Moment equations for rarefied gas-mixtures

Vinay Kumar Gupta and Manuel Torrilhon
Center for Computational Engineering Science,
Department of Mathematics, RWTH Aachen University, Germany

Abstract

Following Grad's moment method [1] for a single gas, we present Grad's $N\times 26$-moment equations and the boundary conditions for N-component monatomic-intert-ideal gas-mixtures. Additionally, to illustrate the capabilities of the model, we study the heat flux problem for a binary gas-mixture confined between two parallel plates having different temperatures and compare the results with those in [2].

Grad's moment equations

Grad's 26-moment equations for α-constituent in a N-component monatomic-intert-ideal gas mixture read

$$\frac{\mathrm{D}\rho_\alpha}{\mathrm{D}t} + \rho_\alpha \frac{\partial v_i}{\partial x_i} + \frac{\partial\big(\rho_\alpha u_i^{(\alpha)}\big)}{\partial x_i} = 0,$$

$$\rho_\alpha\left(\frac{\mathrm{D}u_i^{(\alpha)}}{\mathrm{D}t} + \frac{\mathrm{D}v_i}{\mathrm{D}t}\right) - u_i^{(\alpha)}\frac{\partial\big(\rho_\alpha u_j^{(\alpha)}\big)}{\partial x_j} + \rho_\alpha u_j^{(\alpha)}\frac{\partial v_i}{\partial x_j} + \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{\partial(\rho_\alpha\theta_\alpha)}{\partial x_i} = \mathcal{P}_i^{0(\alpha)},$$

$$\rho_\alpha\left(\frac{3}{2}\frac{\mathrm{D}\theta_\alpha}{\mathrm{D}t} + u_i^{(\alpha)}\frac{\mathrm{D}v_i}{\mathrm{D}t}\right) - \frac{3}{2}\theta_\alpha\frac{\partial\big(\rho_\alpha u_j^{(\alpha)}\big)}{\partial x_j} + \rho_\alpha\theta_\alpha\frac{\partial v_i}{\partial x_i} + \frac{\partial q_i^{(\alpha)}}{\partial x_i} + \sigma_{ij}^{(\alpha)}\frac{\partial v_i}{\partial x_j} = \frac{1}{2}\mathcal{P}^{1(\alpha)},$$

$$\frac{\mathrm{D}\sigma_{ij}^{(\alpha)}}{\mathrm{D}t} + 2\rho_\alpha u_{\langle i}^{(\alpha)}\frac{\mathrm{D}v_{j\rangle}}{\mathrm{D}t} + \sigma_{ij}^{(\alpha)}\frac{\partial v_k}{\partial x_k} + \frac{\partial m_{ijk}^{(\alpha)}}{\partial x_k} + \frac{4}{5}\frac{\partial q_{\langle i}^{(\alpha)}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}^{(\alpha)}\frac{\partial v_{j\rangle}}{\partial x_k} + 2\rho_\alpha\theta_\alpha\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = \mathcal{P}_{ij}^{0(\alpha)},$$

$$\frac{\mathrm{D}q_i^{(\alpha)}}{\mathrm{D}t} + \left(\sigma_{ij}^{(\alpha)} + \frac{5}{2}\rho_\alpha\theta_\alpha\delta_{ij}\right)\frac{\mathrm{D}v_j}{\mathrm{D}t} + \frac{1}{2}\frac{\partial u_{ij}^{1(\alpha)}}{\partial x_j} + \frac{1}{6}\frac{\partial\Delta_\alpha}{\partial x_i} + m_{ijk}^{(\alpha)}\frac{\partial v_j}{\partial x_k}$$
$$+ \frac{5}{2}\theta_\alpha^2\frac{\partial\rho_\alpha}{\partial x_i} + 5\rho_\alpha\theta_\alpha\frac{\partial\theta_\alpha}{\partial x_i} + \frac{7}{5}q_i^{(\alpha)}\frac{\partial v_j}{\partial x_j} + \frac{7}{5}q_j^{(\alpha)}\frac{\partial v_i}{\partial x_j} + \frac{2}{5}q_j^{(\alpha)}\frac{\partial v_j}{\partial x_i} = \frac{1}{2}\mathcal{P}_i^{1(\alpha)},$$

