{ and } k = y, \\ -\frac{2}{15} \frac{\partial \hat{\psi}_{xx}}{\partial \hat{x}} + \frac{8}{15} \frac{\partial \hat{\psi}_{xy}}{\partial \hat{y}} + \frac{1}{3} \frac{\partial \hat{\psi}_{yy}}{\partial \hat{x}} & \text{for } i = x \text{ and } j = k = y, \\ -\frac{2}{5} \frac{\partial \hat{\psi}_{xy}}{\partial \hat{x}} + \frac{3}{5} \frac{\partial \hat{\psi}_{yy}}{\partial \hat{y}} & \text{for } i = j = y. \end{cases}$$

The relevant boundary conditions for the problem are (4.13), (4.16), (4.18), (4.19) in case of $2 \times G13$ equations, and (4.13), (4.16), (4.21)–(4.24), (4.26) in case of $2 \times G26$ equations—all for both the species. The boundary conditions for the present problem in linear-dimensionless form are as follows. Boundary conditions (4.13) and (4.16) read ($\gamma \in \{\alpha, \beta\}$)

$$\int_0^1 \int_0^1 \hat{n}_\gamma \, d\hat{x} \, d\hat{y} = 0, \quad (7.6)$$

$$\hat{u}_x^{(\gamma)}(0, y) = \hat{u}_x^{(\gamma)}(1, y) = \hat{u}_y^{(\gamma)}(x, 0) = \hat{u}_y^{(\gamma)}(x, 1) = 0. \quad (7.7)$$

The remaining boundary conditions for the $2 \times G13$ equations—(eqs. (4.18) and (4.19))—read

$$\hat{\sigma}_{nt}^{(\gamma)} = -\mathbf{n} \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[\frac{v_o}{\sqrt{\theta_\gamma^o}} (\hat{v}_t - \hat{v}_w) + \frac{1}{2} \hat{u}_t^{(\gamma)} + \frac{1}{5} \hat{q}_t^{(\gamma)} \right], \quad (7.8)$$

$$\hat{q}_n^{(\gamma)} = -\mathbf{n} \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[2(\hat{T}_\gamma - \hat{T}_w) + \frac{1}{2} \hat{\sigma}_{nn}^{(\gamma)} \right], \quad (7.9)$$

while the remaining boundary conditions for the 2×G26 equations—(eqs. (4.21)–(4.24) and (4.26))—read

$$\hat{\sigma}_{nt}^{(\gamma)} = -\mathbf{n} \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[\frac{v_o}{\sqrt{\theta_\gamma^o}} (\hat{v}_t - \hat{v}_w) + \frac{1}{2} \hat{u}_t^{(\gamma)} + \frac{1}{5} \hat{q}_t^{(\gamma)} + \frac{1}{2} \hat{m}_{nnt}^{(\gamma)} \right], \quad (7.10)$$

$$\hat{q}_n^{(\gamma)} = -\mathbf{n} \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[2(\hat{T}_\gamma - \hat{T}_w) + \frac{1}{2} \hat{\sigma}_{nn}^{(\gamma)} + \frac{5}{28} \hat{R}_{nn}^{(\gamma)} + \frac{1}{15} \hat{\Delta}_\gamma \right], \quad (7.11)$$

$$\hat{m}_{nnn}^{(\gamma)} = \mathbf{n} \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[\frac{2}{5} (\hat{T}_\gamma - \hat{T}_w) - \frac{7}{5} \hat{\sigma}_{nn}^{(\gamma)} - \frac{1}{14} \hat{R}_{nn}^{(\gamma)} + \frac{1}{75} \hat{\Delta}_\gamma \right], \quad (7.12)$$

$$\hat{m}_{ntt}^{(\gamma)} = -\mathbf{n} \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[\frac{1}{5} (\hat{T}_\gamma - \hat{T}_w) - \frac{1}{5} \hat{\sigma}_{nn}^{(\gamma)} + \hat{\sigma}_{tt}^{(\gamma)} + \frac{1}{14} \hat{R}_{tt}^{(\gamma)} + \frac{1}{150} \hat{\Delta}_\gamma \right], \quad (7.13)$$

$$\hat{R}_{nt}^{(\gamma)} = \mathbf{n} \frac{\chi_\gamma}{2 - \chi_\gamma} \sqrt{\frac{2}{\pi}} \left[\frac{v_o}{\sqrt{\theta_\gamma^o}} (\hat{v}_t - \hat{v}_w) + \frac{13}{2} \hat{u}_t^{(\gamma)} - \frac{11}{5} \hat{q}_t^{(\gamma)} - \frac{1}{2} \hat{m}_{nnt}^{(\gamma)} \right], \quad (7.14)$$

where

$$\gamma \in \{\alpha, \beta\}; \quad \mathbf{n} = \begin{cases} 1 & \text{for left and bottom walls,} \\ -1 & \text{for right and top walls;} \end{cases}$$

$n = x$ and $t = y$ for the left and right walls of the cavity whereas $n = y$ and $t = x$ for the bottom and top walls of the cavity; $\hat{v}_w$, $\hat{T}_w$ denote the dimensionless perturbations in velocity and temperature, respectively, of a wall of the cavity from their respective ground state values. For the present problem, $\hat{v}_w = 0$ for all the walls, and $\hat{T}_w = 0$ for the left, right and top walls while $\hat{T}_w = \hat{T}_H$ for the bottom wall with $\hat{T}_H = \tilde{T}_H/T_o$.

Similar to a single gas case, we include the balance equations for the diffusion velocities of both the constituent into the moment systems while discard the momentum balance equation for the mixture in order to maintain symmetry. Nonetheless, the total velocity of the mixture $\hat{\mathbf{v}}$ is still present in the moment systems. To get rid of the total velocity $\hat{\mathbf{v}}$, we replace the diffusion velocities of the constituents and the total velocity of the mixture in terms of the individual macroscopic velocities $\hat{\mathbf{v}}_\alpha$ and $\hat{\mathbf{v}}_\beta$ by using the dimensionless form of the relations $\mathbf{u}_\alpha = \mathbf{v}_\alpha - \mathbf{v}$, $\rho \mathbf{v} = \rho_\alpha \mathbf{v}_\alpha + \rho_\beta \mathbf{v}_\beta$ and $\rho_\alpha \mathbf{u}_\alpha + \rho_\beta \mathbf{u}_\beta = \mathbf{0}$ in the moment systems and boundary conditions. Again, similar to a single gas case, we need to add some small terms in some of the equations and boundary conditions owing to numerical stability; $\epsilon_1 \hat{n}_\alpha$, $\epsilon_2 \hat{v}_i^{(\alpha)}$ and $\epsilon_3 \hat{T}_\alpha$ are added on the left-hand sides of the balance equations for mass, diffusion velocity and energy of the α -constituent, and analogous terms are also added on the left-hand sides of the balance equations for mass, diffusion velocity and energy of the β -constituent; moreover, boundary conditions (7.7)—which after changing the variables read $\hat{v}_x^{(\gamma)}(0, y) = \hat{v}_x^{(\gamma)}(1, y) = \hat{v}_y^{(\gamma)}(x, 0) = \hat{v}_y^{(\gamma)}(x, 1) = 0$ for $\gamma \in \{\alpha, \beta\}$ —are modified as $\hat{v}_x^{(\gamma)}(0, y) = \hat{v}_x^{(\gamma)}(1, y) = \hat{v}_y^{(\gamma)}(x, 0) = \hat{v}_y^{(\gamma)}(x, 1) = -\epsilon_4 \mathbf{n} \hat{n}_\gamma$ for $\gamma \in \{\alpha, \beta\}$. Obviously, ϵ_1 and ϵ_2 here might be different from those for the one-dimensional problems. We shall discuss the values of small parameters ϵ_i 's after describing the numerical method. Again, owing to the addition of these small terms, boundary conditions (7.6) are not

required for the numerical solution.

7.3.3 Numerical method

The resulting $2 \times G13$ and $2 \times G26$ systems of moment equations can be written as

$$P_1 \frac{\partial \mathbf{U}}{\partial \hat{x}} + P_2 \frac{\partial \mathbf{U}}{\partial \hat{y}} + R \mathbf{U} = \mathbf{0}, \quad (7.15)$$

where P_1 , P_2 and R are constant matrices and $\mathbf{U}$ is the vector containing all the unknowns

$$\mathbf{U} = \{\hat{n}_\alpha, \hat{v}_x^{(\alpha)}, \hat{v}_y^{(\alpha)}, \hat{T}_\alpha, \hat{\sigma}_{xx}^{(\alpha)}, \hat{\sigma}_{xy}^{(\alpha)}, \hat{\sigma}_{yy}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{q}_y^{(\alpha)}, \hat{n}_\beta, \hat{v}_x^{(\beta)}, \hat{v}_y^{(\beta)}, \hat{T}_\beta, \hat{\sigma}_{xx}^{(\beta)}, \hat{\sigma}_{xy}^{(\beta)}, \hat{\sigma}_{yy}^{(\beta)}, \hat{q}_x^{(\beta)}, \hat{q}_y^{(\beta)}\}^\top$$

in case of $2 \times G13$ equations while

$$\mathbf{U} = \{\hat{n}_\alpha, \hat{v}_x^{(\alpha)}, \hat{v}_y^{(\alpha)}, \hat{T}_\alpha, \hat{\sigma}_{xx}^{(\alpha)}, \hat{\sigma}_{xy}^{(\alpha)}, \hat{\sigma}_{yy}^{(\alpha)}, \hat{q}_x^{(\alpha)}, \hat{q}_y^{(\alpha)}, \hat{m}_{xxx}^{(\alpha)}, \hat{m}_{xxy}^{(\alpha)}, \hat{m}_{xyy}^{(\alpha)}, \hat{m}_{yyy}^{(\alpha)}, \hat{R}_{xx}^{(\alpha)}, \hat{R}_{xy}^{(\alpha)}, \hat{R}_{yy}^{(\alpha)}, \hat{\Delta}_\alpha, \\ \hat{n}_\beta, \hat{v}_x^{(\beta)}, \hat{v}_y^{(\beta)}, \hat{T}_\beta, \hat{\sigma}_{xx}^{(\beta)}, \hat{\sigma}_{xy}^{(\beta)}, \hat{\sigma}_{yy}^{(\beta)}, \hat{q}_x^{(\beta)}, \hat{q}_y^{(\beta)}, \hat{m}_{xxx}^{(\beta)}, \hat{m}_{xxy}^{(\beta)}, \hat{m}_{xyy}^{(\beta)}, \hat{m}_{yyy}^{(\beta)}, \hat{R}_{xx}^{(\beta)}, \hat{R}_{xy}^{(\beta)}, \hat{R}_{yy}^{(\beta)}, \hat{\Delta}_\beta\}^\top$$

in case of $2 \times G26$ equations. We now discretize the dimensionless spatial domain of the cavity into $N_x \times N_y$ identical cells using the equispaced grid points $x_i = i \Delta x$ and $y_j = j \Delta y$ where $i = 0, 1, \dots, N_x$ and $j = 0, 1, \dots, N_y$; clearly, $x_0 = 0$, $x_{N_x} = 1$, $y_0 = 0$ and $y_{N_y} = 1$. With this discretization, (7.15) at each point (x_i, y_j) for $i = 0, 1, \dots, N_x$ and $j = 0, 1, \dots, N_y$ assumes the form

$$P_1(\partial_{\hat{x}} \mathbf{U})_{i,j} + P_2(\partial_{\hat{y}} \mathbf{U})_{i,j} + R \mathbf{U}_{i,j} = \mathbf{0}, \quad (7.16)$$

where $\mathbf{U}_{i,j} = \mathbf{U}(x_i, y_j)$, and $(\partial_{\hat{x}} \mathbf{U})_{i,j}$ and $(\partial_{\hat{y}} \mathbf{U})_{i,j}$ are the numerical approximations for the derivatives in (7.15) at point (x_i, y_j) . At the interior grid points, both $\hat{x}$ and $\hat{y}$ derivatives are approximated with the central difference scheme; at the left and right walls, the $\hat{x}$ derivative is approximated with the forward and backward difference schemes, respectively, at all grid points on the wall whereas the $\hat{y}$ derivative is approximated with the central difference scheme at all grid points other than the corners, where it is approximated with forward difference scheme at the bottom and with backward difference scheme at the top; at the bottom and top walls, the $\hat{y}$ derivative is approximated with the forward and backward difference schemes, respectively, at all grid points on the wall whereas the $\hat{x}$ derivative is approximated with the central difference scheme at all points other than the corners, where it is approximated with forward difference scheme at the left and with backward difference scheme at the right. In other words, the derivatives in (7.15) are approximated with

$$(\partial_{\hat{x}} \mathbf{U})_{i,j} = \begin{cases} \frac{U_{i+1,j} - U_{i,j}}{\Delta x} & \text{for } (i, j) \in \{0\} \times \{0, 1, \dots, N_y\}, \\ \frac{U_{i+1,j} - U_{i-1,j}}{2 \Delta x} & \text{for } (i, j) \in \{1, 2, \dots, N_x - 1\} \times \{0, 1, \dots, N_y\}, \\ \frac{U_{i,j} - U_{i-1,j}}{\Delta x} & \text{for } (i, j) \in \{N_x\} \times \{0, 1, \dots, N_y\} \end{cases} \quad (7.17)$$

and

$$(\partial_y \mathbf{U})_{i,j} = \begin{cases} \frac{U_{i,j+1} - U_{i,j}}{\Delta y} & \text{for } (i,j) \in \{0, 1, \dots, N_x\} \times \{0\}, \\ \frac{U_{i,j+1} - U_{i,j-1}}{2\Delta y} & \text{for } (i,j) \in \{0, 1, \dots, N_x\} \times \{1, 2, \dots, N_y - 1\}, \\ \frac{U_{i,j} - U_{i,j-1}}{\Delta y} & \text{for } (i,j) \in \{0, 1, \dots, N_x\} \times \{N_y\}. \end{cases} \quad (7.18)$$

The boundary conditions at the walls are applied in exactly same way as for a single gas by including the boundary condition for a moment in discretized form instead of its balance equation, see § 7.1. Combining all the discrete vectors $\mathbf{U}_{i,j}$'s into a vector $\mathbf{X} = \{\mathbf{U}_{i,j} | (i,j) \in \{0, 1, \dots, N_x\} \times \{0, 1, \dots, N_y\}\}^\top$, the full system of discretized moment equations can again be written in form of $\mathcal{A}\mathbf{X} = \mathbf{b}$ where $\mathbf{b}$ is a known constant vector and $\mathcal{A}$ is a constant matrix consisting of the constants ϵ_i 's. Since, the central difference scheme gives second order convergence (which will be scrutinized below), i.e., the error in numerical results will be at least of order $\mathcal{O}(\max\{\Delta x^2, \Delta y^2\})$, the constants ϵ_i 's are taken proportional to $\min\{\Delta x^2, \Delta y^2\}$ with each proportionality constant having a suitable value such that the error due to extra added terms and the error due to the numerical scheme will be of same order, and thus overall accuracy of the results will not be affected because of additional terms; we have taken $\epsilon_1 = \epsilon_2 = \epsilon_3 = \epsilon_4 = c \times \min\{\Delta x^2, \Delta y^2\}$, with $c < 1$. The algebraic system $\mathcal{A}\mathbf{X} = \mathbf{b}$, can then be solved for $\mathbf{X}$ using any standard iterative method, such as Gauss-Seidel method, for solving a linear system of equations.

Order of convergence: The error in numerical solution for the problem under consideration is computed in L^1 -norm which for a field variable ϱ is given by

$$\|\text{err}(\varrho)\|_1 = \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \Delta x \Delta y |\varrho^{(\text{ex})}(x_i, y_j) - \varrho_{i,j}^{(\text{num})}|, \quad (7.19)$$

where $\varrho^{(\text{ex})}(x_i, y_j)$ and $\varrho_{i,j}^{(\text{num})}$ are the exact and numerical solutions, respectively, for the quantity ϱ at node (i, j) .

The exact solution is again approximated with a reference numerical solution obtained by discretizing the domain of the cavity into 400×400 identical cells. In figure 7.4, we present the convergence results for the shear stress of the lighter component and the number density of the heavier component in He-Xe mixture as examples. Figure 7.4 delineates the $\log_{10}$ - $\log_{10}$ plots of the error in numerical solutions of the shear stress of the lighter component (left column) and the number density of the heavier component (right column) in the mixture over number of discretization intervals in x -direction $N_x = 20, 40, 80, 100$ for Knudsen numbers $\text{Kn} = 0.05, 0.1$ and different moment systems: (top row) $2 \times \text{G13}$ equations with Maxwell interaction potential, (second row from top) $2 \times \text{G13}$ equations with hard-sphere interaction potential, (third row from top) $2 \times \text{G26}$ equations with Maxwell interaction potential, and (bottom row) $2 \times \text{G26}$ equations with hard-sphere interaction potential. The values of other parameters for figure 7.4 are $\hat{T}_H = 0.1$ and $\chi_\alpha = \chi_\beta = 1$. The continuous and dashed black lines in each sub-figure of figure 7.4 have slopes -2 and -1 , respectively, and are included only for comparison. We have also checked the convergence for other field variables of the mixture and found that our numerical method for two-dimensional problems is not second order convergent in general, which is also apparent

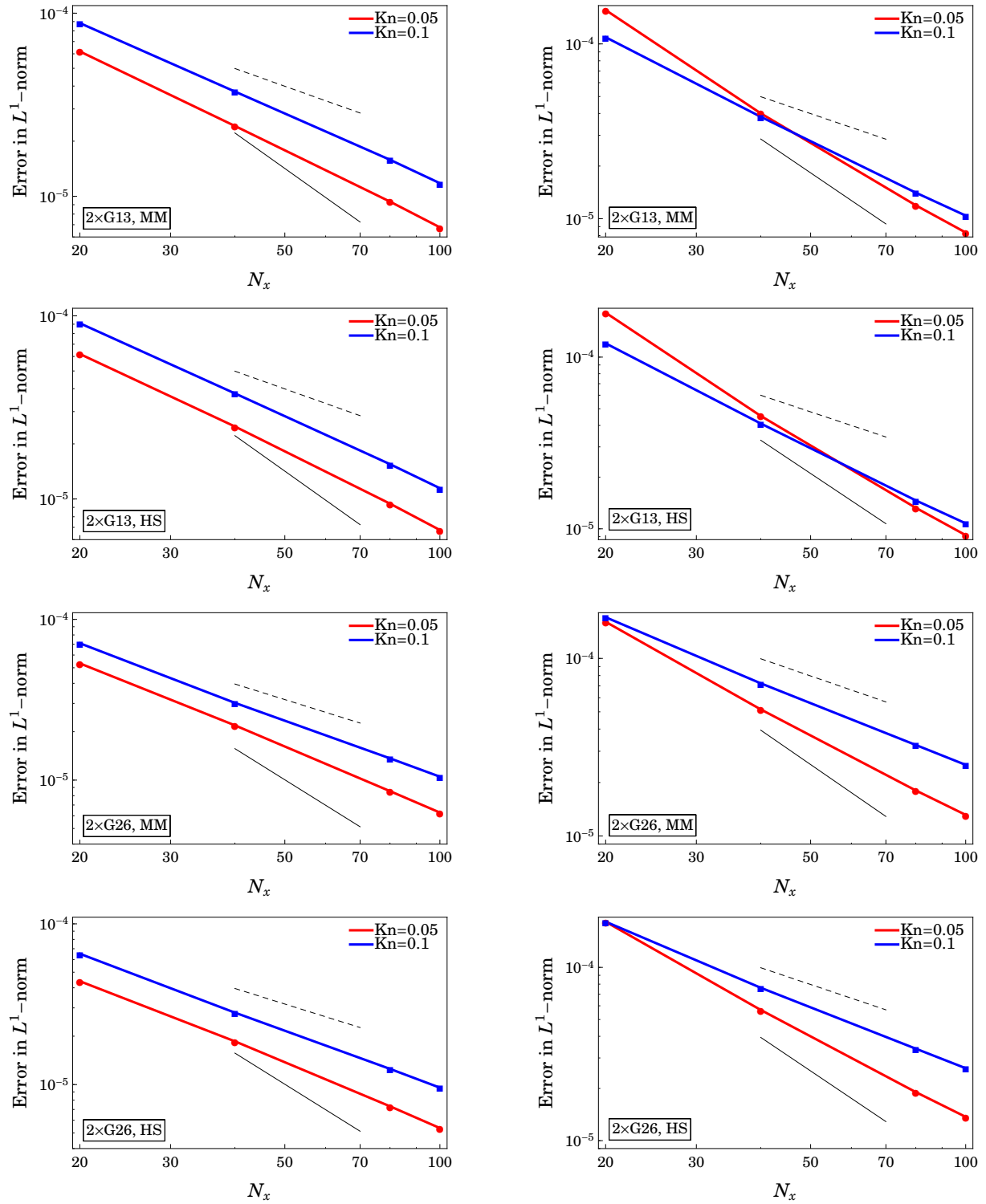


Figure 7.4: Convergence of the numerical method for shear stress of the lighter component (left column) and number density of the heavier component (right column) in He-Xe mixture with $x_{\text{He}}^0 = 0.25$ for different moment systems: (top row) 2xG13 equations with Maxwell interaction potential, (second row from top) 2xG13 equations with hard-sphere interaction potential, (third row from top) 2xG26 equations with Maxwell interaction potential, and (bottom row) 2xG26 equations with hard-sphere interaction potential. The continuous and dashed black lines have slopes -2 and -1 , respectively, and are included only for comparison. The other parameters are $\hat{T}_H = 0.1$ and $\chi_\alpha = \chi_\beta = 1$.

from figure 7.4. The order of convergence is slightly more than one but less than two for most of the field variables. For some field variables, we obtain approximately second order convergence at small Knudsen numbers (see the red lines in the two sub-figures from top in the right column of figure 7.4 for example; also see figure 7.6) but the order of convergence decreases towards one with increasing Knudsen number. The reason for not obtaining the second order convergence could be the discontinuities in temperature at the boundaries as well as the discretization at the boundaries which is of first order (forward/backward differences) in normal directions and the first order errors in solution at the boundaries might be influencing the errors at the interior points. Therefore, we need to investigate the numerical method for two-dimensional problems again in future.

7.4 Flow of a binary gas-mixture in a lid-driven square cavity

The fluid flow in a lid-driven square cavity is another classical problem of fluid dynamics and has been studied by a few authors in the context of a (rarefied) single gas, see e.g., [52, 72, 79]. Unfortunately, the same problem in the context of gaseous mixtures has received much less attention. In this section, we present the numerical convergence results for the problem of binary gaseous mixture flow in a lid driven square cavity. The preliminary results for the same problem are also demonstrated in chapter 9.

7.4.1 Problem description

We anew consider a binary mixture of gases α and β in steady state confined in a square cavity of side length L . Let the temperatures of all the walls of the cavity be same and equal to a constant value $T_w = T_o + \varepsilon \tilde{T}_0$; moreover, let the top wall (lid) of the cavity be moving in positive x -direction with velocity $v_{\text{lid}} = \varepsilon \tilde{v}_0$. The schematic of the problem is shown in figure 7.5. The third dimension z of the cavity is again assumed very long so that the flow takes place essentially in two dimensions (x and y) and thus z -axis in figure 7.5 is also just for illustration purposes. The scales used for non-dimensionalization are same as those for the problem described in § 7.3.

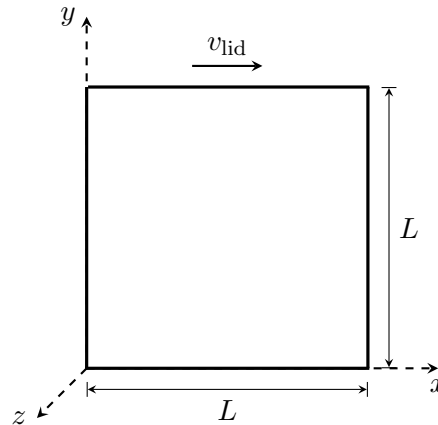


Figure 7.5: Schematic of a two-dimensional lid-driven square cavity; z -axis is included just for illustration purposes.

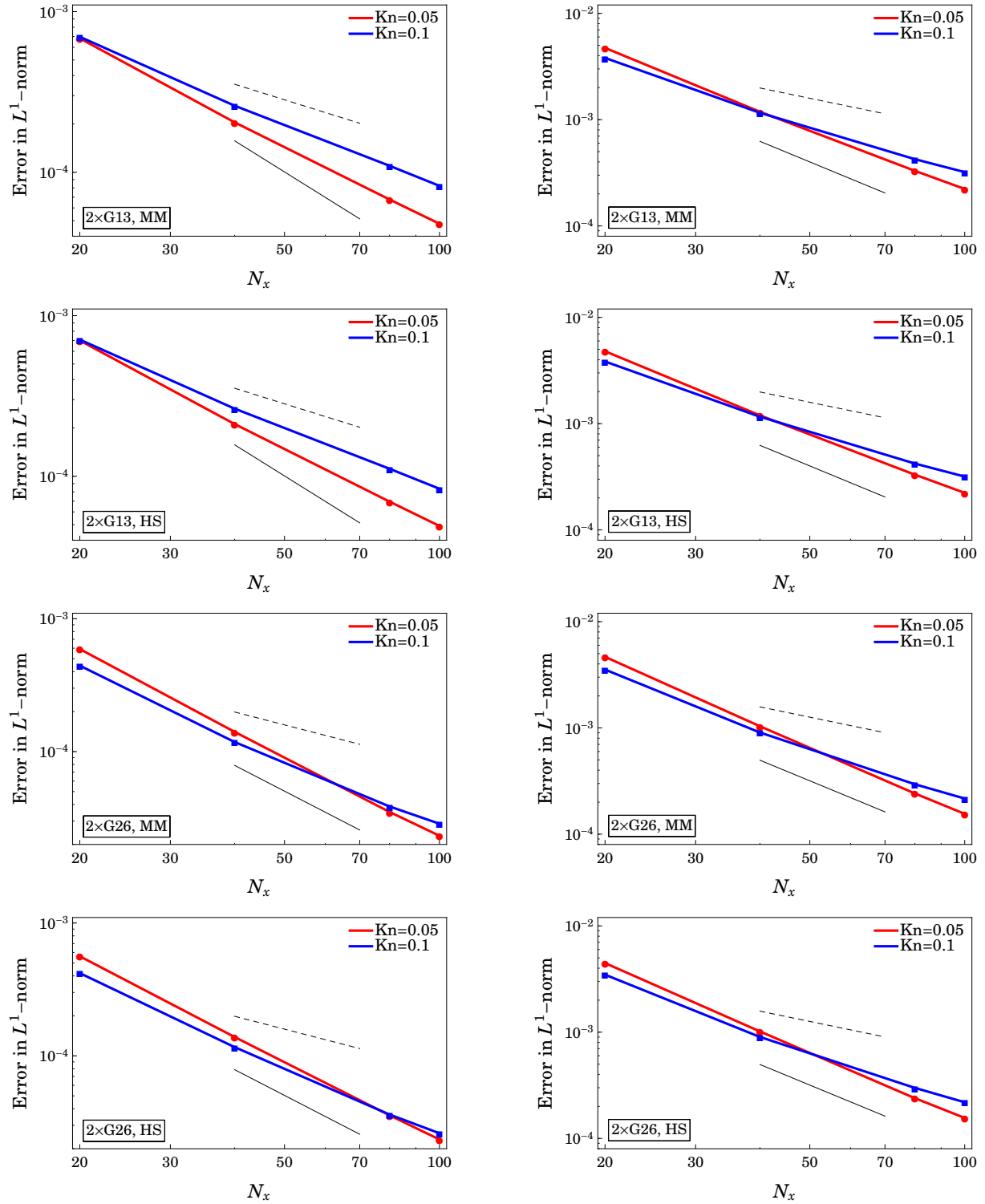


Figure 7.6: Convergence of the numerical method for shear stress of the lighter component (left column) and number density of the heavier component (right column) in He-Xe mixture with $x_{\text{He}}^{\circ} = 0.25$ for different moment systems: (top row) $2 \times \text{G13}$ equations with Maxwell interaction potential, (second row from top) $2 \times \text{G13}$ equations with hard-sphere interaction potential, (third row from top) $2 \times \text{G26}$ equations with Maxwell interaction potential, and (bottom row) $2 \times \text{G26}$ equations with hard-sphere interaction potential. The continuous and dashed black lines have slopes -2 and -1 , respectively, and are included only for comparison. The other parameters are $\hat{v}_w = 1$, $\hat{T}_0 = 0$ and $\chi_{\alpha} = \chi_{\beta} = 1$.

7.4.2 Numerical method and its convergence

The moment equations, the boundary conditions and the numerical method are very similar to those demonstrated in § 7.3; only we need to consider $\hat{v}_w = \hat{v}_0$ for the top wall and $\hat{v}_w = 0$ for the left, right and bottom walls whereas $\hat{T}_w = \hat{T}_0$ for all the walls, where $\hat{v}_0 = \tilde{v}_0/v_o$ and $\hat{T}_0 = \tilde{T}_0/T_o$. Without loss of generality, let $\hat{T}_0 = 0$.

For the present problem, we again consider the He–Xe mixture with $x_{\text{He}}^o = 0.25$ and plot the error in numerical solutions of shear stress of the lighter component (left column) and number density of the heavier component (right column) in the mixture over number of discretization intervals in x -direction $N_x = 20, 40, 80, 100$ —on $\log_{10}$ - $\log_{10}$ scale—for Knudsen numbers $\text{Kn} = 0.05, 0.1$ and different moment systems: (top row) $2 \times \text{G13}$ equations with Maxwell interaction potential, (second row from top) $2 \times \text{G13}$ equations with hard-sphere interaction potential, (third row from top) $2 \times \text{G26}$ equations with Maxwell interaction potential, and (bottom row) $2 \times \text{G26}$ equations with hard-sphere interaction potential in figure 7.6. The reference numerical solution is again obtained by discretizing the domain of the cavity into 400×400 identical cells. The values of other parameters for figure 7.6 are $\hat{v}_w = 1$, $\hat{T}_0 = 0$ and $\chi_\alpha = \chi_\beta = 1$. The continuous and dashed black lines in each sub-figure of figure 7.6 also have slopes -2 and -1 , respectively, and are included only for comparison.

Figure 7.6 shows that this time for the same field variables as considered in figure 7.4, we obtain almost second order convergence for small Knudsen numbers (except in the shear stress computed with $2 \times \text{G13}$ equations for Maxwell interaction potential as well as for hard-sphere interaction potential, where it is slightly less than 2). Moreover, the order of convergence does not significantly decrease (in comparison to figure 7.4) on increasing the Knudsen number. In fact, for most of the other field variables too, we obtain almost second order convergence for small Knudsen numbers, which decreases towards one with increasing Knudsen number.

Chapter 8

Regularized moment equations for binary gas-mixtures

In kinetic theory of single gases, the Chapman–Enskog expansion method and the Grad’s method of moments are the two most avowed techniques for solving the Boltzmann equation approximately. Nonetheless, both the techniques come with shortcomings. Although, the former has great success in educing the constitutive equations of Navier–Stokes and Fourier with explicit expressions for viscosity and heat conductivity, the higher order expansions from it lead to Burnett and super-Burnett equations which are unstable [10, 11, 120]. On the other hand, the equations resulting from the latter are always linearly stable, but they admit unphysical sub-shocks above a critical Mach number due to their hyperbolic nature [71, 122]. In case of a single gas, Struchtrup and Torrilhon [106] derived the regularized 13-moment (R13) equations by coalescing the propitious features of the two methods while avoiding their undesirable features. The R13 equations are always linearly stable and exhibit smooth shock structure for all Mach numbers.

For single gases, Struchtrup [100] further introduced a method, which accounts for the order of magnitude of moments and of each term in moment equations in powers of the Knudsen number. The method provides highly accurate equations and, concurrently, resolves the issue of how many moments need to be considered for describing a process with certain accuracy. For Maxwell molecules and hard spheres, the method has been developed up to third order [100, 108]. The method yields Euler equations at zeroth order, Navier–Stokes equations at first order, Grad’s 13-moment equations (without a non-linear term) at second order and a variant of the original R13 equations [106] at third order. For general interaction potentials, the method has been developed only up to second order, where it provides a generalization to Grad’s 13-moment equations [103].

In this chapter, we shall extend the order of magnitude method to binary gas-mixtures in order to regularize the Grad’s moment equations for them derived in chapter 2. For simplicity, we shall derive the regularized moment equations for binary mixture of gases interacting with *Maxwell* interaction potential only. Moreover, only the derivation of *linear* regularized moment equations will be considered here. The derivation of non-linear regularized moment equations for binary mixture of gases interacting with Maxwell interaction potential as well as the derivation of regularized moment equations for binary mixture of gases interacting with other non-Maxwell interaction potential, including hard-sphere interaction potential, will be considered elsewhere in future.

8.1 Outline of order of magnitude method

The order of magnitude method for finding the proper equations with order of accuracy λ_0 in the Knudsen number comprises of the following three steps [100, 102].

1. Determination of *order of magnitude* λ of the moments:

The goal at this step is to determine the order of magnitude of moments in powers of smallness parameter (ε) which is usually the Knudsen number. To this end, a (non-conserved) moment ϕ is expanded in powers of ε as below.

$$\phi = \phi_0 + \varepsilon\phi_1 + \varepsilon^2\phi_2 + \dots$$

It should be noticed that the above expansion performed on a moment ϕ is somewhat similar to Chapman–Enskog expansion, which is performed on the velocity distribution function. However, unlike the approach of Chapman–Enskog expansion which aims at computing ϕ_i 's ($i = 0, 1, 2, \dots$), the focus in this method is just to find out the leading order of ϕ . The leading order of ϕ is determined by inserting the above expansion into complete set of moment equations. A moment ϕ is said to be of leading order λ if $\phi_i = 0$ for all $i < \lambda$. The leading order of a moment is the order of magnitude of that moment.

2. Construction of a system of moment equations having minimum number of moments at a given order of accuracy λ :

At this step, some of the originally chosen moments are combined linearly in order to introduce new variables in the system. The new variables are constructed in such a way that on replacing the original moments in the moment equations with the new variables, the number of moments at a given order λ is minimum. This step not only provides an unambiguous set of moments at order λ but also guarantees that the final equations will be independent of the initial choice of moments.

3. Deletion of all terms in all equations that would lead to contributions of orders $\lambda > \lambda_0$ in the conservation laws:

At this step, we adopt the following definition of the order of accuracy λ_0 .

Definition 8.1. *A set of equations for binary gas-mixtures is said to be accurate of order λ_0 , when the diffusion velocities (of both the components), total stress and total heat flux in the mixture are known up to the order $\mathcal{O}(\varepsilon^{\lambda_0})$.*

The adoption of this definition relies on the fact that all moment equations are strongly coupled. This connotes that each term in any of the moment equations has some influence on all other equations, particularly on the conservation laws. The influence of each term can be weighted by some power in the Knudsen number, and is related, but not equal to the order of magnitude of the moments present in that term. A theory of order λ_0 considers only those terms—in all the equations—whose leading order of influence in the conservation laws is $\lambda \leq \lambda_0$, and the terms not fulfilling this condition are simply ignored.

In order to apply this condition, it suffices to start with the conservation laws, and add the relevant terms step-by-step, order-by-order. We start with order $\mathcal{O}(\varepsilon^0)$ equations (Euler), then add the relevant terms to obtain order $\mathcal{O}(\varepsilon^1)$ equations (Fick, Navier–Stokes, and Fourier equations) and so on.

8.2 Relevant moment equations

As we shall be deriving the *linear* regularized moment equations for a binary mixture of gases α and β interacting with *Maxwell* interaction potential, it is better to start with linear-dimensionless moment equations of § 5.1.1 for Maxwell molecules. Furthermore, we would also need the mass and energy balance equations of the mixture in linear-dimensionless form, which are obtained from (2.26) by using (5.1), (5.2) and ignoring the external forces.

