DSMC Simulation of Binary Rarefied Gas Flows between Parallel Plates and Comparison to Other Methods

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Abstract. The direct simulation Monte-Carlo (DSMC) method has been developed to solve the Boltzmann equation for binary gas mixtures with hard-sphere molecules. The method is applied for pressure and concentration driven flows between two parallel plates. The flow in both cases is maintained by external force, of which expression is derived from the linearized description of the flow. Simulations have been performed in the low Mach number limit in order to test the method against the accurate solution of the linearzied Boltzmann equation (LBE) with hard-sphere molecules. Very good agreement is obtained between the two situations. The results provided by the present method have also been compared to the corresponding ones of the McCormack kinetic model. It is shown that the agreement between the results obtained from the DSMC method with hard-sphere molecules and the McCormack kinetic model is satisfactory. Hence, it is concluded that the McCormack kinetic model provides reliable results for isothermal flows in comparison to the linearized Boltzmann equation for hard-sphere gases.

Keywords: DSMC, binary gas mixtures, linearized Boltzmann equation, McCormack model, pressure and concentration driven flows
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INTRODUCTION

Over the last decades, rarefied gas flows have attracted much attention in the scientific community. The increasing interest is justified by the appearance of micro- and nano-fluidics besides conventional research fields, such as vacuum technology or high-altitude flows.

From theoretical viewpoint, rarefied gases can be described by extended hydrodynamics at small or moderate rarefactions. The lattice Boltzmann method has also been used for modeling gaseous flows in this domain [1]. However, for the whole range of the rarefaction, kinetic description is necessary. Much effort has been paid to solve the Boltzmann or model kinetic equations mainly in their linearized versions. The direct simulation Monte Carlo method [2] emerged as an alternative approach for modeling and calculating rarefied flows. In principle, the DSMC is a gas model; however, the results provided by the method converge to the solution of the Boltzmann equation [3]. The advantages of the DSMC are its relatively simplicity and applicability for arbitrary geometry. Various research groups have developed DSMC algorithms for general rarefied gas calculations [4, 5].

Single component gas flows have been extensively studied during previous years. Model kinetic equations have been solved for various flow configurations. On the contrary, there are relatively few works on gaseous mixtures.

In this paper, a DSMC method has been developed to calculate pressure and concentration driven binary rarefied gas flows between two parallel plates. The goal of the research is to examine the feasibility of the DSMC to solve the Boltzmann equation for the binary gas and to compare the McCormack kinetic model to hard-sphere gases. An advanced double sampling technique is used in the present DSMC approach. The results obtained from the DSMC methodology is compared to the solution of the linearized Boltzmann equation with binary hard-sphere molecules. On the other hand, a comparative study is carried out between the LBE results provided by the DSMC and the solution of the McCormack linearized kinetic model, which is extensively used in the past for the description of gaseous mixtures. In both cases, results are provided for the flow rates. In addition, representative velocity profiles obtained from the DSMC and the McCormack model are compared to each other.

STATEMENT OF THE PROBLEM

Pressure or concentration driven binary gas flow between two parallel plates is considered. The normal vector of the plates lies in the x coordinate direction, while the flow is in the y direction. The distance between the plates is denoted

by L. The gas mixture consists of the two components $\alpha = 1,2$. The interaction between the particles is assumed to be hard-sphere. The molecular masses, the diameters and the component particle densities are introduced by m_α, d_α and n_α, respectively. It is assumed that the first component is the lighter particle with smaller molecular diameter. The concentration of the first component is introduced by $C = n_\alpha/n$, where $n = n_1 + n_2$ is the total density of the mixture. The flow is driven by pressure or concentration gradients defined by

$$X_P = \frac{\partial P}{\partial y}\frac{L}{P}, \qquad X_C = \frac{\partial C}{\partial y}\frac{L}{C}, \tag{1}$$

where P is the pressure. The DSMC approach will be compared to linearized kinetic calculations; hence, the gradients are assumed to be small $X_P << 1$ and $X_C << 1$ for the comparison. However, it is emphasized that the present DSMC approach can be used beyond the linearized domain.