$$\frac{\mathrm{D}m_{ijk}^{(\alpha)}}{\mathrm{D}t} + 3\sigma_{\langle ij}^{(\alpha)}\frac{\mathrm{D}v_{k\rangle}}{\mathrm{D}t} + m_{ijk}^{(\alpha)}\frac{\partial v_l}{\partial x_l} + \frac{3}{7}\frac{\partial u_{\langle ij}^{1(\alpha)}}{\partial x_{k\rangle}} + 3m_{l\langle ij}^{(\alpha)}\frac{\partial v_{k\rangle}}{\partial x_l} + \frac{12}{5}q_{\langle i}^{(\alpha)}\frac{\partial v_{k\rangle}}{\partial x_j} = \mathcal{P}_{ijk}^{0(\alpha)},$$

$$\frac{\mathrm{D}u_{ij}^{1(\alpha)}}{\mathrm{D}t} + \frac{28}{5}q_{\langle i}^{(\alpha)}\frac{\mathrm{D}v_{j\rangle}}{\mathrm{D}t} + 2m_{ijk}^{(\alpha)}\frac{\mathrm{D}v_k}{\mathrm{D}t} + u_{ij}^{1(\alpha)}\frac{\partial v_k}{\partial x_k} + 9\theta_\alpha\frac{\partial m_{ijk}^{(\alpha)}}{\partial x_k} + 9m_{ijk}^{(\alpha)}\frac{\partial\theta_\alpha}{\partial x_k} + \frac{56}{5}\theta_\alpha\frac{\partial q_{\langle i}^{(\alpha)}}{\partial x_{j\rangle}}$$
$$+ \frac{56}{5}q_{\langle i}^{(\alpha)}\frac{\partial\theta_\alpha}{\partial x_{j\rangle}} - 14\rho_\alpha\theta_\alpha^2\frac{\partial u_{\langle i}^{(\alpha)}}{\partial x_{j\rangle}} - 14\theta_\alpha^2 u_{\langle i}^{(\alpha)}\frac{\partial\rho_\alpha}{\partial x_{j\rangle}} - 28\rho_\alpha\theta_\alpha u_{\langle i}^{(\alpha)}\frac{\partial\theta_\alpha}{\partial x_{j\rangle}} + \frac{6}{7}u_{\langle ij}^{1(\alpha)}\frac{\partial v_{k\rangle}}{\partial x_k}$$
$$+ \frac{4}{5}u_{k\langle i}^{1(\alpha)}\frac{\partial v_k}{\partial x_{j\rangle}} + 2u_{k\langle i}^{1(\alpha)}\frac{\partial v_{j\rangle}}{\partial x_k} + \frac{14}{15}\Delta_\alpha\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + 14\rho_\alpha\theta_\alpha^2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = \mathcal{P}_{ij}^{1(\alpha)},$$

$$\frac{\mathrm{D}\Delta_\alpha}{\mathrm{D}t} + 8\left(q_i^{(\alpha)} - \frac{5}{2}\rho_\alpha\theta_\alpha u_i^{(\alpha)}\right)\frac{\mathrm{D}v_i}{\mathrm{D}t} + \frac{7}{3}\Delta_\alpha\frac{\partial v_i}{\partial x_i} - 20\theta_\alpha\sigma_{ij}^{(\alpha)}\frac{\partial v_i}{\partial x_j} + 8\theta_\alpha\frac{\partial q_i^{(\alpha)}}{\partial x_i} + 28q_i^{(\alpha)}\frac{\partial\theta_\alpha}{\partial x_i}$$
$$- 20\rho_\alpha\theta_\alpha^2\frac{\partial u_i^{(\alpha)}}{\partial x_i} - 20\theta_\alpha^2 u_i^{(\alpha)}\frac{\partial\rho_\alpha}{\partial x_i} - 70\rho_\alpha\theta_\alpha u_i^{(\alpha)}\frac{\partial\theta_\alpha}{\partial x_i} + 4u_{ij}^{1(\alpha)}\frac{\partial v_i}{\partial x_j} = \mathcal{P}^{2(\alpha)} - 10\,\theta_\alpha\mathcal{P}^{1(\alpha)},$$

where $\mathcal{P}_{i_1 i_2\cdots i_n}^{a(\alpha)}$ are the production terms. The conservation laws for the mixture read