Let us introduce the new variables: average temperature T (cf. (2.7)₃) and temperature difference ΔT defined as

$$T = \frac{n_\alpha T_\alpha + n_\beta T_\beta}{n_\alpha + n_\beta} \quad \text{and} \quad \Delta T = T_\alpha - T_\beta.$$

Now, we linearize the average temperature and temperature difference around their respective ground states, i.e., $T = T_o + \varepsilon \tilde{T}$ and $\Delta T = \varepsilon \Delta \tilde{T}$. Thus, $\hat{T} = \tilde{T}/T_o$ and $\Delta \hat{T} = \Delta \tilde{T}/T_o$ denote the linear-dimensionless perturbations to average temperature and temperature difference from their respective ground states, respectively. It is emphasized that all the quantities with over hats except $\hat{t}$ and $\hat{x}_i$'s always mean the linear-dimensionless perturbations to their respective ground states; although in the following, sometimes they are referred with their actual names for simplicity. We shall see below that replacing $\hat{T}_\alpha$ and $\hat{T}_\beta$ with $\hat{T}$ and $\Delta \hat{T}$ in the moment equations is worth because even though the leading orders of $\hat{T}_\alpha$, $\hat{T}_\beta$ and $\hat{T}$ are zero, the leading order of $\Delta \hat{T}$ is two. Moreover, it is also better to use the reduced partial heat fluxes (2.30) instead of usual partial heat fluxes of the constituents, since the right-hand sides of the moment equations for the reduced heat fluxes decouple from the diffusion velocities. The linearization and scaling for the reduced heat fluxes are analogous to the corresponding heat fluxes. The dimensionless reduced heat fluxes for the constituents in the mixture are given by

$$\hat{h}_i^{(\alpha)} = \hat{q}_i^{(\alpha)} - \frac{5}{2} \hat{u}_i^{(\alpha)} \quad \text{and} \quad \hat{h}_i^{(\beta)} = \hat{q}_i^{(\beta)} - \frac{5}{2} \hat{u}_i^{(\beta)}.$$

Additionally, we shall also use the following abbreviations in order to simplify the notations.

$$\frac{v_o}{\sqrt{\theta_\alpha^\circ}} = \varkappa_\alpha, \quad \frac{v_o}{\sqrt{\theta_\beta^\circ}} = \varkappa_\beta, \quad \mathbf{x}_\alpha^\circ \varkappa_\alpha^2 + \mathbf{x}_\beta^\circ \varkappa_\beta^2 = \varkappa.$$

Note that $\varkappa$ becomes 1 on taking the velocity scale as $v_o = \sqrt{kT_o/m}$ with $m = \mathbf{x}_\alpha^\circ m_\alpha + \mathbf{x}_\beta^\circ m_\beta$. In the following, we shall write the moment equations of § 5.1.1 by replacing $\hat{T}_\alpha$, $\hat{T}_\beta$, $\hat{q}_i^{(\alpha)}$ and $\hat{q}_i^{(\beta)}$ with $\hat{T}$, $\Delta \hat{T}$, $\hat{h}_i^{(\alpha)}$ and $\hat{h}_i^{(\beta)}$. Consequently, we shall write the moment equations for the new variables— $\hat{T}$, $\Delta \hat{T}$, $\hat{h}_i^{(\alpha)}$ and $\hat{h}_i^{(\beta)}$ —instead of those for the variables $\hat{T}_\alpha$, $\hat{T}_\beta$, $\hat{q}_i^{(\alpha)}$ and $\hat{q}_i^{(\beta)}$, and we shall also rename Kn to ε . Therefore, hereafter ε is always the Knudsen number. The moment equations for the new variables can be obtained by the appropriate linear combinations of those

for the old ones.

8.2.1 Moment equations in new variables

The mass balance equations for the individual constituents and for the mixture, and the momentum and energy balance equations for the mixture (the conservation laws for the mixture) read

$$\kappa_\alpha \left(\frac{\partial \hat{n}_\alpha}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} \right) + \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} = 0, \quad (8.1)$$

$$\kappa_\beta \left(\frac{\partial \hat{n}_\beta}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} \right) + \frac{\partial \hat{u}_i^{(\beta)}}{\partial \hat{x}_i} = 0, \quad (8.2)$$

$$\frac{\partial}{\partial \hat{t}} (\mu_\alpha x_\alpha^\circ \hat{n}_\alpha + \mu_\beta x_\beta^\circ \hat{n}_\beta) + (\mu_\alpha x_\alpha^\circ + \mu_\beta x_\beta^\circ) \frac{\partial \hat{v}_i}{\partial \hat{x}_i} = 0, \quad (8.3)$$

$$\kappa \frac{\partial \hat{v}_i}{\partial \hat{t}} + \frac{\partial}{\partial \hat{x}_j} \left(x_\alpha^\circ \hat{\sigma}_{ij}^{(\alpha)} + x_\beta^\circ \hat{\sigma}_{ij}^{(\beta)} \right) + \frac{\partial}{\partial \hat{x}_i} (x_\alpha^\circ \hat{n}_\alpha + x_\beta^\circ \hat{n}_\beta) + \frac{\partial \hat{T}}{\partial \hat{x}_i} = 0, \quad (8.4)$$

$$\frac{3}{2} \frac{\partial \hat{T}}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} + \frac{x_\alpha^\circ}{\kappa_\alpha} \left(\frac{\partial \hat{h}_i^{(\alpha)}}{\partial \hat{x}_i} + \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} \right) + \frac{x_\beta^\circ}{\kappa_\beta} \left(\frac{\partial \hat{h}_i^{(\beta)}}{\partial \hat{x}_i} + \frac{\partial \hat{u}_i^{(\beta)}}{\partial \hat{x}_i} \right) = 0. \quad (8.5)$$

The linear-dimensionless balance equation for the temperature difference reads

$$\frac{3}{2} \frac{\partial \Delta \hat{T}}{\partial \hat{t}} + \frac{1}{\kappa_\alpha} \left(\frac{\partial \hat{h}_i^{(\alpha)}}{\partial \hat{x}_i} + \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} \right) - \frac{1}{\kappa_\beta} \left(\frac{\partial \hat{h}_i^{(\beta)}}{\partial \hat{x}_i} + \frac{\partial \hat{u}_i^{(\beta)}}{\partial \hat{x}_i} \right) = -\frac{1}{\varepsilon \Omega} \frac{\delta_5}{\kappa_\alpha} \Delta \hat{T}. \quad (8.6)$$

The other balance equations for the individual constituents read

$$\begin{aligned} & \kappa_\alpha \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{t}} + \frac{x_\beta^\circ}{\kappa} \left[\kappa_\beta^2 \left(\frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{x}_j} + \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} \right) - \kappa_\alpha^2 \left(\frac{\partial \hat{\sigma}_{ij}^{(\beta)}}{\partial \hat{x}_j} + \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} \right) \right] \\ & - \frac{x_\beta^\circ}{\kappa} (\kappa_\alpha^2 - \kappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} + x_\beta^\circ \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} = -\delta_1 \frac{1}{\varepsilon \Omega} x_\beta^\circ \left(\hat{u}_i^{(\alpha)} - \frac{\kappa_\alpha}{\kappa_\beta} \hat{u}_i^{(\beta)} \right), \end{aligned} \quad (8.7)$$

$$\begin{aligned} & \kappa_\beta \frac{\partial \hat{u}_i^{(\beta)}}{\partial \hat{t}} + \frac{x_\alpha^\circ}{\kappa} \left[\kappa_\alpha^2 \left(\frac{\partial \hat{\sigma}_{ij}^{(\beta)}}{\partial \hat{x}_j} + \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} \right) - \kappa_\beta^2 \left(\frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{x}_j} + \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} \right) \right] \\ & - \frac{x_\alpha^\circ}{\kappa} (\kappa_\beta^2 - \kappa_\alpha^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} - x_\alpha^\circ \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} = -\gamma_1 \frac{1}{\varepsilon \Omega} x_\alpha^\circ \left(\hat{u}_i^{(\beta)} - \frac{\kappa_\beta}{\kappa_\alpha} \hat{u}_i^{(\alpha)} \right), \end{aligned} \quad (8.8)$$

$$\begin{aligned} \kappa_\alpha \left(\frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{t}} + 2 \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right) + \frac{\partial \hat{m}_{ijk}^{(\alpha)}}{\partial \hat{x}_k} + \frac{4}{5} \frac{\partial \hat{h}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j \rangle}} + 2 \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j \rangle}} \\ = -\frac{1}{\varepsilon \Omega} \left\{ \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{\sigma}_{ij}^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_{9\beta} \hat{\sigma}_{ij}^{(\alpha)} - \delta_{11\beta} \hat{\sigma}_{ij}^{(\beta)} \right) \right\}, \end{aligned} \quad (8.9)$$

$$\begin{aligned} \kappa_\beta \left(\frac{\partial \hat{\sigma}_{ij}^{(\beta)}}{\partial \hat{t}} + 2 \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right) + \frac{\partial \hat{m}_{ijk}^{(\beta)}}{\partial \hat{x}_k} + \frac{4}{5} \frac{\partial \hat{h}_{\langle i}^{(\beta)}}{\partial \hat{x}_{j \rangle}} + 2 \frac{\partial \hat{u}_{\langle i}^{(\beta)}}{\partial \hat{x}_{j \rangle}} \\ = -\frac{1}{\varepsilon \Omega} \left\{ \mathbf{x}_\beta^\circ \Omega_\beta \hat{\sigma}_{ij}^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_{9\alpha} \hat{\sigma}_{ij}^{(\beta)} - \gamma_{11\alpha} \hat{\sigma}_{ij}^{(\alpha)} \right) \right\}, \end{aligned} \quad (8.10)$$

$$\begin{aligned} \kappa_\alpha \frac{\partial \hat{h}_i^{(\alpha)}}{\partial \hat{t}} + \frac{1}{2} \frac{\partial \hat{R}_{ij}^{(\alpha)}}{\partial \hat{x}_j} + \frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{x}_j} + \frac{1}{6} \frac{\partial \hat{\Delta}_\alpha}{\partial \hat{x}_i} + \frac{5}{2} \frac{\partial \hat{T}}{\partial \hat{x}_i} + \frac{5}{2} \mathbf{x}_\beta^\circ \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \\ = -\frac{1}{\varepsilon \Omega} \left\{ \frac{2}{3} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{h}_i^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_{13\beta} \hat{h}_i^{(\alpha)} - \delta_{15\beta} \hat{h}_i^{(\beta)} \right) \right\}, \end{aligned} \quad (8.11)$$

$$\begin{aligned} \kappa_\beta \frac{\partial \hat{h}_i^{(\beta)}}{\partial \hat{t}} + \frac{1}{2} \frac{\partial \hat{R}_{ij}^{(\beta)}}{\partial \hat{x}_j} + \frac{\partial \hat{\sigma}_{ij}^{(\beta)}}{\partial \hat{x}_j} + \frac{1}{6} \frac{\partial \hat{\Delta}_\beta}{\partial \hat{x}_i} + \frac{5}{2} \frac{\partial \hat{T}}{\partial \hat{x}_i} - \frac{5}{2} \mathbf{x}_\alpha^\circ \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \\ = -\frac{1}{\varepsilon \Omega} \left\{ \frac{2}{3} \mathbf{x}_\beta^\circ \Omega_\beta \hat{h}_i^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_{13\alpha} \hat{h}_i^{(\beta)} - \gamma_{15\alpha} \hat{h}_i^{(\alpha)} \right) \right\}, \end{aligned} \quad (8.12)$$

$$\kappa_\alpha \frac{\partial \hat{m}_{ijk}^{(\alpha)}}{\partial \hat{t}} + \frac{3}{7} \frac{\partial \hat{R}_{ij}^{(\alpha)}}{\partial \hat{x}_k} + 3 \frac{\partial \hat{\sigma}_{ij}^{(\alpha)}}{\partial \hat{x}_k} = -\frac{1}{\varepsilon \Omega} \left\{ \frac{3}{2} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{m}_{ijk}^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_{17\beta} \hat{m}_{ijk}^{(\alpha)} - \delta_{18\beta} \hat{m}_{ijk}^{(\beta)} \right) \right\}, \quad (8.13)$$

$$\kappa_\beta \frac{\partial \hat{m}_{ijk}^{(\beta)}}{\partial \hat{t}} + \frac{3}{7} \frac{\partial \hat{R}_{ij}^{(\beta)}}{\partial \hat{x}_k} + 3 \frac{\partial \hat{\sigma}_{ij}^{(\beta)}}{\partial \hat{x}_k} = -\frac{1}{\varepsilon \Omega} \left\{ \frac{3}{2} \mathbf{x}_\beta^\circ \Omega_\beta \hat{m}_{ijk}^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_{17\alpha} \hat{m}_{ijk}^{(\beta)} - \gamma_{18\alpha} \hat{m}_{ijk}^{(\alpha)} \right) \right\}, \quad (8.14)$$

$$\kappa_\alpha \frac{\partial \hat{R}_{ij}^{(\alpha)}}{\partial \hat{t}} + 2 \frac{\partial \hat{m}_{ijk}^{(\alpha)}}{\partial \hat{x}_k} + \frac{28}{5} \frac{\partial \hat{h}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j \rangle}} = -\frac{1}{\varepsilon \Omega} \left\{ \frac{7}{6} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{R}_{ij}^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_{21\beta} \hat{R}_{ij}^{(\alpha)} - \delta_{23\beta} \hat{R}_{ij}^{(\beta)} \right) \right\}, \quad (8.15)$$

$$\kappa_\beta \frac{\partial \hat{R}_{ij}^{(\beta)}}{\partial \hat{t}} + 2 \frac{\partial \hat{m}_{ijk}^{(\beta)}}{\partial \hat{x}_k} + \frac{28}{5} \frac{\partial \hat{h}_{\langle i}^{(\beta)}}{\partial \hat{x}_{j \rangle}} = -\frac{1}{\varepsilon \Omega} \left\{ \frac{7}{6} \mathbf{x}_\beta^\circ \Omega_\beta \hat{R}_{ij}^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_{21\alpha} \hat{R}_{ij}^{(\beta)} - \gamma_{23\alpha} \hat{R}_{ij}^{(\alpha)} \right) \right\}, \quad (8.16)$$

$$\kappa_\alpha \frac{\partial \hat{\Delta}_\alpha}{\partial \hat{t}} + 8 \frac{\partial \hat{h}_i^{(\alpha)}}{\partial \hat{x}_i} = -\frac{1}{\varepsilon \Omega} \left\{ \frac{2}{3} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{\Delta}_\alpha + \mathbf{x}_\beta^\circ \left(\delta_{25\beta} \hat{\Delta}_\alpha - \delta_{26\beta} \hat{\Delta}_\beta \right) \right\}, \quad (8.17)$$

$$\kappa_\beta \frac{\partial \hat{\Delta}_\beta}{\partial \hat{t}} + 8 \frac{\partial \hat{h}_i^{(\beta)}}{\partial \hat{x}_i} = -\frac{1}{\varepsilon \Omega} \left\{ \frac{2}{3} \mathbf{x}_\beta^\circ \Omega_\beta \hat{\Delta}_\beta + \mathbf{x}_\alpha^\circ \left(\gamma_{25\alpha} \hat{\Delta}_\beta - \gamma_{26\alpha} \hat{\Delta}_\alpha \right) \right\}. \quad (8.18)$$

In (8.6)–(8.8), we have also used the relations

$$\delta_5 = \sqrt{\frac{\mu_\alpha}{\mu_\beta}} \gamma_5 = \frac{\varkappa_\alpha}{\varkappa_\beta} \gamma_5, \quad \delta_3 = \sqrt{\frac{\mu_\alpha}{\mu_\beta}} \delta_1 = \frac{\varkappa_\alpha}{\varkappa_\beta} \delta_1 \quad \text{and} \quad \gamma_3 = \sqrt{\frac{\mu_\beta}{\mu_\alpha}} \gamma_1 = \frac{\varkappa_\beta}{\varkappa_\alpha} \gamma_1.$$

8.3 The order of magnitude of moments

We shall now assign the orders of magnitude to the moments and then construct new sets of moments in such a way that we have minimum number of variables at each order.

In order to examine the order of magnitude of moments, we expand the non-conserved quantities (Ψ) in powers of the Knudsen number (ε) as

$$\Psi = \Psi_{|0} + \varepsilon \Psi_{|1} + \varepsilon^2 \Psi_{|2} + \dots,$$

where $\Psi \in \{\Delta\hat{T}, \hat{u}_i^{(\alpha)}, \hat{u}_i^{(\beta)}, \hat{\sigma}_{ij}^{(\alpha)}, \hat{\sigma}_{ij}^{(\beta)}, \hat{h}_i^{(\alpha)}, \hat{h}_i^{(\beta)}, \hat{m}_{ijk}^{(\alpha)}, \hat{m}_{ijk}^{(\beta)}, \hat{R}_{ij}^{(\alpha)}, \hat{R}_{ij}^{(\beta)}, \hat{\Delta}_\alpha, \hat{\Delta}_\beta\}$, and the quantities $\Psi_{|0}, \Psi_{|1}, \Psi_{|2}, \dots$ are of order $\mathcal{O}(\varepsilon^0)$. Now, we shall substitute the above expansions in (8.6)–(8.18) and compare the coefficients of each power of ε .

Comparing coefficients of ε^{-1} on both sides of (8.6)–(8.18) one readily finds that $\Psi_{|0} = 0$ for all $\Psi \in \{\Delta\hat{T}, \hat{u}_i^{(\alpha)}, \hat{u}_i^{(\beta)}, \hat{\sigma}_{ij}^{(\alpha)}, \hat{\sigma}_{ij}^{(\beta)}, \hat{h}_i^{(\alpha)}, \hat{h}_i^{(\beta)}, \hat{m}_{ijk}^{(\alpha)}, \hat{m}_{ijk}^{(\beta)}, \hat{R}_{ij}^{(\alpha)}, \hat{R}_{ij}^{(\beta)}, \hat{\Delta}_\alpha, \hat{\Delta}_\beta\}$ because there are no terms of order $\mathcal{O}(\varepsilon^{-1})$ on the left-hand sides of the balance equations for these quantities. This concludes that the leading orders of all the non-conserved quantities are at least one.

Comparing coefficients of ε^0 on both sides of (8.6)–(8.18), it turns out that $\hat{u}_{i|1}^{(\alpha)}, \hat{u}_{i|1}^{(\beta)}, \hat{\sigma}_{ij|1}^{(\alpha)}, \hat{\sigma}_{ij|1}^{(\beta)}, \hat{h}_{i|1}^{(\alpha)}, \hat{h}_{i|1}^{(\beta)}$ do not vanish whereas

$$\Delta\hat{T}_{|1} = \hat{m}_{ijk|1}^{(\alpha)} = \hat{m}_{ijk|1}^{(\beta)} = \hat{R}_{ij|1}^{(\alpha)} = \hat{R}_{ij|1}^{(\beta)} = \hat{\Delta}_{\alpha|1} = \hat{\Delta}_{\beta|1} = 0, \quad (8.19)$$

see appendix B for details. In other words, the leading orders of the diffusion velocities, stresses and heat fluxes of the both the constituents are one while the leading orders of temperature difference and other higher moments for both the constituents are at least two.

Comparing the coefficients of ε^1 on both sides of (8.6) and (8.13)–(8.18), it turns out that none of $\Delta\hat{T}_{|2}, \hat{m}_{ijk|2}^{(\alpha)}, \hat{m}_{ijk|2}^{(\beta)}, \hat{R}_{ij|2}^{(\alpha)}, \hat{R}_{ij|2}^{(\beta)}, \hat{\Delta}_{\alpha|2}$, and $\hat{\Delta}_{\beta|2}$ vanish, see appendix B again for details. Therefore, the leading orders of all these quantities are two.

We shall not go further as it would be sufficient for obtaining the third order accurate (regularized) moment equations.

8.4 Minimum number of moments at a given order

8.4.1 Minimum number of moments of $\mathcal{O}(\varepsilon)$

We have established in § 8.3 that $\hat{u}_i^{(\alpha)}, \hat{u}_i^{(\beta)}, \hat{\sigma}_{ij}^{(\alpha)}, \hat{\sigma}_{ij}^{(\beta)}, \hat{h}_i^{(\alpha)}, \hat{h}_i^{(\beta)}$ are the moments of order $\mathcal{O}(\varepsilon)$. In order to have minimum number of moments of order $\mathcal{O}(\varepsilon)$, let us first write down their leading order contributions (by solving (B.2) along with the relation $\rho_\alpha \mathbf{u}_\alpha + \rho_\beta \mathbf{u}_\beta = \mathbf{0}$ in dimensionless

form, (B.3) and (B.4) of appendix B), which read

$$\hat{u}_{i|1}^{(\alpha)} = -x_\beta^\circ \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left[\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right], \quad \hat{u}_{i|1}^{(\beta)} = -\frac{\varkappa_\alpha}{\varkappa_\beta} \frac{x_\alpha^\circ}{x_\beta^\circ} \hat{u}_{i|1}^{(\alpha)}, \quad (8.20)$$

$$\left. \begin{aligned} \hat{\sigma}_{ij|1}^{(\alpha)} &= -2\eta_\alpha \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \quad \text{where} \quad \eta_\alpha = \frac{\Omega \{ \varkappa_\alpha (x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_9) + \varkappa_\beta x_\beta^\circ \delta_{11} \}}{(x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_9)(x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_9) - x_\alpha^\circ x_\beta^\circ \gamma_{11} \delta_{11}}, \\ \hat{\sigma}_{ij|1}^{(\beta)} &= -2\eta_\beta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \quad \text{where} \quad \eta_\beta = \frac{\Omega \{ \varkappa_\beta (x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_9) + \varkappa_\alpha x_\alpha^\circ \gamma_{11} \}}{(x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_9)(x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_9) - x_\alpha^\circ x_\beta^\circ \gamma_{11} \delta_{11}}, \end{aligned} \right\} \quad (8.21)$$

$$\left. \begin{aligned} \hat{h}_{i|1}^{(\alpha)} &= -\kappa_\alpha \frac{\partial \hat{T}}{\partial \hat{x}_i} \quad \text{where} \quad \kappa_\alpha = \frac{\frac{5}{2}\Omega \left\{ \left(\frac{2}{3}x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) + x_\beta^\circ \delta_{15} \right\}}{\left(\frac{2}{3}x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) \left(\frac{2}{3}x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) - x_\alpha^\circ x_\beta^\circ \gamma_{15} \delta_{15}}, \\ \hat{h}_{i|1}^{(\beta)} &= -\kappa_\beta \frac{\partial \hat{T}}{\partial \hat{x}_i} \quad \text{where} \quad \kappa_\beta = \frac{\frac{5}{2}\Omega \left\{ \left(\frac{2}{3}x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) + x_\alpha^\circ \gamma_{15} \right\}}{\left(\frac{2}{3}x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) \left(\frac{2}{3}x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) - x_\alpha^\circ x_\beta^\circ \gamma_{15} \delta_{15}}. \end{aligned} \right\} \quad (8.22)$$

Equations (8.20) are the Fick's law of diffusion (in linearized form) for the mixture. Equations (8.21) represent the Navier–Stokes law for the components in the mixture, with η_α and η_β being the expressions for dimensionless viscosities of the constituents in the mixture. Equations (8.22) represent the Fourier's law for the components in the mixture, with κ_α and κ_β being the expressions for dimensionless heat conductivities of the constituents in the mixture. It should be noted that the usual heat fluxes in case of binary gas-mixtures will depend on the gradients of number densities as well whereas the reduced heat fluxes of the components are proportional to the gradient of the average temperature only, like in Fourier's law for a single gas.

As the diffusion velocities $\hat{u}_i^{(\alpha)}$ and $\hat{u}_i^{(\beta)}$ depend on each other, one can use any one of them in the moment equations. Moreover, the other first order quantities—the stresses $\hat{\sigma}_{ij}^{(\alpha)}$ and $\hat{\sigma}_{ij}^{(\beta)}$, and the reduced heat fluxes $\hat{h}_i^{(\alpha)}$ and $\hat{h}_i^{(\beta)}$ —are linearly combined as below in order to have minimum number of moments of order $\mathcal{O}(\varepsilon)$. We introduce

$$\left. \begin{aligned} \hat{\sigma}_{ij} &= x_\alpha^\circ \hat{\sigma}_{ij}^{(\alpha)} + x_\beta^\circ \hat{\sigma}_{ij}^{(\beta)}, & \Delta \hat{\sigma}_{ij} &= \kappa_1 \hat{\sigma}_{ij}^{(\alpha)} - \kappa_2 \hat{\sigma}_{ij}^{(\beta)}, \\ \hat{h}_i &= \frac{x_\alpha^\circ}{\varkappa_\alpha} \hat{h}_i^{(\alpha)} + \frac{x_\beta^\circ}{\varkappa_\beta} \hat{h}_i^{(\beta)}, & \Delta \hat{h}_i &= \kappa_3 \hat{h}_i^{(\alpha)} - \kappa_4 \hat{h}_i^{(\beta)}, \end{aligned} \right\} \quad (8.23)$$

where $\hat{\sigma}_{ij}$ and $\hat{h}_i$ are the (dimensionless) total stress and the (dimensionless) total reduced heat flux in the mixture, respectively, and

$$\left. \begin{aligned} \kappa_1 &= \varkappa_\beta (x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_9) + \varkappa_\alpha x_\alpha^\circ \gamma_{11}, & \kappa_2 &= \varkappa_\alpha (x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_9) + \varkappa_\beta x_\beta^\circ \delta_{11}, \\ \kappa_3 &= \left(\frac{2}{3}x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) + x_\alpha^\circ \gamma_{15}, & \kappa_4 &= \left(\frac{2}{3}x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) + x_\beta^\circ \delta_{15}, \end{aligned} \right\} \quad (8.24)$$

so that the leading orders of the total stress $\hat{\sigma}_{ij}$ and the total reduced heat flux $\hat{h}_i$ are one while the leading orders of $\Delta \hat{\sigma}_{ij}$ and $\Delta \hat{h}_i$ are two. Notice that the total stress (σ_{ij}) and the total

reduced heat flux (h_i) are scaled as

$$\hat{\sigma}_{ij} = \frac{\sigma_{ij}}{k n_o T_o} \quad \text{and} \quad \hat{h}_i = \frac{h_i}{k n_o T_o v_o}.$$

Thus, the minimum moments of order $\mathcal{O}(\varepsilon)$ are any one of the two diffusion velocities of the constituents, let us say $\hat{u}_i^{(\alpha)}$, the total stress $\hat{\sigma}_{ij}$ and the total reduced heat flux $\hat{h}_i$.

From (8.23), one can obtain the expressions for the stresses and the reduced heat fluxes of the individual components in terms of the other variables. These will be needed in getting the minimum number of moments of order $\mathcal{O}(\varepsilon^2)$, and are as follows.

$$\left. \begin{aligned} \hat{\sigma}_{ij}^{(\alpha)} &= \frac{\kappa_2 \hat{\sigma}_{ij} + x_\beta^\circ \Delta \hat{\sigma}_{ij}}{x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1}, & \hat{\sigma}_{ij}^{(\beta)} &= \frac{\kappa_1 \hat{\sigma}_{ij} - x_\alpha^\circ \Delta \hat{\sigma}_{ij}}{x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1}, \\ \hat{h}_i^{(\alpha)} &= \frac{\varkappa_\alpha (\kappa_4 \varkappa_\beta \hat{h}_i + x_\beta^\circ \Delta \hat{h}_i)}{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha}, & \hat{h}_i^{(\beta)} &= \frac{\varkappa_\beta (\kappa_3 \varkappa_\alpha \hat{h}_i - x_\alpha^\circ \Delta \hat{h}_i)}{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha}. \end{aligned} \right\} \quad (8.25)$$

8.4.2 Minimum number of moments of $\mathcal{O}(\varepsilon^2)$

We have established in § 8.3 that the order $\mathcal{O}(\varepsilon^2)$ quantities are $\Delta \hat{T}$, $\Delta \hat{\sigma}_{ij}$, $\Delta \hat{h}_i$, $\hat{m}_{ijk}^{(\alpha)}$, $\hat{m}_{ijk}^{(\beta)}$, $\hat{R}_{ij}^{(\alpha)}$, $\hat{R}_{ij}^{(\beta)}$, $\hat{\Delta}_\alpha$ and $\hat{\Delta}_\beta$. Notice from the leading order contributions of $\Delta \hat{T}$, $\Delta \hat{\sigma}_{ij}$ and $\Delta \hat{h}_i$ (cf. (B.9), (D.8)₂ and (D.9)₂) that $\Delta \hat{T}$, $\Delta \hat{\sigma}_{ij}$ and $\Delta \hat{h}_i$ can neither be linearly combined among themselves nor with any other moments in order to produce a quantity of order higher than order $\mathcal{O}(\varepsilon^2)$. However, the other moments in the list— $\hat{m}_{ijk}^{(\alpha)}$, $\hat{m}_{ijk}^{(\beta)}$, $\hat{R}_{ij}^{(\alpha)}$, $\hat{R}_{ij}^{(\beta)}$, $\hat{\Delta}_\alpha$ and $\hat{\Delta}_\beta$ —can be linearly combined to produce some quantities of order $\mathcal{O}(\varepsilon^3)$. To this end, let us first write down the leading order contributions of $\hat{m}_{ijk}^{(\alpha)}$, $\hat{m}_{ijk}^{(\beta)}$, $\hat{R}_{ij}^{(\alpha)}$, $\hat{R}_{ij}^{(\beta)}$, $\hat{\Delta}_\alpha$ and $\hat{\Delta}_\beta$ (by solving equations (B.10), (B.11) and (B.12) of appendix B and using (8.25)), which read

$$\left. \begin{aligned} \hat{m}_{ijk|2}^{(\alpha)} &= -c_m^{(\alpha)} \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{x}_k}, & \hat{m}_{ijk|2}^{(\beta)} &= -c_m^{(\beta)} \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{x}_k}, \\ \hat{R}_{ij|2}^{(\alpha)} &= -c_R^{(\alpha)} \frac{\partial \hat{h}_{i|1}}{\partial \hat{x}_j}, & \hat{R}_{ij|2}^{(\beta)} &= -c_R^{(\beta)} \frac{\partial \hat{h}_{i|1}}{\partial \hat{x}_j}, \\ \hat{\Delta}_{\alpha|2} &= -c_\Delta^{(\alpha)} \frac{\partial \hat{h}_{i|1}}{\partial \hat{x}_i}, & \hat{\Delta}_{\beta|2} &= -c_\Delta^{(\beta)} \frac{\partial \hat{h}_{i|1}}{\partial \hat{x}_i}. \end{aligned} \right\} \quad (8.26)$$

For better readability, the coefficients $c_m^{(\alpha)}$, $c_m^{(\beta)}$, $c_R^{(\alpha)}$, $c_R^{(\beta)}$, $c_\Delta^{(\alpha)}$ and $c_\Delta^{(\beta)}$ are given in appendix C. The quantities, $\hat{m}_{ijk}^{(\alpha)}$, $\hat{m}_{ijk}^{(\beta)}$, $\hat{R}_{ij}^{(\alpha)}$, $\hat{R}_{ij}^{(\beta)}$, $\hat{\Delta}_\alpha$ and $\hat{\Delta}_\beta$ are now linearly combined as below in order to have minimum number of moments of order $\mathcal{O}(\varepsilon^2)$. We introduce

$$\left. \begin{aligned} \hat{m}_{ijk} &= \frac{x_\alpha^\circ}{\varkappa_\alpha} \hat{m}_{ijk}^{(\alpha)} + \frac{x_\beta^\circ}{\varkappa_\beta} \hat{m}_{ijk}^{(\beta)}, & \Delta \hat{m}_{ijk} &= \kappa_5 \hat{m}_{ijk}^{(\alpha)} - \kappa_6 \hat{m}_{ijk}^{(\beta)}, \\ \hat{R}_{ij} &= \frac{x_\alpha^\circ}{\varkappa_\alpha^2} \hat{R}_{ij}^{(\alpha)} + \frac{x_\beta^\circ}{\varkappa_\beta^2} \hat{R}_{ij}^{(\beta)}, & \Delta \hat{R}_{ij} &= \kappa_7 \hat{R}_{ij}^{(\alpha)} - \kappa_8 \hat{R}_{ij}^{(\beta)}, \\ \hat{\Delta} &= \frac{x_\alpha^\circ}{\varkappa_\alpha^2} \hat{\Delta}_\alpha + \frac{x_\beta^\circ}{\varkappa_\beta^2} \hat{\Delta}_\beta, & \Delta \hat{\Delta} &= \kappa_9 \hat{\Delta}_\alpha - \kappa_{10} \hat{\Delta}_\beta, \end{aligned} \right\} \quad (8.27)$$

where $\hat{m}_{ijk}$, $\hat{R}_{ij}$ and $\hat{\Delta}$ are the respective (dimensionless) total higher moments in the mixture, and

$$\left. \begin{aligned} \kappa_5 &= \kappa_1 \left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) + \kappa_2 x_\alpha^\circ \gamma_{18}, & \kappa_6 &= \kappa_2 \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) + \kappa_1 x_\beta^\circ \delta_{18}, \\ \kappa_7 &= \kappa_3 \left(\frac{7}{6} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{21} \right) + \kappa_4 x_\alpha^\circ \gamma_{23}, & \kappa_8 &= \kappa_4 \left(\frac{7}{6} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{21} \right) + \kappa_3 x_\beta^\circ \delta_{23}, \\ \kappa_9 &= \kappa_3 \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{25} \right) + \kappa_4 x_\alpha^\circ \gamma_{26}, & \kappa_{10} &= \kappa_4 \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{25} \right) + \kappa_3 x_\beta^\circ \delta_{26}, \end{aligned} \right\} \quad (8.28)$$

so that the leading orders of $\hat{m}_{ijk}$, $\hat{R}_{ij}$ and $\hat{\Delta}$ are two while the leading orders of $\Delta\hat{m}_{ijk}$, $\Delta\hat{R}_{ij}$ and $\Delta\hat{\Delta}$ are three. Thus, the minimum moments of order $\mathcal{O}(\varepsilon^2)$ are $\Delta\hat{T}$, $\Delta\hat{\sigma}_{ij}$, $\Delta\hat{h}_i$, $\hat{m}_{ijk}$, $\hat{R}_{ij}$ and $\hat{\Delta}$. Notice, again, that the total higher order moments (m_{ijk} , R_{ij} , Δ) are scaled as

$$\hat{m}_{ijk} = \frac{m_{ijk}}{k n_o T_o v_o}, \quad \hat{R}_{ij} = \frac{R_{ij}}{k n_o T_o v_o^2} \quad \text{and} \quad \hat{\Delta} = \frac{\Delta}{k n_o T_o v_o^2}.$$

From (8.27), one can obtain the expressions for the higher moments of the individual components in terms of the other variables. These will be needed later and are as follows.

$$\left. \begin{aligned} \hat{m}_{ijk}^{(\alpha)} &= \frac{\varkappa_\alpha (\kappa_6 \varkappa_\beta \hat{m}_{ijk} + x_\beta^\circ \Delta \hat{m}_{ijk})}{x_\alpha^\circ \kappa_6 \varkappa_\beta + x_\beta^\circ \kappa_5 \varkappa_\alpha}, & \hat{m}_{ijk}^{(\beta)} &= \frac{\varkappa_\beta (\kappa_5 \varkappa_\alpha \hat{m}_{ijk} - x_\alpha^\circ \Delta \hat{m}_{ijk})}{x_\alpha^\circ \kappa_6 \varkappa_\beta + x_\beta^\circ \kappa_5 \varkappa_\alpha}, \\ \hat{R}_{ij}^{(\alpha)} &= \frac{\varkappa_\alpha^2 (\kappa_8 \varkappa_\beta^2 \hat{R}_{ij} + x_\beta^\circ \Delta \hat{R}_{ij})}{x_\alpha^\circ \kappa_8 \varkappa_\beta^2 + x_\beta^\circ \kappa_7 \varkappa_\alpha^2}, & \hat{R}_{ij}^{(\beta)} &= \frac{\varkappa_\beta^2 (\kappa_7 \varkappa_\alpha^2 \hat{R}_{ij} - x_\alpha^\circ \Delta \hat{R}_{ij})}{x_\alpha^\circ \kappa_8 \varkappa_\beta^2 + x_\beta^\circ \kappa_7 \varkappa_\alpha^2}, \\ \hat{\Delta}_\alpha &= \frac{\varkappa_\alpha^2 (\kappa_{10} \varkappa_\beta^2 \hat{\Delta} + x_\beta^\circ \Delta \hat{\Delta})}{x_\alpha^\circ \kappa_{10} \varkappa_\beta^2 + x_\beta^\circ \kappa_9 \varkappa_\alpha^2}, & \hat{\Delta}_\beta &= \frac{\varkappa_\beta^2 (\kappa_9 \varkappa_\alpha^2 \hat{\Delta} - x_\alpha^\circ \Delta \hat{\Delta})}{x_\alpha^\circ \kappa_{10} \varkappa_\beta^2 + x_\beta^\circ \kappa_9 \varkappa_\alpha^2}. \end{aligned} \right\} \quad (8.29)$$

8.5 Moment equations with λ^{th} order accuracy

8.5.1 New system of equations

In the following, we shall write (8.3)–(8.18) in new variables $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$, $\Delta\hat{\sigma}_{ij}$, $\hat{h}_i$, $\Delta\hat{h}_i$, $\hat{m}_{ijk}$, $\Delta\hat{m}_{ijk}$, $\hat{R}_{ij}$, $\Delta\hat{R}_{ij}$, $\hat{\Delta}$, $\Delta\hat{\Delta}$ using (8.23) and (8.27). It is emphasized, however, that this change of variables is required only for deriving the third order accurate equations, which we are interested in, and it may not be required to change all the variables for the derivation of zeroth, first and second order accurate equations. Additionally, we shall write each moment by assigning its magnitude in powers of ε (“in gray colour”) in the new equations. These gray coloured ε ’s are included just for finding the terms of correct order while comparing the powers of ε on both sides (see below) and, of course, the value of gray coloured ε is essentially 1.