In the present problem, the primary focus is on the macroscopic velocity of the gas components $\boldsymbol{u}'_\alpha = [0, u'_\alpha, 0]$. For latter purposes, the dimensionless velocities for the pressure or concentration driven flow are introduced by

$$u_\alpha^{(i)} = -\frac{u'_\alpha}{v_0 X_i}, \tag{2}$$

where $v_0 = (2k_BT/m)^{1/2}$ is the characteristic velocity of the problem with k_B, T and $m = Cm_1 + (1-C)m_2$ being Boltzmann constant, the temperature and the average mass. In addition, $i = P,C$ depending whether the flow is driven by pressure or concentration gradient, respectively.

The dimensionless component flow rates are introduced by

$$G_\alpha^{(i)} = \sqrt{\frac{m_\alpha}{m}}\frac{2}{L}\int_0^L u_\alpha^{(i)} dx \tag{3}$$

for $i = P,C$.

EXTERNAL FORCING APPROACH

In the DSMC method, an innovative external forcing approach is used to model the pressure and concentration driven flows. In order to achieve this goal, the driving forces X_P and X_C need to be connected to the external acceleration exerted on the gas molecules. This can be done by using linearized kinetic description.

At the kinetic level, the description of the flow is carried out by the one-particle distribution function $f_\alpha(\boldsymbol{v}, \boldsymbol{r}, t)$ with $\boldsymbol{v} = [v_x, v_y, v_z]$, $\boldsymbol{r} = [x, y, z]$ and t denoting the molecular velocity, the spatial coordinate vector and the time variable. For the present problem, the z coordinate does not appear; hence, it is omitted from our discussion in the following for simplicity. The distribution function obeys the Boltzmann equation

$$\frac{\partial}{\partial t} f_\alpha + v_x \frac{\partial}{\partial x} f_\alpha + v_y \frac{\partial}{\partial y} f_\alpha + a_\alpha \frac{\partial}{\partial v_y} f_\alpha = Q_\alpha, \tag{4}$$

where Q_α denotes the collision operator encoding the molecular interactions between the particles and a_α is a possible external acceleration in the y direction. In the following, the acceleration is determined by employing linearization and matching the resulting terms to the pressure and concentration gradients.

Corresponding to the smallness of the driving terms X_P and X_C, the distribution function can be linearized by

$$f_\alpha(\boldsymbol{v}, x, y, t) = f_\alpha^0(\boldsymbol{v})\left[1 + h_\alpha(\boldsymbol{v}, x, t) + (X_P + \eta_\alpha X_C) y/L\right], \tag{5}$$

where $h_\alpha(\boldsymbol{v}, x, t)$ is the perturbation function and the η_α quantity is defined by $\eta_1 = 1$, $\eta_2 = -C/(1-C)$. In addition, the equilibrium distribution $f_\alpha^0(\boldsymbol{v})$ is given by

$$f_\alpha^0(\boldsymbol{v}) = n_\alpha \left(\frac{m_\alpha}{2\pi k_B T}\right)^{3/2} \exp\left(-\frac{m_\alpha v^2}{2k_B T}\right). \tag{6}$$

By substituting, the linearized form of the distribution function into the Boltzmann equation, Eq. (4), and manipulating the third and fourth terms on the left, the equivalence between the acceleration and the pressure and concentration

gradients can be obtained. The pressure or concentration driven flow is equivalent with the external force driven flow. For the pressure or concentration driven flow, the driving terms can be recovered by the accelerations

$$a_\alpha = -\frac{m}{m_\alpha}\frac{v_0^2}{2L}X_P, \quad a_\alpha = -\frac{m}{m_\alpha}\frac{v_0^2}{2L}\eta_\alpha X_C, \tag{7}$$

respectively. In this way, the external acceleration is determined in the method.