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial v_i}{\partial x_i} = 0,\ \ \rho\frac{\mathrm{D}v_i}{\mathrm{D}t} + \frac{\partial\sigma_{ij}}{\partial x_j} + \frac{\partial p}{\partial x_i} = 0,\ \ \frac{3}{2}nk\frac{\mathrm{D}T}{\mathrm{D}t} + nkT\frac{\partial v_i}{\partial x_i} + \frac{\partial q_i}{\partial x_i} + \sigma_{ij}\frac{\partial v_i}{\partial x_j} = 0,$$

where

$$n = \sum_{\alpha=1}^{N} n_\alpha, \quad p = knT = k\sum_{\alpha=1}^{N} n_\alpha T_\alpha, \quad \sigma_{ij} = \sum_{\alpha=1}^{N}\sigma_{ij}^{(\alpha)}, \quad q_i = \sum_{\alpha=1}^{N} q_i^{(\alpha)},$$

are total number density, total pressure, total stress, total heat flux of the mixture; T is the total temperature of the mixture; and k is the Boltzmann constant.

Production terms

The production terms are evaluated using MATHEMATICA®. For Maxwell molecules, the linear production terms read [3, 4]

$$\mathcal{P}_i^{0(\alpha)} = -\rho_\alpha\sum_{\beta=1}^{N}\nu_{\alpha\beta}\,\delta_1\left(u_i^{(\alpha)} - u_i^{(\beta)}\right), \quad \frac{1}{2}\mathcal{P}^{1(\alpha)} = -n_\alpha k\sum_{\beta=1}^{N}\nu_{\alpha\beta}\delta_2(T_\alpha - T_\beta),$$

$$\mathcal{P}_{ij}^{0(\alpha)} = -\sum_{\beta=1}^{N}\nu_{\alpha\beta}\left(\delta_3\sigma_{ij}^{(\alpha)} - \delta_4\frac{n_\alpha}{n_\beta}\sigma_{ij}^{(\beta)}\right),$$

$$\frac{1}{2}\mathcal{P}_i^{1(\alpha)} = -\sum_{\beta=1}^{N}\nu_{\alpha\beta}\left(\delta_5 q_i^{(\alpha)} - \frac{5}{2}(\delta_5-\delta_1)\rho_\alpha\theta_\alpha u_i^{(\alpha)} - \delta_6\frac{n_\alpha}{n_\beta}q_i^{(\beta)} + \delta_7\rho_\alpha\theta_\alpha u_i^{(\beta)}\right),$$

$$\mathcal{P}_{ijk}^{0(\alpha)} = -\sum_{\beta=1}^{N}\nu_{\alpha\beta}\left(\delta_8 m_{ijk}^{(\alpha)} - \delta_9\frac{n_\alpha}{n_\beta}m_{ijk}^{(\beta)}\right),$$

$$\mathcal{P}_{ij}^{1(\alpha)} = -\sum_{\beta=1}^{N}\nu_{\alpha\beta}\left(\delta_{10}u_{ij}^{1(\alpha)} + \delta_{11}\theta_\alpha\sigma_{ij}^{(\alpha)} - \delta_{12}\frac{n_\alpha}{n_\beta}u_{ij}^{1(\beta)} - \delta_{13}\theta_\alpha\frac{n_\alpha}{n_\beta}\sigma_{ij}^{(\beta)}\right),$$

$$\mathcal{P}^{2(\alpha)} - 10\,\theta_\alpha\mathcal{P}^{1(\alpha)} = -\sum_{\beta=1}^{N}\nu_{\alpha\beta}\left(\delta_{14}\Delta_\alpha - \delta_{15}\frac{n_\alpha}{n_\beta}\Delta_\beta\right).$$

