Flow of binary gas-mixtures in a lid-driven square cavity

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

Abstract

Fluid flow in a lid-driven square cavity is a classical problem of fluid dynamics and has been studied by many researchers in the context of liquids and single monatomic gases. However, the same problem has certainly received much less attention in the context of gas-mixtures. In this work, we employ Grad's moment method to binary mixtures of monatomic-intert-ideal (simple) gases made up of Maxwell molecules in order to study their flow in a lid-driven square cavity.

Problem description

We consider a binary mixture of simple 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 $T_w = T_\circ$, and let the top wall (lid) of the cavity be moving in positive x-direction with velocity $v_{\text{lid}} = \varepsilon\, \tilde{v}_0$, see figure 1.

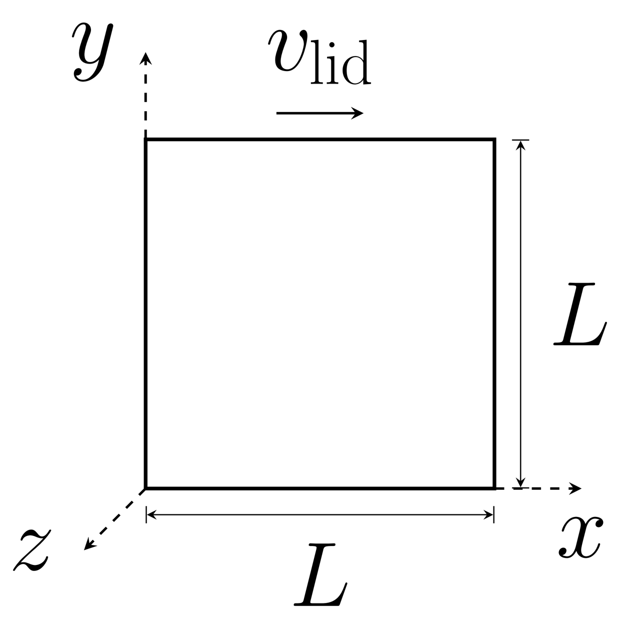

Fig. 1: Schematic of a two-dimensional lid-driven square cavity; z-axis is included just for illustration purposes.

Grad's 2×13-moment equations
(in linearized form)

The system of Grad's 2×13-moment equations consists of 13-moment equations for the α-constituent and 13-moment equations for the β-constituent. The 13-moment equations (in linear-dimensionless form) for the α-constituent in the mixture read [1]

$$\frac{v_\circ}{\sqrt{\theta_\alpha^\circ}}\left(\frac{\partial n_\alpha}{\partial t} + \frac{\partial v_i}{\partial x_i}\right) + \frac{\partial u_i^{(\alpha)}}{\partial x_i} = 0, \tag{1}$$

$$\frac{v_\circ}{\sqrt{\theta_\alpha^\circ}}\frac{\partial u_i^{(\alpha)}}{\partial t} + \frac{v_\circ^2}{\theta_\alpha^\circ}\frac{\partial v_i}{\partial t} + \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{\partial T_\alpha}{\partial x_i} + \frac{\partial n_\alpha}{\partial x_i} = -\frac{1}{\mathrm{Kn}\,\Omega}\mathrm{x}_\beta^\circ\left(\delta_1 u_i^{(\alpha)} - \delta_2 u_i^{(\beta)}\right), \tag{2}$$

$$\frac{v_\circ}{\sqrt{\theta_\alpha^\circ}}\left(\frac{3}{2}\frac{\partial T_\alpha}{\partial t} + \frac{\partial v_i}{\partial x_i}\right) - \frac{3}{2}\frac{\partial u_i^{(\alpha)}}{\partial x_i} + \frac{\partial q_i^{(\alpha)}}{\partial x_i} = -\frac{1}{\mathrm{Kn}\,\Omega}\mathrm{x}_\beta^\circ\delta_3(T_\alpha - T_\beta), \tag{3}$$

$$\frac{v_\circ}{\sqrt{\theta_\alpha^\circ}}\left(\frac{\partial \sigma_{ij}^{(\alpha)}}{\partial t} + 2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right) + \frac{4}{5}\frac{\partial q_{\langle i}^{(\alpha)}}{\partial x_{j\rangle}} = -\frac{1}{\mathrm{Kn}\,\Omega}\left[\mathrm{x}_\alpha^\circ\Omega_\alpha\sigma_{ij}^{(\alpha)} + \mathrm{x}_\beta^\circ\left(\delta_4\sigma_{ij}^{(\alpha)} - \delta_5\sigma_{ij}^{(\beta)}\right)\right], \tag{4}$$