THE DSMC METHOD

The DSMC method is used for modeling the flow and calculating its properties. In the method, the considered geometry is divided into a collection of cells. Because of the symmetry of the problem, the motion of the gas molecules is simulated in one spatial dimension spanned by the coordinate x along the transverse of the channel. The x coordinate axis is divided into N_C number of cells. There is N_{Tot} total number of test particles initially uniformly distributed in the computational domain. The motion of the test particles is simulated by splitting between free motion and collision; the time step of the algorithm is denoted by Δt. The method is based on the No Time Counter scheme. The preselected particles for collision between the components α,β per cell is given by $N_{\alpha\beta} = N_\alpha \bar{n}_\beta \sigma_{T,\alpha\beta}(v_{r,\alpha\beta})_{max}\Delta t/2$, where N_α is the number of particles from component α in the cell, $\bar{n}_\beta$ is the average density of component β in the cell, $\sigma_{T,\alpha\beta}$ is the total cross section and $v_{r,\alpha\beta}$ is the absolute value of the relative velocity for components α and β. In the DSMC algorithm, an acceptance-rejection method is used for the final collision pair generation. From the $N_{\alpha\beta}$ preselected particle pairs, we accept pairs with probability $p = v_{r,\alpha\beta}/(v_{r,\alpha\beta})_{max}$. For hard-spheres, $\sigma_{T,\alpha\beta} = \pi d_{\alpha\beta}^2$ with $d_{\alpha\beta} = (d_\alpha + d_\beta)/2$. In the DSMC scheme, a double sample technique is used. The algorithm consists of the following five repeated steps: 1. free streaming, 2. acceleration, 3. sampling, 4. collision and 5. sampling. This approach is similar to the Strang-splitting [6]. However, in that case, the moving step is halfed and one sampling step is used.

Definition of the rarefaction degree

In the DSMC method, the actual value of the number of preselected collisions $N_{\alpha\beta}$ needs to be determined for the simulations. This can be achieved by the inclusion of the rarefaction degree in the model. The method uses two types of definition of the rarefaction degree depending on other approaches with which the results are compared. First, the method is compared to the linearized Boltzmann equation [7] then to the McCormack model [8].

In the expression of $N_{\alpha\beta}$, the collision cross section needs to be rewritten in units of the problem. In the following, the $\sigma_{T,11}$ collision cross section will be determined by the inclusion of the rarefaction degree for the LBE and McCormack cases. The remaining cross sections from $\sigma_{T,11}$ are obtained by $\sigma_{T,12} = \sigma_{T,21} = \sigma_{T,11}(d_{12}/d_{11})^2$ and $\sigma_{T,22} = \sigma_{T,11}(d_{22}/d_{11})^2$.

Simulation with regard to LBE

In this situation, the channel width L is given by

$$L = l\pi^{-1/2}\frac{1}{n(Cd_1 + (1-C)d_2)^2}, \tag{8}$$

where l is the dimensionless channel width used in the LBE approach [7]. As a result, the cross section of the the first component can be written by

$$\sigma_{T,11} = \pi d_1^2 = l\pi^{1/2}\frac{d_1^2}{nL(Cd_1 + (1-C)d_2)^2} \tag{9}$$

as a function of the *ratio* of d_2/d_1. Using this quantity, the actual value of $N_{\alpha\beta}$ can be determined.

TABLE 1. Flow rates obtained from DSMC and LBE for pressure driven flow.

		DSMC		LBE			
	l	$G_1^{(P)}$	$G_2^{(P)}$	$G_1^{(P)}$	$G_2^{(P)}$	$\Delta_1(\%)$	$\Delta_2(\%)$
Ne/Ar	0.1	3.968	3.350	3.971	3.346	-0.08	0.12
	1	2.802	3.499	2.805	3.503	-0.11	-0.11
	10	5.496	7.685	5.500	7.688	-0.08	-0.04
He/Xe	0.1	3.419	3.623	3.426	3.625	-0.20	-0.06
	1	1.310	4.189	1.311	4.187	-0.08	0.05
	10	1.799	9.927	1.801	9.939	-0.11	-0.12

TABLE 2. Flow rates obtained from DSMC and LBE for concentration driven flow.

