Grad's Moment Equations for Binary Hard Sphere Gas-Mixtures

Vinay Kumar GUPTA ^{1,*}, Neeraj SARNA ¹, Manuel TORRILHON ¹

* Corresponding author: Tel.: +49 (0) 2418098676; Fax: +49 (0) 2418092600; Email: gupta@mathcces.rwth-aachen.de
1: Center for Computational Engineering Science, Department of Mathematics, RWTH Aachen University, Germany

Abstract The derivation of non-linear Grad's 2×26 -moment ($2 \times G26$) equations for a binary gasmixture of monatomic-inert-ideal hard sphere gases is sketched, although—for conciseness—only the linear $2 \times G26$ equations are illustrated and analysed. The linear stability analysis is performed on $2 \times G26$ equations by studying the dispersion relation and by considering the plane wave solution, it is shown that the $2 \times G26$ equations for binary hard sphere gas-mixture are linearly stable.

Keywords: Moment method, Binary mixture, Kinetic theory, Knudsen number

1. Introduction

In the last decade, miniaturizing electronic devices has become an important focus of interest to many industries and, thus, the modelling of gas flows in micro-devices has been an intriguing problem.

As a result of shrinking down the size of devices, the mean-free-path of the gas molecules becomes comparable to the size of the device. This results into the *rarefaction* of gases inside the device. Rarefaction can be characterised by a dimensionless parameter, the Knudsen number Kn, which is defined as the ratio of mean-free-path, λ , of the gas molecules over a characteristic length L. The Knudsen number encountered in microdevices often ranges from 0.01 to 1 [1] which resides in the typical range of the so-called slip flow regime (0.001 \lesssim Kn \lesssim 0.1) and transition regime $(0.1 \lesssim \text{Kn} \lesssim 10)[2]$. The processes in slip flow regime can be described using the well-known Navier-Stokes-Fourier (NSF) equations, provided they are furnished with appropriate velocity slip and temperature jump boundary conditions [3]. However, the NSF equations loose their validity in the transition regime [2, 4] and more sophisticated models are needed to describe the flows in this regime.

The processes in all flow regimes can be well-described by the Boltzmann equation, which is the evolution equation for the distribution function of the gas particles. However, the direct solutions of the Boltzmann equation are computationally expensive, particularly, in the transition regime.

The approximation methods in kinetic theory offer an alternative for solving the Boltzmann equation. In kinetic theory, the two most celebrated approximation methods for solving the Boltzmann equation are *Grad's method of moments* [5–7] and the *Chapman– Enskog expansion method* [8]. Nevertheless, the equations resulting from higher-order approximation in Chapman–Enskog expansion method suffer from instability [9], hence their applicability is questionable. On the other hand, the moment equations resulting from Grad's method of moments, in case of a single gas, are always linearly stable.

Despite the success of Grad's method of moments and its variants, e.g. [4], in describing many rarefaction effects for a single gas, they have not been used enough for the mixtures, perhaps, because the production terms—the right-hand sides resulting from the collision term in the Boltzmann equation—in the moment equations are not easy to evaluate. To the best of our knowledge, the fully non-linear Grad's 26-moment (G26) equations for each component of a multi-temperature Maxwell gas-mixture are derived and a linear stability of Grad's 2×26 moment ($2\times G26$) equations for binary gasmixture of Maxwell gases has been analysed for the first time in [10].

Since the hard sphere molecule model is more realistic, we analyse the linear stability of $2 \times G26$ equations for binary mixture of gases with hard sphere interaction potential in this paper. Also, it is commonly believed that the more moments one includes, the better approximation to the Boltzmann equation one obtains. That is why we chose 26 moments for each constituent in the mixture instead of 13 moments.

2. Boltzmann Equation

We consider a mixture of two monatomicinert-ideal hard sphere gases α and β . Let the molecular masses of the two gases be m_{α} and m_{β} , and the diameters be d_{α} and d_{β} . The state of the binary mixture of α and β gases is characterised by the two velocity distribution functions $f_{\gamma} \equiv f_{\gamma}(t, \boldsymbol{x}, \boldsymbol{c}_{\gamma}), \gamma \in \{\alpha, \beta\}$, where \boldsymbol{x} is the position vector and \boldsymbol{c}_{γ} is the instantaneous velocity of the γ -molecule at time t. The evolutions of these distribution functions are governed by the Boltzmann equations

$$\frac{\partial f_{\gamma}}{\partial t} + c_i^{(\gamma)} \frac{\partial f_{\gamma}}{\partial x_i} + F_i^{(\gamma)} \frac{\partial f_{\gamma}}{\partial c_i^{(\gamma)}} = S_{\gamma\alpha} + S_{\gamma\beta} \quad (1)$$

for $\gamma \in \{\alpha, \beta\}$, where F_{γ} is the external force per unit mass acting on γ -species and

$$S_{\gamma\delta} = \left(\frac{d_{\gamma} + d_{\delta}}{2}\right)^2 \int (f_{\gamma}' f_{\delta}' - f_{\gamma} f_{\delta}) |\boldsymbol{k}_{\gamma\delta} \cdot \boldsymbol{g}_{\gamma\delta}| \\ \times \Theta(\boldsymbol{k}_{\gamma\delta} \cdot \boldsymbol{g}_{\gamma\delta}) \,\mathrm{d}^2 \boldsymbol{k}_{\gamma\delta} \,\mathrm{d}^3 \boldsymbol{c}_{\delta}$$
(2)

for $\gamma, \delta \in \{\alpha, \beta\}$ are the collision terms. In (2), $\boldsymbol{g}_{\gamma\delta} = \boldsymbol{c}_{\gamma} - \boldsymbol{c}_{\delta}$ is the relative velocity between two colliding molecules, $\boldsymbol{k}_{\gamma\delta}$ is the unit contact vector between the centres of two colliding molecules, $\Theta(x)$ is the Heaviside stepfunction and primes are used to denote the distribution functions with post-collisional velocities $(\mathbf{c}'_{\alpha}, \mathbf{c}'_{\beta})$ [11], e.g. $f'_{\alpha} \equiv f_{\alpha}(t, \mathbf{x}, \mathbf{c}'_{\alpha})$. Furthermore, the integration over velocity in (2) and in rest of the paper covers the whole velocity space \mathbb{R}^3 whereas the integration over solid angle covers the unit sphere associated with the unit contact vector $\mathbf{k}_{\gamma\delta}$.