The conservation laws (eqs. (8.1)–(8.5)) in new variables read

$$\varkappa_\alpha \left(\frac{\partial \hat{n}_\alpha}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} \right) + \varepsilon \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} = 0, \quad (8.30)$$

$$\frac{\partial}{\partial t}(\mu_\alpha x_\alpha^\circ \hat{n}_\alpha + \mu_\beta x_\beta^\circ \hat{n}_\beta) + (\mu_\alpha x_\alpha^\circ + \mu_\beta x_\beta^\circ) \frac{\partial \hat{v}_i}{\partial \hat{x}_i} = 0, \quad (8.31)$$

$$\varkappa \frac{\partial \hat{v}_i}{\partial \hat{t}} + \varepsilon \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + x_\alpha^\circ \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} + x_\beta^\circ \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} + \frac{\partial \hat{T}}{\partial \hat{x}_i} = 0, \quad (8.32)$$

$$\frac{3}{2} \frac{\partial \hat{T}}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} + \varepsilon \frac{\partial \hat{h}_i}{\partial \hat{x}_i} + \varsigma_1 \varepsilon \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} = 0. \quad (8.33)$$

Note that the mass balance equation for the β -constituent, (8.2), is not included in this system as it can be obtained from (8.30) and (8.31). The other equations in new variables read

$$\begin{aligned} & \varkappa_\alpha \varepsilon \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{t}} + \varsigma_2 \varepsilon \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \varsigma_3 \varepsilon^2 \frac{\partial \Delta \hat{\sigma}_{ij}}{\partial \hat{x}_j} + x_\beta^\circ \varepsilon^2 \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \\ &= -\delta_1 \frac{1}{\varepsilon \Omega} \frac{\varkappa}{\varkappa_\beta^2} \left[\varepsilon \hat{u}_i^{(\alpha)} + x_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) \right], \end{aligned} \quad (8.34)$$

$$\frac{3}{2} \varepsilon^2 \frac{\partial \Delta \hat{T}}{\partial \hat{t}} + \varsigma_4 \varepsilon \frac{\partial \hat{h}_i}{\partial \hat{x}_i} + \varsigma_5 \varepsilon^2 \frac{\partial \Delta \hat{h}_i}{\partial \hat{x}_i} + \varsigma_6 \varepsilon \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} = -\frac{1}{\varepsilon \Omega} \frac{\delta_5}{\varkappa_\alpha} \varepsilon^2 \Delta \hat{T}, \quad (8.35)$$

$$\varepsilon \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{t}} + \varepsilon^2 \frac{\partial \hat{m}_{ijk}}{\partial \hat{x}_k} + \frac{4}{5} \varepsilon \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j \rangle}} + 2 \varsigma_1 \varepsilon \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j \rangle}} = -\frac{1}{\varepsilon \Omega} \left[\varpi_1 \left(\varepsilon \hat{\sigma}_{ij} + 2 \varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right) + \varpi_2 \varepsilon^2 \Delta \hat{\sigma}_{ij} \right], \quad (8.36)$$

$$\begin{aligned} & \varepsilon^2 \frac{\partial \Delta \hat{\sigma}_{ij}}{\partial \hat{t}} + \varsigma_7 \varepsilon^2 \frac{\partial \hat{m}_{ijk}}{\partial \hat{x}_k} + \varsigma_8 \varepsilon^3 \frac{\partial \Delta \hat{m}_{ijk}}{\partial \hat{x}_k} + \frac{4}{5} \varsigma_9 \varepsilon \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j \rangle}} + \frac{4}{5} \varsigma_{10} \varepsilon^2 \frac{\partial \Delta \hat{h}_{\langle i}}{\partial \hat{x}_{j \rangle}} + 2 \varsigma_{11} \varepsilon \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j \rangle}} \\ &= -\frac{1}{\varepsilon \Omega} \left[\varpi_3 \left(\varepsilon \hat{\sigma}_{ij} + 2 \varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right) + \varpi_4 \varepsilon^2 \Delta \hat{\sigma}_{ij} \right], \end{aligned} \quad (8.37)$$

$$\begin{aligned} & \varepsilon \frac{\partial \hat{h}_i}{\partial \hat{t}} + \varsigma_{12} \varepsilon \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \varsigma_{13} \varepsilon^2 \frac{\partial \Delta \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \frac{1}{2} \varepsilon^2 \frac{\partial \hat{R}_{ij}}{\partial \hat{x}_j} + \frac{1}{6} \varepsilon^2 \frac{\partial \hat{\Delta}}{\partial \hat{x}_i} + \frac{5}{2} \varsigma_{14} \varepsilon^2 \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \\ &= -\frac{1}{\varepsilon \Omega} \left[\varpi_5 \left(\varepsilon \hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) + \varpi_6 \varepsilon^2 \Delta \hat{h}_i \right], \end{aligned} \quad (8.38)$$

$$\begin{aligned} & \varepsilon^2 \frac{\partial \Delta \hat{h}_i}{\partial \hat{t}} + \varsigma_{15} \varepsilon \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \varsigma_{16} \varepsilon^2 \frac{\partial \Delta \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \frac{1}{2} \varsigma_{17} \varepsilon^2 \frac{\partial \hat{R}_{ij}}{\partial \hat{x}_j} + \frac{1}{2} \varsigma_{18} \varepsilon^3 \frac{\partial \Delta \hat{R}_{ij}}{\partial \hat{x}_j} \\ &+ \frac{1}{6} \varsigma_{19} \varepsilon^2 \frac{\partial \hat{\Delta}}{\partial \hat{x}_i} + \frac{1}{6} \varsigma_{20} \varepsilon^3 \frac{\partial \Delta \hat{\Delta}}{\partial \hat{x}_i} + \frac{5}{2} \varsigma_{21} \varepsilon^2 \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} = -\frac{1}{\varepsilon \Omega} \left[\varpi_7 \left(\varepsilon \hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) + \varpi_8 \varepsilon^2 \Delta \hat{h}_i \right]. \end{aligned} \quad (8.39)$$

$$\varepsilon^2 \frac{\partial \hat{m}_{ijk}}{\partial \hat{t}} + \frac{3}{7} \varepsilon^2 \frac{\partial \hat{R}_{\langle ij}}{\partial \hat{x}_{k\rangle}} + 3\varsigma_{13} \varepsilon^2 \frac{\partial \Delta \hat{\sigma}_{\langle ij}}{\partial \hat{x}_{k\rangle}} = -\frac{1}{\varepsilon \Omega} \left[\varpi_9 \left(\varepsilon^2 \hat{m}_{ijk} + \varepsilon \varsigma_m \varepsilon \frac{\partial \hat{\sigma}_{\langle ij}}{\partial \hat{x}_{k\rangle}} \right) + \varpi_{10} \varepsilon^3 \Delta \hat{m}_{ijk} \right], \quad (8.40)$$

$$\begin{aligned} & \varepsilon^3 \frac{\partial \Delta \hat{m}_{ijk}}{\partial \hat{t}} + \frac{3}{7} \varsigma_{22} \varepsilon^2 \frac{\partial \hat{R}_{\langle ij}}{\partial \hat{x}_{k\rangle}} + \frac{3}{7} \varsigma_{23} \varepsilon^3 \frac{\partial \Delta \hat{R}_{\langle ij}}{\partial \hat{x}_{k\rangle}} + 3\varsigma_{24} \varepsilon^2 \frac{\partial \Delta \hat{\sigma}_{\langle ij}}{\partial \hat{x}_{k\rangle}} \\ &= -\frac{1}{\varepsilon \Omega} \left[\varpi_{11} \left(\varepsilon^2 \hat{m}_{ijk} + \varepsilon \varsigma_m \varepsilon \frac{\partial \hat{\sigma}_{\langle ij}}{\partial \hat{x}_{k\rangle}} \right) + \varpi_{12} \varepsilon^3 \Delta \hat{m}_{ijk} \right], \end{aligned} \quad (8.41)$$

$$\begin{aligned} & \varepsilon^2 \frac{\partial \hat{R}_{ij}}{\partial \hat{t}} + 2\varsigma_{25} \varepsilon^2 \frac{\partial \hat{m}_{ijk}}{\partial \hat{x}_k} + 2\varsigma_{26} \varepsilon^3 \frac{\partial \Delta \hat{m}_{ijk}}{\partial \hat{x}_k} + \frac{28}{5} \varsigma_{27} \varepsilon^2 \frac{\partial \Delta \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} \\ &= -\frac{1}{\varepsilon \Omega} \left[\varpi_{13} \left(\varepsilon^2 \hat{R}_{ij} + \varepsilon \varsigma_R \varepsilon \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) + \varpi_{14} \varepsilon^3 \Delta \hat{R}_{ij} \right], \end{aligned} \quad (8.42)$$

$$\begin{aligned} & \varepsilon^3 \frac{\partial \Delta \hat{R}_{ij}}{\partial \hat{t}} + 2\varsigma_{28} \varepsilon^2 \frac{\partial \hat{m}_{ijk}}{\partial \hat{x}_k} + 2\varsigma_{29} \varepsilon^3 \frac{\partial \Delta \hat{m}_{ijk}}{\partial \hat{x}_k} + \frac{28}{5} \varsigma_{30} \varepsilon^2 \frac{\partial \Delta \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} \\ &= -\frac{1}{\varepsilon \Omega} \left[\varpi_{15} \left(\varepsilon^2 \hat{R}_{ij} + \varepsilon \varsigma_R \varepsilon \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) + \varpi_{16} \varepsilon^3 \Delta \hat{R}_{ij} \right], \end{aligned} \quad (8.43)$$

$$\varepsilon^2 \frac{\partial \hat{\Delta}}{\partial \hat{t}} + 8\varsigma_{27} \varepsilon^2 \frac{\partial \Delta \hat{h}_i}{\partial \hat{x}_i} = -\frac{1}{\varepsilon \Omega} \left[\varpi_{17} \left(\varepsilon^2 \hat{\Delta} + \varepsilon \varsigma_{\Delta} \varepsilon \frac{\partial \hat{h}_i}{\partial \hat{x}_i} \right) + \varpi_{18} \varepsilon^3 \Delta \hat{\Delta} \right], \quad (8.44)$$

$$\varepsilon^3 \frac{\partial \Delta \hat{\Delta}}{\partial \hat{t}} + 8\varsigma_{31} \varepsilon^2 \frac{\partial \Delta \hat{h}_i}{\partial \hat{x}_i} = -\frac{1}{\varepsilon \Omega} \left[\varpi_{19} \left(\varepsilon^2 \hat{\Delta} + \varepsilon \varsigma_{\Delta} \varepsilon \frac{\partial \hat{h}_i}{\partial \hat{x}_i} \right) + \varpi_{20} \varepsilon^3 \Delta \hat{\Delta} \right], \quad (8.45)$$

where

$$\eta = \frac{\Omega}{\varpi_1} = x_{\alpha}^{\circ} \eta_{\alpha} + x_{\beta}^{\circ} \eta_{\beta} \quad \text{and} \quad \kappa = \frac{5}{2} \frac{\Omega}{\varpi_5} \left(\frac{x_{\alpha}^{\circ}}{\varkappa_{\alpha}^2} + \frac{x_{\beta}^{\circ}}{\varkappa_{\beta}^2} \right) = \frac{x_{\alpha}^{\circ}}{\varkappa_{\alpha}} \kappa_{\alpha} + \frac{x_{\beta}^{\circ}}{\varkappa_{\beta}} \kappa_{\beta} \quad (8.46)$$

are the dimensionless viscosity and the dimensionless heat conductivity of the whole mixture, respectively, and all other coefficients are given in appendix C for better readability.

λ^{th} order accuracy: Clearly, the conservation laws (8.30)–(8.33) do not form a closed set of equations for $\hat{n}_{\alpha}$, $\hat{n}_{\beta}$, $\hat{v}_i$, $\hat{T}$ because they contain the additional variables $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$, $\hat{h}_i$. We shall speak of a theory with λ^{th} order accuracy, when $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$ and $\hat{h}_i$ are accurately known up to order $\mathcal{O}(\varepsilon^{\lambda})$.

8.5.2 Zeroth order accuracy: Euler equations

The equations with zeroth order accuracy result by setting the first order quantities to zero, i.e., by ignoring the terms with the factor ε in the conservation laws (8.30)–(8.33). This yields the

(linearized) Euler equations for the binary gas-mixture:

$$\left. \begin{aligned} \frac{\partial \hat{n}_\alpha}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} &= 0, \\ \frac{\partial}{\partial \hat{t}} (\mu_\alpha x_\alpha^\circ \hat{n}_\alpha + \mu_\beta x_\beta^\circ \hat{n}_\beta) + (\mu_\alpha x_\alpha^\circ + \mu_\beta x_\beta^\circ) \frac{\partial \hat{v}_i}{\partial \hat{x}_i} &= 0, \\ \varkappa \frac{\partial \hat{v}_i}{\partial \hat{t}} + x_\alpha^\circ \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} + x_\beta^\circ \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} + \frac{\partial \hat{T}}{\partial \hat{x}_i} &= 0, \\ \frac{3}{2} \frac{\partial \hat{T}}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} &= 0. \end{aligned} \right\} \quad (8.47)$$

8.5.3 First order accuracy: Fick, Navier–Stokes, and Fourier equations

For first order accuracy, one needs to include all the terms with factor ε^0 and ε^1 . That means all the terms in the conservation laws (8.30)–(8.33) are retained and therefore, the conservation laws at this order (on setting gray coloured ε to 1) read

$$\left. \begin{aligned} \varkappa_\alpha \left(\frac{\partial \hat{n}_\alpha}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} \right) + \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} &= 0, \\ \frac{\partial}{\partial \hat{t}} (\mu_\alpha x_\alpha^\circ \hat{n}_\alpha + \mu_\beta x_\beta^\circ \hat{n}_\beta) + (\mu_\alpha x_\alpha^\circ + \mu_\beta x_\beta^\circ) \frac{\partial \hat{v}_i}{\partial \hat{x}_i} &= 0, \\ \varkappa \frac{\partial \hat{v}_i}{\partial \hat{t}} + \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + x_\alpha^\circ \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} + x_\beta^\circ \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} + \frac{\partial \hat{T}}{\partial \hat{x}_i} &= 0, \\ \frac{3}{2} \frac{\partial \hat{T}}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} + \frac{\partial \hat{h}_i}{\partial \hat{x}_i} + \varsigma_1 \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} &= 0, \end{aligned} \right\} \quad (8.48)$$

where we need to find $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$ and $\hat{h}_i$ accurately up to first order, i.e., to their leading orders. For the leading orders of these quantities, only the terms up to order $\mathcal{O}(\varepsilon^0)$ in the balance equations for these quantities (in eqs. (8.34), (8.36) and (8.38)) need to be considered and, obviously, there are no terms of order $\mathcal{O}(\varepsilon^0)$ on the left-hand sides of (8.34), (8.36) and (8.38). Thus, we readily obtain the first order accurate $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$ and $\hat{h}_i$, which are the laws of Fick, Navier–Stokes, and Fourier:

$$\left. \begin{aligned} \hat{u}_i^{(\alpha)} &= -x_\beta^\circ \frac{\varepsilon}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right), \\ \hat{\sigma}_{ij} &= -2\varepsilon\eta \frac{\partial \hat{v}_{(i}}{\partial \hat{x}_{j)}}, \\ \hat{h}_i &= -\varepsilon\kappa \frac{\partial \hat{T}}{\partial \hat{x}_i}. \end{aligned} \right\} \quad (8.49)$$

8.5.4 Second order accuracy: 17 equations

At this order, we need to find $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$ and $\hat{h}_i$, appearing in the conservation laws, with second order accuracy. Therefore, one needs to consider all terms having factors ε^0 and ε^1 in the balance equations of these quantities (i.e., in eqs. (8.34), (8.36) and (8.38)), we have (on setting gray

coloured ε to 1)

$$\varkappa_\alpha \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{t}} + \varsigma_2 \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} = -\delta_1 \frac{1}{\varepsilon \Omega} \frac{\varkappa}{\varkappa_\beta^2} \left[\hat{u}_i^{(\alpha)} + \mathbf{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) \right], \quad (8.50)$$

$$\frac{\partial \hat{\sigma}_{ij}}{\partial \hat{t}} + \frac{4}{5} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + 2\varsigma_1 \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} = -\frac{1}{\varepsilon \Omega} \left[\varpi_1 \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) + \varpi_2 \Delta \hat{\sigma}_{ij} \right], \quad (8.51)$$

$$\frac{\partial \hat{h}_i}{\partial \hat{t}} + \varsigma_{12} \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} = -\frac{1}{\varepsilon \Omega} \left[\varpi_5 \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) + \varpi_6 \Delta \hat{h}_i \right], \quad (8.52)$$

where $\Delta \hat{\sigma}_{ij}$ and $\Delta \hat{h}_i$ are needed to be second order accurate. The second order accurate $\Delta \hat{\sigma}_{ij}$ and $\Delta \hat{h}_i$ follow from their respective balance equations (eqs. (8.37) and (8.39)) on considering terms up to order $\mathcal{O}(\varepsilon)$, we have

$$\Delta \hat{\sigma}_{ij} \approx \Delta \hat{\sigma}_{ij}^{(2)} = -\frac{\varpi_3}{\varpi_4} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) - \frac{\varepsilon \Omega}{\varpi_4} \left(\frac{4}{5} \varsigma_9 \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + 2\varsigma_{11} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} \right), \quad (8.53)$$

$$\Delta \hat{h}_i \approx \Delta \hat{h}_i^{(2)} = -\frac{\varpi_7}{\varpi_8} \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) - \frac{\varepsilon \Omega}{\varpi_8} \varsigma_{15} \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j}. \quad (8.54)$$

where the superscript ‘(2)’ denotes the second order accurate contributions.

Thus, in the system of second order accurate equations, we have the conservation laws (8.48) and the governing equations for $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$ and $\hat{h}_i$ (eqs. (8.50)–(8.52))—total 17 equations in 3D—and the system is closed with the second order accurate contributions of $\Delta \hat{\sigma}_{ij}$ and $\Delta \hat{h}_i$, given by (8.53) and (8.54). The second order accurate equations in the closed form read

$$\left. \begin{aligned} \varkappa_\alpha \left(\frac{\partial \hat{n}_\alpha}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} \right) + \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} &= 0, \\ \frac{\partial}{\partial \hat{t}} (\mu_\alpha \mathbf{x}_\alpha^\circ \hat{n}_\alpha + \mu_\beta \mathbf{x}_\beta^\circ \hat{n}_\beta) + (\mu_\alpha \mathbf{x}_\alpha^\circ + \mu_\beta \mathbf{x}_\beta^\circ) \frac{\partial \hat{v}_i}{\partial \hat{x}_i} &= 0, \\ \varkappa \frac{\partial \hat{v}_i}{\partial \hat{t}} + \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \mathbf{x}_\alpha^\circ \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} + \mathbf{x}_\beta^\circ \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} + \frac{\partial \hat{T}}{\partial \hat{x}_i} &= 0, \\ \frac{3}{2} \frac{\partial \hat{T}}{\partial \hat{t}} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} + \frac{\partial \hat{h}_i}{\partial \hat{x}_i} + \varsigma_1 \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} &= 0, \end{aligned} \right\} \quad (8.55)$$

$$\varkappa_\alpha \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{t}} + \mathbf{a}_0 \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} = -\frac{1}{\varepsilon \Omega} \mathbf{a}_1 \left[\hat{u}_i^{(\alpha)} + \mathbf{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) \right], \quad (8.56)$$

$$\frac{\partial \hat{\sigma}_{ij}}{\partial \hat{t}} + \mathbf{a}_2 \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + \mathbf{a}_3 \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} = -\frac{1}{\varepsilon \Omega} \mathbf{a}_4 \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right), \quad (8.57)$$

$$\frac{\partial \hat{h}_i}{\partial \hat{t}} + \mathfrak{a}_5 \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} = -\frac{1}{\varepsilon \Omega} \mathfrak{a}_6 \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right). \quad (8.58)$$

The coefficients $\mathfrak{a}_0, \mathfrak{a}_2, \dots, \mathfrak{a}_6$ are given in appendix C for better readability.

8.5.5 Third order accuracy: regularized moment equations

8.5.5.1 Intermediate result: 25 equations

At this order, we need to find $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$ and $\hat{h}_i$, appearing in the conservation laws, with third order accuracy. Therefore, one need to consider all terms having factors ε^0 , ε^1 and ε^2 in the balance equations of these quantities (i.e., in eqs. (8.34), (8.36) and (8.38)), we get (on setting gray coloured ε to 1)

$$\begin{aligned} & \varkappa_\alpha \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{t}} + \varsigma_2 \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \varsigma_3 \frac{\partial \Delta \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \mathfrak{x}_\beta^\circ \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \\ &= -\delta_1 \frac{1}{\varepsilon \Omega} \frac{\varkappa}{\varkappa_\beta^2} \left[\hat{u}_i^{(\alpha)} + \mathfrak{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) \right], \end{aligned} \quad (8.59)$$

$$\frac{\partial \hat{\sigma}_{ij}}{\partial \hat{t}} + \frac{\partial \hat{m}_{ijk}}{\partial \hat{x}_k} + \frac{4}{5} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + 2\varsigma_1 \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} = -\frac{1}{\varepsilon \Omega} \left[\varpi_1 \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) + \varpi_2 \Delta \hat{\sigma}_{ij} \right], \quad (8.60)$$

$$\begin{aligned} & \frac{\partial \hat{h}_i}{\partial \hat{t}} + \varsigma_{12} \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \varsigma_{13} \frac{\partial \Delta \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \frac{1}{2} \frac{\partial \hat{R}_{ij}}{\partial \hat{x}_j} + \frac{1}{6} \frac{\partial \hat{\Delta}}{\partial \hat{x}_i} + \frac{5}{2} \varsigma_{14} \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \\ &= -\frac{1}{\varepsilon \Omega} \left[\varpi_5 \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) + \varpi_6 \Delta \hat{h}_i \right]. \end{aligned} \quad (8.61)$$

Now, we have the additional variables $\Delta \hat{T}$, $\Delta \hat{\sigma}_{ij}$, $\Delta \hat{h}_i$, $\hat{m}_{ijk}$, $\hat{R}_{ij}$ and $\hat{\Delta}$ in the system. The variables $\Delta \hat{\sigma}_{ij}$ and $\Delta \hat{h}_i$ not only appear on the left-hand sides of (8.59)–(8.61) where only their leading order contributions are required but also on the right-hand sides of (8.60) and (8.61) where they are required up to order $\mathcal{O}(\varepsilon^3)$. Therefore, we need to include the terms up to order $\mathcal{O}(\varepsilon^2)$ in the balance equations for them (eqs. (8.37) and (8.39)), which gives

$$\begin{aligned} & \frac{\partial \Delta \hat{\sigma}_{ij}}{\partial \hat{t}} + \varsigma_7 \frac{\partial \hat{m}_{ijk}}{\partial \hat{x}_k} + \frac{4}{5} \varsigma_9 \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + \frac{4}{5} \varsigma_{10} \frac{\partial \Delta \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + 2\varsigma_{11} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} \\ &= -\frac{1}{\varepsilon \Omega} \left[\varpi_3 \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) + \varpi_4 \Delta \hat{\sigma}_{ij} \right], \end{aligned} \quad (8.62)$$

$$\begin{aligned} & \frac{\partial \Delta \hat{h}_i}{\partial \hat{t}} + \varsigma_{15} \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \varsigma_{16} \frac{\partial \Delta \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \frac{1}{2} \varsigma_{17} \frac{\partial \hat{R}_{ij}}{\partial \hat{x}_j} + \frac{1}{6} \varsigma_{19} \frac{\partial \hat{\Delta}}{\partial \hat{x}_i} + \frac{5}{2} \varsigma_{21} \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \\ &= -\frac{1}{\varepsilon \Omega} \left[\varpi_7 \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) + \varpi_8 \Delta \hat{h}_i \right]. \end{aligned} \quad (8.63)$$

Fortunately, all other additional variables— $\Delta\hat{T}$, $\hat{m}_{ijk}$, $\hat{R}_{ij}$ and $\hat{\Delta}$ —appear only on the left-hand sides of (8.59)–(8.63). Therefore, for the third order accurate $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$, $\hat{h}_i$, $\Delta\hat{\sigma}_{ij}$, $\Delta\hat{h}_i$, only the second order accurate contributions of $\Delta\hat{T}$, $\hat{m}_{ijk}$, $\hat{R}_{ij}$ and $\hat{\Delta}$ are needed and these follow from their respective balance equations (eqs. (8.35), (8.40), (8.42), (8.44), respectively) by considering only the terms up to order $\mathcal{O}(\varepsilon)$, we have

$$\left. \begin{aligned} \Delta\hat{T} &= -\varepsilon \Omega \frac{\varkappa_\alpha}{\delta_5} \left(\varsigma_4 \frac{\partial \hat{h}_i}{\partial \hat{x}_i} + \varsigma_6 \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} \right), \\ \hat{m}_{ijk} &= -\varepsilon \zeta_m \frac{\partial \hat{\sigma}_{\langle ij}}{\partial \hat{x}_k}, \quad \hat{R}_{ij} = -\varepsilon \zeta_R \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_j}, \quad \hat{\Delta} = -\varepsilon \zeta_\Delta \frac{\partial \hat{h}_i}{\partial \hat{x}_i}. \end{aligned} \right\} \quad (8.64)$$

Thus, the system of third order accurate equations consists of the conservation laws (8.48) and the governing equations for $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$, $\hat{h}_i$, $\Delta\hat{\sigma}_{ij}$ and $\Delta\hat{h}_i$ (eqs. (8.59)–(8.63))—total 25 equations in 3D—and the system is closed with the second order accurate contributions of $\Delta\hat{T}$, $\hat{m}_{ijk}$, $\hat{R}_{ij}$ and $\hat{\Delta}$, given by (8.64).

8.5.5.2 Further reduction

As one can notice that (8.62) and (8.63) have been included in the system of third order accurate equations just because $\Delta\hat{\sigma}_{ij}$ and $\Delta\hat{h}_i$ are present on the right-hand sides of (8.60) and (8.61). Nevertheless, the explicit *third* order accurate expressions for $\Delta\hat{\sigma}_{ij}$ and $\Delta\hat{h}_i$ can be obtained by using ideas somewhat similar to Chapman–Enskog expansion, also used in [108], so that we only have 17 equations and the third order accurate values of $\Delta\hat{\sigma}_{ij}$ and $\Delta\hat{h}_i$ can be included in the closures.

For finding the third order accurate $\Delta\hat{\sigma}_{ij}$ and $\Delta\hat{h}_i$, it suffices to consider their second order accurate contributions on the left-hand sides of (8.62) and (8.63). In other words, (8.62) and (8.63) can be rewritten as

$$\begin{aligned} \frac{\partial \Delta\hat{\sigma}_{ij}^{(2)}}{\partial \hat{t}} + \varsigma_7 \frac{\partial \hat{m}_{ijk}}{\partial \hat{x}_k} + \frac{4}{5} \varsigma_9 \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_j} + \frac{4}{5} \varsigma_{10} \frac{\partial \Delta\hat{h}_{\langle i}^{(2)}}{\partial \hat{x}_j} + 2\varsigma_{11} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_j} \\ = -\frac{1}{\varepsilon \Omega} \left[\varpi_3 \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_j} \right) + \varpi_4 \Delta\hat{\sigma}_{ij} \right], \end{aligned} \quad (8.65)$$

$$\begin{aligned} \frac{\partial \Delta\hat{h}_i^{(2)}}{\partial \hat{t}} + \varsigma_{15} \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \varsigma_{16} \frac{\partial \Delta\hat{\sigma}_{ij}^{(2)}}{\partial \hat{x}_j} + \frac{1}{2} \varsigma_{17} \frac{\partial \hat{R}_{ij}}{\partial \hat{x}_j} + \frac{1}{6} \varsigma_{19} \frac{\partial \hat{\Delta}}{\partial \hat{x}_i} + \frac{5}{2} \varsigma_{21} \frac{\partial \Delta\hat{T}}{\partial \hat{x}_i} \\ = -\frac{1}{\varepsilon \Omega} \left[\varpi_7 \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) + \varpi_8 \Delta\hat{h}_i \right]. \end{aligned} \quad (8.66)$$

From (8.53) and (8.54), we have

$$\left. \begin{aligned} \frac{\partial \Delta\hat{\sigma}_{ij}^{(2)}}{\partial \hat{t}} &= -\frac{\varpi_3}{\varpi_4} \frac{\partial}{\partial \hat{t}} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_j} \right) - \frac{\varepsilon \Omega}{\varpi_4} \left(\frac{4}{5} \varsigma_9 \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{t}} + 2\varsigma_{11} \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{t}} \right), \\ \frac{\partial \Delta\hat{h}_i^{(2)}}{\partial \hat{t}} &= -\frac{\varpi_7}{\varpi_8} \frac{\partial}{\partial \hat{t}} \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) - \frac{\varepsilon \Omega}{\varpi_8} \varsigma_{15} \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{t}}. \end{aligned} \right\} \quad (8.67)$$

As we want to evaluate the time derivatives of the second order accurate $\Delta\hat{\sigma}_{ij}$ and $\Delta\hat{h}_i$, it is natural to use the second order accurate balance equations for $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$ and $\hat{h}_i$ (eqs. (8.50), (8.57) and (8.58)) for replacing the time derivatives in the underlined terms in (8.67). Moreover, the underbraced terms in (8.67) are order $\mathcal{O}(\varepsilon^2)$ contributions to the total stress and the total reduced heat flux and it suffices to use only the precise values of order $\mathcal{O}(\varepsilon^2)$ contributions of these quantities in (8.67). The precise values of order $\mathcal{O}(\varepsilon^2)$ contributions to the total stress and the total reduced heat flux can be obtained by performing Chapman–Enskog like expansion either on the second order accurate balance equations (eqs. (8.50), (8.57) and (8.58)) or on the full system of moment equations (eqs. (8.34)–(8.45)) and we get (cf. (D.12) and (D.14))

$$\left. \begin{aligned} \hat{\sigma}_{ij} + 2\varepsilon\eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} &= -\varepsilon^2 \frac{\partial^2}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} (\mathbf{b}_1 \hat{n}_\alpha + \mathbf{b}_2 \hat{n}_\beta + \mathbf{b}_3 \hat{T}) + \mathcal{O}(\varepsilon^3), \\ \hat{h}_i + \varepsilon\kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} &= -\varepsilon^2 \frac{\Omega}{\mathbf{a}_6} \left(\frac{2}{3} \kappa \frac{\partial^2 \hat{v}_j}{\partial \hat{x}_i \partial \hat{x}_j} - 2\eta \mathbf{a}_5 \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) + \mathcal{O}(\varepsilon^3). \end{aligned} \right\} \quad (8.68)$$

The values of the coefficients $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ are given in appendix D. For second order accurate underbraced terms in (8.67), we can use $\hat{\sigma}_{ij} \approx -2\varepsilon\eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}}$ in the right-hand side of (8.68)₂ and it will not affect the accuracy. Thus, we have

$$\left. \begin{aligned} \hat{\sigma}_{ij} + 2\varepsilon\eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} &\approx -\varepsilon^2 \frac{\partial^2}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} (\mathbf{b}_1 \hat{n}_\alpha + \mathbf{b}_2 \hat{n}_\beta + \mathbf{b}_3 \hat{T}), \\ \hat{h}_i + \varepsilon\kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} &\approx -\frac{\Omega}{\mathbf{a}_6} \left(\frac{2}{3} \kappa \varepsilon^2 \frac{\partial^2 \hat{v}_j}{\partial \hat{x}_i \partial \hat{x}_j} + \mathbf{a}_5 \varepsilon \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} \right). \end{aligned} \right\} \quad (8.69)$$

Now, we apply the time derivative and immediately replace the time derivative of the total stress with its second order accurate balance equation (8.51) and the time derivatives of number densities, velocity and temperature using the conservation laws with $\hat{u}_i^{(\alpha)} = \hat{u}_i^{(\beta)} = \hat{\sigma}_{ij} = \hat{h}_i = 0$ (i.e., using Euler equations) to get

$$\left. \begin{aligned} \frac{\partial}{\partial \hat{t}} \left(\hat{\sigma}_{ij} + 2\varepsilon\eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) &\approx \left(\mathbf{b}_1 + \mathbf{b}_2 + \frac{2}{3} \mathbf{b}_3 \right) \varepsilon^2 \frac{\partial^2}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} \frac{\partial \hat{v}_k}{\partial \hat{x}_k}, \\ \frac{\partial}{\partial \hat{t}} \left(\hat{h}_i + \varepsilon\kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) &\approx \frac{2}{3} \frac{\Omega}{\mathbf{a}_6} \frac{\kappa}{\varkappa} \varepsilon^2 \frac{\partial^2}{\partial \hat{x}_i \partial \hat{x}_j} \frac{\partial}{\partial \hat{x}_j} (\mathbf{x}_\alpha^\circ \hat{n}_\alpha + \mathbf{x}_\beta^\circ \hat{n}_\beta + \hat{T}) \\ &\quad + \frac{\Omega}{\mathbf{a}_6} \mathbf{a}_5 \varepsilon \frac{\partial}{\partial \hat{x}_j} \left[\mathbf{a}_2 \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + \mathbf{a}_3 \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} + \frac{1}{\varepsilon \Omega} \mathbf{a}_4 \left(\hat{\sigma}_{ij} + 2\varepsilon\eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) \right]. \end{aligned} \right\} \quad (8.70)$$

The temperature gradient in (8.70) is replaced by heat flux as before, however, the elimination of gradients of number densities is a bit tricky. The trick is the following. Similar to above, without affecting the accuracy, one can use

$$\hat{u}_i^{(\alpha)} \approx -\mathbf{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) \quad \text{and} \quad \hat{h}_i \approx -\varepsilon\kappa \frac{\partial \hat{T}}{\partial \hat{x}_i}$$

in order to get

$$-\varepsilon \frac{1}{\mathbf{x}_\beta^\circ} \frac{\delta_1}{\Omega} \frac{\kappa^2}{\kappa_\beta^2} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} - \varepsilon (\kappa_\alpha^2 - \kappa_\beta^2) \frac{1}{\kappa} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} \approx \varepsilon^2 \left(\kappa_\beta^2 \frac{\partial^2 \hat{n}_\alpha}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} - \kappa_\alpha^2 \frac{\partial^2 \hat{n}_\beta}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} \right). \quad (8.71)$$

Moreover, one can again use $\hat{h}_i \approx -\varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i}$ in (8.69)₁ to obtain

$$\left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) \approx -\varepsilon^2 \frac{\partial^2}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} \left(\mathbf{b}_1 \hat{n}_\alpha + \mathbf{b}_2 \hat{n}_\beta \right) + \varepsilon \frac{\mathbf{b}_3}{\kappa} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}}, \quad (8.72)$$

On solving (8.71) with (8.72), one obtains

$$\begin{aligned} \varepsilon^2 \frac{\partial^2 \hat{n}_\alpha}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} &\approx \frac{1}{(\mathbf{b}_1 \kappa_\alpha^2 + \mathbf{b}_2 \kappa_\beta^2)} \left[-\varepsilon \frac{1}{\mathbf{x}_\beta^\circ} \frac{\delta_1}{\Omega} \frac{\kappa^2}{\kappa_\beta^2} \mathbf{b}_2 \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} + \varepsilon \{ \mathbf{b}_3 \kappa_\alpha^2 - \mathbf{b}_2 (\kappa_\alpha^2 - \kappa_\beta^2) \} \frac{1}{\kappa} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right. \\ &\quad \left. - \kappa_\alpha^2 \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) \right], \end{aligned} \quad (8.73)$$

$$\begin{aligned} \varepsilon^2 \frac{\partial^2 \hat{n}_\beta}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} &\approx \frac{1}{(\mathbf{b}_1 \kappa_\alpha^2 + \mathbf{b}_2 \kappa_\beta^2)} \left[\varepsilon \frac{1}{\mathbf{x}_\beta^\circ} \frac{\delta_1}{\Omega} \frac{\kappa^2}{\kappa_\beta^2} \mathbf{b}_1 \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} + \varepsilon \{ \mathbf{b}_1 (\kappa_\alpha^2 - \kappa_\beta^2) + \mathbf{b}_3 \kappa_\beta^2 \} \frac{1}{\kappa} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right. \\ &\quad \left. - \kappa_\beta^2 \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) \right]. \end{aligned} \quad (8.74)$$

