Rarefied gas mixture flow between plates of arbitrary length due to small pressure difference

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Abstract. The linearized flow of a binary gas mixture between two parallel plates of any length driven by a small pressure difference is numerically solved based on the McCormack kinetic model. In this case the flow is not fully developed and the simulated flow field includes, in addition to the channel, efficiently large upstream and downstream regions significantly increasing the required computational effort. In the present work results are provided for one gas mixture, namely He-Ne with a specific concentration of 0.5 in a wide range of gas rarefaction. The ratio of the length over the height of the channel is taken to be equal to 0, 1 and 5 corresponding to flow through channels of very short (slit), short and moderate lengths respectively. Results are provided for the two kinetic coefficients related to Poiseuille and barodiffusion flow rates and the velocity profiles of each species. The effect of the length to height ratio and of the gas rarefaction on the flow quantities is investigated deducing that as the ratio in increased the separation phenomenon becomes more dominant, while a Knudsen minimum is observed at the ratio equal to 5.

1. Introduction
Most of the work of gas mixture flows through micro channels is based on the assumption that the channel is long enough to introduce a fully developed flow approach [1-4]. The corresponding work through short micro channels is very limited mainly due to the involved computational cost. When the flow is fully developed the pressure varies only in the flow direction and it is possible to simulate the flow field in several cross sections along the channel. Then, following a well known integrating procedure based on the mass conservation principal yields the flow rate through the channel [4]. Contrary, when the fully developed assumption is not valid as in the case of channels of short and moderate lengths the whole flow field including the channel with adequate large inlet and outlet regions must be simulated.

In the latter case when the flow field is driven by large pressure differences the DSMC method may be implemented in an efficient manner [5]. However, when small pressure differences are imposed the flow velocity is rather small and the DSMC method becomes computationally inefficient due to the introduced statistical noise. It has been shown that in the case of low-speed flows linearized kinetic theory is the most suitable computational approach.

In the present work a system of linearized Boltzmann equations is solved via a fully deterministic approach to simulate the flow of a binary gas mixture between parallel plates of arbitrary length. The McCormack kinetic model [6] is introduced to replace the complicated collision term of the Boltzmann equation. Purely diffuse boundary conditions at the wall boundaries are assumed. The
proposed algorithm is initially validated by comparing the present results for the flow through a slit with corresponding ones available in the literature [7] and then it is used to simulate binary gas flow between parallel plates of finite length. Preliminary results are provided for one mixture and a limited number of channel lengths in a wide range of the Knudsen number. A more complete investigation of the effect of all involved geometric and flow parameters will be performed in the short future.

2. Formulation

Consider two large reservoirs connected by a channel of length $L$. The reservoirs contain a binary gas mixture having a reference concentration $C_0$ and they are maintained at pressures $P_o + \Delta P$ and $P_o$ with $\Delta P / P_o \ll 1$, while the temperature in both reservoirs is equal to $T_o$. Due to the pressure difference there is a gas mixture flow through the channel. The height of the channel is denoted by $H$, while the width of the channel is much larger than its height in order to ignore the end effects in that direction. However, the end effects in the flow direction are taken into account with the present formulation and channels of arbitrary length may be studied provided that the pressure difference is adequately small to justify a linear treatment. In Figure 1 the flow configuration is shown. The coordinate system is $(x, y)$, with $x$ denoting the flow direction and $y$ the direction vertical to the plates.

The concentration of the mixture is defined as

$$C(x, y) = n_a(x, y) / n(x, y)$$

where $n_a(x, y)$, $a=1,2$ is the number density of the species and $n = n_1 + n_2$ is the number density of the mixture. Always the number density of light species is denoted by “1”. The reference concentration $C_0$ is defined as

$$C_0 = n_{b1} / n_b$$

where $n_{b1}$ and $n_b$ are the number density of the light species and of the mixture respectively at the downstream container. In the present configuration the concentrations of the mixture in the downstream and upstream containers are equal. The molecular mass of the mixture is

$$m = C m_1 + (1 - C) m_2$$

where $m_a$, $a=1,2$ is the molecular mass of each species.
The formulation of the McCormack kinetic equation is identical to the one described in [6,7] and therefore only the final projected kinetic equations, as implemented in the present work, are provided. In particular starting from the second order McCormack model and introducing the well known projection procedure yields the following set of four coupled kinetic equations:

\[
\frac{\partial R_a}{\partial y} + c_p \cos \theta \frac{\partial R_a}{\partial x} = \delta \frac{\alpha}{\gamma_{a\beta}} \sum_{\beta=1}^{2} \left( -R_{a\alpha} + \gamma_{a\alpha} V_{a\alpha} \right) + 2 \left[ \gamma_{a\alpha} u_{a\alpha} - \left( \frac{m_{a\beta}}{m_p} u_{a\beta} \right) \left( \frac{\partial}{\partial x} \left( \frac{\partial}{\partial y} \right) \right) \right] c_p \cos \theta + 2 \left[ \gamma_{a\alpha} u_{a\alpha} - \left( \frac{m_{a\beta}}{m_p} u_{a\beta} \right) \left( \frac{\partial}{\partial y} \left( \frac{\partial}{\partial x} \right) \right) \right] c_p \sin \theta
\]

\[
+ 2 \left[ \gamma_{a\alpha} u_{a\alpha} - \left( \frac{m_{a\beta}}{m_p} u_{a\beta} \right) \left( \frac{\partial}{\partial z} \left( \frac{\partial}{\partial x} \right) \right) \right] c_p \cos \theta + 2 \left[ \gamma_{a\alpha} u_{a\alpha} - \left( \frac{m_{a\beta}}{m_p} u_{a\beta} \right) \left( \frac{\partial}{\partial z} \left( \frac{\partial}{\partial y} \right) \right) \right] c_p \sin \theta
\]

\[
\sum_{\alpha=1}^{2} \left[ \gamma_{a\alpha} u_{a\alpha} - \left( \frac{m_{a\beta}}{m_p} u_{a\beta} \right) \left( \frac{\partial}{\partial z} \left( \frac{\partial}{\partial x} \right) \right) \right] c_p \cos \theta \sin \theta
\]

\[
\frac{\partial S_a}{\partial y} + c_p \cos \theta \frac{\partial S_a}{\partial x} = \delta \frac{\alpha}{\gamma_{a\beta}} \sum_{\beta=1}^{2} \left( -S_{a\alpha} + 2 \left( \gamma_{a\alpha} - \gamma_{a\alpha} V_{a\alpha} \right) + \gamma_{a\alpha} V_{a\alpha} \right) c_p \cos \theta
\]

\[
+ 2 \left[ \gamma_{a\alpha} - \gamma_{a\alpha} V_{a\alpha} + \gamma_{a\alpha} V_{a\alpha} \right] \cos \theta + 2 \left[ \gamma_{a\alpha} - \gamma_{a\alpha} V_{a\alpha} + \gamma_{a\alpha} V_{a\alpha} \right] \sin \theta
\]

\[
\sum_{\alpha=1}^{2} \left[ \gamma_{a\alpha} - \gamma_{a\alpha} V_{a\alpha} + \gamma_{a\alpha} V_{a\alpha} \right] \cos \theta \sin \theta
\]

All quantities are in dimensionless form. Here \( R_a(x,y,c_p,\theta) \) and \( S_a(x,y,c_p,\theta) \), \( \alpha=1,2 \) are the unknown projected distribution functions, \( (x,y) \) the two spatial independent variables and \( (c_p,\theta) \) the magnitude and the polar angle of the molecular velocity. The quantities \( \gamma_{a\alpha}, \gamma_{a\beta} \) and \( \nu_{a\alpha} \) are model parameters described in [6,7]. At the right hand side the dimensionless perturbed macroscopic quantities of number density \( \nu_{a\alpha} \), bulk velocity \( u_{a\alpha} \) and shear stress tensor \( \Pi_{a\alpha\beta} \) of each species are given by the moments of \( R_a \) and \( S_a \) according to

\[
\nu_{a\alpha} = \frac{1}{\pi} \int_0^{2\pi} \int_0^\infty c_p R_{a\alpha} e^{-c_p^2} dc_p d\theta
\]

\[
u_{a\alpha\beta} = \frac{1}{\pi} \int_0^{2\pi} \int_0^\infty c_p \sin \theta R_{a\alpha} e^{-c_p^2} dc_p d\theta
\]