3. Moment Equations

The general form of moment of velocity distribution function f_{γ} ($\gamma \in \{\alpha, \beta\}$) is

$$u_{i_1\cdots i_n}^{a(\gamma)} = m_{\gamma} \int C_{\gamma}^{2a} C_{\langle i_1}^{(\gamma)} C_{i_2}^{(\gamma)} \cdots C_{i_n\rangle}^{(\gamma)} f_{\gamma} \,\mathrm{d}\boldsymbol{c}_{\gamma},$$
(3)

where $a, n \in \mathbb{N}_0$, $C_{\gamma} = c_{\gamma} - v$ is the peculiar velocity of γ -constituent with respect to the whole mixture and angular brackets around the indices denote the symmetrictraceless quantities [2]; v is the barycentric velocity of the mixture. The physical quantities—density ρ_{γ} , diffusion velocity $u_{\gamma} = v_{\gamma} - v$ (where v_{γ} is the mean velocity of γ -component), temperature T_{γ} , stress tensor σ_{γ} and heat flux q_{γ} ($\gamma \in \{\alpha, \beta\}$)—relate with the first few moments defined by (3) as

$$\rho_{\gamma} = m_{\gamma} n_{\gamma} = m_{\gamma} \int f_{\gamma} \, \mathrm{d}\boldsymbol{c}_{\gamma} = u^{0(\gamma)},$$

$$\rho_{\gamma} u_{i}^{(\gamma)} = m_{\gamma} \int C_{i}^{(\gamma)} f_{\gamma} \, \mathrm{d}\boldsymbol{c}_{\gamma} = u_{i}^{0(\gamma)},$$

$$\frac{3}{2} \rho_{\gamma} \theta_{\gamma} = \frac{1}{2} m_{\gamma} \int C_{\gamma}^{2} f_{\gamma} \, \mathrm{d}\boldsymbol{c}_{\gamma} = \frac{1}{2} u^{1(\gamma)}, \quad (4)$$

$$\sigma_{ij}^{(\gamma)} = m_{\gamma} \int C_{\langle i}^{(\gamma)} C_{j\rangle}^{(\gamma)} f_{\gamma} \, \mathrm{d}\boldsymbol{c}_{\gamma} = u_{ij}^{0(\gamma)},$$

$$q_{i}^{(\gamma)} = \frac{1}{2} m_{\gamma} \int C_{\gamma}^{2} C_{i}^{(\gamma)} f_{\gamma} \, \mathrm{d}\boldsymbol{c}_{\gamma} = \frac{1}{2} u_{i}^{1(\gamma)},$$

where n_{γ} is the number density, $\theta_{\gamma} = kT_{\gamma}/m_{\gamma}$ is the temperature in energy units, and k is the Boltzmann constant. The other higher moments defined by (3) do not represent physical quantities in general. Additionally, the barycentric velocities of the individual components are defined as

$$\rho_{\gamma} v_i^{(\gamma)} = m_{\gamma} \int c_i^{(\gamma)} f_{\gamma} \, \mathrm{d} \boldsymbol{c}_{\gamma}, \quad \gamma \in \{\alpha, \beta\}$$

so that the expression for momentum density of the mixture, $(\rho_{\alpha} + \rho_{\beta})v_i = \rho_{\alpha}v_i^{(\alpha)} + \rho_{\beta}v_i^{(\beta)}$, implies that

$$\rho_{\alpha}u_i^{(\alpha)} + \rho_{\beta}u_i^{(\beta)} = 0.$$
 (5)

Note that in non-equilibrium individual gases in a mixture have different temperatures [12–14], although most of the times in literature all the gases in a mixture are assumed to have a common temperature for simplicity, see e.g. [8, 11–13, 15–18]. In this paper, we consider different temperatures for different gases and, therefore, the equations presented in this paper are expected to deliver more feasible results. The total temperature of the mixture T, if required, can be evaluated using the relation for total pressure, i.e., $k(n_{\alpha} + n_{\beta})T = k n_{\alpha}T_{\alpha} + k n_{\beta}T_{\beta}$.