The relation

$$\frac{\partial}{\partial \hat{x}_j} \frac{\partial^2}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} (\cdot) = \frac{2}{3} \frac{\partial^2}{\partial \hat{x}_i \partial \hat{x}_j} \frac{\partial}{\partial \hat{x}_j} (\cdot),$$

is also used for replacing the gradients of number densities and temperature in (8.70). Furthermore, the right-hand side of (8.70)₁ is simplified by using an expression obtained by taking the deviatoric gradient of (8.69)₂. After all replacements and some algebra, we finally get

$$\begin{aligned} \frac{\partial}{\partial \hat{t}} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) &\approx -\varepsilon \Omega \frac{\mathbf{a}_5}{\mathbf{a}_4} \frac{1}{\kappa} \left(5 \frac{\eta}{\kappa} - \mathbf{a}_2 \kappa + \frac{\varsigma_{32}}{\kappa} \right) \frac{\partial}{\partial \hat{x}_k} \frac{\partial \hat{\sigma}_{k\langle i}}{\partial \hat{x}_{j\rangle}} \\ &\quad - \frac{\mathbf{a}_6}{\mathbf{a}_4} \frac{1}{\kappa} \left(5 \frac{\eta}{\kappa} - \mathbf{a}_2 \kappa + \frac{\varsigma_{32}}{\kappa} \right) \frac{\partial}{\partial \hat{x}_{j\rangle}} \left(\hat{h}_{\langle i} + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_{\langle i}} \right), \end{aligned} \quad (8.75)$$

$$\begin{aligned} \frac{\partial}{\partial \hat{t}} \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) &\approx \varepsilon \Omega \frac{\mathbf{a}_2}{\mathbf{a}_6} \left(\mathbf{a}_5 - \frac{\kappa}{2\eta} \right) \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + \varepsilon \Omega \frac{\mathbf{a}_3}{\mathbf{a}_6} \left(\mathbf{a}_5 - \frac{\kappa}{2\eta} \right) \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} \\ &\quad + \frac{\mathbf{a}_4}{\mathbf{a}_6} \left(\mathbf{a}_5 - \frac{\kappa}{2\eta} \right) \frac{\partial}{\partial \hat{x}_j} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right), \end{aligned} \quad (8.76)$$

where the coefficient ς_{32} is also given in appendix C for better readability. Therefore, equa-

tions (8.67) on using (8.50), (8.57), (8.58), (8.75) and (8.76) yield

$$\begin{aligned} \frac{\partial \Delta \hat{\sigma}_{ij}^{(2)}}{\partial \hat{t}} &\approx \frac{\Omega}{\varpi_4} \left[2 \frac{\varsigma_{2\varsigma_{11}}}{\varkappa_\alpha} + \mathfrak{a}_5 \left\{ \frac{4}{5} \varsigma_9 + \frac{\varpi_3}{\mathfrak{a}_4} \frac{1}{\varkappa} \left(5 \frac{\eta}{\kappa} - \mathfrak{a}_2 \varkappa + \frac{\varsigma_{32}}{\kappa} \right) \right\} \right] \varepsilon \frac{\partial}{\partial \hat{x}_k} \frac{\partial \hat{\sigma}_{k\langle i}}{\partial \hat{x}_{j\rangle}} \\ &\quad + 2\delta_1 \frac{\varkappa}{\varkappa_\alpha \varkappa_\beta^2} \frac{\varsigma_{11}}{\varpi_4} \frac{\partial}{\partial \hat{x}_{j\rangle}} \left[\hat{u}_{\langle i}^{(\alpha)} + \mathfrak{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_{\langle i}} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_{\langle i}} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_{\langle i}} \right) \right] \\ &\quad + \frac{\mathfrak{a}_6}{\varpi_4} \left[\frac{4}{5} \varsigma_9 + \frac{\varpi_3}{\mathfrak{a}_4} \frac{1}{\varkappa} \left(5 \frac{\eta}{\kappa} - \mathfrak{a}_2 \varkappa + \frac{\varsigma_{32}}{\kappa} \right) \right] \frac{\partial}{\partial \hat{x}_{j\rangle}} \left(\hat{h}_{\langle i} + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_{\langle i}} \right), \end{aligned} \quad (8.77)$$

$$\begin{aligned} \frac{\partial \Delta \hat{h}_i^{(2)}}{\partial \hat{t}} &\approx \frac{\Omega}{\varpi_8} \left[\varsigma_{15} - \frac{\varpi_7}{\mathfrak{a}_6} \left(\mathfrak{a}_5 - \frac{\kappa}{2\eta} \right) \right] \left(\mathfrak{a}_2 \varepsilon \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + \mathfrak{a}_3 \varepsilon \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} \right) \\ &\quad + \frac{\mathfrak{a}_4}{\varpi_8} \left[\varsigma_{15} - \frac{\varpi_7}{\mathfrak{a}_6} \left(\mathfrak{a}_5 - \frac{\kappa}{2\eta} \right) \right] \frac{\partial}{\partial \hat{x}_j} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right). \end{aligned} \quad (8.78)$$

On using (8.53), (8.54), (8.77) and (8.78), equations (8.65) and (8.66) provide the third order accurate expressions for $\Delta \hat{\sigma}_{ij}$ and $\Delta \hat{h}_i$:

$$\begin{aligned} \Delta \hat{\sigma}_{ij} &\approx -\frac{\varpi_3}{\varpi_4} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) - \frac{\varepsilon \Omega}{\varpi_4} \left(\frac{4}{5} \varsigma_9 \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + 2\varsigma_{11} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} \right) - \frac{\varepsilon \Omega}{\varpi_4} \varsigma_7 \frac{\partial \hat{m}_{ijk}}{\partial \hat{x}_k} \\ &\quad - \varepsilon^2 \frac{\Omega^2}{\varpi_4^2} \left[2 \frac{\varsigma_{2\varsigma_{11}}}{\varkappa_\alpha} + \mathfrak{a}_5 \left\{ \frac{4}{5} \varsigma_9 + \frac{\varpi_3}{\mathfrak{a}_4} \frac{1}{\varkappa} \left(5 \frac{\eta}{\kappa} - \mathfrak{a}_2 \varkappa + \frac{\varsigma_{32}}{\kappa} \right) \right\} - \frac{4}{5} \frac{\varpi_4}{\varpi_8} \varsigma_{10} \varsigma_{15} \right] \frac{\partial}{\partial \hat{x}_k} \frac{\partial \hat{\sigma}_{k\langle i}}{\partial \hat{x}_{j\rangle}} \\ &\quad - 2\varepsilon \Omega \delta_1 \frac{\varkappa}{\varkappa_\alpha \varkappa_\beta^2} \frac{\varsigma_{11}}{\varpi_4} \frac{\partial}{\partial \hat{x}_{j\rangle}} \left[\hat{u}_{\langle i}^{(\alpha)} + \mathfrak{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_{\langle i}} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_{\langle i}} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_{\langle i}} \right) \right] \\ &\quad - \frac{\varepsilon \Omega}{\varpi_4} \left[\frac{\mathfrak{a}_6}{\varpi_4} \left\{ \frac{4}{5} \varsigma_9 + \frac{\varpi_3}{\mathfrak{a}_4} \frac{1}{\varkappa} \left(5 \frac{\eta}{\kappa} - \mathfrak{a}_2 \varkappa + \frac{\varsigma_{32}}{\kappa} \right) \right\} - \frac{4}{5} \frac{\varpi_7}{\varpi_8} \varsigma_{10} \right] \frac{\partial}{\partial \hat{x}_{j\rangle}} \left(\hat{h}_{\langle i} + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_{\langle i}} \right), \end{aligned} \quad (8.79)$$

$$\begin{aligned} \Delta \hat{h}_i &\approx -\frac{\varpi_7}{\varpi_8} \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) - \frac{\varepsilon \Omega}{\varpi_8} \varsigma_{15} \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} - \frac{\varepsilon \Omega}{\varpi_8} \left(\frac{1}{2} \varsigma_{17} \frac{\partial \hat{R}_{ij}}{\partial \hat{x}_j} + \frac{1}{6} \varsigma_{19} \frac{\partial \hat{\Delta}}{\partial \hat{x}_i} + \frac{5}{2} \varsigma_{21} \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \right) \\ &\quad - \frac{\varepsilon^2 \Omega^2}{\varpi_8} \left[\frac{\mathfrak{a}_2}{\varpi_8} \left\{ \varsigma_{15} - \frac{\varpi_7}{\mathfrak{a}_6} \left(\mathfrak{a}_5 - \frac{\kappa}{2\eta} \right) \right\} - \frac{4}{5} \frac{\varsigma_9 \varsigma_{16}}{\varpi_4} \right] \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} \\ &\quad - \frac{\varepsilon^2 \Omega^2}{\varpi_8} \left[\frac{\mathfrak{a}_3}{\varpi_8} \left\{ \varsigma_{15} - \frac{\varpi_7}{\mathfrak{a}_6} \left(\mathfrak{a}_5 - \frac{\kappa}{2\eta} \right) \right\} - 2 \frac{\varsigma_{11} \varsigma_{16}}{\varpi_4} \right] \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} \\ &\quad - \frac{\varepsilon \Omega}{\varpi_8} \left[\frac{\mathfrak{a}_4}{\varpi_8} \left\{ \varsigma_{15} - \frac{\varpi_7}{\mathfrak{a}_6} \left(\mathfrak{a}_5 - \frac{\kappa}{2\eta} \right) \right\} - \varsigma_{16} \frac{\varpi_3}{\varpi_4} \right] \frac{\partial}{\partial \hat{x}_j} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right). \end{aligned} \quad (8.80)$$

Now, inserting the second order accurate value of $\Delta \hat{\sigma}_{ij}$ from (8.53) into (8.59), we obtain the third order accurate balance equation for the diffusion velocity of the α -constituent

$$\begin{aligned} \varkappa_\alpha \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{t}} + \varsigma_2 \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} - \mathfrak{a}_7 \frac{\partial}{\partial \hat{x}_j} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) - \mathfrak{a}_8 \varepsilon \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} - \mathfrak{a}_9 \varepsilon \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + \mathfrak{x}_\beta^\circ \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \\ = -\delta_1 \frac{1}{\varepsilon \Omega} \frac{\varkappa}{\varkappa_\beta^2} \left[\hat{u}_i^{(\alpha)} + \mathfrak{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) \right], \end{aligned} \quad (8.81)$$

The coefficients $\mathbf{a}_7$, $\mathbf{a}_8$ and $\mathbf{a}_9$ are given in appendix C for better readability. Inserting the second order accurate value of $\Delta\hat{\sigma}_{ij}$ from (8.53) and the third order accurate values of $\Delta\hat{\sigma}_{ij}$ and $\Delta\hat{h}_i$ from (8.79) and (8.80), respectively, into (8.60) and (8.61), we obtain the third order accurate balance equations for the total stress and the total reduced heat flux:

$$\begin{aligned}
& \frac{\partial \hat{\sigma}_{ij}}{\partial t} + \left(1 - \frac{\varpi_2}{\varpi_4}\varsigma_7\right) \frac{\partial \hat{m}_{ijk}}{\partial \hat{x}_k} + \mathbf{a}_2 \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} + \mathbf{a}_3 \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} \\
& - \varepsilon \Omega \frac{\varpi_2}{\varpi_4} \left[2 \frac{\varsigma_{211}}{\kappa_\alpha} + \mathbf{a}_5 \left\{ \frac{4}{5}\varsigma_9 + \frac{\varpi_3}{\mathbf{a}_4} \frac{1}{\kappa} \left(5 \frac{\eta}{\kappa} - \mathbf{a}_2 \kappa + \frac{\varsigma_{32}}{\kappa} \right) \right\} - \frac{4}{5} \frac{\varpi_4}{\varpi_8} \varsigma_{10} \varsigma_{15} \right] \frac{\partial}{\partial \hat{x}_k} \frac{\partial \hat{\sigma}_{k\langle i}}{\partial \hat{x}_{j\rangle}} \\
& - 2\delta_1 \frac{\kappa}{\kappa_\alpha \kappa_\beta^2} \frac{\varsigma_{11} \varpi_2}{\varpi_4} \frac{\partial}{\partial \hat{x}_{j\rangle}} \left[\hat{u}_{\langle i}^{(\alpha)} + \mathbf{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\kappa_\beta^2}{\kappa^2} \left(\kappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_{\langle i}} - \kappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_{\langle i}} - (\kappa_\alpha^2 - \kappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_{\langle i}} \right) \right] \\
& - \frac{\varpi_2}{\varpi_4} \left[\frac{\mathbf{a}_6}{\varpi_4} \left\{ \frac{4}{5}\varsigma_9 + \frac{\varpi_3}{\mathbf{a}_4} \frac{1}{\kappa} \left(5 \frac{\eta}{\kappa} - \mathbf{a}_2 \kappa + \frac{\varsigma_{32}}{\kappa} \right) \right\} - \frac{4}{5} \frac{\varpi_7}{\varpi_8} \varsigma_{10} \right] \frac{\partial}{\partial \hat{x}_{j\rangle}} \left(\hat{h}_{\langle i} + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_{\langle i}} \right) \\
& = -\frac{1}{\varepsilon \Omega} \mathbf{a}_4 \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right), \tag{8.82}
\end{aligned}$$

$$\begin{aligned}
& \frac{\partial \hat{h}_i}{\partial t} + \mathbf{a}_5 \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \frac{1}{2} \left(1 - \frac{\varpi_6}{\varpi_8} \varsigma_{17} \right) \frac{\partial \hat{R}_{ij}}{\partial \hat{x}_j} + \frac{1}{6} \left(1 - \frac{\varpi_6}{\varpi_8} \varsigma_{19} \right) \frac{\partial \hat{\Delta}}{\partial \hat{x}_i} + \frac{5}{2} \left(\varsigma_{14} - \frac{\varpi_6}{\varpi_8} \varsigma_{21} \right) \frac{\partial \Delta \hat{T}}{\partial \hat{x}_i} \\
& - \varepsilon \Omega \left[\mathbf{a}_2 \frac{\varpi_6}{\varpi_8^2} \left\{ \varsigma_{15} - \frac{\varpi_7}{\mathbf{a}_6} \left(\mathbf{a}_5 - \frac{\kappa}{2\eta} \right) \right\} + \frac{4}{5} \frac{\varsigma_9}{\varpi_4} \left(\varsigma_{13} - \frac{\varpi_6}{\varpi_8} \varsigma_{16} \right) \right] \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j\rangle}} \\
& - \varepsilon \Omega \left[\mathbf{a}_3 \frac{\varpi_6}{\varpi_8^2} \left\{ \varsigma_{15} - \frac{\varpi_7}{\mathbf{a}_6} \left(\mathbf{a}_5 - \frac{\kappa}{2\eta} \right) \right\} + 2 \frac{\varsigma_{11}}{\varpi_4} \left(\varsigma_{13} - \frac{\varpi_6}{\varpi_8} \varsigma_{16} \right) \right] \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} \\
& - \left[\mathbf{a}_4 \frac{\varpi_6}{\varpi_8^2} \left\{ \varsigma_{15} - \frac{\varpi_7}{\mathbf{a}_6} \left(\mathbf{a}_5 - \frac{\kappa}{2\eta} \right) \right\} + \frac{\varpi_3}{\varpi_4} \left(\varsigma_{13} - \frac{\varpi_6}{\varpi_8} \varsigma_{16} \right) \right] \frac{\partial}{\partial \hat{x}_j} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j\rangle}} \right) \\
& = -\frac{1}{\varepsilon \Omega} \mathbf{a}_6 \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right). \tag{8.83}
\end{aligned}$$

8.5.5.3 Regularized 17-moment equations

The system of regularized 17-moment (R17) equations for binary gas-mixtures consists of the conservation laws (8.48) and the governing equations for $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$, $\hat{h}_i$ (eqs. (8.81)–(8.83))—total 17 equations in 3D—and the system is closed with the second order accurate contributions of $\Delta \hat{T}$, $\hat{m}_{ijk}$, $\hat{R}_{ij}$ and $\hat{\Delta}$, given by (8.64). We write the system of regularized 17-moment equations in the closed form—using (8.64) for the unknowns and the relation $\frac{\partial}{\partial \hat{x}_k} \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_k} = \frac{2}{5} \frac{\partial}{\partial \hat{x}_k} \frac{\partial \hat{\sigma}_{k\langle i}}{\partial \hat{x}_{j\rangle}} + \frac{1}{3} \frac{\partial^2 \hat{\sigma}_{ij}}{\partial \hat{x}_k^2}$ —below. It reads

$$\left. \begin{aligned}
& \kappa_\alpha \left(\frac{\partial \hat{n}_\alpha}{\partial t} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} \right) + \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} = 0, \\
& \frac{\partial}{\partial t} (\mu_\alpha \mathbf{x}_\alpha^\circ \hat{n}_\alpha + \mu_\beta \mathbf{x}_\beta^\circ \hat{n}_\beta) + (\mu_\alpha \mathbf{x}_\alpha^\circ + \mu_\beta \mathbf{x}_\beta^\circ) \frac{\partial \hat{v}_i}{\partial \hat{x}_i} = 0, \\
& \kappa \frac{\partial \hat{v}_i}{\partial t} + \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} + \mathbf{x}_\alpha^\circ \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} + \mathbf{x}_\beta^\circ \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} + \frac{\partial \hat{T}}{\partial \hat{x}_i} = 0, \\
& \frac{3}{2} \frac{\partial \hat{T}}{\partial t} + \frac{\partial \hat{v}_i}{\partial \hat{x}_i} + \frac{\partial \hat{h}_i}{\partial \hat{x}_i} + \varsigma_1 \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_i} = 0,
\end{aligned} \right\} \tag{8.84}$$

$$\begin{aligned}
& \underline{\underline{\kappa_\alpha \frac{\partial \hat{u}_i^{(\alpha)}}{\partial t} + \mathbf{a}_0 \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} - \mathbf{a}_7 \frac{\partial}{\partial \hat{x}_j} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right) - \mathbf{a}_8 \varepsilon \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_{j \rangle} - \mathbf{a}_9 \varepsilon \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j \rangle} - \mathbf{a}_{10} \varepsilon \frac{\partial}{\partial \hat{x}_i} \frac{\partial \hat{u}_j^{(\alpha)}}{\partial \hat{x}_j}}}} \\
& - \underline{\underline{\mathbf{a}_{11} \varepsilon \frac{\partial}{\partial \hat{x}_i} \frac{\partial \hat{h}_j}{\partial \hat{x}_j}}} = - \frac{1}{\varepsilon \Omega} \mathbf{a}_1 \left[\hat{u}_i^{(\alpha)} + \mathbf{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\kappa_\beta^2}{\kappa^2} \left(\kappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \kappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\kappa_\alpha^2 - \kappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right) \right], \quad (8.85)
\end{aligned}$$

$$\begin{aligned}
& \underline{\underline{\frac{\partial \hat{\sigma}_{ij}}{\partial t} + \mathbf{a}_2 \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_j} + \mathbf{a}_3 \frac{\partial \hat{u}_{\langle i}^{(\alpha)}}{\partial \hat{x}_j} - \mathbf{a}_{12} \frac{\partial}{\partial \hat{x}_j} \left(\hat{h}_{\langle i} + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_{\langle i}} \right)}}} \\
& - \underline{\underline{\mathbf{a}_{13} \frac{\partial}{\partial \hat{x}_j} \left[\hat{u}_{\langle i}^{(\alpha)} + \mathbf{x}_\beta^\circ \frac{\varepsilon \Omega}{\delta_1} \frac{\kappa_\beta^2}{\kappa^2} \left(\kappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_{\langle i}} - \kappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_{\langle i}} - (\kappa_\alpha^2 - \kappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_{\langle i}} \right) \right]}}} \\
& - \underline{\underline{\mathbf{a}_{14} \varepsilon \frac{\partial}{\partial \hat{x}_k} \frac{\partial \hat{\sigma}_{k\langle i}}{\partial \hat{x}_j} - \mathbf{a}_{15} \varepsilon \frac{\partial^2 \hat{\sigma}_{ij}}{\partial \hat{x}_k^2}}} = - \frac{1}{\varepsilon \Omega} \mathbf{a}_4 \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right), \quad (8.86)
\end{aligned}$$

$$\begin{aligned}
& \underline{\underline{\frac{\partial \hat{h}_i}{\partial t} + \mathbf{a}_5 \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} - \mathbf{a}_{16} \frac{\partial}{\partial \hat{x}_j} \left(\hat{\sigma}_{ij} + 2\varepsilon \eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right) - \mathbf{a}_{17} \varepsilon \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{h}_{\langle i}}{\partial \hat{x}_{j \rangle} - \mathbf{a}_{18} \varepsilon \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{u}_i^{(\alpha)}}{\partial \hat{x}_j}}}} \\
& - \underline{\underline{\mathbf{a}_{19} \varepsilon \frac{\partial}{\partial \hat{x}_i} \frac{\partial \hat{h}_j}{\partial \hat{x}_j} - \mathbf{a}_{20} \varepsilon \frac{\partial}{\partial \hat{x}_i} \frac{\partial \hat{u}_j^{(\alpha)}}{\partial \hat{x}_j}}} = - \frac{1}{\varepsilon \Omega} \mathbf{a}_6 \left(\hat{h}_i + \varepsilon \kappa \frac{\partial \hat{T}}{\partial \hat{x}_i} \right). \quad (8.87)
\end{aligned}$$

The coefficients $\mathbf{a}_0, \mathbf{a}_1, \dots, \mathbf{a}_{20}$ in the R17 equations are also given in appendix C for better readability. The underlining in (8.85)–(8.87) is used for distinguishing terms of different order in ε , the single underline denotes the terms of order $\mathcal{O}(\varepsilon)$ and the double underlines denote the terms of order $\mathcal{O}(\varepsilon^2)$. For zeroth order accuracy, obviously, the conservation laws (8.84) are closed by setting $\hat{u}_i^{(\alpha)}$, $\hat{\sigma}_{ij}$ and $\hat{h}_i$ to zero, which leads to the Euler equations for binary gas-mixtures (8.47). For first order accuracy in the Knudsen number, it suffices to consider the non-underlined terms in (8.85)–(8.87), i.e., the terms on the left-hand sides of these equations are set to zero, which leads to the laws of Fick, Navier–Stokes, and Fourier (8.49). For second order accuracy, one also needs to consider the single-underlined terms along with right-hand sides in (8.85)–(8.87), which indeed leads to the second order accurate equations (8.55)–(8.58). For third order accuracy, the double underlined terms should also be considered, and then the third order accurate equations are the full R17 equations. Thus, the zeroth, first and second order accurate equations for the binary gas-mixtures are inherently contained in the third order accurate R17 equations for binary gas-mixtures.

Interestingly, in the limiting case when the binary mixture reduces to just a single gas, the R17 equations for binary gas-mixtures (eqs. (8.84)–(8.87)) reduce to the well-known R13 equations (in linear form) of Struchtrup and Torrilhon [106] and of Struchtrup [100] for Maxwell molecules. The limiting case arises when either the mole fraction of any component in the mixture is zero (i.e., $\mathbf{x}_\alpha^\circ = 0$ or $\mathbf{x}_\beta^\circ = 0$) or when one component is replaced with the other (i.e., $\beta \rightarrow \alpha$ or $\alpha \rightarrow \beta$). In all the possible four cases, it suffices to consider the mass balance equation for the mixture (8.84)₂ and, therefore, one can ignore (8.84)₁. Moreover, the coefficient $\mathbf{c}_1$ in (8.84)₄ vanishes that means we do not need the balance equation for the diffusion velocity (8.85)

in the system any more, this agrees with the fact that there should not be any term/equation of the diffusion velocity in single gas case because there is no diffusion in single gases. Furthermore, owing to same reason, the reduced heat flux $\hat{h}_i$ in the mixture changes to the usual heat flux $\hat{q}_i$ in single gas case (see the definition of reduced heat flux). In all these limiting cases, all the coefficients except $\mathbf{a}_{18}$ and $\mathbf{a}_{20}$ in (8.86) and (8.87) immediately reduce to the coefficients in R13 equations for Maxwell molecules, i.e., they reduce to

$$\mathbf{a}_2 = \mathbf{a}_{14} = \frac{4}{5}, \quad \mathbf{a}_3 = \mathbf{a}_{12} = \mathbf{a}_{13} = \mathbf{a}_{16} = 0, \quad \mathbf{a}_4 = \mathbf{a}_5 = 1, \quad \mathbf{a}_6 = \mathbf{a}_{15} = \frac{2}{3}, \quad \mathbf{a}_{17} = \frac{12}{5}, \quad \mathbf{a}_{19} = 2.$$

For $x_\alpha^\circ = 0$ or $\beta \rightarrow \alpha$ or $\alpha \rightarrow \beta$ cases, one immediately gets $\mathbf{a}_{18} = \mathbf{a}_{20} = 0$. Although, for the case of $x_\beta^\circ = 0$, both $\mathbf{a}_{18}$ and $\mathbf{a}_{20}$ themselves are non-zero, but together with $\hat{u}_i^{(\alpha)}$ they let the whole terms vanish, i.e., $\mathbf{a}_{18}\hat{u}_i^{(\alpha)} = \mathbf{a}_{20}\hat{u}_i^{(\alpha)} = 0$, since the diffusion velocities for both the components in the mixture vanish.

8.6 Discussion on linear stability of the equations

The Euler equations (8.47) for binary gas-mixtures are always linearly stable for all gas-mixtures. It is trivial to check their linear stability, therefore we omit the details of their stability analysis. In order to scrutinize the linear stability of other sets of equations derived in this chapter, we follow exactly the same procedure as detailed in § 5.2 and assume a plane wave solution of the form (5.25) for each set in one dimension. Recall from § 5.2 that the length scale L used for non-dimensionalization of equations is taken as inverse of the wavenumber so that the wavenumber is proportional to the Knudsen number ε (here) and stability requires damping ς to be non-positive, i.e., $\varsigma \leq 0$ for stability. For the other sets of equations (except Euler equations), owing to large number of parameters, it is not easy to check the stability for all gas-mixtures. Nevertheless, we have checked the linear stability by considering many different permissible values of the parameters and found *empirically* that the first order accurate equations (eqs. (8.48) and (8.49))—i.e., Fick, Navier–Stokes, and Fourier equations—as well as the second order accurate equations (eqs. (8.55)–(8.58)) are linearly stable for all gas-mixtures. As an example, we plot the dimensionless damping over the Knudsen number for He–Xe mixture with $x_{\text{He}}^\circ = 0.75$ in figure 8.1, in which figure 8.1(a) illustrates the dispersion modes obtained with the first order accurate (Fick, Navier–Stokes, and Fourier) equations (eqs. (8.48) and (8.49)) while figure 8.1(b) depicts the dispersion modes obtained with the second order accurate equations (eqs. (8.55)–(8.58)). Figure 8.1(a) delineates four modes where two modes coincide with each other for small Knudsen numbers (for $\varepsilon \lesssim 0.323$) and for large Knudsen numbers they split into two distinct modes. Similarly, figure 8.1(b) displays seven modes where three modes have quite small damping for very small Knudsen numbers and two modes coincide. For large Knudsen numbers some of the modes coincide with each other. It can be seen from figure 8.1 that the damping remains always non-positive resulting into stability for both first and second order accurate equations.

The R17 equations (eqs. (8.84)–(8.87)), on the other hand, turn out to be stable for the mixtures with small or moderate mass differences but, unfortunately, unstable for the mixtures with large mass differences. We have analyzed the stability for three mixtures: Ne–Ar, He–Ar,

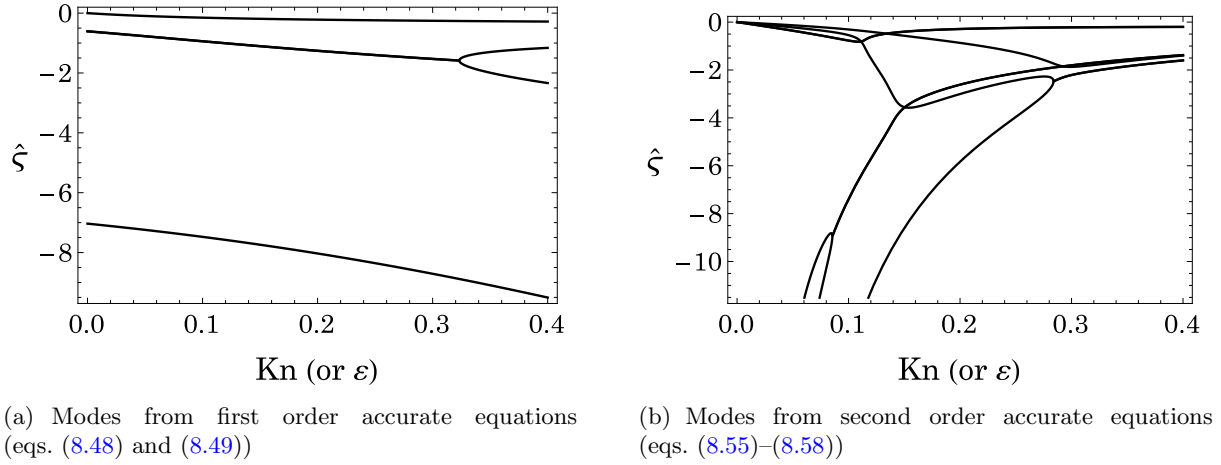


Figure 8.1: Dispersion modes in He–Xe mixture with $x_{\text{He}}^o = 0.75$ obtained with (a) first order accurate (Fick, Navier–Stokes, and Fourier) equations (eqs. (8.48) and (8.49)), and (b) second order accurate equations (eqs. (8.55)–(8.58)).

He–Xe with mole fraction of the lighter component in each mixture as $x_{\alpha}^o \in \{0.25, 0.5, 0.75\}$ and found that the R17 equations are stable for Ne–Ar and He–Ar mixtures with any mole fraction from the above list while unstable for He–Xe mixture. Figure 8.2 illustrates the dimensionless damping in the dispersion modes from the R17 equations for the three mixtures (a) Ne–Ar, (b) He–Ar and (c) He–Xe with mole fraction of each gas in each mixture being 0.5. Each sub-figure of figure 8.2 displays seven modes, three of them have quite small damping at very small Knudsen numbers and two modes coincide with each other. It is also clear from figure 8.2 that the R17 equations are not stable for He–Xe mixture since it is the mixture with large mass difference but they are stable for the other two mixtures. In order to have more insight into region of instability, we plot the zero contours of maximum (dimensionless) damping in figure 8.3 which illustrates them in $(x_{\alpha}^o, \mu_{\alpha})$ plane for fixed values of Ω_{α} and Ω_{β} : (a) $\Omega_{\alpha} = 1$, $\Omega_{\beta} = 1$ and (b) $\Omega_{\alpha} = 0.5$, $\Omega_{\beta} = 1.5$. The Knudsen number (ε) varies from 0.001 to 5000. The white color represents the regions in which the R17 equations are stable while the gray color portrays the regions in which they are unstable. Of course, in the limiting cases of $\mu_{\alpha} \approx 0$ and $\mu_{\alpha} \approx 1$, the R17 equations reduce to the linearized R13 equations for a single gas and become stable. It

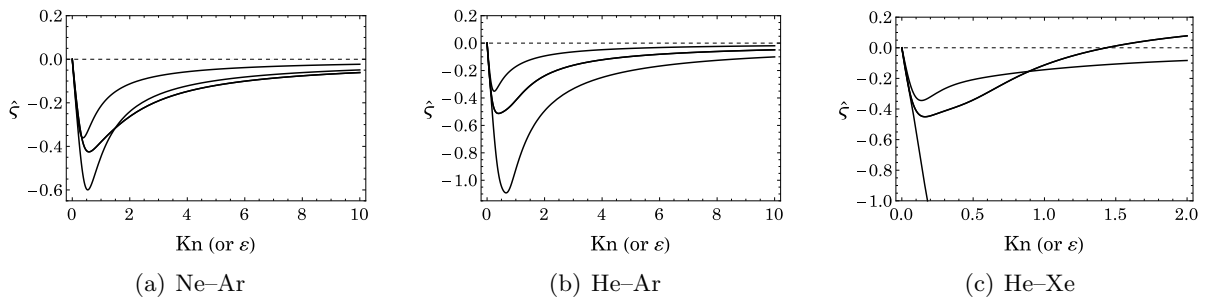


Figure 8.2: Dispersion modes in different binary gas-mixtures computed with R17 equations (eqs. (8.84)–(8.87)): (a) Ne–Ar ($x_{\text{Ne}}^o = 0.5$), (b) He–Ar ($x_{\text{He}}^o = 0.5$) and (c) He–Xe ($x_{\text{He}}^o = 0.5$).

can be stated from figure 8.3 that for plausible values of Ω_{α} and Ω_{β} , the R17 equations seem to

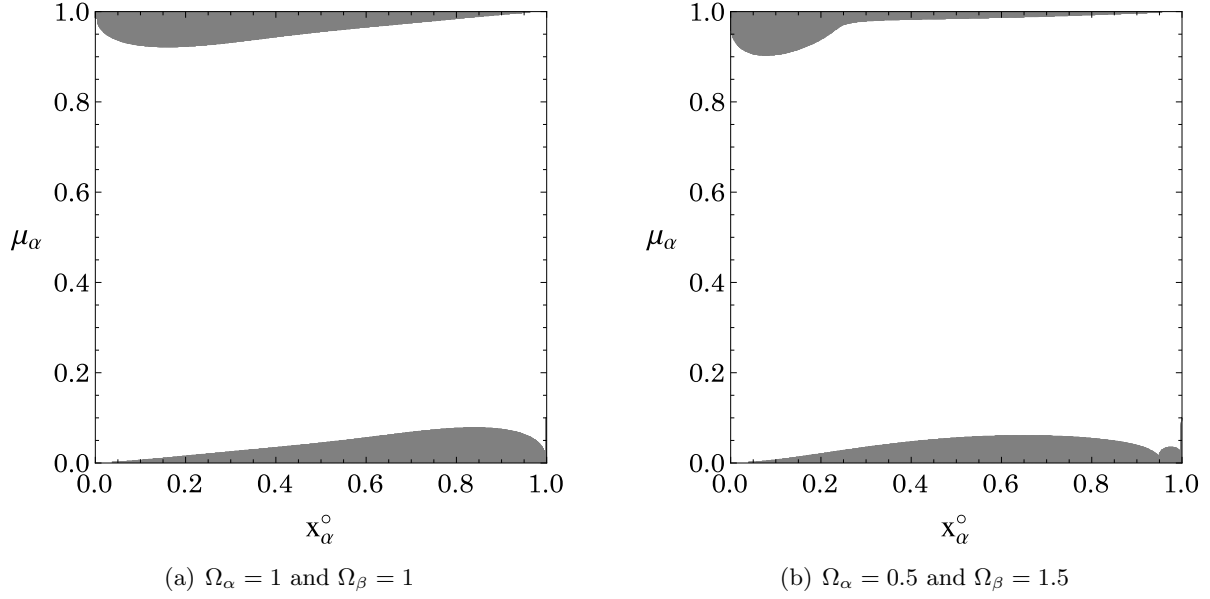


Figure 8.3: Zero contours of maximum (dimensionless) damping for different mole fractions (x_α^o) and different mass ratios (μ_α) with fixed values of Ω_α and Ω_β : (a) $\Omega_\alpha = 1$, $\Omega_\beta = 1$ and (b) $\Omega_\alpha = 0.5$, $\Omega_\beta = 1.5$. The Knudsen number (ε) varies from 0.001 to 5000. The white color represents the regions in which the R17 equations are stable while the gray color portrays the regions in which they are unstable.

be stable for the mixtures with mass ratios $0.1 \lesssim \mu_\alpha \lesssim 0.9$ for any mole fractions.

On investigating closely, we find that the third order accurate 25 equations (eqs. (8.48) and (8.59)–(8.64)) at intermediate step themselves are not stable for any of the three mixtures above and luckily the R17 equations have come out stable for mixtures with small and moderate mass differences. We have noticed that if we include the equation for temperature difference with these 25 equations, the resulting 26 equations become stable. The equation for temperature difference may be included in the system of 25 equations by modifying definition 8.1 for the order of accuracy; one will have to say that a set of equations for binary gas-mixtures is said to be accurate of order λ_0 , when the diffusion velocities (of both the components), temperature difference, total stress and total heat flux in the mixture are known up to the order $\mathcal{O}(\varepsilon^{\lambda_0})$. However, this modification of the definition too does not stabilize the final 18 equations (R17 equations + equation for the temperature difference). Furthermore, we have also scrutinized the case of single temperature theory. In this case, the third order accurate 25 equations (eqs. (8.48) and (8.59)–(8.64)) are stable for most of the binary mixtures, at least for all the mixtures considered in this chapter. However, the R17 equations are again unstable for He–Xe mixture, although they are stable for Ne–Ar and He–Ar mixtures.

Chapter 9

Conclusion and outlook

9.1 Summary

Unlike single gases, the existing kinetic theory for gaseous mixtures is not so mature. The present study is an attempt to ameliorate the kinetic theory for gaseous mixtures and has been concerned with developing models—based on moment equations—for describing processes in rarefied gaseous mixtures. Some of the models have been applied to some benchmark problems of fluid mechanics in simple geometries and it has been demonstrated that these models can serve as exemplary alternates to the computationally expensive particle-based methods (such as DSMC method) for studying processes in (moderately) rarefied gaseous mixtures. Original contributions of the present thesis are as follows.

- The full non-linear $N \times G13$ and $N \times G26$ equations for a mixture of N monatomic-inert-ideal gases have been derived.
- The methodology for computing the Boltzmann collision integrals associated with the moment equations for gaseous mixtures interacting with any interaction potential has been demonstrated and employed to obtain the explicit expressions of the non-linear production terms associated with the $N \times G13$ and $N \times G26$ equations, both for Maxwell as well as hard-sphere interaction potentials.
- The boundary conditions for $N \times G13$ and $N \times G26$ equations have been derived through Maxwell's accommodation model by writing the boundary conditions for each component in the mixture separately.
- The moment equations and the boundary conditions have then been restricted to binary gas mixtures and the linear stability analysis has been performed to examine the stability of the $2 \times G13$ and $2 \times G26$ equations for binary gas-mixtures and it has been found *empirically* that $2 \times G13$ and $2 \times G26$ equations are linearly stable for both Maxwell as well as hard-sphere interaction potentials.
- Some benchmark problems of fluid mechanics in simple geometries have been studied through all four types of moment systems ($2 \times G13$ and $2 \times G26$ equations, both for Maxwell and hard-sphere interaction potentials) and derived boundary conditions. Heat transfer in a binary gas-mixture confined between two infinite parallel plates having different temperatures has been analyzed with all four types of moment systems, and the results are compared with those in [87] obtained via the direct discretization of the Boltzmann equation with the implementation of realistic potential. The results have been found in good agreement with those in [87]. Furthermore, a one-dimensional problem of binary gas-mixture having one component infinitely diluted has been solved *analytically* with all four

types of moment systems in order to study the flow of diluted component, which acts as a contaminant, in the mixture. Heat transfer problems of binary gaseous mixtures confined in bottom-heated and lid-driven square cavities have also been studied (see below) and the preliminary results have been presented.