Boundary conditions

The boundary conditions have been derived using the Maxwell accommodation model [5] for each component in the mixture. For α-constituent, they read

$$u_n^{(\alpha)} = 0, \qquad \sigma_{nt_i}^{(\alpha)} = -\tau_\alpha\left[P_\alpha V_{t_i} + \frac{1}{2}\rho_\alpha\theta_\alpha u_{t_i}^{(\alpha)} + \frac{1}{5}q_{t_i}^{(\alpha)} + \frac{1}{2}m_{nnt_i}^{(\alpha)}\right],$$

$$q_n^{(\alpha)} = -\tau_\alpha\left[2P_\alpha\{\theta_\alpha - \theta_w^{(\alpha)}\} - \frac{3}{4}\theta_\alpha\sigma_{nn}^{(\alpha)} + \frac{5}{28}u_{nn}^{1(\alpha)} + \frac{1}{15}\Delta_\alpha - \frac{1}{2}P_\alpha V^2\right],$$

$$m_{nnn}^{(\alpha)} = \tau_\alpha\left[\frac{2}{5}P_\alpha\{\theta_\alpha - \theta_w^{(\alpha)}\} - \frac{9}{10}\theta_\alpha\sigma_{nn}^{(\alpha)} - \frac{1}{14}u_{nn}^{1(\alpha)} + \frac{1}{75}\Delta_\alpha - \frac{3}{5}P_\alpha V^2\right],$$

$$m_{nt_1t_2}^{(\alpha)} = -\tau_\alpha\left[\frac{1}{2}\theta_\alpha\sigma_{t_1t_2}^{(\alpha)} + \frac{1}{14}u_{t_1t_2}^{1(\alpha)} - P_\alpha V_{t_1}V_{t_2}\right],$$

$$m_{nt_it_i}^{(\alpha)} = -\tau_\alpha\left[\frac{1}{5}P_\alpha\{\theta_\alpha - \theta_w^{(\alpha)}\} - \frac{1}{5}\theta_\alpha\sigma_{nn}^{(\alpha)} + \frac{1}{2}\theta_\alpha\sigma_{t_it_i}^{(\alpha)} + \frac{1}{14}u_{t_it_i}^{1(\alpha)} + \frac{1}{150}\Delta_\alpha + \frac{1}{5}P_\alpha V^2 - P_\alpha V_{t_i}^2\right],$$

$$u_{nt_i}^{1(\alpha)} = \tau_\alpha\left[6P_\alpha\{\theta_\alpha - \theta_w^{(\alpha)}\}V_{t_i} - 6P_\alpha\theta_\alpha V_{t_i} + 3\rho_\alpha\theta_\alpha^2 u_{t_i}^{(\alpha)} - \frac{18}{5}\theta_\alpha q_{t_i}^{(\alpha)} - 4\theta_\alpha m_{nnt_i}^{(\alpha)} - P_\alpha V^2 V_{t_i}\right],$$