Finally, the quantity \( \delta_{a\alpha} \) is the rarefaction parameter of each species defined as

\[
\delta_{a\alpha} = \frac{H_{a\alpha} \mu_{a\alpha}}{\nu_{a\alpha}} \quad \alpha=1,2
\]
where $H$ is the distance between the plates, $P_\alpha$ is the local pressure of each species, $v_{0\alpha} = \sqrt{2kT_0 / m_\alpha}$ is a characteristic velocity and $\mu_\alpha$ the viscosity at temperature $T_0$. For the purposes of the present work the reference rarefaction parameter is defined as

$$\delta_\alpha = \frac{H P_{0\alpha}}{v_{0\alpha} \mu_\alpha}$$

Next, the boundary conditions associated with the governing kinetic equations (4) and (5) are described. At the open boundaries of the computational domain defined in figure 1 by the letters A, B, F, G the gas is considered to be in local equilibrium and the distributions representing particles coming inside the computational field are described by their Maxwellian characterized by the local temperature $T_0$. The distributions representing particles departing from the computational field are unknown and part of the solution. At the wall boundaries of the computation domain defined in figure 1 by the letters C, D, E the Maxwell purely diffuse reflection interaction model is assumed satisfying the no penetration condition. Finally, along the symmetry axis $y = 0$ defined in figure 1 by the letter I the reflection is specular. Based on above the boundary condition are

- A, B: $R^+_\alpha = 1$, $S^+_\alpha = 0$  \hspace{1cm} (9.1)
- F, G: $R^-_\alpha = 0$, $S^-_\alpha = 0$  \hspace{1cm} (9.2)
- C, D, E: $R^+_\alpha = \nu_{\alpha,wall}$, $S^+_\alpha = 0$  \hspace{1cm} (9.3)
- I: $R^+_\alpha (x,0,c_p,\theta) = R^-_\alpha (x,0,c_p,-\theta)$  \hspace{1cm} (9.4)

where $\nu_{\alpha,wall}$, $\alpha = 1,2$ are parameters, which are defined by the impermeability condition. The superscript ($+)$ denotes distributions departing from the boundaries.

The main quantities of practical interest in the present work are the so called “kinetic coefficients” $\Lambda_{pp}$ and $\Lambda_{cp}$ [1,2]. The first one is related to the mass flow rate and it corresponds to the classical Poiseuille flow, while the second one is related to the diffusion flux and is known as barodiffusion. Both of them are caused by the pressure difference with $\Lambda_{pp}$ to be a direct effect, and $\Lambda_{cp}$ to be a cross effect. The two kinetic coefficients are computed by [7]:

$$\Lambda_{pp} = C_0 \langle u_{sz} \rangle (1 - C_0) \sqrt{m_1 / m_2} \langle u_{sz} \rangle \langle u_{sz} \rangle$$

$$\Lambda_{cp} = C_0 \left( \langle u_{sz} \rangle - \sqrt{m_1 / m_2} \langle u_{sz} \rangle \right)$$

where $\langle u_{sz} \rangle$ is obtained by integrating $u_{sz}$ at any cross section of the channel. The objective is to numerically solve equations (4) and (5) subject to boundary conditions (9) and compute the macroscopic quantities of practical interest given by equations (6).

### 3. Numerical scheme

The implement numerical scheme is based on the discrete velocity method and on a typical second order finite volume scheme. The continuum spectrum of molecular velocities is replaced by a discrete set of velocities which are defined by their magnitude $c_r$ and polar angle $\theta$. The discretized version of equations (4), (5) and (6) is solved in an iterative manner. The convergence is fast at small rarefaction parameters and then is gradually slows down as $\delta_\alpha$ is increased. The set of numerical parameters used in the results section is shown in Table 1.
Table 1. Numerical parameters used in the simulations.

| Parameters                                      | Values                                      |
|------------------------------------------------|---------------------------------------------|
| Nodes / unit length in dense areas (N_x = N_y) | 100 (L/H = 0); 50 (L/H = 1.5)               |
| Size of inlet and outlet region                 | 16 x 16                                     |
| Discrete angles θ in (0,2π)                    | 64                                          |
| Discrete magnitudes M                           | 16                                          |
| Max. Value of velocity magnitude (max c_p)     | 5                                           |
| Convergence criterion                           | 10^7                                        |

4. Results and discussion

Results are provided for one mixture, namely He-Ne, with a reference concentration of C_0 = 0.50, flowing between two parallel plates in a wide range of the rarefaction parameter 0 ≤ δ_1 ≤ 10. The ratio of the length L over the height H is taken to be equal to 0, 1 and 5. In all cases the hard sphere intermolecular potential model is applied.