- The numerical methods based on finite differences for solving one- and two-dimensional problems through the moment systems considered in the present thesis have been demonstrated and employed to various benchmark problems in order to study the convergence of numerical methods. The convergence has been analyzed for all the aforementioned one- and two-dimensional problems. For one-dimensional problems, the method has been found to be second order convergent in L^∞ -norm for any moment system considered. However, for two-dimensional problems, the method has been found slightly more than first order convergent in L^1 -norm, in general.
- Grad's moment equations for a binary gas-mixture with Maxwell interaction potential have then been regularized by employing the order of magnitude method and the (linear) regularized 17-moment (R17) equations for a binary gas-mixture interacting with Maxwell interaction potential have been derived; the R17 equations are third order accurate in the Knudsen number. The linear stability of R17 equation has also been analyzed in order to conclude *empirically* that the R17 equations with Maxwell interaction potential are linearly stable for binary gas-mixtures with small and moderate mass differences while unstable for those with large mass differences.

The models derived in this thesis can provide a better understanding of processes in gaseous mixtures at low computational cost. For example, it can be seen from figures 6.2 and 6.3 that on the one hand, the results from moment equations for the problem of heat transfer in a binary gas-mixture confined between two infinite parallel plates having different temperatures agree with those in [87] fairly well even for high Knudsen numbers (see also tables in [45]), at least qualitatively; on the other hand, the results for this problem from any moment system considered in the present thesis just take a couple of seconds to be computed. By comparing the results for the same problem from moment equations with those in [87], it may be stated that as an alternative to the realistic potential, the Maxwell interaction potential could be a preferable choice over the hard-sphere interaction potential in the hydrodynamic/slip-flow regime whereas the hard-sphere interaction potential could be a preferable choice over the Maxwell interaction potential in the transition regime. Furthermore, the models derived in this thesis are capable of describing the flow of a contaminant in a gas-mixture (see § 6.2.1), which the particle-based methods may not describe due to insufficient number of molecules of the contaminant in the mixture.

In the following, we shall also present the preliminary results on the problems of bottom-heated and lid-driven square cavities described in § 7.3 and § 7.4, although these results require further investigation and comparison with those obtained with highly accurate methods, such as DSMC method. All the quantities plotted and described below are the dimensionless perturbations from their respective ground states. All the results for both the cavity problems presented here have been computed by discretizing the domain of the cavity in 100×100 identical cells.

Each computation shown below with (unoptimized) MATHEMATICA[®] code on a standard computer takes around 2 minutes with $2 \times G13$ equations for Maxwell molecules and 15–20 minutes with other moment systems. A similar computation with DSMC method takes days even in case of a single gas [79].

9.2 Heat transfer in a bottom-heated square cavity

9.2.1 Problem description

We consider a binary mixture of gases α and β in steady state confined in a square cavity of side length L . Let the temperature of the bottom of the cavity be $T_H = T_o + \varepsilon \tilde{T}_H$ while the temperatures of its all other sides be $T_C = T_o$; and let all the walls of the cavity are stationary (i.e., $\mathbf{v}_w = \mathbf{0}$ for all the walls). The schematic of the problem is shown in figure 9.1. The third dimension z of the cavity is assumed very long so that heat transfer takes place essentially in two dimensions (x and y) and thus z -axis in figure 9.1 is just for illustration purposes. The moment equations and the boundary conditions for the problem are exactly same as in § 7.3.

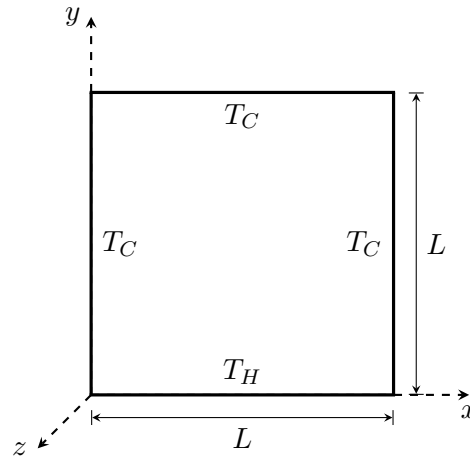


Figure 9.1: Schematic of a two-dimensional bottom heated square cavity; z -axis is included just for illustration purposes.

9.2.2 Preliminary results

As an example, we compute the results for He–Xe mixture with $x_{\text{He}}^o = 0.25$. The other parameters for the problem are taken as $\text{Kn} = 0.05$, $\hat{T}_H = 0.1$ and $\chi_\alpha = \chi_\beta = 1$. Similar preliminary results for Ne–Ar gas mixture can be found in [43].

Figure 9.2 exhibits the velocity streamlines superimposed over the temperature contours of the lighter component (He) in the mixture for different moment systems considered in the present thesis. Each sub-figure of figure 9.2 delineates four (two primary and two secondary) antipodal-rotating vortices, symmetrical about yz -plane passing through the center of the cavity. The primary vortices are induced due to acute temperature differences at the lower corners of the cavity—leading to thermal transpiration—while the secondary vortices are generated due to the coupling of the shear stress with velocity slip and tangential component of the heat flux

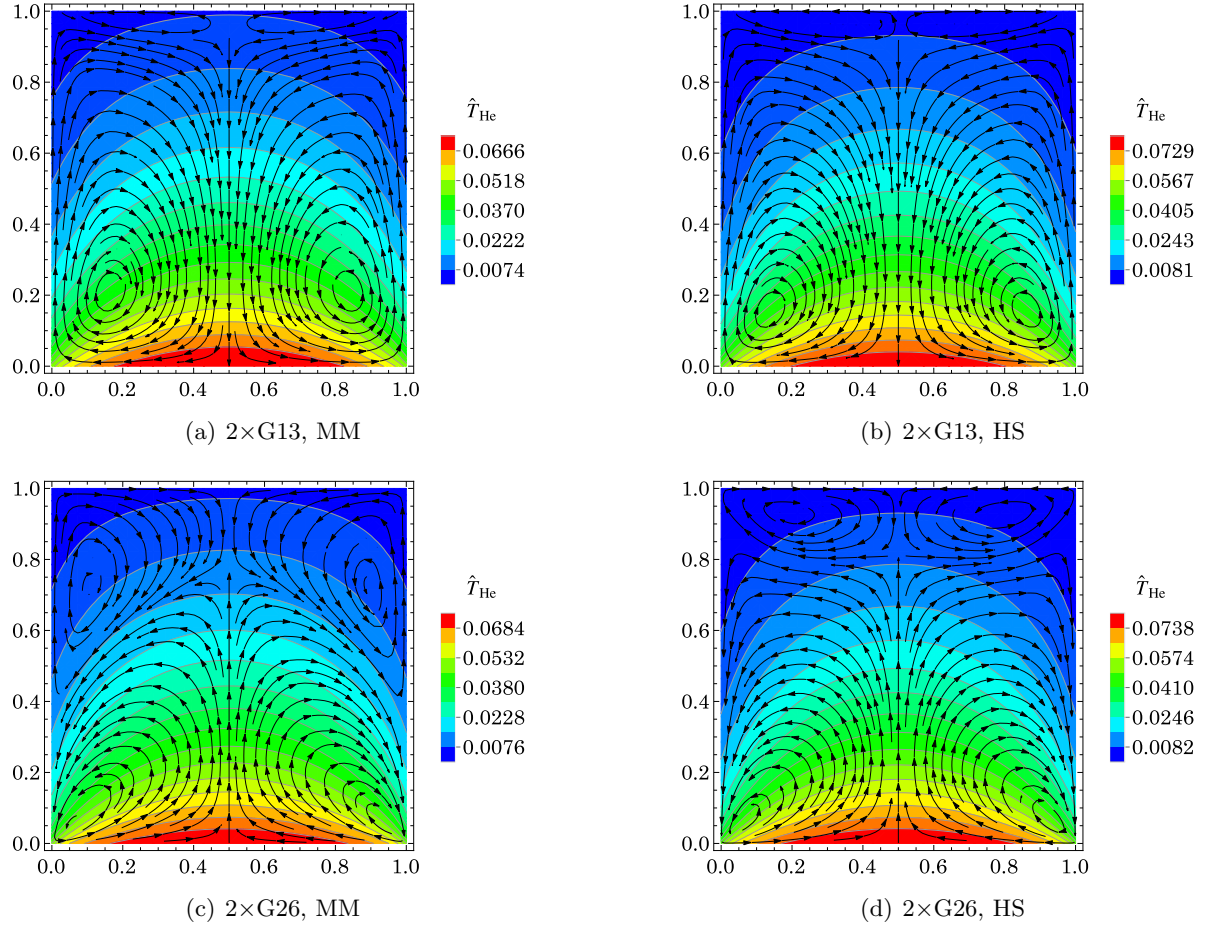


Figure 9.2: Velocity streamlines and temperature contours for He in He-Xe mixture with $x_{\text{He}}^o = 0.25$ computed with different moment systems at $\text{Kn} = 0.05$: (a) $2 \times \text{G13}$ equations for Maxwell molecules, (b) $2 \times \text{G13}$ equations for hard spheres, (c) $2 \times \text{G26}$ equations for Maxwell molecules and (d) $2 \times \text{G26}$ equations for hard spheres. The other parameters are $\hat{T}_H = 0.1$ and $\chi_\alpha = \chi_\beta = 1$.

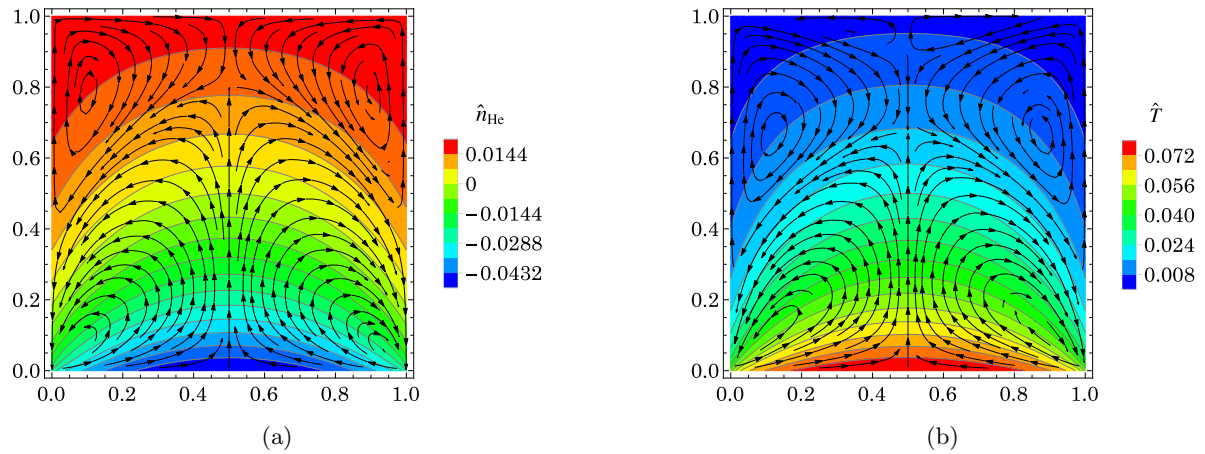


Figure 9.3: Plots of various field variables in He-Xe mixture with $x_{\text{He}}^o = 0.25$ computed with $2 \times \text{G26}$ equations for Maxwell molecules at $\text{Kn} = 0.05$: (a) number density contours and diffusion velocity lines for He and (b) average temperature and hydrodynamic velocity streamlines of the mixture. The other parameters are $\hat{T}_H = 0.1$ and $\chi_\alpha = \chi_\beta = 1$.

in the velocity slip boundary condition (boundary conditions (7.8) and (7.10)), see [81]. The secondary vortices are prominent for $2\times G26$ equations (figures 9.2(c) and 9.2(d)) but not so much for $2\times G13$ equations (figures 9.2(a) and 9.2(b)). Furthermore, the DSMC and R13 results of [81] in case of a single gas show that the secondary vortices are induced only along the vertical walls at $Kn = 0.05$, in that sense the result only with $2\times G26$ equations for Maxwell molecules is somewhat close to that of [81]. This again asserts that the hard-sphere interaction potential may not be a suitable choice for low Knudsen number processes. Nevertheless, it should be kept in mind that the results of [81] are computed with non-linear moment equations and boundary conditions whereas the results presented here are computed only with linear moment equations and boundary conditions.

Figure 9.3 illustrates the plots of various field variables computed with $2\times G26$ equations for Maxwell molecules. Figure 9.3(a) depicts the diffusion velocity lines of the lighter component (He) in the mixture superposed over the contours of its number density. Figure 9.3(a) shows that the gas molecules tend to stay towards colder sides of the cavity. Furthermore, the diffusion velocity at the bottom of the cavity is directed upwards, i.e., from the region of low density towards the region of high density which is due to the strong temperature gradient between the hot and cold plates. It should be noted that by Fick's law of diffusion in case of gaseous mixtures, the diffusion velocity of a constituent not only depends on its number density gradient but also on the number density gradients of the other constituents in the mixture as well as on the average temperature of the mixture, see (8.49)₁. Figure 9.3(b) delineates the hydrodynamic velocity streamlines of the whole mixture superposed over the average temperature of the mixture. In addition to primary and secondary vortices, figure 9.3(b) also shows two tertiary counter-rotating vortices. These tertiary vortices have also been observed in case of a single gas through R13 equations as well as through DSMC method (see [81]), but at relatively high Knudsen numbers ($Kn \gtrsim 0.1$).

9.3 Heat transfer in a lid-driven square cavity

9.3.1 Problem description

We again consider a binary mixture of gases α and β in steady state confined in a square cavity of side length L . Let the temperatures of all the walls of the cavity be same and equal to a constant value $T_w = T_o + \varepsilon \tilde{T}_0$; moreover, let the top wall (lid) of the cavity be moving in positive x -direction with velocity $v_{\text{lid}} = \varepsilon \tilde{v}_0$. The schematic of the problem is shown in figure 9.4. The third dimension z of the cavity is again assumed very long so that the flow takes place essentially in two dimensions (x and y) and thus z -axis in figure 9.4 is also just for illustration purposes. The moment equations and the boundary conditions for the problem are exactly same as in § 7.4.

9.3.2 Preliminary results

As an example, we again compute the results for He–Xe mixture with $x_{\text{He}}^o = 0.25$. The other parameters for the problem are taken as $Kn = 0.05$, $\hat{v}_w = 1$, $\hat{T}_0 = 0$ and $\chi_\alpha = \chi_\beta = 1$ (see

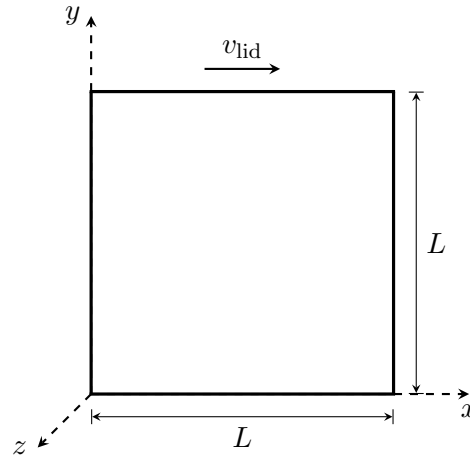


Figure 9.4: Schematic of a two-dimensional lid-driven square cavity; z -axis is included just for illustration purposes.

§ 7.4.2).

Figure 9.5 delineates the total heat flux lines superimposed over the temperature contours of the lighter component (He) in the mixture for different moment systems considered in the present thesis. Owing to the motion of the lid in positive x -direction, the gases in the cavity expand at the top-left corner while compress at the top-right corner, resulting into low temperature at the top-left corner while high temperature at the top-right corner. Each sub-figure of figure 9.5 depicts that the heat flows from cold to hot. This is a non-Fourier effect, which the Fick, Navier–Stokes and Fourier equations cannot capture, and have been confirmed by DSMC as well as by R13 equations in case of a single gas, see [79]. The reason for the non-Fourier heat transfer is the coupling of heat flux not only with the temperature gradient but also with the stress gradient in the moment equations for heat fluxes of the constituents; when the stress gradient dominates over the temperature gradient, the heat may flow from cold to hot; and owing to the moving lid, the stress gradient for the present problem is strong near the top wall of the cavity. The $2\times G13$ equations show the low and high temperatures only at the top-left and top-right corners, respectively, see figures 9.5(a) and 9.5(b), whereas the $2\times G26$ equations show them somewhat below the top-left and top-right corners, respectively, and tiny areas with opposite temperatures (high and low temperatures at the top-left and top-right corners, respectively), see figures 9.5(c) and 9.5(d); these opposite temperatures in case of $2\times G26$ equations may be due to our treatment of boundary conditions at corners which need to be analyzed further. In fact, the DSMC and R13 results of [79] for a single gas also show that the heat flux lines are not symmetric about yz -plane passing through the center of the cavity whereas they are apparently symmetric in our results. The asymmetry in heat flux lines of [79] is due to the non-linear moment equations and boundary conditions used in that work.

Figure 9.6 illustrates the plots of various field variables computed with $2\times G26$ equations for Maxwell molecules. Figure 9.6(a) depicts the diffusion velocity lines of the lighter component (He) in the mixture superposed over the contours of its number density. Figure 9.6(a) shows that the gas molecules of He in the mixture diffuse from their high density region towards low density region along the walls of the cavity while the other way round in the bulk of the cavity.

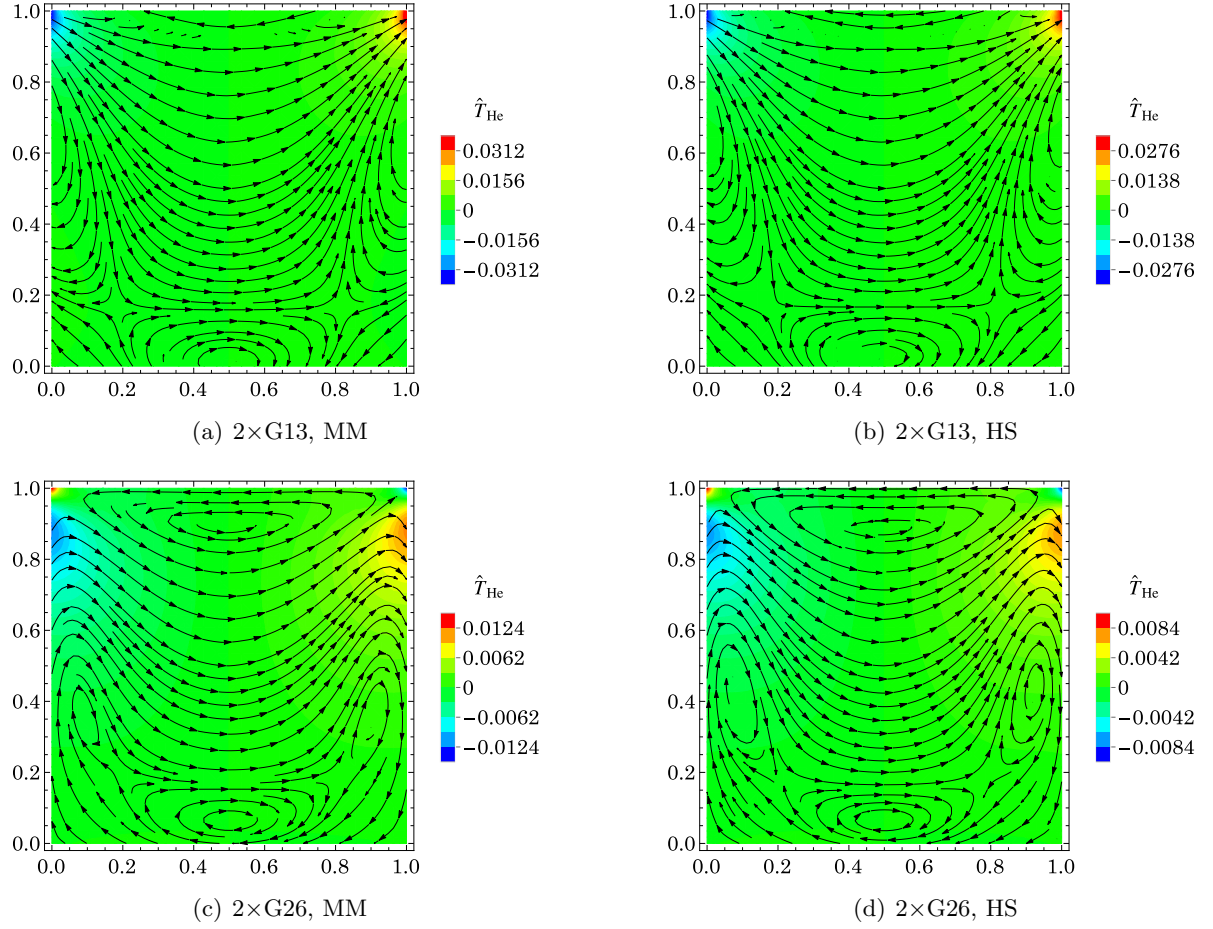


Figure 9.5: Heat flux lines and temperature contours for He in He–Xe mixture with $x_{\text{He}}^0 = 0.25$ computed with different moment systems at $\text{Kn} = 0.05$: (a) $2 \times G13$ equations for Maxwell molecules, (b) $2 \times G13$ equations for hard spheres, (c) $2 \times G26$ equations for Maxwell molecules and (d) $2 \times G26$ equations for hard spheres. The other parameters are $\hat{T}_0 = 0$, $\hat{v}_w = \chi_\alpha = \chi_\beta = 1$.

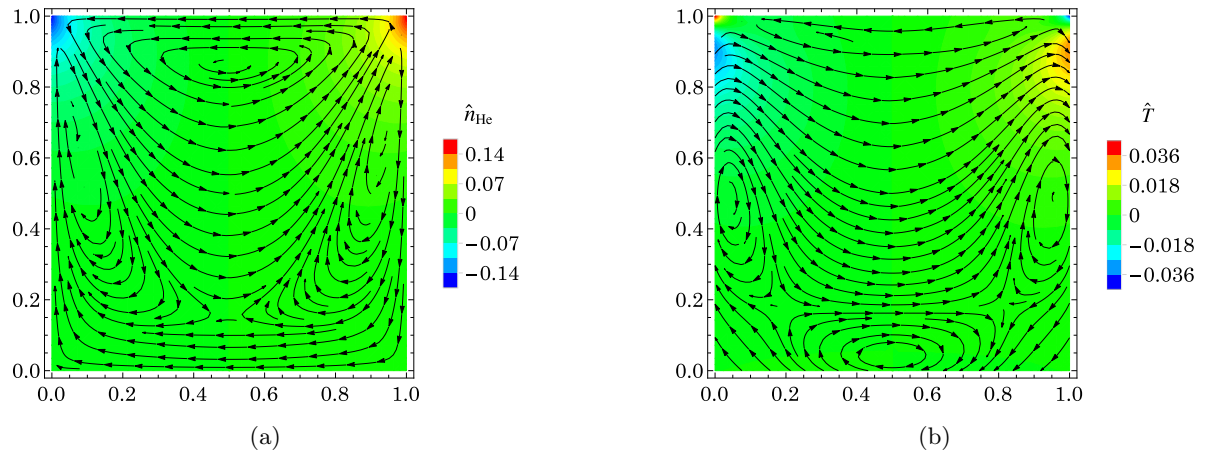


Figure 9.6: Plots of various field variables in He–Xe mixture with $x_{\text{He}}^0 = 0.25$ computed with $2 \times G26$ equations for Maxwell molecules at $\text{Kn} = 0.05$: (a) number density contours and diffusion velocity lines for He and (b) average temperature and total heat flux lines of the mixture. The other parameters are $\hat{T}_0 = 0$, $\hat{v}_w = \chi_\alpha = \chi_\beta = 1$.

For this problem, the diffusion is dominated mainly by the number density gradients of the constituents since the temperature gradients are very small. Figure 9.6(b) delineates the hydrodynamic velocity streamlines of the whole mixture superposed over the average temperature of the mixture. Again, the figure shows that the heat flows from cold to hot which is a non-Fourier effect as explained above.

9.4 Outlook

Based on this work, there are many possibilities which are to be explored in future. Some of them are listed below.

- For the bottom-heated square cavity and lid-driven square cavity problems, a detailed investigation and comparison with highly accurate results from DSMC or some other method will be considered in future.
- In this thesis, we mainly focused on solving the problems with linear equations in steady state and in simple geometries (one- and two-dimensional problems in Cartesian coordinate system). A glance at our results on lid-driven square cavity problem and those in [79] immediately demands extending the numerical method to non-linear problems. It remains to extend the method for solving the problems in 3D, in curvilinear coordinate systems, for non-linear processes and for time-dependent problems.
- It has been learned in chapter 7 that our numerical method based on finite differences is not second order convergent for large Knudsen numbers in case of two-dimensional problems mainly due to the discretization at the boundaries which was performed with one-sided finite (forward or backward) difference schemes in normal directions. The discretization at the boundaries (and corners of the square cavity), perhaps, can be performed more ingeniously in order to get convergence of order close to two. Therefore, the numerical method for two-dimensional problems will be scrutinized again.
- Also, it motivates to develop more advanced numerical methods, such as finite volume method, with structured and unstructured grids for the moment systems derived in this thesis in order to solve the problems in complex geometries.
- The system of Grad's moment equations derived in the present thesis can further be extended by including the full fourth order moment in order to describe the processes with high Knudsen numbers.
- The R17 equations for binary gas-mixtures are derived only for Maxwell molecules and only in linearized form, although one may concur that the derivation of linear R17 equations for binary gas-mixtures of Maxwell molecules is already not so straightforward, see chapter 8. Moreover, the derivation of the regularized moment equations for hard spheres is so intricate even in case of single gas that they have been derived only in linearized form till now, see [104]. Therefore, the derivation of non-linear R17 equations for binary gas-mixtures of Maxwell molecules as well as the derivation of linear and non-linear R17 equations for hard-sphere gas-mixtures will be considered elsewhere in future. Moreover,

the R17 equations for Maxwell interaction potential derived in this thesis are not stable for all binary gas-mixtures. The procedure for the derivation will be investigated again in prospect of stabilizing the R17 equations for all binary gas-mixtures.

- The R13 equations for a single gas have been very successful in describing many non-equilibrium effects and several processes in early transition regime. Nevertheless, owing to time constraint, no problems have been studied through R17 equations for binary gas-mixtures in the present thesis, and the application of R17 equations for binary gas-mixtures will be explored in future.
- After deriving the $N \times G13$ and $N \times G26$ equations and their associated boundary conditions, we promptly switched to binary gas-mixtures. In future, the gas-mixtures comprised of more than two gases may also be explored using these equations.
- It can be taken as a motivation and challenge to develop and exploit the higher order and regularized moment equations for polyatomic and granular gas-mixtures.

Apparently, the moment equations derived in this thesis appear to be promising alternatives to the computationally expensive particle based methods for studying the processes in gaseous mixtures in the transition regime since they help in understanding the non-intuitive behaviours—for instance, the non-Fourier heat flow—in rarefied gases, at least qualitatively, although many things are yet to be explored.

Appendix A

Additional results on the problem of § 6.2.1

Figures A.1–A.4 illustrate the number density, temperature, normal stress and heat flux, respectively, of the infinitely diluted component in Ne-Ar mixture with Ar being the diluted component. Furthermore, figures A.5–A.8 show the same quantities, respectively, for the infinitely diluted component in He-Ar mixture with He being the diluted component whereas figures A.9–A.12 display them, respectively, for the same mixture with Ar being the diluted component. Similarly, figures A.13–A.16 depict the same quantities, respectively, for the infinitely diluted component in He-Xe mixture with He being the diluted component whereas figures A.17–A.20 delineate them, respectively, for the same mixture with Xe being the diluted component.

All the plots in each figure are shown in the right half of the channel and the values of other parameters for all the figures are $\Delta\hat{T}_w = 0.5$, $\chi_\alpha = 1$ and $\chi_\beta = 0.1$. In all the figures, the top and bottom rows show the plots for the 2×G13 and 2×G26 equations, respectively, whereas the left and right columns depict them for Maxwell and hard-sphere interaction potentials, respectively. Moreover, in each figure, the continuous and dashed lines denote the analytical and first order Chapman–Enskog solutions, respectively. The dashed lines for all Knudsen numbers are overlapped in all the figures except in the figures for heat flux (figures A.4, A.8, A.12, A.16 and A.20) since the number density, temperature and normal stress of the diluted component do not vary with the Knudsen number. Moreover, the (constant) values of the heat flux from the first order Chapman–Enskog solution for Knudsen numbers 0.5 and 1 are higher than the plot ranges shown, and therefore the green and pink dashed lines do not appear in figures A.4, A.8, A.12, A.16 and A.20. The plot ranges are taken this way for clarity.

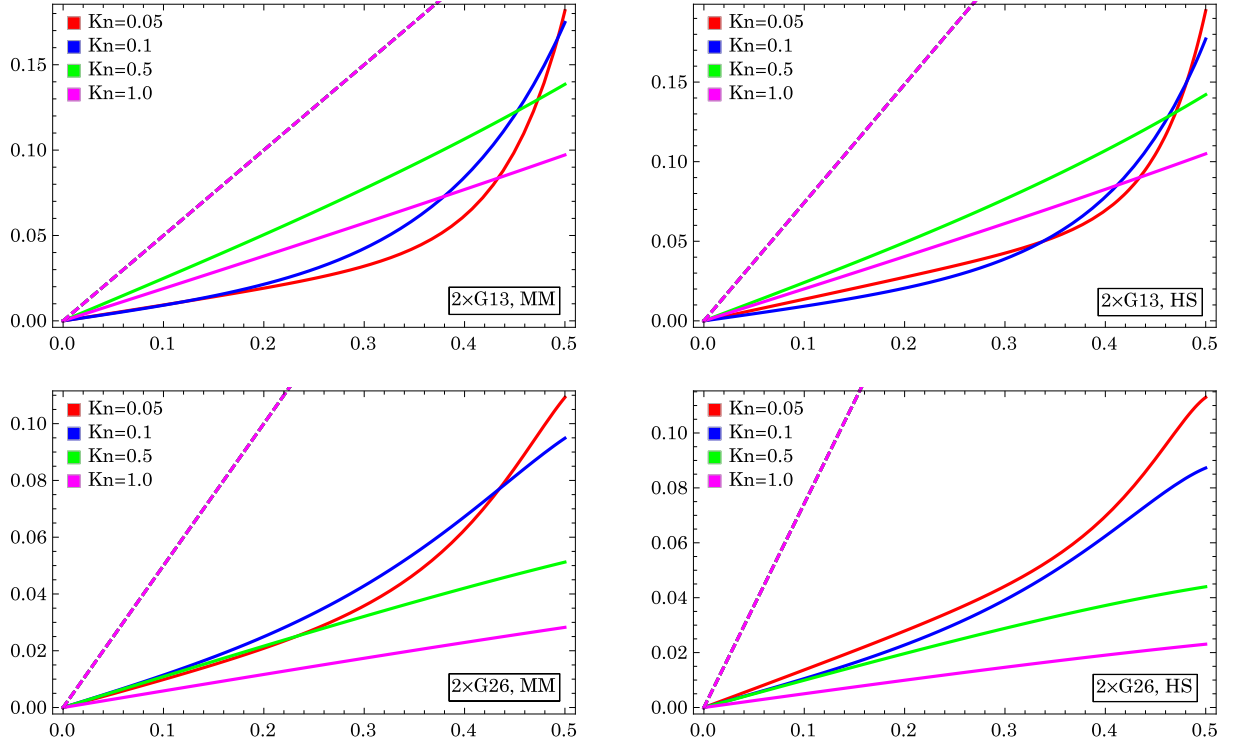


Figure A.1: Number density of the infinitely diluted (heavier) component in Ne-Ar mixture, $\hat{n}_{Ar}(\hat{x})$, plotted in right half of the channel for different moment systems.

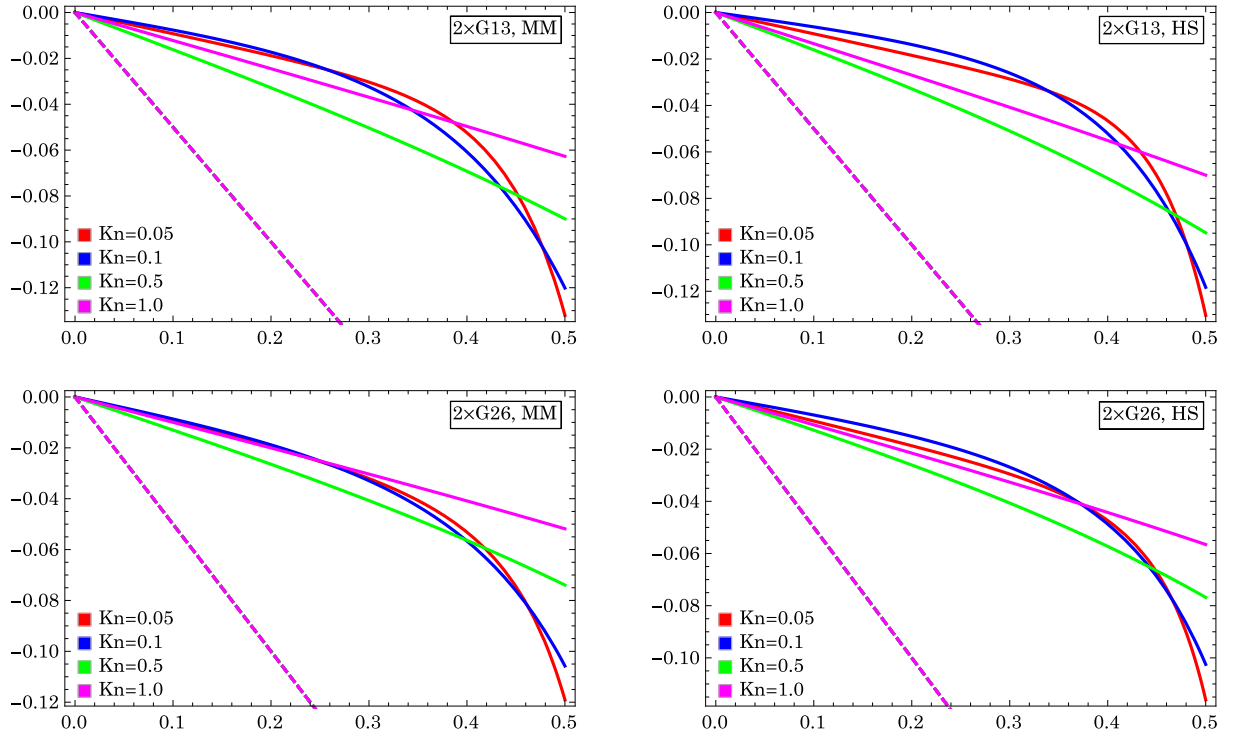


Figure A.2: Temperature of the infinitely diluted (heavier) component in Ne-Ar mixture, $\hat{T}_{Ar}(\hat{x})$, plotted in right half of the channel for different moment systems.

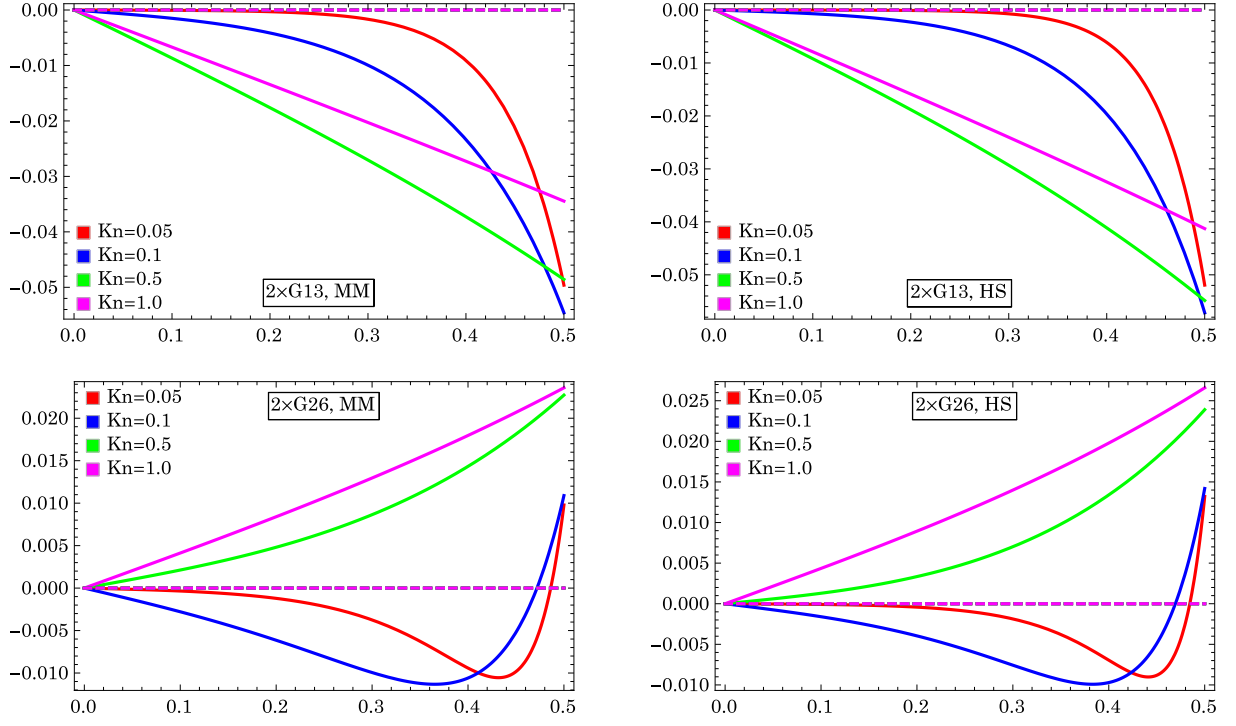


Figure A.3: Normal stress of the infinitely diluted (heavier) component in Ne-Ar mixture, $\hat{\sigma}_{xx}^{(Ar)}(\hat{x})$, plotted in right half of the channel for different moment systems.