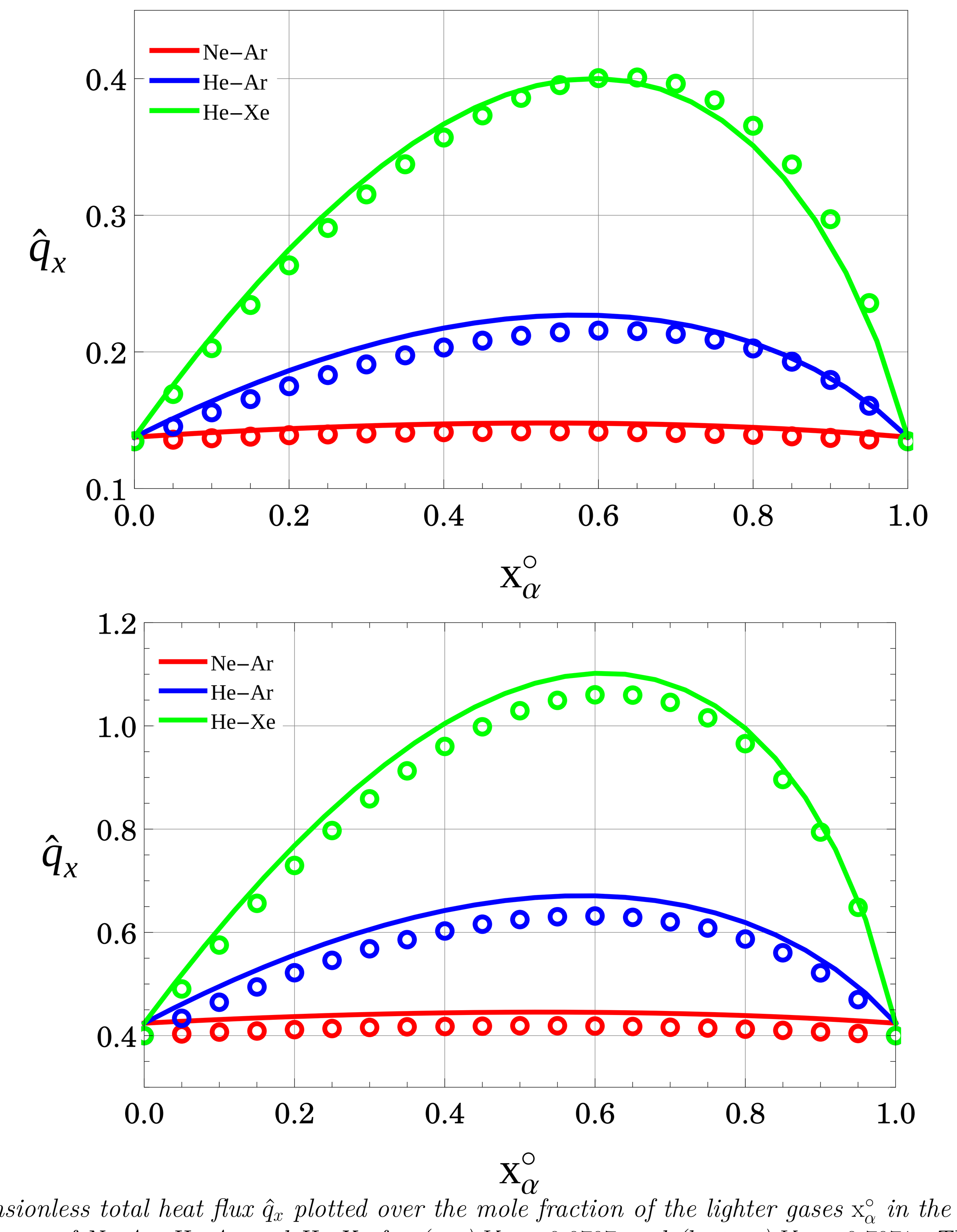
where

$$P_\alpha = \rho_\alpha\theta_\alpha + \frac{3}{4}\sigma_{nn}^{(\alpha)} - \frac{1}{28}\frac{u_{nn}^{1(\alpha)}}{\theta_\alpha} - \frac{1}{120}\frac{\Delta_\alpha}{\theta_\alpha}; \quad \tau_\alpha = \frac{\chi_\alpha}{2-\chi_\alpha}\sqrt{\frac{2}{\pi\,\theta_\alpha}}; \quad \boldsymbol{V} = \boldsymbol{v} - \boldsymbol{v}_w$$

is the slip velocity and χ_α is the accommodation coefficient of the α-constituent.

Results

We solve the linear-dimensionless-steady state-1D Grad's 2×26-moment equations along with the boundary conditions using the finite differences and compare the results with those in [2] obtained using the realistic interaction potential. See [4] for more details.



Dimensionless total heat flux $\hat{q}_x$ plotted over the mole fraction of the lighter gases x_α° in the binary gas-mixtures of Ne-Ar, He-Ar and He-Xe for (top) Kn = 0.0707 and (bottom) Kn = 0.7071. The circles denote the data from [2] obtained by direct discretization of the Boltzmann equation using realistic potential.

References

[1] Grad, H. 1949 On the kinetic theory of rarefied gases. *Comm. Pure Appl. Math.*, **2**, 331–407.

[2] Sharipov, F., Cumin, L. M. G. & Kalempa, D. 2007 Heat flux between parallel plates through a binary gaseous mixture over the whole range of the knudsen number. *Physica A*, **378**, 183–193.

[3] Gupta, V. K. & Torrilhon, M. 2012 Automated Boltzmann collision integrals for moment equations. vol. 1501 of *AIP Conference Proceedings*, pp. 67–74.

[4] Gupta, V. K. & Torrilhon, M. 2014 Higher order moment equations for rarefied gas-mixtures. (Submitted to Proc. Roy. Soc. A).

[5] Maxwell, J. C. 1879 On stresses in rarefied gases arising from inequalities of temperature. *Phil. Trans. R. Soc. Lond.*, **170**, 231–256.