		DSMC		LBE			
	l	$G_1^{(C)}$	$-G_2^{(C)}$	$G_1^{(C)}$	$-G_2^{(C)}$	$\Delta_1(\%)$	$\Delta_2(\%)$
Ne/Ar	0.1	2.813	1.142	2.815	1.146	-0.06	-0.32
	1	5.695E-1	2.393E-1	5.698E-1	2.395E-1	-0.06	-0.07
	10	6.402E-2	2.735E-2	6.405E-2	2.747E-2	-0.04	-0.44
He/Xe	0.1	3.097	1.170	3.100	1.171	-0.11	-0.09
	1	6.485E-1	2.607E-1	6.485E-1	2.605E-1	0.00	0.06
	10	7.463E-2	3.160E-2	7.412E-2	3.155E-2	0.70	0.16

Simulation with regard to McCormack

In the case of the McCormack model, the cross section of the first component is determined from the rarefaction parameter through the viscosity. The rarefaction parameter of the mixture is given by $\delta = PL/(\mu v_0)$, where $\mu = \mu(C)$ is the mixture viscosity. The viscosity depends on the concentration. The component viscosities are introduced by $\mu_1 = \mu(1)$ and $\mu_2 = \mu(0)$.

The hard-sphere viscosity of the first component [9] can be written by

$$\mu_1 = 1.016034 \frac{5}{16} \frac{\sqrt{\pi m_1 k_B T}}{\sigma_{T,11}}. \tag{10}$$

By using the rarefaction parameter, the characteristic velocity and the ideal gas law together with Eq. (10), the cross section of the first component is obtained by

$$\sigma_{T,11} = 1.016034 \frac{5}{16} (2\pi)^{1/2} \left(\frac{m_1}{m}\right)^{1/2} \frac{\delta}{nL} \frac{\mu}{\mu_1}. \tag{11}$$

It can be seen that this expression requires the *ratio* of the mixture viscosity to the viscosity of the first component. This ratio for hard-spheres can be obtained in a standard manner. Using this information, the actual value of $N_{\alpha\beta}$ can be determined.

RESULTS

First, simulations have been performed to compare the DSMC results to the LBE for binary hard-sphere gases. In the simulations, the flow rate has been computed and compared to the results available in Ref. [7]. The results are characterized by the dimensionless channel width given in Ref. [7]. It is mentioned that the $G_\alpha^{(i)}$ values are exactly the same in the DSMC and the LBE for the pressure driven flow. However, the flow rate in Ref. [7] must be multiplied with $(1-C)^{-1}$ to be compatible with the present DSMC for the concentration driven flow. The following channel width cases are investigated $l = [0.1, 1, 10]$. The concentration is $C = 0.4$ in all situations. Diffuse-specular boundary condition is assumed at the channel walls. The accommodation coefficients are $\gamma = [0.2, 0.4]$ for the first and the second components at the left wall, while $\gamma = [0.6, 0.8]$ for the first and second components at the right wall. The parameters in the simulations are given as follows: $N_C = 100$ for $l = [0.1, 1]$ and $N_C = 200$ for $l = 10$. The total number of particles

TABLE 3. Flow rates obtained from DSMC and McCormack for pressure driven flow.

		DSMC		McCormack			
	δ	$G_1^{(P)}$	$G_2^{(P)}$	$G_1^{(P)}$	$G_2^{(P)}$	$\Delta_1(\%)$	$\Delta_2(\%)$
Ne/Ar	0.1	1.981	1.932	2.039	2.058	-2.84	-6.12
	1	1.385	1.632	1.421	1.688	-2.53	-3.32
	10	2.271	3.151	2.315	3.210	-1.90	-1.84
He/Xe	0.1	2.097	2.013	2.065	2.232	1.55	-9.81
	1	1.117	1.956	1.114	2.025	0.27	-3.41
	10	8.584E-1	4.040	8.706E-1	4.111	-1.40	-1.73

TABLE 4. Flow rates flow obtained from DSMC and McCormack for concentration driven.