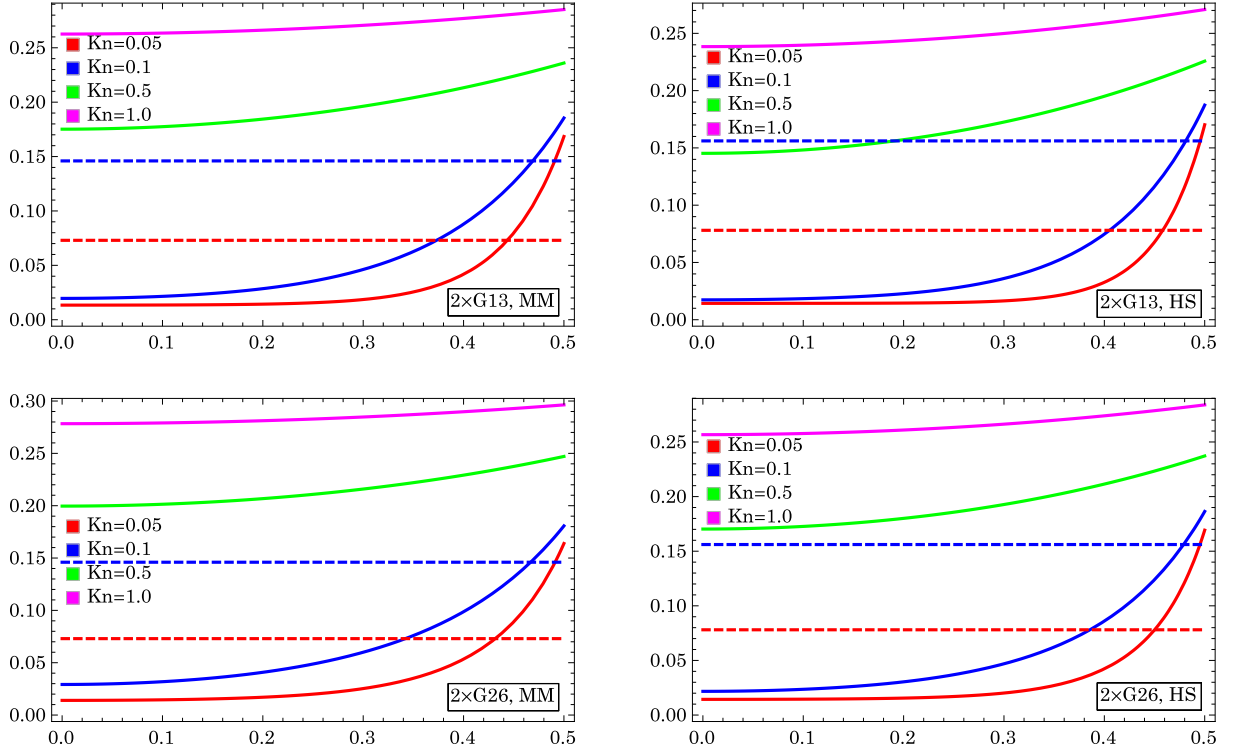


Figure A.4: Heat flux of the infinitely diluted (heavier) component in Ne-Ar mixture, $\hat{q}_x^{(Ar)}(\hat{x})$, plotted in right half of the channel for different moment systems.

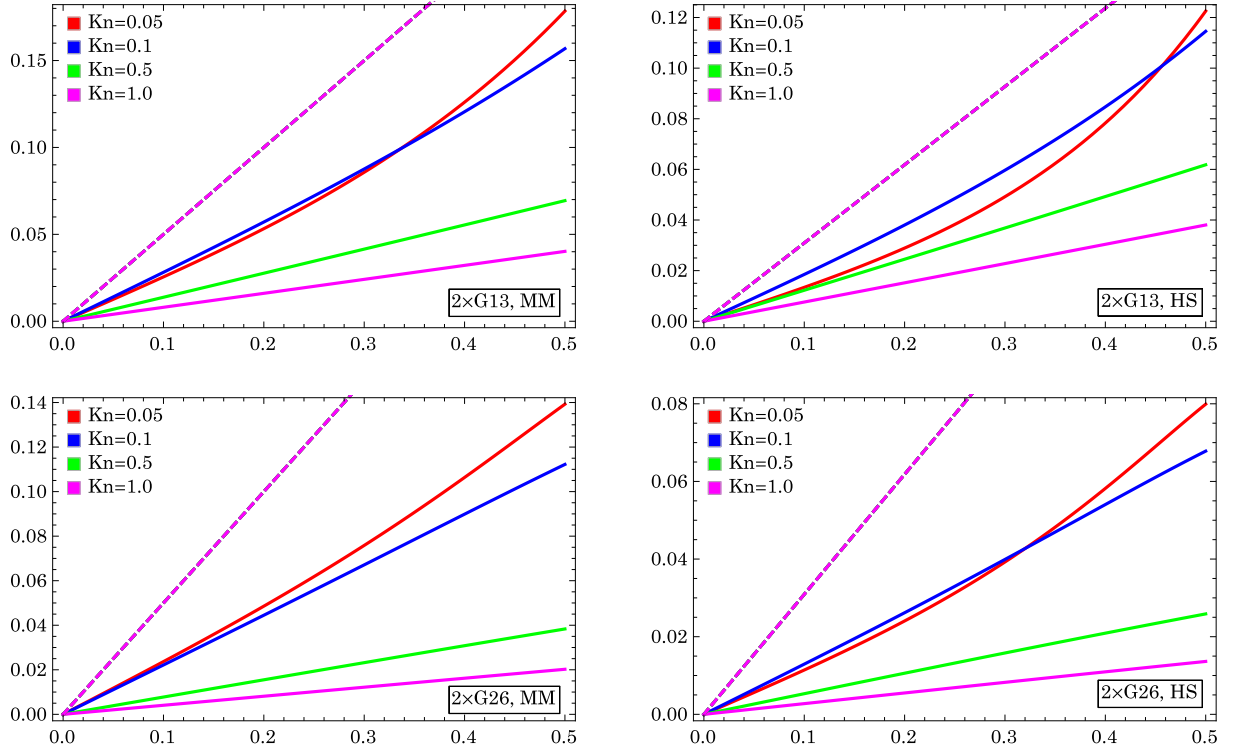


Figure A.5: Number density of the infinitely diluted (lighter) component in He-Ar mixture, $\hat{n}_{\text{He}}(\hat{x})$, plotted in right half of the channel for different moment systems.

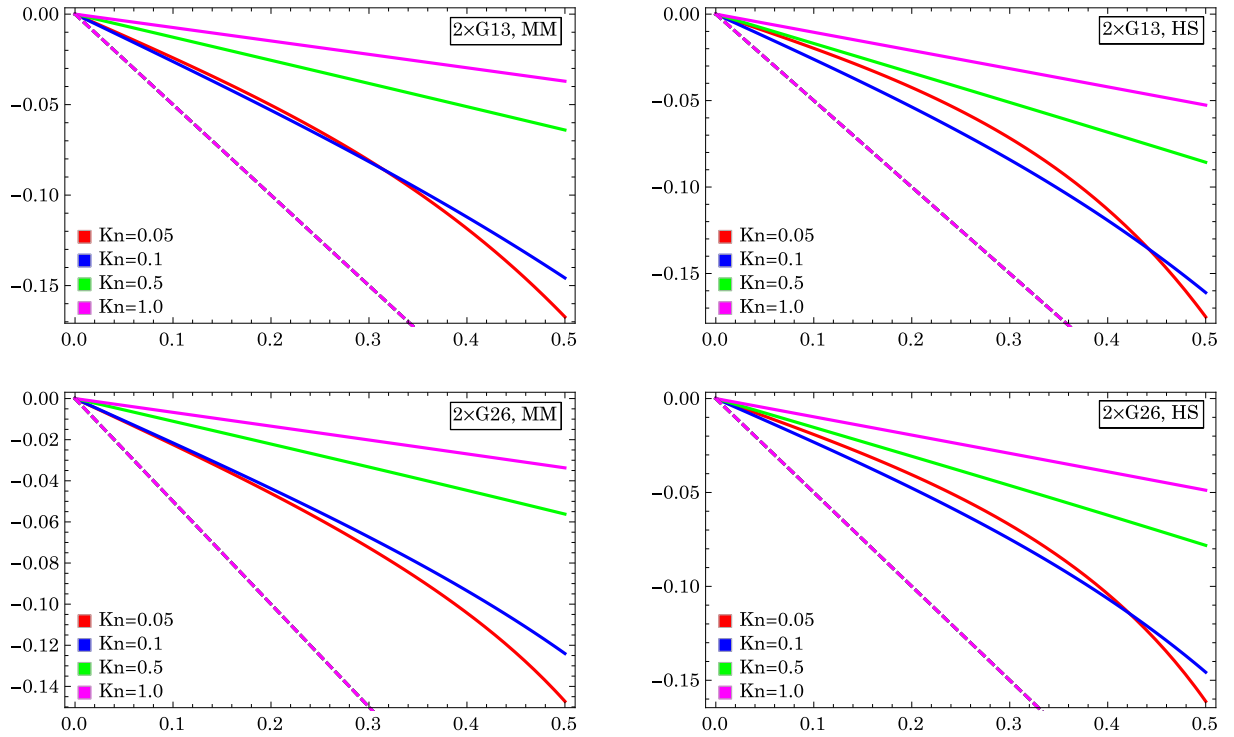


Figure A.6: Temperature of the infinitely diluted (lighter) component in He-Ar mixture, $\hat{T}_{\text{He}}(\hat{x})$, plotted in right half of the channel for different moment systems.

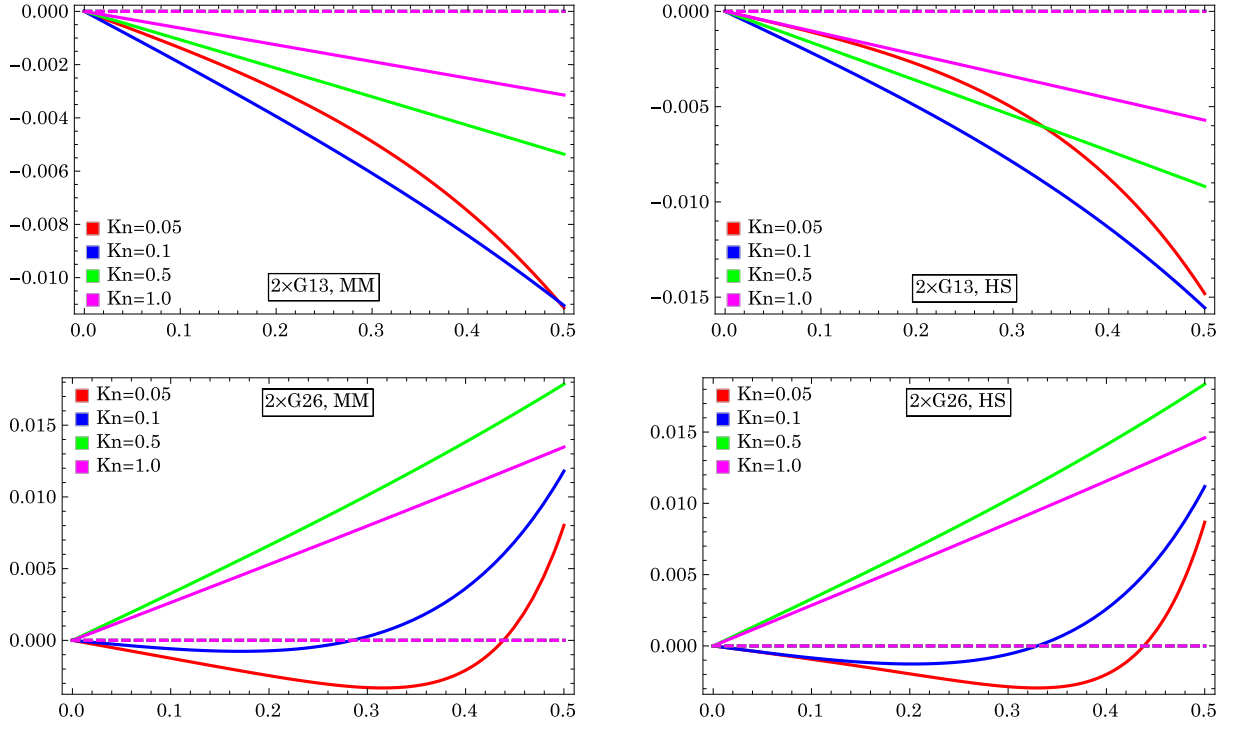


Figure A.7: Normal stress of the infinitely diluted (lighter) component in He-Ar mixture, $\hat{\sigma}_{xx}^{(\text{He})}(\hat{x})$, plotted in right half of the channel for different moment systems.

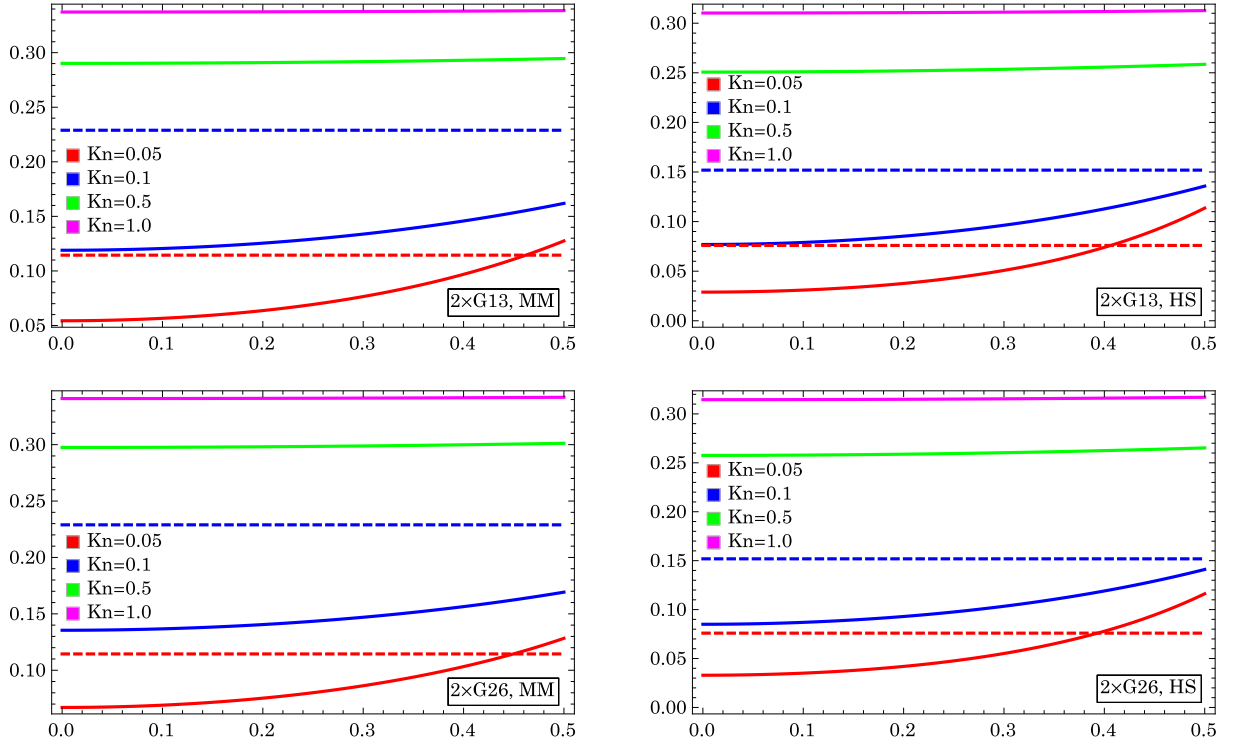


Figure A.8: Heat flux of the infinitely diluted (lighter) component in He-Ar mixture, $\hat{q}_x^{(\text{He})}(\hat{x})$, plotted in right half of the channel for different moment systems.

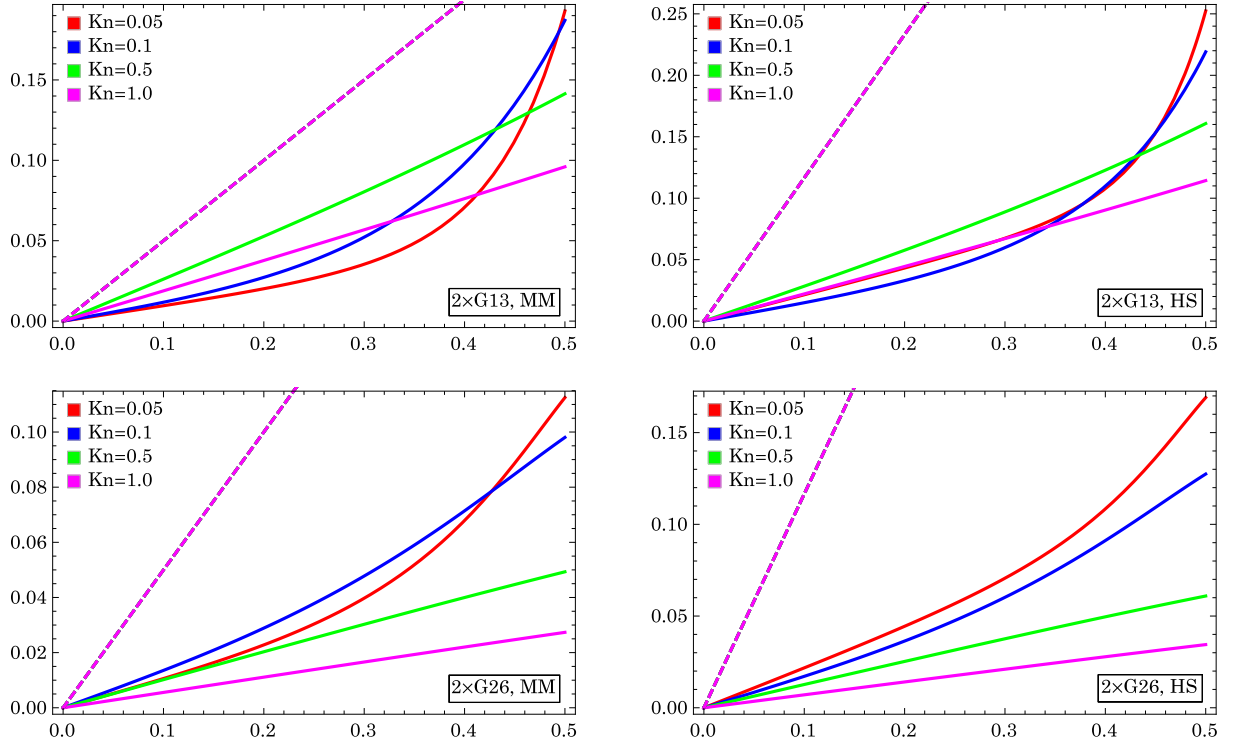


Figure A.9: Number density of the infinitely diluted (heavier) component in He-Ar mixture, $\hat{n}_{Ar}(\hat{x})$, plotted in right half of the channel for different moment systems.

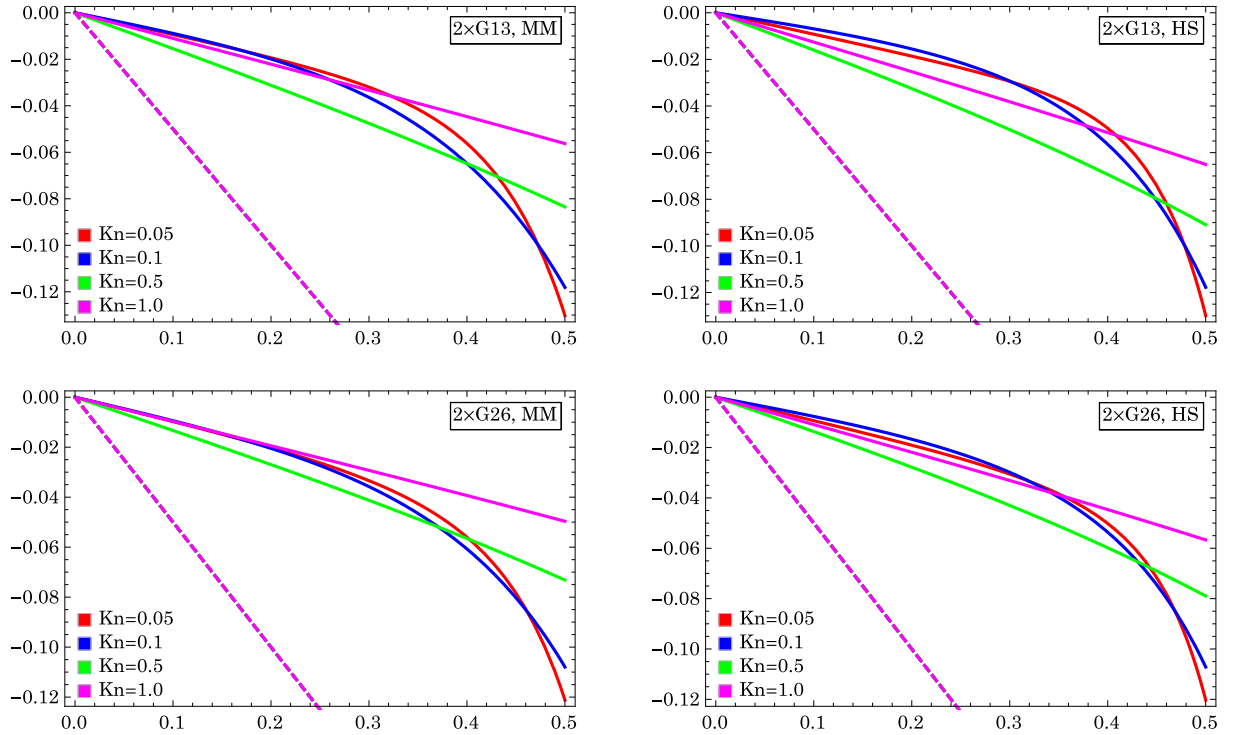


Figure A.10: Temperature of the infinitely diluted (heavier) component in He-Ar mixture, $\hat{T}_{Ar}(\hat{x})$, plotted in right half of the channel for different moment systems.

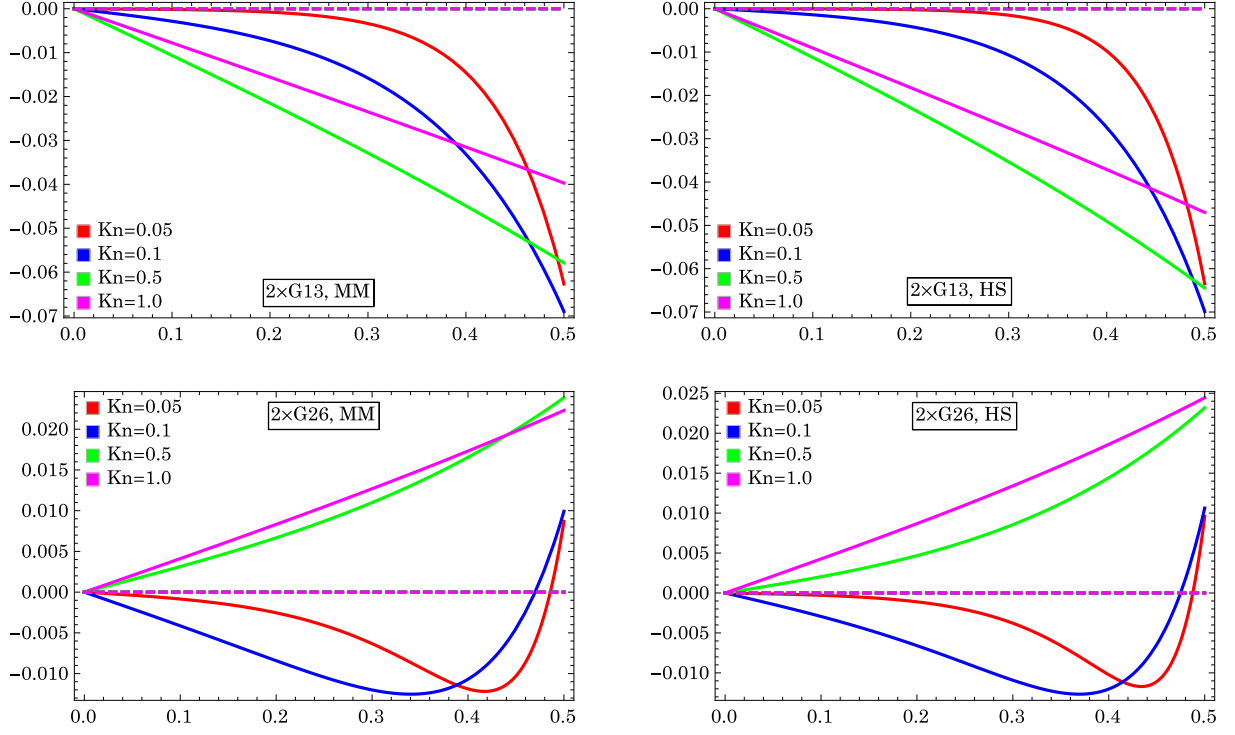


Figure A.11: Normal stress of the infinitely diluted (heavier) component in He-Ar mixture, $\hat{\sigma}_{xx}^{(Ar)}(\hat{x})$, plotted in right half of the channel for different moment systems.

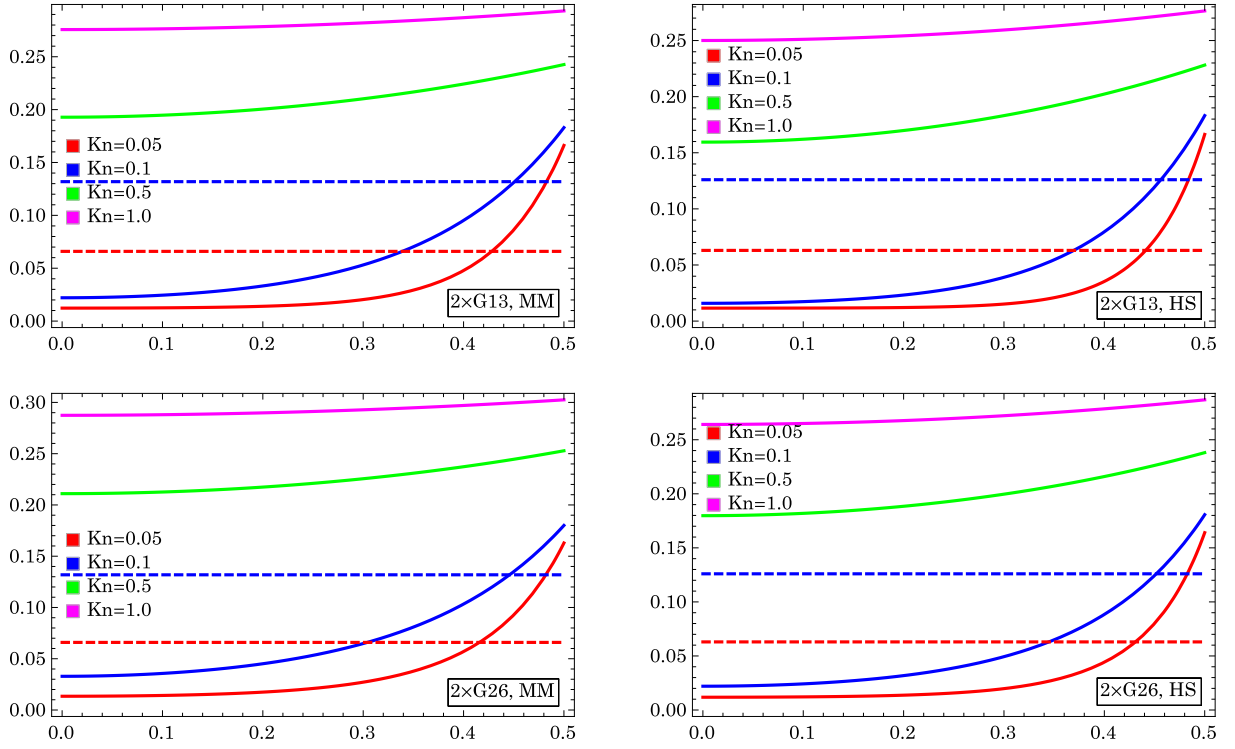


Figure A.12: Heat flux of the infinitely diluted (heavier) component in He-Ar mixture, $\hat{q}_x^{(Ar)}(\hat{x})$, plotted in right half of the channel for different moment systems.

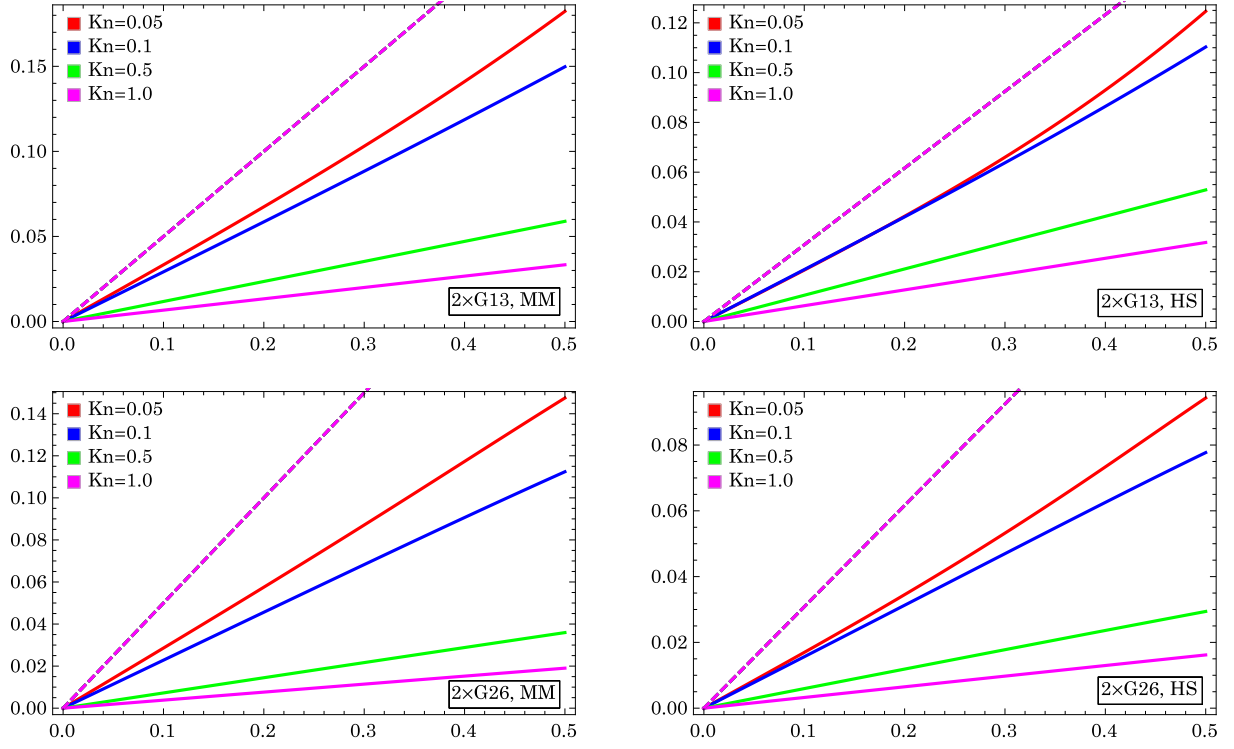


Figure A.13: Number density of the infinitely diluted (lighter) component in He-Xe mixture, $\hat{n}_{\text{He}}(\hat{x})$, plotted in right half of the channel for different moment systems.

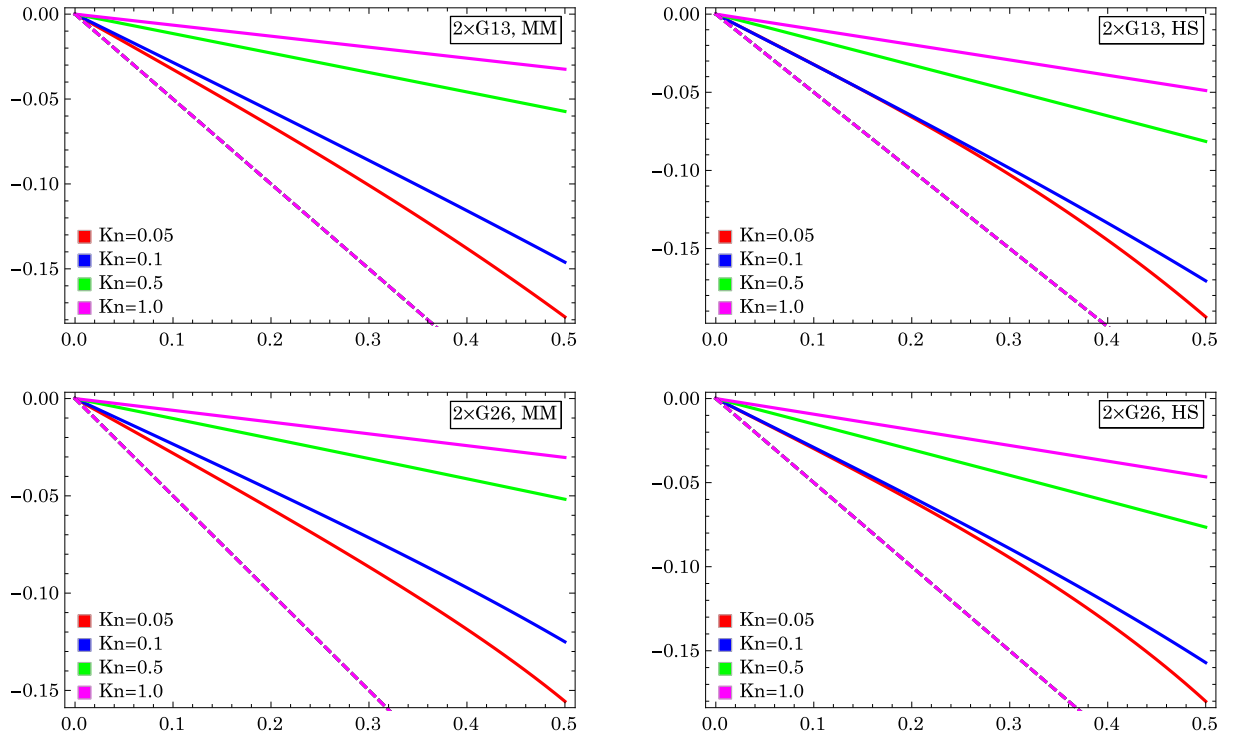


Figure A.14: Temperature of the infinitely diluted (lighter) component in He-Xe mixture, $\hat{T}_{\text{He}}(\hat{x})$, plotted in right half of the channel for different moment systems.

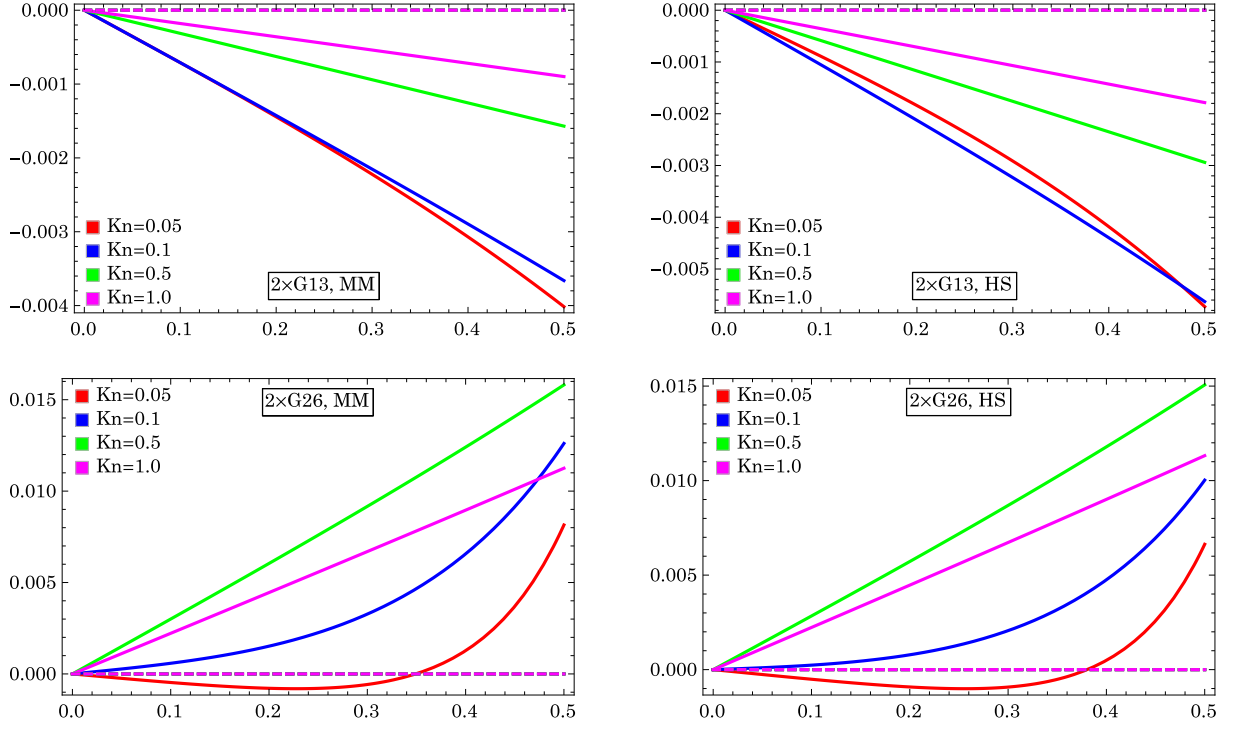


Figure A.15: Normal stress of the infinitely diluted (lighter) component in He-Xe mixture, $\hat{\sigma}_{xx}^{(\text{He})}(\hat{x})$, plotted in right half of the channel for different moment systems.