$$\begin{aligned}&\frac{v_\circ}{\sqrt{\theta_\alpha^\circ}}\frac{\partial q_i^{(\alpha)}}{\partial t} + \frac{5 v_\circ^2}{2\theta_\alpha^\circ}\frac{\partial v_i}{\partial t} + \frac{7}{2}\frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + 5\frac{\partial T_\alpha}{\partial x_i} + \frac{5}{2}\frac{\partial n_\alpha}{\partial x_i} \\ &= -\frac{1}{\mathrm{Kn}\,\Omega}\left[\frac{2}{3}\mathrm{x}_\alpha^\circ\Omega_\alpha\left(q_i^{(\alpha)} - \frac{5}{2}u_i^{(\alpha)}\right) + \mathrm{x}_\beta^\circ\left(\delta_6 q_i^{(\alpha)} - \delta_7 u_i^{(\alpha)} - \delta_8 q_i^{(\beta)} - \delta_9 u_i^{(\beta)}\right)\right],\end{aligned} \tag{5}$$

where all the moments are dimensionless and have their usual meanings, Kn is the Knudsen number for the mixture, $\theta_{\alpha,\beta}^\circ = \sqrt{k\,T_\circ/m_{\alpha,\beta}}$ with k being the Boltzmann constant, $v_\circ = \sqrt{k\,T_\circ/m}$—with $m = \mathrm{x}_\alpha^\circ m_\alpha + \mathrm{x}_\beta^\circ m_\beta$—is a velocity scale, $\mathrm{x}_{\alpha,\beta}^\circ = n_{\alpha,\beta}^\circ/(n_\alpha^\circ + n_\beta^\circ)$ are the mole fractions of the constituents in the ground state, Ω_α and Ω_β are the ratios of different *Omega integrals* [2, 3]: $\Omega_\alpha = \Omega_{\alpha\alpha}^{(2,2)}/\Omega_{\alpha\beta}^{(2,2)}$ and $\Omega_\beta = \Omega_{\beta\beta}^{(2,2)}/\Omega_{\alpha\beta}^{(2,2)}$, $\Omega = \mathrm{x}_\alpha^\circ\Omega_\alpha + \mathrm{x}_\beta^\circ\Omega_\beta$, and the coefficients δ_i's depend only on the mass ratios $\mu_{\alpha,\beta} = m_{\alpha,\beta}/(m_\alpha + m_\beta)$.

The 13-moment equations for the β-constituent can be obtained by interchanging α and β in (1)–(5). Furthermore, since the diffusion velocities in a binary gas-mixture are not independent ($\mathrm{x}_\alpha^\circ\sqrt{\mu_\alpha}u_i^{(\alpha)} + \mathrm{x}_\beta^\circ\sqrt{\mu_\beta}u_i^{(\beta)} = 0$), we discard the moment equation for $u_i^{(\beta)}$ and replace it in terms of $u_i^{(\alpha)}$ in the other equations. Owing to the presence of hydrodynamic velocity of the mixture v_i in this system, one also needs to include momentum balance equation for the mixture which in dimensionless form reads

$$\mathrm{x}_\alpha^\circ\left(\frac{v_\circ^2}{\theta_\alpha^\circ}\frac{\partial v_i}{\partial t} + \frac{\partial \sigma_{ij}^{(\alpha)}}{\partial x_j} + \frac{\partial n_\alpha}{\partial x_i} + \frac{\partial T_\alpha}{\partial x_i}\right) + \mathrm{x}_\beta^\circ\left(\frac{v_\circ^2}{\theta_\beta^\circ}\frac{\partial v_i}{\partial t} + \frac{\partial \sigma_{ij}^{(\beta)}}{\partial x_j} + \frac{\partial n_\beta}{\partial x_i} + \frac{\partial T_\beta}{\partial x_i}\right) = 0. \tag{6}$$

Boundary conditions

The boundary conditions are obtained through the Maxwell accommodation model, see [1]. The required boundary conditions for the problem under consideration in linear-dimensionless form read

$$\int_0^1\!\!\int_0^1 n_\gamma \,\mathrm{d}x\,\mathrm{d}y = 0, \tag{7}$$

$$u_x^{(\gamma)}(0,y) = u_x^{(\gamma)}(1,y) = u_y^{(\gamma)}(x,0) = u_y^{(\gamma)}(x,1) = 0, \tag{8}$$

$$\sigma_{nt}^{(\gamma)} = -\mathfrak{n}\frac{\chi_\gamma}{2-\chi_\gamma}\sqrt{\frac{2}{\pi}}\left[\frac{v_\circ}{\sqrt{\theta_\gamma^\circ}}(v_t - v_w) + \frac{1}{2}u_t^{(\gamma)} + \frac{1}{5}q_t^{(\gamma)}\right], \tag{9}$$

$$q_n^{(\gamma)} = -\mathfrak{n}\frac{\chi_\gamma}{2-\chi_\gamma}\sqrt{\frac{2}{\pi}}\left[2\big(T_\gamma - T_w\big) + \frac{1}{2}\sigma_{nn}^{(\gamma)}\right], \tag{10}$$

where

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

Results

The above system of linearized 2×G13 equations and boundary condition is solved numerically using finite difference method. The reference solution is obtained by discretizing the domain of the cavity into 400×400 cells of equal size. The method is more than first order convergent in L^1-norm for all field variables. As an example, figure 2 illustrates the convergence results for the number density of Xe in He–Xe mixture.