Moment equations for γ -component $(\gamma \in \{\alpha, \beta\})$ in the mixture are obtained by multiplying the Boltzmann equation (1)with $\psi_{\gamma} \equiv \psi(t, \boldsymbol{x}, \boldsymbol{c}_{\gamma})$ and integrating over velocity space c_{γ} . For 26-moment theory,
$$\begin{split} \psi_{\gamma} \text{ is chosen from } m_{\gamma} \big\{ 1, C_i^{(\gamma)}, C_{\gamma}^2/2, C_{\langle i}^{(\gamma)} C_{j\rangle}^{(\gamma)}, \\ C_{\gamma}^2 C_i^{(\gamma)}/2, C_{\langle i}^{(\gamma)} C_j^{(\gamma)} C_{k\rangle}^{(\gamma)}, C_{\gamma}^2 C_{\langle i}^{(\gamma)} C_{j\rangle}^{(\gamma)}, C_{\gamma}^4 \big\} & \text{ in } \end{split}$$
order to obtain the 26-moment equations for γ -constituent corresponding to 26 variables $\{n_{\gamma}, u_{i}^{(\gamma)}, T_{\gamma}, \sigma_{ij}^{(\gamma)}, q_{i}^{(\gamma)}, m_{ijk}^{(\gamma)} = u_{ijk}^{0(\gamma)},$ $u_{ii}^{1(\gamma)}, u^{2(\gamma)}$. The 2×26-moment equations obtained in this way are not closed since the flux term (second term on the left-hand side) in the Boltzmann equation (1) produces the moments which are an order higher than the moments used. Additionally, the production terms in each moment equation (except the mass balance equation) are also unknown and all the moment equations contain an extra variable—the barycentric velocity of the mixture \boldsymbol{v} .

The system of 2×26 -moment equations is closed by assuming Grad-type velocity distribution function for each component $\gamma \in$ $\{\alpha,\beta\}$ based on first 26 moments of respective component:

$$f_{\gamma|G26} = f_0^{(\gamma)} \left[1 + \frac{\Delta_{\gamma}}{8\rho_{\gamma}\theta_{\gamma}^2} \left(1 - \frac{2}{3}\frac{C_{\gamma}^2}{\theta_{\gamma}} + \frac{1}{15}\frac{C_{\gamma}^4}{\theta_{\gamma}^2} \right) + \frac{q_i^{(\gamma)}C_i^{(\gamma)}}{5\rho_{\gamma}\theta_{\gamma}^2} \left(\frac{C_{\gamma}^2}{\theta_{\gamma}} - 5 \right) - \frac{u_i^{(\gamma)}C_i^{(\gamma)}}{2\rho_{\gamma}\theta_{\gamma}} \left(\frac{C_{\gamma}^2}{\theta_{\gamma}} - 7 \right) + \frac{\sigma_{ij}^{(\gamma)}}{2\rho_{\gamma}\theta_{\gamma}^2} C_{\langle i}^{(\gamma)}C_{j\rangle}^{(\gamma)} + \frac{m_{ijk}^{(\gamma)}}{6\rho_{\gamma}\theta_{\gamma}^3} C_{\langle i}^{(\gamma)}C_j^{(\gamma)}C_{k\rangle}^{(\gamma)} + \left(\frac{u_{ij}^{1(\gamma)} - 7\theta_{\gamma}\sigma_{ij}^{(\gamma)}}{28\rho_{\gamma}\theta_{\gamma}^3} \right) C_{\langle i}^{(\gamma)}C_{j\rangle}^{(\gamma)} \left(\frac{C_{\gamma}^2}{\theta_{\gamma}} - 7 \right) \right],$$

$$(6)$$

where

$$f_0^{(\gamma)} = n_\gamma \left(\frac{1}{2\pi\theta_\gamma}\right)^{3/2} \exp\left(-\frac{C_\gamma^2}{2\theta_\gamma}\right) \qquad (7)$$

is Maxwellian distribution function and $\Delta_{\gamma} = u^{2(\gamma)} - 15\rho_{\gamma}\theta_{\gamma}^2$. With this closure, the unknown higher-order moments as well as the production terms (for any interaction potential) are expressed in terms of the moments considered. For the extra variable v, one needs the momentum balance equation for the mixture which may be obtained by adding the balance equations for both the diffusion velocities. Including the momentum balance equation for mixture one gets a closed system of $(2 \times 26 + 1)$ equations. However, it is clear from (5) that the diffusion velocities of the two components in the mixture are not independent and one of them could be replaced by other using (5). Therefore, one equation for any diffusion velocity could be removed from the $(2 \times 26 + 1)$ equations and one gets closed system of 2×26 equations. We still refer to them as $2 \times G26$ equations.

In principle, one can obtain the fully nonlinear $2 \times G26$ moment equations with any general interaction potential. However, evaluating the production terms for a general potential and expressing them in a nice form is not easy. Therefore, we restrict ourselves to Maxwell and hard sphere interaction potentials. The fully non-linear $N \times G26$ equations with the production terms for Maxwell molecules are detailed in [10] and the linear production terms for a binary gas-mixture of hard spheres are given in [19]. For better readability, we shall present only the linear $2 \times G26$ equations for a binary gas-mixture of hard spheres with $\mathbf{F}_{\alpha} = \mathbf{F}_{\beta} = \mathbf{0}$.

The non-linear $2 \times G26$ equations are linearised by perturbing the field variables around their corresponding ground states:

$$\begin{split} v_i &= \varepsilon \, \tilde{v}_i, \quad n_\gamma = n_\gamma^\circ + \varepsilon \, \tilde{n}_\gamma, \quad T_\gamma = T_\circ + \varepsilon \, \tilde{T}_\gamma, \\ u_i^{(\gamma)} &= \varepsilon \, \tilde{u}_i^{(\gamma)}, \quad \sigma_{ij}^{(\gamma)} = \varepsilon \, \tilde{\sigma}_{ij}^{(\gamma)}, \quad q_i^{(\gamma)} = \varepsilon \, \tilde{q}_i^{(\gamma)}, \\ m_{ijk}^{(\gamma)} &= \varepsilon \, \tilde{m}_{ijk}^{(\gamma)}, \quad u_{ij}^{1(\gamma)} = \varepsilon \, \tilde{u}_{ij}^{1(\gamma)}, \quad \Delta_\gamma = \varepsilon \, \tilde{\Delta}_\gamma, \end{split}$$