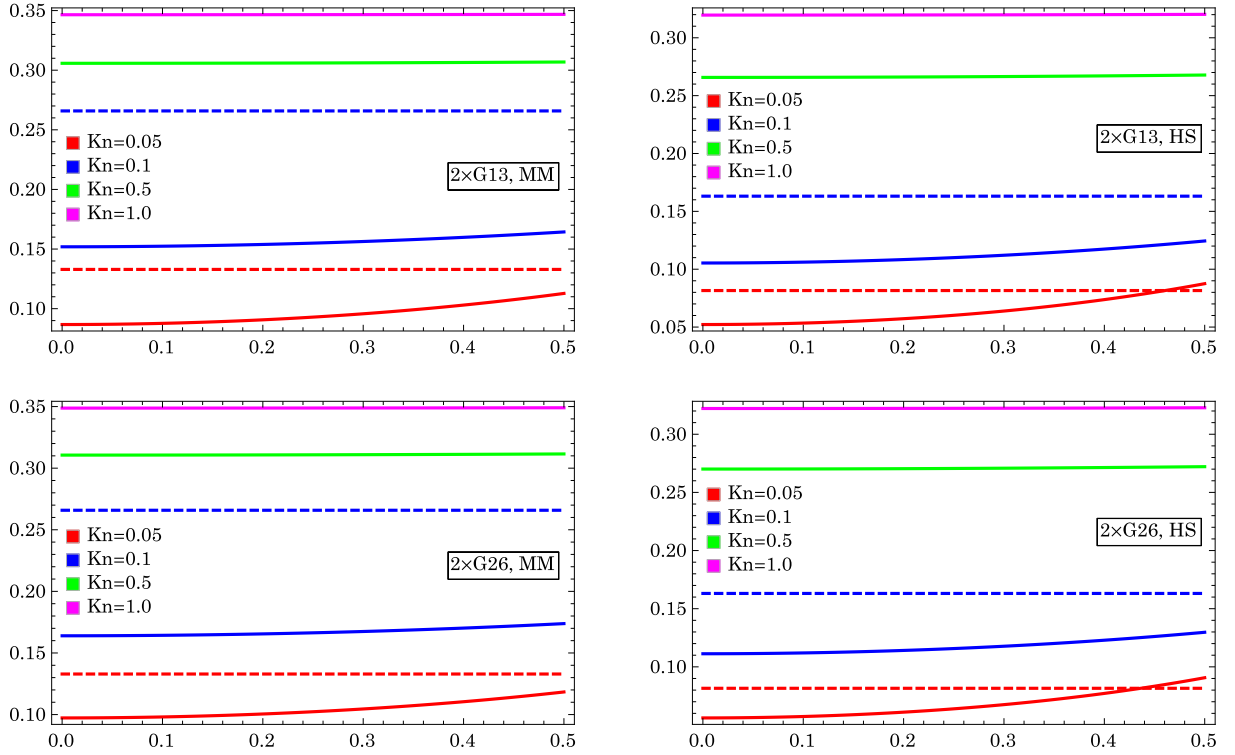


Figure A.16: Heat flux of the infinitely diluted (lighter) component in He-Xe mixture, $\hat{q}_x^{(\text{He})}(\hat{x})$, plotted in right half of the channel for different moment systems.

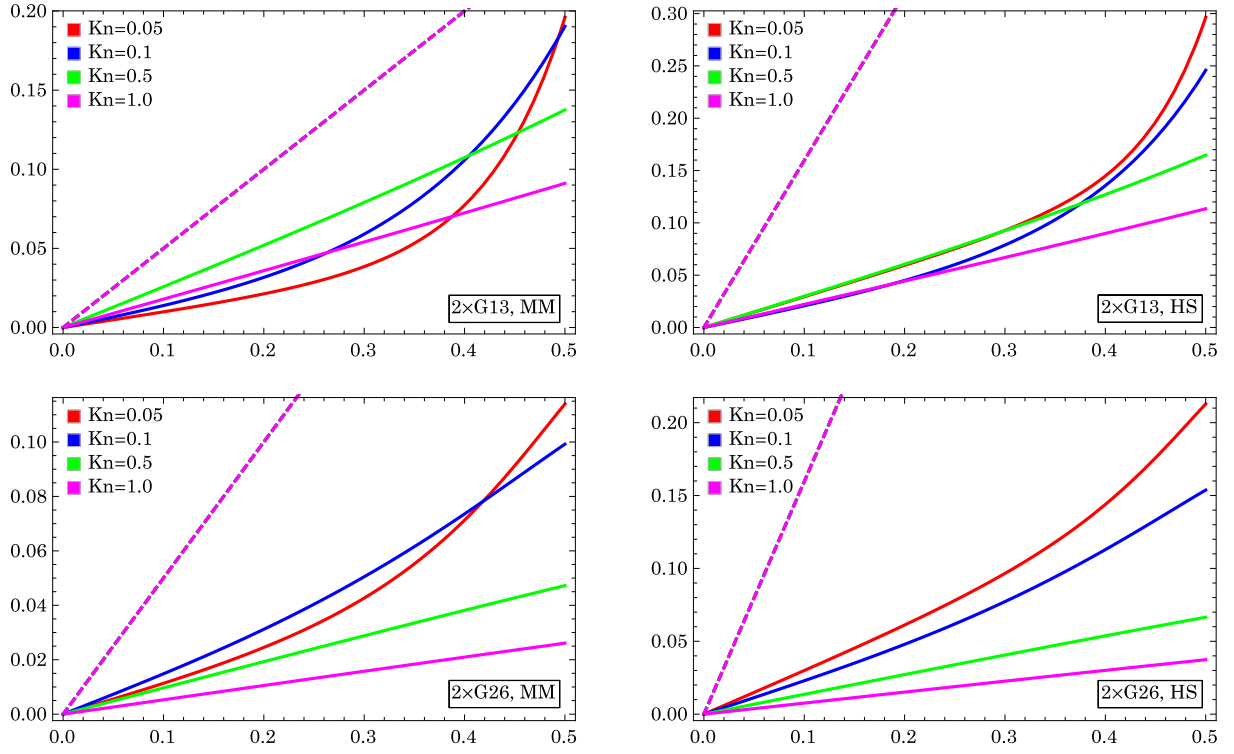


Figure A.17: Number density of the infinitely diluted (heavier) component in He-Xe mixture, $\hat{n}_{\text{Xe}}(\hat{x})$, plotted in right half of the channel for different moment systems.

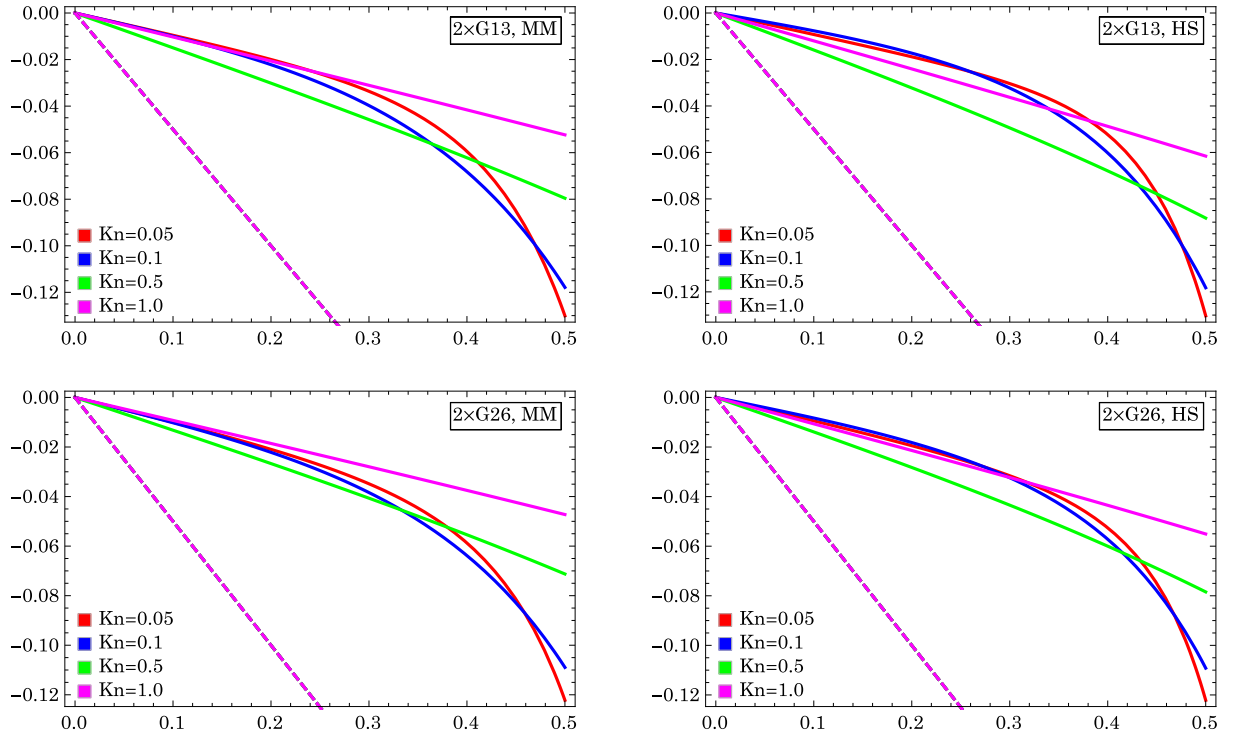


Figure A.18: Temperature of the infinitely diluted (heavier) component in He-Xe mixture, $\hat{T}_{\text{Xe}}(\hat{x})$, plotted in right half of the channel for different moment systems.

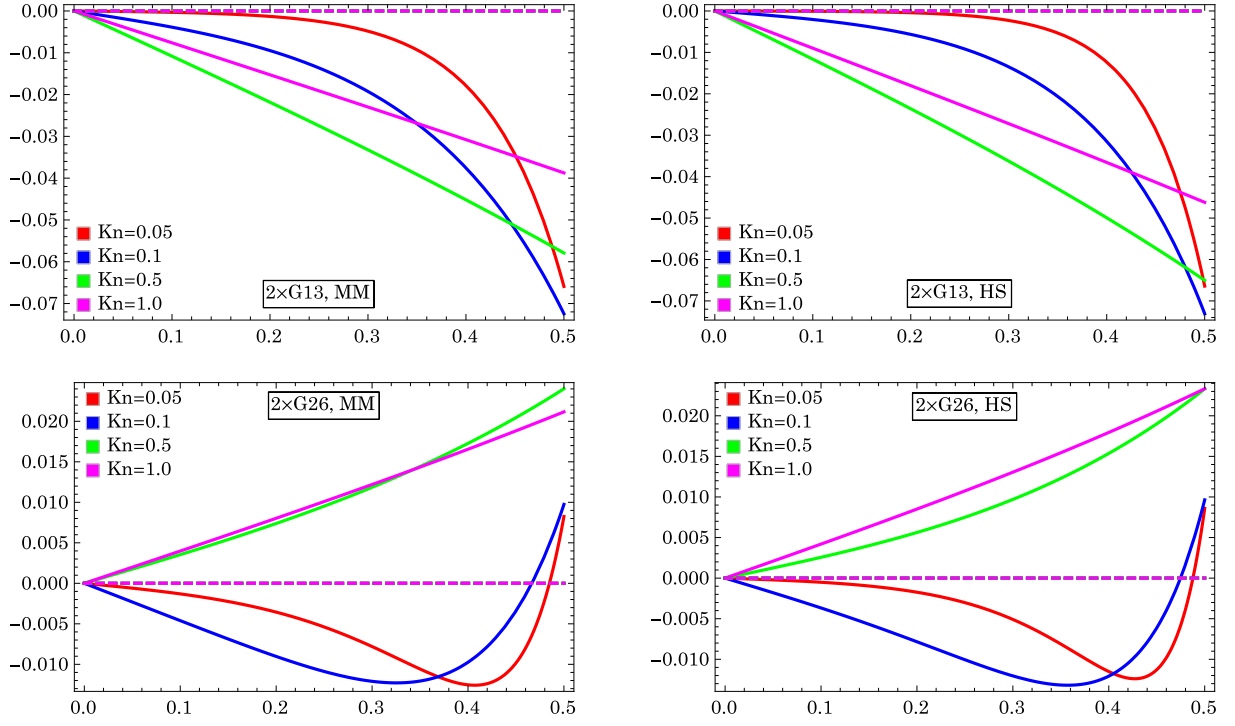


Figure A.19: Normal stress of the infinitely diluted (heavier) component in He-Xe mixture, $\hat{\sigma}_{xx}^{(\text{He})}(\hat{x})$, plotted in right half of the channel for different moment systems.

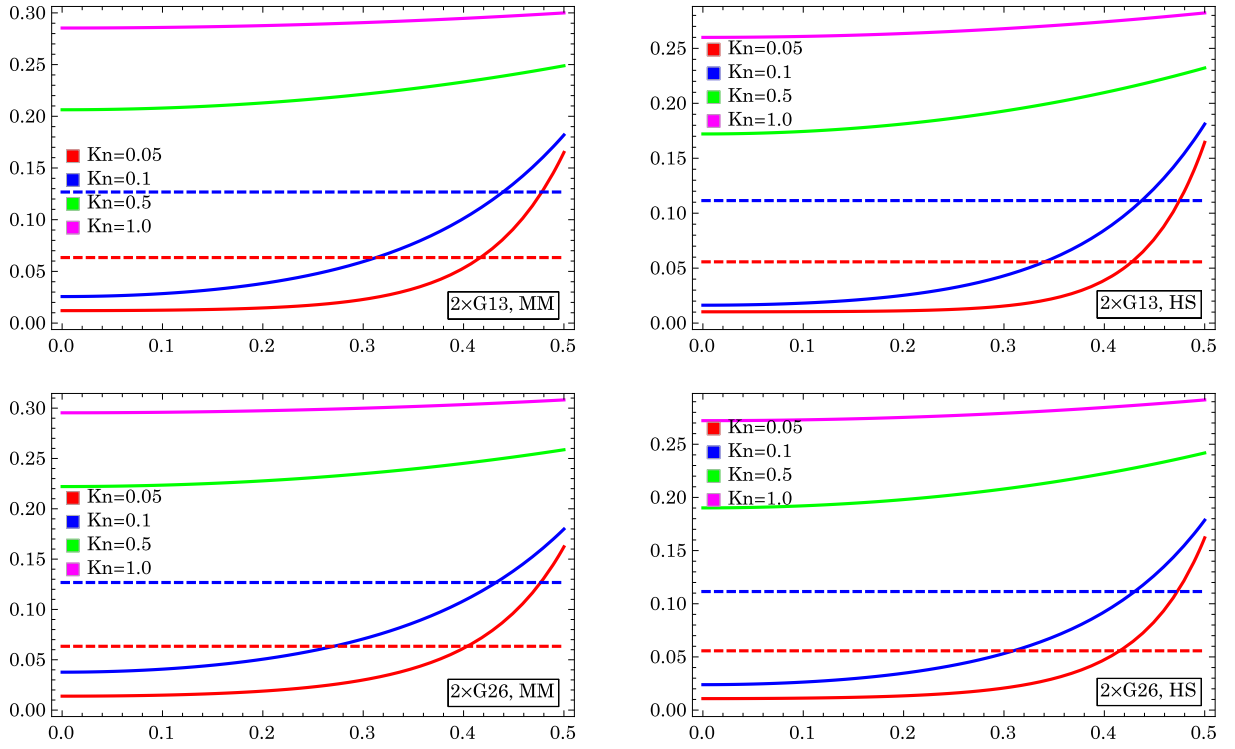


Figure A.20: Heat flux of the infinitely diluted (heavier) component in He-Xe mixture, $\hat{q}_x^{(\text{He})}(\hat{x})$, plotted in right half of the channel for different moment systems.

Appendix B

Leading orders of higher moments

Comparing coefficients of ε^0 on both sides of (8.6) and (8.7)–(8.18), one obtains:

$$\Delta \hat{T}_{|1} = 0, \quad (\text{B.1})$$

$$\begin{aligned} \frac{1}{\varkappa} \left[\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right] &= -\frac{\delta_1}{\Omega} \left(\hat{u}_{i|1}^{(\alpha)} - \frac{\varkappa_\alpha}{\varkappa_\beta} \hat{u}_{i|1}^{(\beta)} \right), \\ \frac{1}{\varkappa} \left[\varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - \varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - (\varkappa_\beta^2 - \varkappa_\alpha^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right] &= -\frac{\gamma_1}{\Omega} \left(\hat{u}_{i|1}^{(\beta)} - \frac{\varkappa_\beta}{\varkappa_\alpha} \hat{u}_{i|1}^{(\alpha)} \right), \end{aligned} \quad (\text{B.2})$$

$$\begin{aligned} 2\varkappa_\alpha \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} &= -\frac{1}{\Omega} \left\{ \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{\sigma}_{ij|1}^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_9 \hat{\sigma}_{ij|1}^{(\alpha)} - \delta_{11} \hat{\sigma}_{ij|1}^{(\beta)} \right) \right\}, \\ 2\varkappa_\beta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} &= -\frac{1}{\Omega} \left\{ \mathbf{x}_\beta^\circ \Omega_\beta \hat{\sigma}_{ij|1}^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_9 \hat{\sigma}_{ij|1}^{(\beta)} - \gamma_{11} \hat{\sigma}_{ij|1}^{(\alpha)} \right) \right\}, \end{aligned} \quad (\text{B.3})$$

$$\begin{aligned} \frac{5}{2} \frac{\partial \hat{T}}{\partial \hat{x}_i} &= -\frac{1}{\Omega} \left\{ \frac{2}{3} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{h}_{i|1}^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_{13} \hat{h}_{i|1}^{(\alpha)} - \delta_{15} \hat{h}_{i|1}^{(\beta)} \right) \right\}, \\ \frac{5}{2} \frac{\partial \hat{T}}{\partial \hat{x}_i} &= -\frac{1}{\Omega} \left\{ \frac{2}{3} \mathbf{x}_\beta^\circ \Omega_\beta \hat{h}_{i|1}^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_{13} \hat{h}_{i|1}^{(\beta)} - \gamma_{15} \hat{h}_{i|1}^{(\alpha)} \right) \right\}, \end{aligned} \quad (\text{B.4})$$

$$\begin{aligned} 0 &= -\frac{1}{\Omega} \left\{ \frac{3}{2} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{m}_{ijk|1}^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_{17} \hat{m}_{ijk|1}^{(\alpha)} - \delta_{18} \hat{m}_{ijk|1}^{(\beta)} \right) \right\}, \\ 0 &= -\frac{1}{\Omega} \left\{ \frac{3}{2} \mathbf{x}_\beta^\circ \Omega_\beta \hat{m}_{ijk|1}^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_{17} \hat{m}_{ijk|1}^{(\beta)} - \gamma_{18} \hat{m}_{ijk|1}^{(\alpha)} \right) \right\}, \end{aligned} \quad (\text{B.5})$$

$$\begin{aligned} 0 &= -\frac{1}{\Omega} \left\{ \frac{7}{6} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{R}_{ij|1}^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_{21} \hat{R}_{ij|1}^{(\alpha)} - \delta_{23} \hat{R}_{ij|1}^{(\beta)} \right) \right\}, \\ 0 &= -\frac{1}{\Omega} \left\{ \frac{7}{6} \mathbf{x}_\beta^\circ \Omega_\beta \hat{R}_{ij|1}^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_{21} \hat{R}_{ij|1}^{(\beta)} - \gamma_{23} \hat{R}_{ij|1}^{(\alpha)} \right) \right\}, \end{aligned} \quad (\text{B.6})$$

$$\begin{aligned} 0 &= -\frac{1}{\Omega} \left\{ \frac{2}{3} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{\Delta}_{\alpha|1} + \mathbf{x}_\beta^\circ \left(\delta_{25} \hat{\Delta}_{\alpha|1} - \delta_{26} \hat{\Delta}_{\beta|1} \right) \right\}, \\ 0 &= -\frac{1}{\Omega} \left\{ \frac{2}{3} \mathbf{x}_\beta^\circ \Omega_\beta \hat{\Delta}_{\beta|1} + \mathbf{x}_\alpha^\circ \left(\gamma_{25} \hat{\Delta}_{\beta|1} - \gamma_{26} \hat{\Delta}_{\alpha|1} \right) \right\}. \end{aligned} \quad (\text{B.7})$$

Equations (B.1)–(B.7) on using the relation $\rho_\alpha \mathbf{u}_\alpha + \rho_\beta \mathbf{u}_\beta = \mathbf{0}$ in dimensionless form imply that $\hat{u}_{i|1}^{(\alpha)}$, $\hat{u}_{i|1}^{(\beta)}$, $\hat{\sigma}_{ij|1}^{(\alpha)}$, $\hat{\sigma}_{ij|1}^{(\beta)}$, $\hat{h}_{i|1}^{(\alpha)}$, $\hat{h}_{i|1}^{(\beta)}$ do not vanish, whereas

$$\Delta \hat{T}_{|1} = \hat{m}_{ijk|1}^{(\alpha)} = \hat{m}_{ijk|1}^{(\beta)} = \hat{R}_{ij|1}^{(\alpha)} = \hat{R}_{ij|1}^{(\beta)} = \hat{\Delta}_{\alpha|1} = \hat{\Delta}_{\beta|1} = 0. \quad (\text{B.8})$$

Thus, the leading orders of the diffusion velocities, stresses and heat fluxes of both the constituents are one while the leading orders of temperature difference and other higher moments for both the constituents are at least two.

Comparing the coefficients of ε^1 on both sides of (8.6) and (8.13)–(8.18), one obtains

$$\frac{1}{\varkappa_\alpha} \left(\frac{\partial \hat{h}_{i|1}^{(\alpha)}}{\partial \hat{x}_i} + \frac{\partial \hat{u}_{i|1}^{(\alpha)}}{\partial \hat{x}_i} \right) - \frac{1}{\varkappa_\beta} \left(\frac{\partial \hat{h}_{i|1}^{(\beta)}}{\partial \hat{x}_i} + \frac{\partial \hat{u}_{i|1}^{(\beta)}}{\partial \hat{x}_i} \right) = -\frac{1}{\Omega} \frac{\delta_5}{\varkappa_\alpha} \Delta \hat{T}_{|2}, \quad (\text{B.9})$$

$$\left. \begin{aligned} 3 \frac{\partial \hat{\sigma}_{ij|1}^{(\alpha)}}{\partial \hat{x}_k} &= -\frac{1}{\Omega} \left\{ \frac{3}{2} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{m}_{ijk|2}^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_{17} \hat{m}_{ijk|2}^{(\alpha)} - \delta_{18} \hat{m}_{ijk|2}^{(\beta)} \right) \right\}, \\ 3 \frac{\partial \hat{\sigma}_{ij|1}^{(\beta)}}{\partial \hat{x}_k} &= -\frac{1}{\Omega} \left\{ \frac{3}{2} \mathbf{x}_\beta^\circ \Omega_\beta \hat{m}_{ijk|2}^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_{17} \hat{m}_{ijk|2}^{(\beta)} - \gamma_{18} \hat{m}_{ijk|2}^{(\alpha)} \right) \right\}, \end{aligned} \right\} \quad (\text{B.10})$$

$$\left. \begin{aligned} \frac{28}{5} \frac{\partial \hat{h}_{i|1}^{(\alpha)}}{\partial \hat{x}_j} &= -\frac{1}{\Omega} \left\{ \frac{7}{6} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{R}_{ij|2}^{(\alpha)} + \mathbf{x}_\beta^\circ \left(\delta_{21} \hat{R}_{ij|2}^{(\alpha)} - \delta_{23} \hat{R}_{ij|2}^{(\beta)} \right) \right\}, \\ \frac{28}{5} \frac{\partial \hat{h}_{i|1}^{(\beta)}}{\partial \hat{x}_j} &= -\frac{1}{\Omega} \left\{ \frac{7}{6} \mathbf{x}_\beta^\circ \Omega_\beta \hat{R}_{ij|2}^{(\beta)} + \mathbf{x}_\alpha^\circ \left(\gamma_{21} \hat{R}_{ij|2}^{(\beta)} - \gamma_{23} \hat{R}_{ij|2}^{(\alpha)} \right) \right\}, \end{aligned} \right\} \quad (\text{B.11})$$

$$\left. \begin{aligned} 8 \frac{\partial \hat{h}_{i|1}^{(\alpha)}}{\partial \hat{x}_i} &= -\frac{1}{\Omega} \left\{ \frac{2}{3} \mathbf{x}_\alpha^\circ \Omega_\alpha \hat{\Delta}_{\alpha|2} + \mathbf{x}_\beta^\circ \left(\delta_{25} \hat{\Delta}_{\alpha|2} - \delta_{26} \hat{\Delta}_{\beta|2} \right) \right\}, \\ 8 \frac{\partial \hat{h}_{i|1}^{(\beta)}}{\partial \hat{x}_i} &= -\frac{1}{\Omega} \left\{ \frac{2}{3} \mathbf{x}_\beta^\circ \Omega_\beta \hat{\Delta}_{\beta|2} + \mathbf{x}_\alpha^\circ \left(\gamma_{25} \hat{\Delta}_{\beta|2} - \gamma_{26} \hat{\Delta}_{\alpha|2} \right) \right\}. \end{aligned} \right\} \quad (\text{B.12})$$

From (B.10)–(B.12), it is clear that $\hat{m}_{ijk|2}^{(\alpha)}$, $\hat{m}_{ijk|2}^{(\beta)}$, $\hat{R}_{ij|2}^{(\alpha)}$, $\hat{R}_{ij|2}^{(\beta)}$, $\hat{\Delta}_{\alpha|2}$, and $\hat{\Delta}_{\beta|2}$ do not vanish and therefore the leading orders of these quantities are two. Also, one can verify from (B.9)—by inserting the values of $\hat{u}_{i|1}^{(\alpha)}$, $\hat{u}_{i|1}^{(\beta)}$, $\hat{h}_{i|1}^{(\alpha)}$ and $\hat{h}_{i|1}^{(\beta)}$ from (8.20) and (8.22)—that $\Delta \hat{T}_{|2}$ is also non-zero. Therefore, the leading order of $\Delta \hat{T}_{|2}$ is two as well.

Appendix C

Coefficients in chapter 8

The coefficients in (8.26) are as follows.

$$\left. \begin{aligned} c_m^{(\alpha)} &= \frac{3\Omega}{(x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)} \left[\frac{\kappa_2 \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) + \kappa_1 x_\beta^\circ \delta_{18}}{\left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) - x_\alpha^\circ x_\beta^\circ \delta_{18} \gamma_{18}} \right], \\ c_m^{(\beta)} &= \frac{3\Omega}{(x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)} \left[\frac{\kappa_1 \left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) + \kappa_2 x_\alpha^\circ \gamma_{18}}{\left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) - x_\alpha^\circ x_\beta^\circ \delta_{18} \gamma_{18}} \right] \end{aligned} \right\} \quad (C.1)$$

$$\left. \begin{aligned} c_R^{(\alpha)} &= \frac{28}{5} \Omega \frac{\varkappa_\alpha \varkappa_\beta}{(x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha)} \left[\frac{\kappa_4 \left(\frac{7}{6} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{21} \right) + \kappa_3 x_\beta^\circ \delta_{23}}{\left(\frac{7}{6} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{21} \right) \left(\frac{7}{6} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{21} \right) - x_\alpha^\circ x_\beta^\circ \delta_{23} \gamma_{23}} \right], \\ c_R^{(\beta)} &= \frac{28}{5} \Omega \frac{\varkappa_\alpha \varkappa_\beta}{(x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha)} \left[\frac{\kappa_3 \left(\frac{7}{6} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{21} \right) + \kappa_4 x_\alpha^\circ \gamma_{23}}{\left(\frac{7}{6} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{21} \right) \left(\frac{7}{6} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{21} \right) - x_\alpha^\circ x_\beta^\circ \delta_{23} \gamma_{23}} \right] \end{aligned} \right\} \quad (C.2)$$

$$\left. \begin{aligned} c_\Delta^{(\alpha)} &= 8\Omega \frac{\varkappa_\alpha \varkappa_\beta}{(x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha)} \left[\frac{\kappa_4 \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{25} \right) + \kappa_3 x_\beta^\circ \delta_{26}}{\left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{25} \right) \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{25} \right) - x_\alpha^\circ x_\beta^\circ \delta_{26} \gamma_{26}} \right], \\ c_\Delta^{(\beta)} &= 8\Omega \frac{\varkappa_\alpha \varkappa_\beta}{(x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha)} \left[\frac{\kappa_3 \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{25} \right) + \kappa_4 x_\alpha^\circ \gamma_{26}}{\left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{25} \right) \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{25} \right) - x_\alpha^\circ x_\beta^\circ \delta_{26} \gamma_{26}} \right] \end{aligned} \right\} \quad (C.3)$$

The coefficients ζ_m , ζ_R and ζ_Δ are as follows.

$$\left. \begin{aligned} \zeta_m &= 3\Omega \frac{\varsigma_{12}}{\varpi_9} = \frac{x_\alpha^\circ}{\varkappa_\alpha} c_m^{(\alpha)} + \frac{x_\beta^\circ}{\varkappa_\beta} c_m^{(\beta)}, \\ \zeta_R &= \frac{28}{5} \Omega \frac{\varsigma_{33}}{\varpi_{13}} = \frac{x_\alpha^\circ}{\varkappa_\alpha^2} c_R^{(\alpha)} + \frac{x_\beta^\circ}{\varkappa_\beta^2} c_R^{(\beta)}, \\ \zeta_\Delta &= 8\Omega \frac{\varsigma_{33}}{\varpi_{17}} = \frac{x_\alpha^\circ}{\varkappa_\alpha^2} c_\Delta^{(\alpha)} + \frac{x_\beta^\circ}{\varkappa_\beta^2} c_\Delta^{(\beta)}. \end{aligned} \right\} \quad (C.4)$$

The coefficients ς_i 's are as follows.

$$\varsigma_1 = \frac{x_\alpha^\circ}{\varkappa_\alpha} \left(1 - \frac{\varkappa_\alpha^2}{\varkappa_\beta^2} \right), \quad \varsigma_2 = \frac{x_\beta^\circ (\kappa_2 \varkappa_\beta^2 - \kappa_1 \varkappa_\alpha^2)}{\varkappa (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)}, \quad \varsigma_3 = \frac{x_\beta^\circ}{x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1}, \quad \varsigma_4 = \frac{\kappa_4 \varkappa_\beta - \kappa_3 \varkappa_\alpha}{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha},$$

$$\begin{aligned}
\varsigma_5 &= \frac{1}{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha}, \quad \varsigma_6 = \frac{\varkappa}{x_\beta^\circ \varkappa_\alpha \varkappa_\beta^2}, \quad \varsigma_7 = \frac{\kappa_1 \kappa_6 \varkappa_\beta - \kappa_2 \kappa_5 \varkappa_\alpha}{x_\alpha^\circ \kappa_6 \varkappa_\beta + x_\beta^\circ \kappa_5 \varkappa_\alpha}, \quad \varsigma_8 = \frac{x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1}{x_\alpha^\circ \kappa_6 \varkappa_\beta + x_\beta^\circ \kappa_5 \varkappa_\alpha}, \\
\varsigma_9 &= \frac{\kappa_1 \kappa_4 \varkappa_\beta - \kappa_2 \kappa_3 \varkappa_\alpha}{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha}, \quad \varsigma_{10} = \frac{x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1}{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha}, \quad \varsigma_{11} = \frac{x_\alpha^\circ \kappa_2 \varkappa_\alpha^2 + x_\beta^\circ \kappa_1 \varkappa_\beta^2}{x_\beta^\circ \varkappa_\alpha \varkappa_\beta^2}, \\
\varsigma_{12} &= \frac{x_\alpha^\circ \kappa_2 \varkappa_\beta^2 + x_\beta^\circ \kappa_1 \varkappa_\alpha^2}{\varkappa_\alpha^2 \varkappa_\beta^2 (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)}, \quad \varsigma_{13} = \frac{x_\alpha^\circ x_\beta^\circ}{(x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)} \left(\frac{1}{\varkappa_\alpha^2} - \frac{1}{\varkappa_\beta^2} \right), \quad \varsigma_{14} = x_\alpha^\circ x_\beta^\circ \left(\frac{1}{\varkappa_\alpha^2} - \frac{1}{\varkappa_\beta^2} \right), \\
\varsigma_{15} &= \frac{\kappa_2 \kappa_3 \varkappa_\beta - \kappa_1 \kappa_4 \varkappa_\alpha}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)}, \quad \varsigma_{16} = \frac{x_\alpha^\circ \kappa_4 \varkappa_\alpha + x_\beta^\circ \kappa_3 \varkappa_\beta}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)}, \quad \varsigma_{17} = \frac{\varkappa_\alpha \varkappa_\beta (\kappa_8 \kappa_3 \varkappa_\beta - \kappa_7 \kappa_4 \varkappa_\alpha)}{x_\alpha^\circ \kappa_8 \varkappa_\beta^2 + x_\beta^\circ \kappa_7 \varkappa_\alpha^2}, \\
\varsigma_{18} &= \frac{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha}{x_\alpha^\circ \kappa_8 \varkappa_\beta^2 + x_\beta^\circ \kappa_7 \varkappa_\alpha^2}, \quad \varsigma_{19} = \frac{\varkappa_\alpha \varkappa_\beta (\kappa_{10} \kappa_3 \varkappa_\beta - \kappa_9 \kappa_4 \varkappa_\alpha)}{x_\alpha^\circ \kappa_{10} \varkappa_\beta^2 + x_\beta^\circ \kappa_9 \varkappa_\alpha^2}, \quad \varsigma_{20} = \frac{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha}{x_\alpha^\circ \kappa_{10} \varkappa_\beta^2 + x_\beta^\circ \kappa_9 \varkappa_\alpha^2}, \\
\varsigma_{21} &= \frac{x_\alpha^\circ \kappa_4 \varkappa_\alpha + x_\beta^\circ \kappa_3 \varkappa_\beta}{\varkappa_\alpha \varkappa_\beta}, \quad \varsigma_{22} = \frac{\varkappa_\alpha \varkappa_\beta (\kappa_5 \kappa_8 \varkappa_\beta - \kappa_6 \kappa_7 \varkappa_\alpha)}{x_\alpha^\circ \kappa_8 \varkappa_\beta^2 + x_\beta^\circ \kappa_7 \varkappa_\alpha^2}, \quad \varsigma_{23} = \frac{x_\alpha^\circ \kappa_6 \varkappa_\beta + x_\beta^\circ \kappa_5 \varkappa_\alpha}{x_\alpha^\circ \kappa_8 \varkappa_\beta^2 + x_\beta^\circ \kappa_7 \varkappa_\alpha^2}, \\
\varsigma_{24} &= \frac{x_\alpha^\circ \kappa_6 \varkappa_\alpha + x_\beta^\circ \kappa_5 \varkappa_\beta}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)}, \quad \varsigma_{25} = \frac{x_\alpha^\circ \kappa_6 \varkappa_\beta^3 + x_\beta^\circ \kappa_5 \varkappa_\alpha^3}{\varkappa_\alpha^2 \varkappa_\beta^2 (x_\alpha^\circ \kappa_6 \varkappa_\beta + x_\beta^\circ \kappa_5 \varkappa_\alpha)}, \\
\varsigma_{26} &= \frac{x_\alpha^\circ x_\beta^\circ}{(x_\alpha^\circ \kappa_6 \varkappa_\beta + x_\beta^\circ \kappa_5 \varkappa_\alpha)} \left(\frac{1}{\varkappa_\alpha^2} - \frac{1}{\varkappa_\beta^2} \right), \quad \varsigma_{27} = \frac{x_\alpha^\circ x_\beta^\circ}{(x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha)} \left(\frac{1}{\varkappa_\alpha^2} - \frac{1}{\varkappa_\beta^2} \right), \\
\varsigma_{28} &= \frac{\kappa_7 \kappa_6 \varkappa_\beta - \kappa_8 \kappa_5 \varkappa_\alpha}{x_\alpha^\circ \kappa_6 \varkappa_\beta + x_\beta^\circ \kappa_5 \varkappa_\alpha}, \quad \varsigma_{29} = \frac{x_\alpha^\circ \kappa_8 + x_\beta^\circ \kappa_7}{x_\alpha^\circ \kappa_6 \varkappa_\beta + x_\beta^\circ \kappa_5 \varkappa_\alpha}, \quad \varsigma_{30} = \frac{x_\alpha^\circ \kappa_8 + x_\beta^\circ \kappa_7}{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha}, \\
\varsigma_{31} &= \frac{x_\alpha^\circ \kappa_{10} + x_\beta^\circ \kappa_9}{x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha}, \quad \varsigma_{32} = \frac{5}{2} x_\beta^\circ \mathfrak{a}_3 (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa}, \quad \varsigma_{33} = \frac{x_\alpha^\circ \kappa_4 \varkappa_\beta^3 + x_\beta^\circ \kappa_3 \varkappa_\alpha^3}{\varkappa_\alpha^2 \varkappa_\beta^2 (x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha)}.
\end{aligned}$$