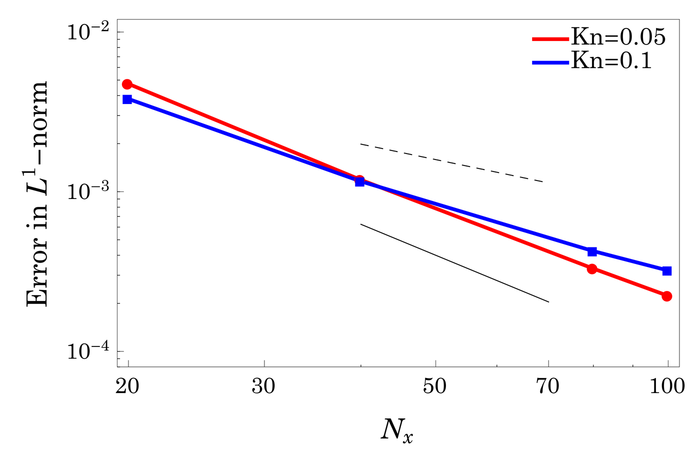

Fig. 2: Convergence of the numerical method for the number density of Xe in He–Xe mixture with $\mathrm{x}_{\mathrm{He}}^\circ = 0.25$. The continuous and dashed black lines have slopes -2 and -1, respectively, and are included only for comparison. The other parameters are $v_w = \chi_\alpha = \chi_\beta = 1$.

Figure 3 illustrates the total heat flux lines plotted over average temperature contours for He–Xe mixture with $\mathrm{x}_{\mathrm{He}}^\circ = 0.25$ at $\mathrm{Kn} = 0.05$. It can be seen from figure 3 that heat flows from cold region to hot region which is a non-Fourier effect and cannot be captured with traditional Navier–Stokes and Fourier equations.

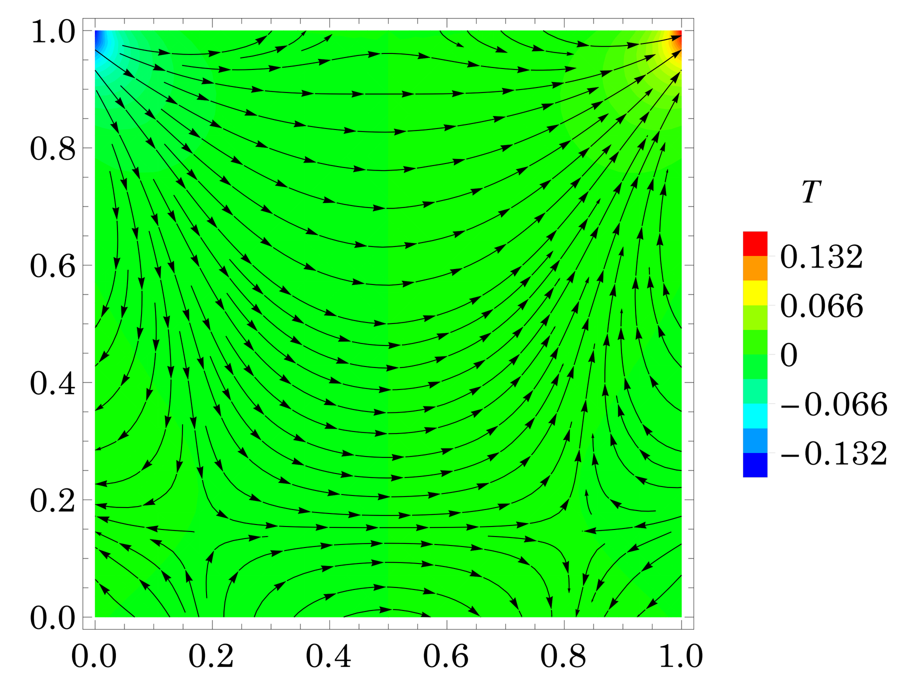

Fig. 3: Total heat flux lines and average temperature contours in He–Xe mixture with $\mathrm{x}_{\mathrm{He}}^\circ = 0.25$ at $\mathrm{Kn} = 0.05$. The other parameters are $v_w = \chi_\alpha = \chi_\beta = 1$.

References

[1] Gupta, V. K. & Torrilhon, M. 2015 Higher order moment equations for rarefied gas mixtures. *Proc. Roy. Soc. A*, **471**, 20140754.

[2] Kremer, G. M. 2010 *An Introduction to the Boltzmann Equation and Transport Processes in Gases.* Berlin: Springer.

[3] Gupta, V. K. & Torrilhon, M. 2015 Comparison of relaxation phenomena in binary gas-mixtures of Maxwell molecules and hard spheres. *Comput. Math. Appl.*, **70**, 73–88.