for $\gamma \in \{\alpha, \beta\}$, where n_{γ}° and T_{\circ} are the number density of the γ -constituent and the common temperature, respectively, in the ground state; the ground state values of other quantities are assumed to be zero. The quantities with tilde are the corresponding perturbations from the ground state and ε is a small parameter. Next, the equations are rewritten in a dimensionless form by employing the length scale L, velocity scale $v_0 = \sqrt{k T_{\circ}/m_{\beta}}$ for the barycentric velocity of the mixture and time scale $t_0 = v_0/L$; the number densities and temperatures are scaled with their respective ground state values and the other moments including diffusion velocities for γ constituent ($\gamma \in \{\alpha, \beta\}$) are scaled with appropriate powers of $(m_{\gamma}n_{\gamma}^{\circ})$ and (kT_{\circ}/m_{γ}) . Note that the velocity scale v_0 is chosen in such a way that if one considers the gasmixture with infinitely diluted α -component, the G26 equations for β -constituent reduces to those for a single gas.

Here onwards, all the quantities will be in dimensionless form unless otherwise stated. The linear G26 equations for α -constituent in the mixture read

$$\sqrt{r_m} \left(\frac{\partial n_\alpha}{\partial t} + \frac{\partial v_i}{\partial x_i} \right) + \frac{\partial u_i^{(\alpha)}}{\partial x_i} = 0, \quad (8)$$

$$\sqrt{r_m} \frac{\partial u_i^{(\alpha)}}{\partial t} + r_m \frac{\partial v_i}{\partial t} + \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{\partial n_\alpha}{\partial x_i} + \frac{\partial T_\alpha}{\partial x_i} \\
= -\frac{\Omega}{\mathrm{Kn}} \Big[\delta_1 u_i^{(\alpha)} + \delta_2 q_i^{(\alpha)} - \delta_3 u_i^{(\beta)} - \delta_4 q_i^{(\beta)} \Big], \tag{9}$$

$$\sqrt{r_m} \left(\frac{3}{2} \frac{\partial T_\alpha}{\partial t} + \frac{\partial v_i}{\partial x_i} \right) - \frac{3}{2} \frac{\partial u_i^{(\alpha)}}{\partial x_i} + \frac{\partial q_i^{(\alpha)}}{\partial x_i} \\ = -\frac{\Omega}{\mathrm{Kn}} \left[\delta_5 (T_\alpha - T_\beta) + \delta_6 \Delta_\alpha - \delta_7 \Delta_\beta \right], \quad (10)$$

$$\begin{split} \sqrt{r_m} & \left(\frac{\partial \sigma_{ij}^{(\alpha)}}{\partial t} + 2 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right) + \frac{\partial m_{ijk}^{(\alpha)}}{\partial x_k} + \frac{4}{5} \frac{\partial q_{\langle i}^{(\alpha)}}{\partial x_{j \rangle}} \\ &= -\frac{1}{28} \frac{r_n r_d^2}{\mathrm{Kn}} \left[21 \sigma_{ij}^{(\alpha)} + u_{ij}^{1(\alpha)} \right] \\ &- \frac{\Omega}{\mathrm{Kn}} \left[\delta_8 \sigma_{ij}^{(\alpha)} + \delta_9 u_{ij}^{1(\alpha)} - \delta_{10} \sigma_{ij}^{(\beta)} - \delta_{11} u_{ij}^{1(\beta)} \right], \end{split}$$
(11)

$$\sqrt{r_m} \frac{\partial q_i^{(\alpha)}}{\partial t} + \frac{5}{2} r_m \frac{\partial v_i}{\partial t} + \frac{1}{2} \frac{\partial u_{ij}^{1(\alpha)}}{\partial x_j} + \frac{1}{6} \frac{\partial \Delta_{\alpha}}{\partial x_i} \\
+ \frac{5}{2} \frac{\partial n_{\alpha}}{\partial x_i} + 5 \frac{\partial T_{\alpha}}{\partial x_i} = -\frac{1}{3} \frac{r_n r_d^2}{\mathrm{Kn}} \Big[2q_i^{(\alpha)} - 5u_i^{(\alpha)} \Big] \\
- \frac{\Omega}{\mathrm{Kn}} \Big[\delta_{12} q_i^{(\alpha)} - \delta_{13} u_i^{(\alpha)} - \delta_{14} q_i^{(\beta)} - \delta_{15} u_i^{(\beta)} \Big],$$
(12)

$$\sqrt{r_m} \frac{\partial m_{ijk}^{(\alpha)}}{\partial t} + \frac{3}{7} \frac{\partial u_{\langle ij}^{1(\alpha)}}{\partial x_{k\rangle}} = -\frac{3}{2} \frac{r_n r_d^2}{\mathrm{Kn}} m_{ijk}^{(\alpha)}$$
$$-\frac{\Omega}{\mathrm{Kn}} \left[\delta_{16} m_{ijk}^{(\alpha)} - \delta_{17} m_{ijk}^{(\beta)} \right], \qquad (13)$$