The coefficients ϖ_i 's are as follows.

$$\begin{aligned}
\varpi_1 &= \frac{x_\alpha^\circ \varkappa_\beta \{ \kappa_2 (x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_9) - \kappa_1 x_\beta^\circ \delta_{11} \} + x_\beta^\circ \varkappa_\alpha \{ \kappa_1 (x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_9) - \kappa_2 x_\alpha^\circ \gamma_{11} \}}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)} \\
&= \frac{(x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_9)(x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_9) - x_\alpha^\circ x_\beta^\circ \delta_{11} \gamma_{11}}{x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1}, \\
\varpi_2 &= \frac{x_\alpha^\circ x_\beta^\circ [\varkappa_\beta \{ (x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_9) + x_\alpha^\circ \delta_{11} \} - \varkappa_\alpha \{ (x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_9) + x_\beta^\circ \gamma_{11} \}]}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)} \\
&= \frac{x_\alpha^\circ x_\beta^\circ \{ (\kappa_1 - \kappa_2) + \varkappa_\beta \delta_{11} - \varkappa_\alpha \gamma_{11} \}}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)}, \\
\varpi_3 &= \frac{\kappa_1 \varkappa_\beta \{ \kappa_2 (x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_9) - \kappa_1 x_\beta^\circ \delta_{11} \} - \kappa_2 \varkappa_\alpha \{ \kappa_1 (x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_9) - \kappa_2 x_\alpha^\circ \gamma_{11} \}}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)} = (\kappa_1 - \kappa_2) \varpi_1 \\
\varpi_4 &= \frac{\kappa_1 \varkappa_\beta x_\beta^\circ \{ (x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_9) + x_\alpha^\circ \delta_{11} \} + \kappa_2 \varkappa_\alpha x_\alpha^\circ \{ (x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_9) + x_\beta^\circ \gamma_{11} \}}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)} \\
&= \frac{x_\alpha^\circ \kappa_2^2 + x_\beta^\circ \kappa_1^2 + x_\alpha^\circ x_\beta^\circ (\kappa_1 - \kappa_2) (\varkappa_\beta \delta_{11} - \varkappa_\alpha \gamma_{11})}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_2 + x_\beta^\circ \kappa_1)}, \\
\varpi_5 &= \frac{x_\alpha^\circ \varkappa_\beta^2 \left\{ \kappa_4 \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) - \kappa_3 x_\beta^\circ \delta_{15} \right\} + x_\beta^\circ \varkappa_\alpha^2 \left\{ \kappa_3 \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) - \kappa_4 x_\alpha^\circ \gamma_{15} \right\}}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_4 \varkappa_\beta + x_\beta^\circ \kappa_3 \varkappa_\alpha)}
\end{aligned}$$

$$\begin{aligned}
&= \frac{(x_\alpha^\circ \kappa_\beta^2 + x_\beta^\circ \kappa_\alpha^2) \left\{ \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) - x_\alpha^\circ x_\beta^\circ \delta_{15} \gamma_{15} \right\}}{\kappa_\alpha \kappa_\beta (x_\alpha^\circ \kappa_4 \kappa_\beta + x_\beta^\circ \kappa_3 \kappa_\alpha)}, \\
\varpi_6 &= \frac{x_\alpha^\circ x_\beta^\circ \left[\kappa_\beta^2 \left\{ \kappa_\alpha \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) + \kappa_\beta x_\alpha^\circ \delta_{15} \right\} - \kappa_\alpha^2 \left\{ \kappa_\beta \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) + \kappa_\alpha x_\beta^\circ \gamma_{15} \right\} \right]}{\kappa_\alpha^2 \kappa_\beta^2 (x_\alpha^\circ \kappa_4 \kappa_\beta + x_\beta^\circ \kappa_3 \kappa_\alpha)} \\
&= \frac{x_\alpha^\circ x_\beta^\circ \{ \kappa_\alpha \kappa_\beta (\kappa_3 \kappa_\beta - \kappa_4 \kappa_\alpha) + (x_\alpha^\circ \kappa_\beta^2 + x_\beta^\circ \kappa_\alpha^2) (\kappa_\beta \delta_{15} - \kappa_\alpha \gamma_{15}) \}}{\kappa_\alpha^2 \kappa_\beta^2 (x_\alpha^\circ \kappa_4 \kappa_\beta + x_\beta^\circ \kappa_3 \kappa_\alpha)}, \\
\varpi_7 &= \frac{\kappa_3 \kappa_\beta \left\{ \kappa_4 \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) - \kappa_3 x_\beta^\circ \delta_{15} \right\} - \kappa_4 \kappa_\alpha \left\{ \kappa_3 \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) - \kappa_4 x_\alpha^\circ \gamma_{15} \right\}}{x_\alpha^\circ \kappa_4 \kappa_\beta + x_\beta^\circ \kappa_3 \kappa_\alpha} \\
&= \frac{(\kappa_3 \kappa_\beta - \kappa_4 \kappa_\alpha) \left\{ \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) - x_\alpha^\circ x_\beta^\circ \delta_{15} \gamma_{15} \right\}}{x_\alpha^\circ \kappa_4 \kappa_\beta + x_\beta^\circ \kappa_3 \kappa_\alpha} \\
&= \frac{\kappa_\alpha \kappa_\beta (\kappa_3 \kappa_\beta - \kappa_4 \kappa_\alpha)}{(x_\alpha^\circ \kappa_\beta^2 + x_\beta^\circ \kappa_\alpha^2)} \varpi_5, \\
\varpi_8 &= \frac{\kappa_3 \kappa_\beta x_\beta^\circ \left\{ \kappa_\alpha \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{13} \right) + \kappa_\beta x_\alpha^\circ \delta_{15} \right\} + \kappa_4 \kappa_\alpha x_\alpha^\circ \left\{ \kappa_\beta \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{13} \right) + \kappa_\alpha x_\beta^\circ \gamma_{15} \right\}}{\kappa_\alpha \kappa_\beta (x_\alpha^\circ \kappa_4 \kappa_\beta + x_\beta^\circ \kappa_3 \kappa_\alpha)} \\
&= \frac{\kappa_\alpha \kappa_\beta (x_\alpha^\circ \kappa_4^2 + x_\beta^\circ \kappa_3^2) + x_\alpha^\circ x_\beta^\circ (\kappa_3 \kappa_\beta - \kappa_4 \kappa_\alpha) (\kappa_\beta \delta_{15} - \kappa_\alpha \gamma_{15})}{\kappa_\alpha \kappa_\beta (x_\alpha^\circ \kappa_4 \kappa_\beta + x_\beta^\circ \kappa_3 \kappa_\alpha)}, \\
\varpi_9 &= \frac{x_\alpha^\circ \kappa_\beta^2 \left\{ \kappa_6 \left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) - \kappa_5 x_\beta^\circ \delta_{18} \right\} + x_\beta^\circ \kappa_\alpha^2 \left\{ \kappa_5 \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) - \kappa_6 x_\alpha^\circ \gamma_{18} \right\}}{\kappa_\alpha \kappa_\beta (x_\alpha^\circ \kappa_6 \kappa_\beta + x_\beta^\circ \kappa_5 \kappa_\alpha)} \\
&= \frac{(x_\alpha^\circ \kappa_2 \kappa_\beta^2 + x_\beta^\circ \kappa_1 \kappa_\alpha^2) \left\{ \left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) - x_\alpha^\circ x_\beta^\circ \delta_{18} \gamma_{18} \right\}}{\kappa_\alpha \kappa_\beta (x_\alpha^\circ \kappa_6 \kappa_\beta + x_\beta^\circ \kappa_5 \kappa_\alpha)}, \\
\varpi_{10} &= \frac{x_\alpha^\circ x_\beta^\circ \left[\kappa_\beta^2 \left\{ \kappa_\alpha \left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) + \kappa_\beta x_\alpha^\circ \delta_{18} \right\} - \kappa_\alpha^2 \left\{ \kappa_\beta \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) + \kappa_\alpha x_\beta^\circ \gamma_{18} \right\} \right]}{\kappa_\alpha^2 \kappa_\beta^2 (x_\alpha^\circ \kappa_6 \kappa_\beta + x_\beta^\circ \kappa_5 \kappa_\alpha)} \\
&= \frac{x_\alpha^\circ x_\beta^\circ \{ \kappa_\alpha \kappa_\beta (\kappa_5 \kappa_2 \kappa_\beta - \kappa_6 \kappa_1 \kappa_\alpha) + (x_\alpha^\circ \kappa_2 \kappa_\beta^2 + x_\beta^\circ \kappa_1 \kappa_\alpha^2) (\kappa_1 \kappa_\beta \delta_{18} - \kappa_2 \kappa_\alpha \gamma_{18}) \}}{\kappa_1 \kappa_2 \kappa_\alpha^2 \kappa_\beta^2 (x_\alpha^\circ \kappa_6 \kappa_\beta + x_\beta^\circ \kappa_5 \kappa_\alpha)}, \\
\varpi_{11} &= \frac{\kappa_5 \kappa_\beta \left\{ \kappa_6 \left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) - \kappa_5 x_\beta^\circ \delta_{18} \right\} - \kappa_6 \kappa_\alpha \left\{ \kappa_5 \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) - \kappa_6 x_\alpha^\circ \gamma_{18} \right\}}{x_\alpha^\circ \kappa_6 \kappa_\beta + x_\beta^\circ \kappa_5 \kappa_\alpha} \\
&= \frac{(\kappa_5 \kappa_2 \kappa_\beta - \kappa_6 \kappa_1 \kappa_\alpha) \left\{ \left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) - x_\alpha^\circ x_\beta^\circ \delta_{18} \gamma_{18} \right\}}{x_\alpha^\circ \kappa_6 \kappa_\beta + x_\beta^\circ \kappa_5 \kappa_\alpha} \\
&= \frac{\kappa_\alpha \kappa_\beta (\kappa_5 \kappa_2 \kappa_\beta - \kappa_6 \kappa_1 \kappa_\alpha)}{(x_\alpha^\circ \kappa_2 \kappa_\beta^2 + x_\beta^\circ \kappa_1 \kappa_\alpha^2)} \varpi_9, \\
\varpi_{12} &= \frac{\kappa_5 \kappa_\beta x_\beta^\circ \left\{ \kappa_\alpha \left(\frac{3}{2} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{17} \right) + \kappa_\beta x_\alpha^\circ \delta_{18} \right\} + \kappa_6 \kappa_\alpha x_\alpha^\circ \left\{ \kappa_\beta \left(\frac{3}{2} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{17} \right) + \kappa_\alpha x_\beta^\circ \gamma_{18} \right\}}{\kappa_\alpha \kappa_\beta (x_\alpha^\circ \kappa_6 \kappa_\beta + x_\beta^\circ \kappa_5 \kappa_\alpha)}
\end{aligned}$$

$$\begin{aligned}
&= \frac{\varkappa_\alpha \varkappa_\beta (\kappa_9 \kappa_4 \varkappa_\beta - \kappa_{10} \kappa_3 \varkappa_\alpha) \left\{ \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{25} \right) \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{25} \right) - x_\alpha^\circ x_\beta^\circ \delta_{26} \gamma_{26} \right\}}{(x_\alpha^\circ \kappa_{10} \varkappa_\beta^2 + x_\beta^\circ \kappa_9 \varkappa_\alpha^2)} \\
&= \frac{\varkappa_\alpha^2 \varkappa_\beta^2 (\kappa_9 \kappa_4 \varkappa_\beta - \kappa_{10} \kappa_3 \varkappa_\alpha)}{(x_\alpha^\circ \kappa_4 \varkappa_\beta^3 + x_\beta^\circ \kappa_3 \varkappa_\alpha^3)} \varpi_{17}, \\
\varpi_{20} &= \frac{\kappa_9 \varkappa_\beta x_\beta^\circ \left\{ \varkappa_\alpha^2 \left(\frac{2}{3} x_\alpha^\circ \Omega_\alpha + x_\beta^\circ \delta_{25} \right) + \varkappa_\beta^2 x_\alpha^\circ \delta_{26} \right\} + \kappa_{10} \varkappa_\alpha x_\alpha^\circ \left\{ \varkappa_\beta^2 \left(\frac{2}{3} x_\beta^\circ \Omega_\beta + x_\alpha^\circ \gamma_{25} \right) + \varkappa_\alpha^2 x_\beta^\circ \gamma_{26} \right\}}{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_{10} \varkappa_\beta^2 + x_\beta^\circ \kappa_9 \varkappa_\alpha^2)} \\
&= \frac{\varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_3 \kappa_{10}^2 \varkappa_\beta + x_\beta^\circ \kappa_4 \kappa_9^2 \varkappa_\alpha) + x_\alpha^\circ x_\beta^\circ (\kappa_9 \kappa_4 \varkappa_\beta - \kappa_{10} \kappa_3 \varkappa_\alpha) (\kappa_3 \varkappa_\beta^2 \delta_{26} - \kappa_4 \varkappa_\alpha^2 \gamma_{26})}{\kappa_3 \kappa_4 \varkappa_\alpha \varkappa_\beta (x_\alpha^\circ \kappa_{10} \varkappa_\beta^2 + x_\beta^\circ \kappa_9 \varkappa_\alpha^2)}.
\end{aligned}$$

The coefficients $\mathbf{a}_0, \mathbf{a}_1, \dots, \mathbf{a}_{20}$ are as follows.

$$\begin{aligned}
\mathbf{a}_0 &= \varsigma_2, & \mathbf{a}_1 &= \delta_1 \frac{\varkappa}{\varkappa_\beta^2}, & \mathbf{a}_2 &= \frac{4}{5} \left(1 - \frac{\varpi_2}{\varpi_4} \varsigma_9 \right), \\
\mathbf{a}_3 &= 2 \left(\varsigma_1 - \frac{\varpi_2}{\varpi_4} \varsigma_{11} \right), & \mathbf{a}_4 &= \frac{1}{\varpi_4} (\varpi_1 \varpi_4 - \varpi_2 \varpi_3), & \mathbf{a}_5 &= \varsigma_{12} - \frac{\varpi_6}{\varpi_8} \varsigma_{15}, \\
\mathbf{a}_6 &= \frac{1}{\varpi_8} (\varpi_5 \varpi_8 - \varpi_6 \varpi_7), & \mathbf{a}_7 &= \frac{\varpi_3}{\varpi_4} \varsigma_3, & \mathbf{a}_8 &= 2 \Omega \frac{\varsigma_3 \varsigma_{11}}{\varpi_4}, \\
\mathbf{a}_9 &= \frac{4}{5} \Omega \frac{\varsigma_3 \varsigma_9}{\varpi_4}, & \mathbf{a}_{10} &= \Omega x_\beta^\circ \varkappa_\alpha \frac{\varsigma_6}{\delta_5}, & \mathbf{a}_{11} &= \Omega x_\beta^\circ \varkappa_\alpha \frac{\varsigma_4}{\delta_5}, \\
\mathbf{a}_{12} &= \frac{\varpi_2}{\varpi_4} \left[\frac{\mathbf{a}_6}{\varpi_4} \left\{ \frac{4}{5} \varsigma_9 + \frac{\varpi_3}{\mathbf{a}_4} \frac{1}{\varkappa} \left(5 \frac{\eta}{\kappa} - \mathbf{a}_2 \varkappa + \frac{\varsigma_{32}}{\kappa} \right) \right\} - \frac{4}{5} \frac{\varpi_7}{\varpi_8} \varsigma_{10} \right], \\
\mathbf{a}_{13} &= 2 \delta_1 \frac{\varkappa}{\varkappa_\alpha \varkappa_\beta^2} \frac{\varsigma_{11} \varpi_2}{\varpi_4^2}, \\
\mathbf{a}_{14} &= \Omega \frac{\varpi_2}{\varpi_4} \left[2 \frac{\varsigma_2 \varsigma_{11}}{\varpi_4} \frac{1}{\varkappa_\alpha} + \frac{\mathbf{a}_5}{\varpi_4} \left\{ \frac{4}{5} \varsigma_9 + \frac{\varpi_3}{\mathbf{a}_4} \frac{1}{\varkappa} \left(5 \frac{\eta}{\kappa} - \mathbf{a}_2 \varkappa + \frac{\varsigma_{32}}{\kappa} \right) \right\} - \frac{4}{5} \frac{\varsigma_{10} \varsigma_{15}}{\varpi_8} \right] + \frac{2}{5} \left(1 - \frac{\varpi_2}{\varpi_4} \varsigma_7 \right) \zeta_m, \\
\mathbf{a}_{15} &= \frac{1}{3} \left(1 - \frac{\varpi_2}{\varpi_4} \varsigma_7 \right) \zeta_m, \\
\mathbf{a}_{16} &= \mathbf{a}_4 \frac{\varpi_6}{\varpi_8^2} \left\{ \varsigma_{15} - \frac{\varpi_7}{\mathbf{a}_6} \left(\mathbf{a}_5 - \frac{\kappa}{2\eta} \right) \right\} + \frac{\varpi_3}{\varpi_4} \left(\varsigma_{13} - \frac{\varpi_6}{\varpi_8} \varsigma_{16} \right), \\
\mathbf{a}_{17} &= \Omega \left[\mathbf{a}_2 \frac{\varpi_6}{\varpi_8^2} \left\{ \varsigma_{15} - \frac{\varpi_7}{\mathbf{a}_6} \left(\mathbf{a}_5 - \frac{\kappa}{2\eta} \right) \right\} + \frac{4}{5} \frac{\varsigma_9}{\varpi_4} \left(\varsigma_{13} - \frac{\varpi_6}{\varpi_8} \varsigma_{16} \right) \right] + \frac{1}{2} \left(1 - \frac{\varpi_6}{\varpi_8} \varsigma_{17} \right) \zeta_R, \\
\mathbf{a}_{18} &= \Omega \left[\mathbf{a}_3 \frac{\varpi_6}{\varpi_8^2} \left\{ \varsigma_{15} - \frac{\varpi_7}{\mathbf{a}_6} \left(\mathbf{a}_5 - \frac{\kappa}{2\eta} \right) \right\} + 2 \frac{\varsigma_{11}}{\varpi_4} \left(\varsigma_{13} - \frac{\varpi_6}{\varpi_8} \varsigma_{16} \right) \right], \\
\mathbf{a}_{19} &= \frac{5}{2} \Omega \varkappa_\alpha \frac{\varsigma_4}{\delta_5} \left(\varsigma_{14} - \frac{\varpi_6}{\varpi_8} \varsigma_{21} \right) + \frac{1}{6} \left(1 - \frac{\varpi_6}{\varpi_8} \varsigma_{19} \right) \zeta_\Delta, \\
\mathbf{a}_{20} &= \frac{5}{2} \Omega \varkappa_\alpha \frac{\varsigma_6}{\delta_5} \left(\varsigma_{14} - \frac{\varpi_6}{\varpi_8} \varsigma_{21} \right).
\end{aligned}$$

Appendix D

Burnett order equations: second order contributions to $\hat{\sigma}_{ij}$ and $\hat{h}_i$

To obtain the precise values of second order contributions to $\hat{\sigma}_{ij}$ and $\hat{h}_i$, let us perform the Chapman-Enskog like expansion on the new system of moment equations (8.34)–(8.45). We again expand the non-conserved quantities (Ψ) in powers of the Knudsen number (ε) as

$$\Psi = \Psi_{|0} + \varepsilon \Psi_{|1} + \varepsilon^2 \Psi_{|2} + \dots,$$

where $\Psi \in \{\hat{u}_i^{(\alpha)}, \Delta \hat{T}, \hat{\sigma}_{ij}, \Delta \hat{\sigma}_{ij}, \hat{h}_i, \Delta \hat{h}_i, \hat{m}_{ijk}, \Delta \hat{m}_{ijk}, \hat{R}_{ij}, \Delta \hat{R}_{ij}, \hat{\Delta}, \Delta \hat{\Delta}\}$ and the quantities $\Psi_{|0}, \Psi_{|1}, \Psi_{|2}, \dots$ are of order $\mathcal{O}(\varepsilon^0)$. Now, we shall substitute the above expansions in the new system of moment equations (8.34)–(8.45) and compare the coefficients of each power of ε .

Comparing coefficients of ε^{-1} on both sides of (8.34)–(8.45), it immediately follows that $\Psi_{|0} = 0$ for all $\Psi \in \{\hat{u}_i^{(\alpha)}, \Delta \hat{T}, \hat{\sigma}_{ij}, \Delta \hat{\sigma}_{ij}, \hat{h}_i, \Delta \hat{h}_i, \hat{m}_{ijk}, \Delta \hat{m}_{ijk}, \hat{R}_{ij}, \Delta \hat{R}_{ij}, \hat{\Delta}, \Delta \hat{\Delta}\}$.

Comparing coefficients of ε^0 on both sides of (8.34)–(8.45), it follows that

$$\left. \begin{aligned} \hat{u}_{i|1}^{(\alpha)} &= -x_\beta^\circ \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{x}_i} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{x}_i} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{x}_i} \right), \\ \hat{\sigma}_{ij|1} &= -2\eta \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}}, \quad \hat{h}_{i|1} = -\kappa \frac{\partial \hat{T}}{\partial \hat{x}_i}, \\ \Delta \hat{T}_{|1} &= \Delta \hat{\sigma}_{ij|1} = \Delta \hat{h}_{i|1} = \hat{m}_{ijk|1} = \hat{R}_{ij|1} = \hat{\Delta}_{|1} = \Delta \hat{m}_{ijk|1} = \Delta \hat{R}_{ij|1} = \Delta \hat{\Delta}_{|1} = 0. \end{aligned} \right\} \quad (\text{D.1})$$

Comparing coefficients of ε^1 on both sides of (8.34)–(8.45), it follows that

$$\begin{aligned} \hat{u}_{i|2}^{(\alpha)} &= -\frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa} \left(\varkappa_\alpha \frac{\partial \hat{u}_{i|1}^{(\alpha)}}{\partial \hat{t}} + \varsigma_2 \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{x}_j} \right) \\ &= \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa} \left[x_\beta^\circ \frac{\Omega}{\delta_1} \frac{\varkappa_\alpha \varkappa_\beta^2}{\varkappa^2} \frac{\partial}{\partial \hat{x}_i} \left(\varkappa_\beta^2 \frac{\partial \hat{n}_\alpha}{\partial \hat{t}} - \varkappa_\alpha^2 \frac{\partial \hat{n}_\beta}{\partial \hat{t}} - (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial \hat{T}}{\partial \hat{t}} \right) + 2\eta \varsigma_2 \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right] \\ &= \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa} \left[\frac{5}{3} x_\beta^\circ \frac{\Omega}{\delta_1} \frac{\varkappa_\alpha \varkappa_\beta^2}{\varkappa^2} (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\partial}{\partial \hat{x}_i} \frac{\partial \hat{v}_j}{\partial \hat{x}_j} + 2\eta \varsigma_2 \frac{\partial}{\partial \hat{x}_j} \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} \right], \end{aligned} \quad (\text{D.2})$$

$$\begin{aligned} \Delta \hat{T}_{|2} &= -\Omega \frac{\varkappa_\alpha}{\delta_5} \left(\varsigma_4 \frac{\partial \hat{h}_{i|1}}{\partial \hat{x}_i} + \varsigma_6 \frac{\partial \hat{u}_{i|1}^{(\alpha)}}{\partial \hat{x}_i} \right) \\ &= \Omega \frac{\varkappa_\alpha}{\delta_5} \left[\varsigma_4 \kappa \frac{\partial^2 \hat{T}}{\partial \hat{x}_i^2} + \varsigma_6 x_\beta^\circ \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \frac{\partial^2}{\partial \hat{x}_i^2} \left(\varkappa_\beta^2 \hat{n}_\alpha - \varkappa_\alpha^2 \hat{n}_\beta - (\varkappa_\alpha^2 - \varkappa_\beta^2) \hat{T} \right) \right], \end{aligned} \quad (\text{D.3})$$

$$\left. \begin{aligned} \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{t}} + \frac{4}{5} \frac{\partial \hat{h}_{\langle i|1}}{\partial \hat{x}_{j\rangle}} + 2\varsigma_1 \frac{\partial \hat{u}_{\langle i|1}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} &= -\frac{1}{\Omega} (\varpi_1 \hat{\sigma}_{ij|2} + \varpi_2 \Delta \hat{\sigma}_{ij|2}), \\ \frac{4}{5} \varsigma_9 \frac{\partial \hat{h}_{\langle i|1}}{\partial \hat{x}_{j\rangle}} + 2\varsigma_{11} \frac{\partial \hat{u}_{\langle i|1}^{(\alpha)}}{\partial \hat{x}_{j\rangle}} &= -\frac{1}{\Omega} (\varpi_3 \hat{\sigma}_{ij|2} + \varpi_4 \Delta \hat{\sigma}_{ij|2}), \end{aligned} \right\} \quad (\text{D.4})$$

$$\left. \begin{aligned} \frac{\partial \hat{h}_{i|1}}{\partial \hat{t}} + \varsigma_{12} \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{x}_j} &= -\frac{1}{\Omega} (\varpi_5 \hat{h}_{i|2} + \varpi_6 \Delta \hat{h}_{i|2}), \\ \varsigma_{15} \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{x}_j} &= -\frac{1}{\Omega} (\varpi_7 \hat{h}_{i|2} + \varpi_8 \Delta \hat{h}_{i|2}), \end{aligned} \right\} \quad (\text{D.5})$$

$$\hat{m}_{ijk|2} = -\zeta_m \frac{\partial \hat{\sigma}_{\langle ij|1}}{\partial \hat{x}_k}, \quad \hat{R}_{ij|2} = -\zeta_R \frac{\partial \hat{h}_{\langle i|1}}{\partial \hat{x}_j}, \quad \hat{\Delta}_{|2} = -\zeta_\Delta \frac{\partial \hat{h}_i}{\partial \hat{x}_i} \quad (\text{D.6})$$

and

$$\Delta \hat{m}_{ijk|2} = \Delta \hat{R}_{ij|2} = \Delta \hat{\Delta}_{|2} = 0. \quad (\text{D.7})$$

From (D.4) and (D.5), we have

$$\left. \begin{aligned} \hat{\sigma}_{ij|2} &= -\frac{\Omega}{(\varpi_1 \varpi_4 - \varpi_2 \varpi_3)} \left[\varpi_4 \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{t}} + \frac{4}{5} (\varpi_4 - \varpi_2 \varsigma_9) \frac{\partial \hat{h}_{\langle i|1}}{\partial \hat{x}_j} + 2(\varpi_4 \varsigma_1 - \varpi_2 \varsigma_{11}) \frac{\partial \hat{u}_{\langle i|1}^{(\alpha)}}{\partial \hat{x}_j} \right], \\ \Delta \hat{\sigma}_{ij|2} &= \frac{\Omega}{(\varpi_1 \varpi_4 - \varpi_2 \varpi_3)} \left[\varpi_3 \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{t}} + \frac{4}{5} (\varpi_3 - \varpi_1 \varsigma_9) \frac{\partial \hat{h}_{\langle i|1}}{\partial \hat{x}_j} + 2(\varpi_3 \varsigma_1 - \varpi_1 \varsigma_{11}) \frac{\partial \hat{u}_{\langle i|1}^{(\alpha)}}{\partial \hat{x}_j} \right], \end{aligned} \right\} \quad (\text{D.8})$$

$$\left. \begin{aligned} \hat{h}_{i|2} &= -\frac{\Omega}{(\varpi_5 \varpi_8 - \varpi_6 \varpi_7)} \left[\varpi_8 \frac{\partial \hat{h}_{i|1}}{\partial \hat{t}} + (\varpi_8 \varsigma_{12} - \varpi_6 \varsigma_{15}) \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{x}_j} \right], \\ \Delta \hat{h}_{i|2} &= \frac{\Omega}{(\varpi_5 \varpi_8 - \varpi_6 \varpi_7)} \left[\varpi_7 \frac{\partial \hat{h}_{i|1}}{\partial \hat{t}} + (\varpi_7 \varsigma_{12} - \varpi_5 \varsigma_{15}) \frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{x}_j} \right]. \end{aligned} \right\} \quad (\text{D.9})$$

From (D.1)_{2,3} on using momentum and energy balance equations (eqs. (8.32) and (8.33)) with $\hat{u}_i^{(\alpha)} = \hat{\sigma}_{ij} = \hat{q}_i = 0$ (i.e., on using the Euler equations), we have

$$\frac{\partial \hat{\sigma}_{ij|1}}{\partial \hat{t}} = -2\eta \frac{\partial}{\partial \hat{x}_{j\rangle}} \frac{\partial \hat{v}_{\langle i}}{\partial \hat{t}} = 2\frac{\eta}{\kappa} \frac{\partial^2}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} \left(x_\alpha^\circ \hat{n}_\alpha + x_\beta^\circ \hat{n}_\beta + \hat{T} \right), \quad (\text{D.10})$$

$$\frac{\partial \hat{h}_{i|1}}{\partial \hat{t}} = -\kappa \frac{\partial}{\partial \hat{x}_i} \frac{\partial \hat{T}}{\partial \hat{t}} = \frac{2}{3} \kappa \frac{\partial^2 \hat{v}_j}{\partial \hat{x}_i \partial \hat{x}_j}. \quad (\text{D.11})$$

Therefore, equations (D.8) and (D.9) on using (D.1) yield

$$\hat{\sigma}_{ij|2} = -\frac{\partial^2}{\partial \hat{x}_{\langle i} \partial \hat{x}_{j\rangle}} \left(\mathfrak{b}_1 \hat{n}_\alpha + \mathfrak{b}_2 \hat{n}_\beta + \mathfrak{b}_3 \hat{T} \right), \quad (\text{D.12})$$

$$\Delta\hat{\sigma}_{ij|2} = \frac{\partial^2}{\partial\hat{x}_{\langle i}\partial\hat{x}_{j\rangle}} \left(\mathbf{b}_4\hat{n}_\alpha + \mathbf{b}_5\hat{n}_\beta + \mathbf{b}_6\hat{T} \right), \quad (\text{D.13})$$

$$\hat{h}_{i|2} = -\mathbf{b}_7 \frac{\partial^2 \hat{v}_j}{\partial\hat{x}_i\partial\hat{x}_j} - 2\eta\mathbf{b}_8 \frac{\partial}{\partial\hat{x}_j} \frac{\partial\hat{v}_{\langle i}}{\partial\hat{x}_{j\rangle}}, \quad (\text{D.14})$$

$$\Delta\hat{h}_{i|2} = \mathbf{b}_9 \frac{\partial^2 \hat{v}_j}{\partial\hat{x}_i\partial\hat{x}_j} - 2\eta\mathbf{b}_{10} \frac{\partial}{\partial\hat{x}_j} \frac{\partial\hat{v}_{\langle i}}{\partial\hat{x}_{j\rangle}}, \quad (\text{D.15})$$

where

$$\begin{aligned} \mathbf{b}_1 &= \frac{2\Omega}{(\varpi_1\varpi_4 - \varpi_2\varpi_3)} \left\{ \mathbf{x}_\alpha^\circ \varpi_4 \frac{\eta}{\varkappa} - \mathbf{x}_\beta^\circ (\varpi_4\varsigma_1 - \varpi_2\varsigma_{11}) \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^4}{\varkappa^2} \right\} = \frac{\Omega}{\mathbf{a}_4} \left\{ \mathbf{x}_\alpha^\circ \frac{2\eta}{\varkappa} - \mathbf{x}_\beta^\circ \mathbf{a}_3 \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^4}{\varkappa^2} \right\}, \\ \mathbf{b}_2 &= \frac{2\Omega}{(\varpi_1\varpi_4 - \varpi_2\varpi_3)} \mathbf{x}_\beta^\circ \left\{ \varpi_4 \frac{\eta}{\varkappa} + (\varpi_4\varsigma_1 - \varpi_2\varsigma_{11}) \frac{\Omega}{\delta_1} \frac{\varkappa_\alpha^2 \varkappa_\beta^2}{\varkappa^2} \right\} = \frac{\Omega}{\mathbf{a}_4} \mathbf{x}_\beta^\circ \left\{ \frac{2\eta}{\varkappa} + \mathbf{a}_3 \frac{\Omega}{\delta_1} \frac{\varkappa_\alpha^2 \varkappa_\beta^2}{\varkappa^2} \right\}, \\ \mathbf{b}_3 &= \frac{2\Omega}{(\varpi_1\varpi_4 - \varpi_2\varpi_3)} \left\{ \varpi_4 \frac{\eta}{\varkappa} - \frac{2}{5} \kappa (\varpi_4 - \varpi_2\varsigma_9) + \mathbf{x}_\beta^\circ (\varpi_4\varsigma_1 - \varpi_2\varsigma_{11}) (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \right\} \\ &= \frac{\Omega}{\mathbf{a}_4} \left\{ \frac{2\eta}{\varkappa} - \mathbf{a}_2 \kappa + \mathbf{x}_\beta^\circ \mathbf{a}_3 (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \right\}, \\ \mathbf{b}_4 &= \frac{2\Omega}{(\varpi_1\varpi_4 - \varpi_2\varpi_3)} \left\{ \mathbf{x}_\alpha^\circ \varpi_3 \frac{\eta}{\varkappa} - \mathbf{x}_\beta^\circ (\varpi_3\varsigma_1 - \varpi_1\varsigma_{11}) \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^4}{\varkappa^2} \right\}, \\ \mathbf{b}_5 &= \frac{2\Omega}{(\varpi_1\varpi_4 - \varpi_2\varpi_3)} \mathbf{x}_\beta^\circ \left\{ \varpi_3 \frac{\eta}{\varkappa} + (\varpi_3\varsigma_1 - \varpi_1\varsigma_{11}) \frac{\Omega}{\delta_1} \frac{\varkappa_\alpha^2 \varkappa_\beta^2}{\varkappa^2} \right\}, \\ \mathbf{b}_6 &= \frac{2\Omega}{(\varpi_1\varpi_4 - \varpi_2\varpi_3)} \left\{ \varpi_3 \frac{\eta}{\varkappa} - \frac{2}{5} \kappa (\varpi_3 - \varpi_1\varsigma_9) + \mathbf{x}_\beta^\circ (\varpi_3\varsigma_1 - \varpi_1\varsigma_{11}) (\varkappa_\alpha^2 - \varkappa_\beta^2) \frac{\Omega}{\delta_1} \frac{\varkappa_\beta^2}{\varkappa^2} \right\}, \\ \mathbf{b}_7 &= \frac{2}{3} \frac{\Omega}{(\varpi_5\varpi_8 - \varpi_6\varpi_7)} \varpi_8 \kappa = \frac{2}{3} \frac{\Omega}{\mathbf{a}_6} \kappa, \\ \mathbf{b}_8 &= -\frac{\Omega}{(\varpi_5\varpi_8 - \varpi_6\varpi_7)} (\varpi_8\varsigma_{12} - \varpi_6\varsigma_{15}) = -\frac{\Omega}{\mathbf{a}_6} \mathbf{a}_5, \\ \mathbf{b}_9 &= \frac{2}{3} \frac{\Omega}{(\varpi_5\varpi_8 - \varpi_6\varpi_7)} \varpi_7 \kappa, \\ \mathbf{b}_{10} &= \frac{\Omega}{(\varpi_5\varpi_8 - \varpi_6\varpi_7)} (\varpi_7\varsigma_{12} - \varpi_5\varsigma_{15}). \end{aligned}$$

Therefore, if the conservation laws for mixture are closed with up to second order corrections in the diffusion velocity (of one constituent), total stress and total reduced heat flux, i.e., with

$$\hat{u}_i^{(\alpha)} = \varepsilon \hat{u}_{i|1}^{(\alpha)} + \varepsilon^2 \hat{u}_{i|2}^{(\alpha)}, \quad \hat{\sigma}_{ij} = \varepsilon \hat{\sigma}_{ij|1} + \varepsilon^2 \hat{\sigma}_{ij|2}, \quad \hat{h}_i = \varepsilon \hat{h}_{i|1} + \varepsilon^2 \hat{h}_{i|2}, \quad (\text{D.16})$$

where $\hat{u}_{i|1}^{(\alpha)}$, $\hat{\sigma}_{ij|1}$, $\hat{h}_{i|1}$, $\hat{u}_{i|2}^{(\alpha)}$, $\hat{\sigma}_{ij|2}$ and $\hat{h}_{i|2}$ are given by (D.1)_{1,2,3}, (D.2), (D.12) (D.14), we essentially get the (linear) Burnett order equations for a binary gas-mixture made up of Maxwell molecules.

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