In Table 2 the kinetic coefficients Λ_{pp} and Λ_{cp} are presented for L/H = 0. The corresponding results from [7] are also tabulated for comparison purposes. It is seen that for all values of δ_1 tested the agreement is very good. The observed small deviations between the present results and the ones in [7] may be contributed the different intermolecular model (in [7] the LJ potential is applied) and in the involved numerical parameters including the size of the computational domain before and after the slit.

In Table 3 the kinetic coefficients Λ_{pp} and Λ_{cp} are shown for the cases of L/H = 1 and L/H = 5. Observing the behavior of the two kinetic coefficients with regard to L/H and δ_1 the following remarks can be made. It is clearly seen that as L/H is increased both flow rates (Λ_{pp} and Λ_{cp}) are decreased. It is expected that as L/H is further increased the results will tend to the corresponding fully developed solution [2]. As δ_1 is increased it is seen that the behavior of Λ_{pp} is not monotonic for all lengths. In particular, it is seen that for L/H = 0 and 1 as δ_1 is increased Λ_{pp} is monotonically increased. However, for L/H = 5 the kinetic coefficient Λ_{pp} is initially decreased up to δ_1 = 0.4 and then as δ_1 is further increased Λ_{pp} is also increased. It is clearly seen that a Knudsen minimum is observed for a channel length which is relatively small compared to the corresponding single gas flow [8]. The coefficient Λ_{cp} related to barodiffusion in all cases, as expected, is reduced as δ_1 is increased. This type of flow is diminishing in the hydrodynamic regime.

Table 2. Kinetic coefficients for various δ_1 with L/H = 0 and comparison with [7].

| δ_1 | Λ_{pp} | Λ_{cp} | Λ_{pp} | Λ_{cp} |
|-----|--------|--------|--------|--------|
| 0   | 0.203  | 0.078  | 0.204  | 0.078  |
| 0.1 | 0.210  | 0.072  | 0.213  | 0.073  |
| 0.4 | 0.226  | 0.057  | 0.229  | 0.058  |
| 1   | 0.258  | 0.039  | 0.262  | 0.044  |
| 10  | 0.724  | 0.0040 | 0.680  | 0.011  |
In Figure 2 the $x$-component of the bulk velocity vector for each species at the center of the channel is shown versus the vertical distance between plates. The velocities of Ne produced by the code have been divided by the factor $\sqrt{m_{Ne}/m_{He}} = 2.24$ in order to be directly comparable with the ones of He. Results are provided for $\delta_1=0.1, 1, 10$ and $L/H = 1, 5$. In all cases the bulk velocity of the light species is higher than the velocity of the heavy one. The differences between the velocities of the two species are increased as $\delta_1$ is decreased, i.e. as the flow becomes more rarefied. This behavior of the two species creates the separation phenomenon which is also more dominant as the length of the channel is increased. Also, as the ratio $L/H$ is increased the magnitude of the velocity in all cases is decreased.

5. Concluding remarks
The flow of a binary gas mixture between two parallel plates of any length due to small pressure differences has been simulated based on the McCormack kinetic model. Results are provided for the binary gas mixture of He-Ne, with a reference concentration of 0.5 and three different channel lengths. A Knudsen minimum is observed at $L/H=5$. The presence of the separation phenomenon is confirmed by plotting the velocity profiles of each species.

The present work is considered as preliminary and it will be extended in the short future in order to investigate in a more complete and detailed manner the effect of the type of the mixture, its concentration and the length of the channel on the flow characteristics.

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Figure 2. Figure with axial velocity profiles for each species for $L/H = 1$ and 5 with $\delta_1 = 0.1$ (top), $\delta_1 = 1$ (middle) and $\delta_1 = 10$ (bottom).