$$\sqrt{r_m} \left(\frac{\partial u_{ij}^{1(\alpha)}}{\partial t} + 14 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right) + 9 \frac{\partial m_{ijk}^{(\alpha)}}{\partial x_k} + \frac{56}{5} \frac{\partial q_{\langle i}^{(\alpha)}}{\partial x_{j \rangle}}
- 14 \frac{\partial u_{\langle i}^{(\alpha)}}{\partial x_{j \rangle}} = -\frac{1}{168} \frac{r_n r_d^2}{\mathrm{Kn}} \left[247 u_{ij}^{1(\alpha)} - 469 \sigma_{ij}^{(\alpha)} \right]
- \frac{\Omega}{\mathrm{Kn}} \left[\delta_{18} u_{ij}^{1(\alpha)} - \delta_{19} \sigma_{ij}^{(\alpha)} - \delta_{20} u_{ij}^{1(\beta)} - \delta_{21} \sigma_{ij}^{(\beta)} \right],$$
(14)

$$\sqrt{r_m} \frac{\partial \Delta_\alpha}{\partial t} + 8 \frac{\partial q_i^{(\alpha)}}{\partial x_i} - 20 \frac{\partial u_i^{(\alpha)}}{\partial x_i} = -\frac{2}{3} \frac{r_n r_d^2}{\mathrm{Kn}} \Delta_\alpha - \frac{\Omega}{\mathrm{Kn}} \Big[\delta_{22} \Delta_\alpha - \delta_{23} \Delta_\beta + \delta_{24} (T_\alpha - T_\beta) \Big],$$
(15)

where $r_n = n_{\alpha}^{\circ}/n_{\beta}^{\circ}$, $r_m = m_{\alpha}/m_{\beta}$ and $r_d = d_{\alpha}/d_{\beta}$ are the ratio of ground state number densities, the ratio of masses and the ratio of diameters, respectively; Kn =

 $5/(16\sqrt{\pi}n_{\beta}^{\circ}d_{\beta}^{2}L)$ is the Knudsen number for β -constituent; and $\Omega = (1 + r_{d})^{2}$. Further, δ_{i} 's in (9)–(15) depend only on the masses of the gas molecules through the relation $\delta_{i} = \bar{\delta}_{i}\sqrt{2\mu_{\beta}}$ for all i, where $\mu_{\gamma} = m_{\gamma}/(m_{\alpha} + m_{\beta})$ for $\gamma \in \{\alpha, \beta\}$ are the mass ratios [20] and

$$\begin{split} \bar{\delta}_{1} &= \frac{5(1+\mu_{\alpha})}{48}, \ \bar{\delta}_{2} &= \frac{\mu_{\beta}}{24}, \ \bar{\delta}_{3} &= \frac{5(1+\mu_{\beta})\sqrt{r_{m}}}{48} \\ \bar{\delta}_{4} &= \frac{\mu_{\alpha}\sqrt{r_{m}}}{24}, \ \bar{\delta}_{5} &= \frac{5\mu_{\alpha}}{8}, \ \bar{\delta}_{6} &= \frac{\mu_{\alpha}\mu_{\beta}}{48}, \\ \bar{\delta}_{7} &= \frac{\mu_{\alpha}^{2}}{48}, \ \bar{\delta}_{8} &= \frac{3+3\mu_{\alpha}+4\mu_{\alpha}^{2}}{24}, \\ \bar{\delta}_{9} &= \frac{\mu_{\beta}(3+4\mu_{\alpha})}{168}, \ \bar{\delta}_{10} &= 8 \ \bar{\delta}_{6}, \ \bar{\delta}_{11} &= \frac{8 \ \bar{\delta}_{7}}{7}, \\ \bar{\delta}_{12} &= \frac{6-5\mu_{\alpha}+9\mu_{\alpha}^{2}}{16}, \\ \bar{\delta}_{13} &= \frac{5(6-13\mu_{\alpha}+27\mu_{\alpha}^{2})}{96}, \\ \bar{\delta}_{14} &= \frac{\bar{\delta}_{4}(5+27\mu_{\beta})}{2}, \\ \bar{\delta}_{15} &= \frac{5(12-34\mu_{\alpha}+27\mu_{\alpha}^{2})\sqrt{r_{m}}}{96}, \\ \bar{\delta}_{15} &= \frac{5(12-34\mu_{\alpha}+27\mu_{\alpha}^{2})\sqrt{r_{m}}}{96}, \\ \bar{\delta}_{16} &= \frac{16+10\mu_{\alpha}+9\mu_{\alpha}^{2}}{56}, \\ \bar{\delta}_{16} &= \frac{16+10\mu_{\alpha}+9\mu_{\alpha}^{2}}{56}, \\ \bar{\delta}_{16} &= \frac{72+39\mu_{\alpha}-91\mu_{\alpha}^{2}+120\mu_{\alpha}^{3}}{168}, \\ \bar{\delta}_{19} &= \frac{24+9\mu_{\alpha}-83\mu_{\alpha}^{2}+120\mu_{\alpha}^{3}}{24}, \\ \bar{\delta}_{20} &= \frac{\mu_{\alpha}(13-18\mu_{\alpha}+15\mu_{\alpha}^{2})}{12}, \ \bar{\delta}_{23} &= \frac{5\mu_{\alpha}^{2}\mu_{\beta}}{4}, \\ \bar{\delta}_{24} &= 120 \ \bar{\delta}_{6}. \end{split}$$

The linear-dimensionless G26 equations for the β -constituent follow by setting $r_m =$ 1, replacing $r_n r_d^2$ by 1 and Ω by $r_n \Omega$, and interchanging α and β on both sides of (8)– (15). The dimensionless momentum balance equation for the mixture reads

$$\frac{\partial v_i}{\partial t} = -\frac{r_n}{r_m r_n + 1} \left(\frac{\partial n_\alpha}{\partial x_i} + \frac{\partial T_\alpha}{\partial x_i} + \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} \right) - \frac{1}{r_m r_n + 1} \left(\frac{\partial n_\beta}{\partial x_i} + \frac{\partial T_\beta}{\partial x_i} + \frac{\partial \sigma_{ij}^{(\beta)}}{\partial x_j} \right).$$
(16)

Thus, we shall have total $(2 \times 26 + 1)$ equations in three dimensions and we shall simply ignore the equation for diffusion velocity of β -constituent because of the aforementioned reason.

4. Dispersion Relation

In this section, we discuss the behaviour of linear waves predicted by $2 \times G26$ equations for hard sphere gases. In order to verify the linear stability of $2 \times G26$ equations, we consider them in one dimension (1D). For α -constituent, they read

$$\sqrt{r_m} \left(\frac{\mathrm{d}n_\alpha}{\mathrm{d}t} + \frac{\mathrm{d}v_x}{\mathrm{d}x} \right) + \frac{\mathrm{d}u_x^{(\alpha)}}{\mathrm{d}x} = 0, \qquad (17)$$

$$\sqrt{r_m} \frac{\mathrm{d}u_x^{(\alpha)}}{\mathrm{d}t} + r_m \frac{\mathrm{d}v_x}{\mathrm{d}t} + \frac{\mathrm{d}\sigma_{xx}^{(\alpha)}}{\mathrm{d}x} + \frac{\mathrm{d}n_\alpha}{\mathrm{d}x} + \frac{\mathrm{d}T_\alpha}{\mathrm{d}x} \\
= -\frac{\Omega}{\mathrm{Kn}} \left[\delta_1 u_x^{(\alpha)} + \delta_2 q_x^{(\alpha)} - \delta_3 u_x^{(\beta)} - \delta_4 q_x^{(\beta)} \right], \tag{18}$$

$$\sqrt{r_m} \left(\frac{3}{2} \frac{\mathrm{d}T_\alpha}{\mathrm{d}t} + \frac{\mathrm{d}v_x}{\mathrm{d}x} \right) - \frac{3}{2} \frac{\mathrm{d}u_x^{(\alpha)}}{\mathrm{d}x} + \frac{\mathrm{d}q_x^{(\alpha)}}{\mathrm{d}x} = -\frac{\Omega}{\mathrm{Kn}} \left[\delta_5 (T_\alpha - T_\beta) + \delta_6 \Delta_\alpha - \delta_7 \Delta_\beta \right], \quad (19)$$

$$\sqrt{r_m} \left(\frac{\mathrm{d}\sigma_{xx}^{(\alpha)}}{\mathrm{d}t} + \frac{4}{3} \frac{\mathrm{d}v_x}{\mathrm{d}x} \right) + \frac{\mathrm{d}m_{xxx}^{(\alpha)}}{\mathrm{d}x} + \frac{8}{15} \frac{\mathrm{d}q_x^{(\alpha)}}{\mathrm{d}x} \\
= -\frac{1}{28} \frac{r_n r_d^2}{\mathrm{Kn}} \left[21\sigma_{xx}^{(\alpha)} + u_{xx}^{1(\alpha)} \right] \\
- \frac{\Omega}{\mathrm{Kn}} \left[\delta_8 \sigma_{xx}^{(\alpha)} + \delta_9 u_{xx}^{1(\alpha)} - \delta_{10} \sigma_{xx}^{(\beta)} - \delta_{11} u_{xx}^{1(\beta)} \right], \tag{20}$$

$$\sqrt{r_m} \frac{\mathrm{d}q_x^{(\alpha)}}{\mathrm{d}t} + \frac{5}{2} r_m \frac{\mathrm{d}v_x}{\mathrm{d}t} + \frac{1}{2} \frac{\mathrm{d}u_{xx}^{1(\alpha)}}{\mathrm{d}x} + \frac{1}{6} \frac{\mathrm{d}\Delta_{\alpha}}{\mathrm{d}x} \\
+ \frac{5}{2} \frac{\mathrm{d}n_{\alpha}}{\mathrm{d}x} + 5 \frac{\mathrm{d}T_{\alpha}}{\mathrm{d}x} = -\frac{1}{3} \frac{r_n r_d^2}{\mathrm{Kn}} \left[2q_x^{(\alpha)} - 5u_x^{(\alpha)} \right] \\
- \frac{\Omega}{\mathrm{Kn}} \left[\delta_{12} q_x^{(\alpha)} - \delta_{13} u_x^{(\alpha)} - \delta_{14} q_x^{(\beta)} - \delta_{15} u_x^{(\beta)} \right],$$
(21)

$$\sqrt{r_m} \frac{\mathrm{d}m_{xxx}^{(\alpha)}}{\mathrm{d}t} + \frac{9}{35} \frac{\mathrm{d}u_{xx}^{1(\alpha)}}{\mathrm{d}x} = -\frac{3}{2} \frac{r_n r_d^2}{\mathrm{Kn}} m_{xxx}^{(\alpha)} - \frac{\Omega}{\mathrm{Kn}} \left[\delta_{16} m_{xxx}^{(\alpha)} - \delta_{17} m_{xxx}^{(\beta)} \right], \qquad (22)$$

$$\sqrt{r_m} \left(\frac{\mathrm{d}u_{xx}^{1(\alpha)}}{\mathrm{d}t} + \frac{28}{3} \frac{\mathrm{d}v_x}{\mathrm{d}x} \right) + 9 \frac{\mathrm{d}m_{xxx}^{(\alpha)}}{\mathrm{d}x} + \frac{112}{15} \frac{\mathrm{d}q_x^{(\alpha)}}{\mathrm{d}x} \\
- \frac{28}{3} \frac{\mathrm{d}u_x^{(\alpha)}}{\mathrm{d}x} = -\frac{1}{168} \frac{r_n r_d^2}{\mathrm{Kn}} \left[247 u_{xx}^{1(\alpha)} - 469 \sigma_{xx}^{(\alpha)} \right] \\
- \frac{\Omega}{\mathrm{Kn}} \left[\delta_{18} u_{xx}^{1(\alpha)} - \delta_{19} \sigma_{xx}^{(\alpha)} - \delta_{20} u_{xx}^{1(\beta)} - \delta_{21} \sigma_{xx}^{(\beta)} \right], \tag{23}$$

$$\sqrt{r_m} \frac{\mathrm{d}\Delta_\alpha}{\mathrm{d}t} + 8 \frac{\mathrm{d}q_i^{(\alpha)}}{\mathrm{d}x_i} - 20 \frac{\mathrm{d}u_i^{(\alpha)}}{\mathrm{d}x_i} = -\frac{2}{3} \frac{r_n r_d^2}{\mathrm{Kn}} \Delta_\alpha$$
$$- \frac{\Omega}{\mathrm{Kn}} \left[\delta_{22} \Delta_\alpha - \delta_{23} \Delta_\beta + \delta_{24} (T_\alpha - T_\beta) \right].$$
(24)

The 1D equations for β -constituent can be written in a similar way. The momentum balance equation for the mixture (16) in 1D reads

$$\frac{\mathrm{d}v_x}{\mathrm{d}t} = -\frac{r_n}{r_m r_n + 1} \left(\frac{\mathrm{d}n_\alpha}{\mathrm{d}x} + \frac{\mathrm{d}T_\alpha}{\mathrm{d}x} + \frac{\mathrm{d}\sigma_{xx}^{(\alpha)}}{\mathrm{d}x} \right) - \frac{1}{r_m r_n + 1} \left(\frac{\mathrm{d}n_\beta}{\mathrm{d}x} + \frac{\mathrm{d}T_\beta}{\mathrm{d}x} + \frac{\mathrm{d}\sigma_{xx}^{(\beta)}}{\mathrm{d}x} \right).$$
(25)

For the field variables

$$\boldsymbol{U} = \left\{ n_{\alpha}, u_{x}^{(\alpha)}, T_{\alpha}, \sigma_{xx}^{(\alpha)}, q_{x}^{(\alpha)}, m_{xxx}^{(\alpha)}, u_{xx}^{1(\alpha)}, \Delta_{\alpha}, \\ n_{\beta}, T_{\beta}, \sigma_{xx}^{(\beta)}, q_{x}^{(\beta)}, m_{xxx}^{(\beta)}, u_{xx}^{1(\beta)}, \Delta_{\beta}, v_{x} \right\}^{\mathsf{T}},$$

we consider the plane wave ansatz

$$\boldsymbol{U} = \boldsymbol{U}_A \exp\left\{i(x - \hat{\omega}t)\right\},\tag{26}$$

where we have assumed that the length scale L is the inverse of the wave number κ , $\hat{\omega} = \omega/(\kappa v_0)$ is the dimensionless complex frequency of the wave with ω as the conventional complex frequency and U_A is the vector consisting of complex ampli-In this case, the Knudsen number tudes. Kn = $(5\kappa)/(16\sqrt{\pi}n_{\beta}^{\circ}d_{\beta}^{2})$ takes the role of a dimensionless wave number. Substitution of the ansatz (26) into the above 1D moment equations yields an algebraic equation $\mathcal{A}(\hat{\omega}, \mu_{\alpha}, r_d, r_n, \operatorname{Kn}) U = 0.$ For non-trivial solutions U, the determinant of matrix \mathcal{A} should vanish, i.e., det $\mathcal{A} = 0$. The condition det $\mathcal{A} = 0$ gives the so-called dispersion relation relating $\hat{\omega}$ and dimensionless wave number Kn (here).

4.1 Temporal Stability

For temporal stability, the wave number κ is assumed to be real whereas the frequency ω is assumed to be complex. The associated wave travels with phase velocity $v_{\rm ph} = \text{Re}(\omega)/\kappa$ and the growth rate of the amplitudes is characterised by the damping coefficient $\varsigma = \text{Im}(\omega)$. Temporal stability requires $\varsigma \leq 0$.

5. Results

In order to illustrate the linear stability, we plot the dimensionless damping coefficient $\hat{\varsigma} = (5\varsigma)/(16\sqrt{\pi}n_{\beta}^{\circ}d_{\beta}^2v_0)$ over the Knudsen number Kn for parameters $\mu_{\alpha} = 0.3$, $r_n = 0.005$ in figure 1. Figures 1(a) and 1(b) show the damping coefficients of all the modes of the $2 \times G26$ equations for hard spheres and Maxwell molecules, respectively; for hard spheres the diameter ratio r_d is taken as 1 and for Maxwell molecules the ratios of all collision cross sections are taken as 1. The equations for Maxwell molecules can be found in [10]. The red curves in figure 1 show the modes for single gas by considering $r_n = 0$ while the blue curves show the modes for binary gas-mixture. The red curves are included only for comparison. Clearly, for all the modes damping is non-positive. Moreover, for all permissible values of the parameters, damping remains non-positive for both hard spheres and Maxwell molecules. Therefore, we conclude empirically that the $2 \times G26$ equations for hard spheres as well as Maxwell molecules are linearly stable.

To have more insight into the dispersion modes in figure 1, we plot the dimensionless damping $\hat{\varsigma}$ over the dimensionless phase velocity $\hat{v}_{\rm ph}$ for (a) hard spheres and (b) Maxwell molecules in figure 2. The Knudsen number in figure 2 varies between 0 and 20, and the other parameters are same as those in figure 1. Again, the red curves represent the modes for single gas whereas the blue curves represent the modes for binary gasmixture, and the black dots depict the start-





(b) Maxwell molecules

Figure 1: Damping coefficients $\hat{\varsigma}$ of all the modes of 2×G26 equations for (a) hard spheres and (b) Maxwell molecules plotted over the Knudsen number Kn.

ing point of the modes at $\text{Kn} = \kappa = 0$. At $\text{Kn} = \kappa = 0$, four sound modes commence with non-zero velocities, two of them have zero damping and other two have non-zero damping at the start. One sound mode begins with zero damping and zero velocity. All other modes are pure diffusion modes which start with zero velocity and have non-zero damping. Some of the diffusion modes (8 in each figure) bifurcate into propagating waves with damping.

6. Conclusion

In this paper, the derivation of fully non-linear $2 \times G26$ equations for a binary gas-mixture of monatomic-inert-ideal hard

Figure 2: Damping coefficients $\hat{\varsigma}$ of all the modes of 2×G26 equations for (a) hard spheres and (b) Maxwell molecules plotted over the phase velocity $\hat{v}_{\rm ph}$ for $0 \leq {\rm Kn} \leq 20$.

sphere gases has been outlined, though for brevity—the full non-linear $2 \times G26$ equations have not been shown and only the linear $2 \times G26$ equations are presented. In order to obtain the dispersion relation for stability analysis, the linear $2 \times G26$ equations have been restricted to 1D. Assuming the plane wave solution, it has been concluded empirically as well as with the plots for some parameter values that the $2 \times G26$ equations for binary mixture of hard sphere gases are linearly stable.

References

 Zhang, W.-M., Meng, G. & Wei, X. 2012 A review on slip models for gas microflows. *Microfluid.*, **13**, 845–882. doi:10.1007/s10404-012-1012-9.

- [2] Struchtrup, H. 2005 Macroscopic Transport Equations for Rarefied Gas Flows. Berlin: Springer.
- [3] Colin, S. 2012 Gas microflows in the slip flow regime: A critical review on convective heat transfer. J. Heat Transfer, 134, 020908. doi:10.1115/1.4005063.
- [4] Struchtrup, H. & Torrilhon, M. 2003 Regularization of Grad's 13 moment equations: Derivation and linear analysis. *Phys. Fluids*, **15**(9), 2668–2680. doi: 10.1063/1.1597472.
- [5] Grad, H. 1949 On the kinetic theory of rarefied gases. *Comm. Pure Appl. Math.*, 2, 331–407. doi: 10.1002/cpa.3160020403.
- [6] Kremer, G. M. 1987 Extended thermodynamics of mixtures of ideal gases. *Int. J. Eng. Sci.*, **25**, 95–115. doi: 10.1016/0020-7225(87)90137-6.
- [7] Barbera, E. & Brini, F. 2011 Heat transfer in gas mixtures: Advantages of an extended thermodynamics approach. *Phys. Lett. A*, **375**, 827–831. doi: 10.1016/j.physleta.2010.12.043.
- [8] Chapman, S. & Cowling, T. G. 1970 The Mathematical Theory of Non-Uniform Gases. Cambridge University Press.
- [9] Bobylev, A. V. 1982 The Chapman-Enskog and Grad methods for solving the Boltzmann equation. Sov. Phys. Dokl., 27, 29–31.
- [10] Gupta, V. K. & Torrilhon, M. (Submitted) Moment equations for rarefied gasmixtures. *Proc. Roy. Soc. A.*
- [11] Kremer, G. M. 2010 An Introduction to the Boltzmann Equation and Transport Processes in Gases. Berlin: Springer.

- [12] Heckl, M. & Müller, I. 1983 Frame dependence, entropy, entropy flux, and wave speeds in mixtures of gases. Acta Mech., 50, 71–95. doi: 10.1007/BF01170442.
- [13] Zhdanov, V. M. 2002 Transport Processes in Multicomponent Plasma. London: Taylor & Francis.
- [14] Ruggeri, T. & Lou, J. 2009 Heat conduction in multi-temperature mixtures of fluids: the role of the average temperature. *Phys. Lett. A*, **373**, 3052–3055. doi:10.1016/j.physleta.2009.06.037.
- [15] Müller, I. & Ruggeri, T. 1998 Rational Extended Thermodynamics. New York: Springer.
- [16] Naris, S., Valougeorgis, D., Kalempa, D. & Sharipov, F. 2005 Flow of gaseous mixtures through rectangular microchannels driven by pressure, temperature, and concentration gradients. *Phys. Fluids*, **17**, 100607. doi: 10.1063/1.1896986.
- [17] Barbera, E. & Brini, F. 2012 An extended thermodynamics description of stationary heat transfer in binary gas mixtures confined in radial symmetric bounded domains. *Continuum Mech. Thermodyn.*, 24, 313–331. doi: 10.1007/s00161-011-0200-2.
- [18] Sharipov, F. & Strapasson, J. L. 2013 Benchmark problems for mixtures of rarefied gases. I. Couette flow. *Phys. Fluids*, **25**, 037102. doi: 10.1063/1.4791604.
- [19] Gupta, V. K. & Torrilhon, M. 2012 Automated Boltzmann collision integrals for moment equations. vol. 1501 of AIP Conf. Proc., pp. 67–74. doi: 10.1063/1.4769474.
- [20] Ferziger, J. H. & Kaper, H. G. 1972 Mathematical Theory of transport processes in gases. Amsterdam, London: North-Holland Pub. Co.