		DSMC		McCormack			
	δ	$G_1^{(C)}$	$-G_2^{(C)}$	$G_1^{(C)}$	$-G_2^{(C)}$	$\Delta_1(\%)$	$\Delta_2(\%)$
Ne/Ar	0.1	1.763	1.628	1.811	1.737	-2.65	-6.30
	1	7.106E-1	6.834E-1	7.220E-1	7.042E-1	-1.58	-2.95
	10	1.175E-1	1.198E-1	1.199E-1	1.219E-1	-2.00	-1.69
He/Xe	0.1	2.044	1.698	2.006	1.891	1.89	-10.20
	1	9.232E-1	8.432E-1	9.122E-1	8.702E-1	1.21	-3.10
	10	1.861E-1	1.919E-1	1.856E-1	1.878E-1	0.28	2.17

is $N_{Tot} = 10^5$ and the the time step is $\Delta t = 0.005L/v_0$ in all cases. Samples have been calculated over 5×10^7 time steps after the system has reached its steady state. The average velocity of the lighter particle between the plates is fixed at $\bar{u}_1' = 0.015v_0$.

In Tables 1-2, the flow rates are presented for both DSMC and LBE. The difference between $G_\alpha^{(i)}$ for the DSMC and LBE is defined by $\Delta_\alpha = (G_{\alpha,DSMC}^{(i)} - G_{\alpha,LBE}^{(i)})/G_{\alpha,LBE}^{(i)}$. In Table 1, the results for the pressure driven flow is presented. It can be seen that good agreement is obtained between the two approaches. The absolute discrepancy between the two situations is less than 0.20%. In Table 2, the flow rate for the concentration driven flow is presented. Again, good agreement is found between the DSMC simulations and LBE calculations. The absolute deviation between the two approaches is less than 0.70%.

Secondly, the flow rate provided by the DSMC simulation is compared to the results of McCormack given by Ref. [8]. Now, the results are characterized by the rarefaction parameter. It is noted that the rarefaction parameter is $\delta = l$, where l is the dimensionless channel width in Ref. [8]. Again, the values of $G_\alpha^{(i)}$ are exactly the same for the DSMC and McCormack considering the pressure driven flow. However, the flow rate must be multiplied with $(1-C)^{-1}$ in Ref. [8] for the concentration driven flow. The rarefaction parameters for the simulation cases are $\delta = [0.1, 1, 10]$. The concentration is $C = 0.5$, and the wall is fully diffuse in all situations, $\gamma = 1$. The parameters in the simulations are the same as in the LBE situation. However, the average velocity of the lighter particle is chosen as $\bar{u}_1' = 0.03v_0$.

In Tables 3-4, the flow rates are tabulated for DSMC and McCormack. The difference between the results of the two approaches is also introduced as $\Delta_\alpha = (G_{\alpha,DSMC}^{(i)} - G_{\alpha,McCormack}^{(i)})/G_{\alpha,McCormack}^{(i)}$. Table 3 presents the results of the pressure driven flow. It is clearly seen that the absolute difference between the DSMC, which actually solves the LBE for the hard-sphere gas, and the McCormack is less than 9.81%. In Table 4, the corresponding results for the concentration driven flow is presented. Here, the absolute deviation between the two approaches is less than 10.20%. The discrepancy for both flows is the largest in the rarefied region $\delta = 0.1$ as it is expected. From these data, it can be concluded that the agreement between the DSMC (LBE hard-sphere) and the McCormack is relatively good. This means that the McCormack can replace the binary hard-sphere system in actual calculations. Here, it is mentioned that the McCormack has recently been compared to flow rate measurements under isothermal conditions [10]. Very good agreement has been obtained between the two situations. These results indeed indicate the McCormack can be considered a good model for binary gases and provide satisfactory results for isothermal situations.

In Fig. 1, the velocity profiles for the McCormack simulations are presented for the case of $\delta = 1$ in order to demonstrate the results. It can be seen that the difference between the McCormack and the LBE results is relatively small. The agreement between the two approaches is considered very good.

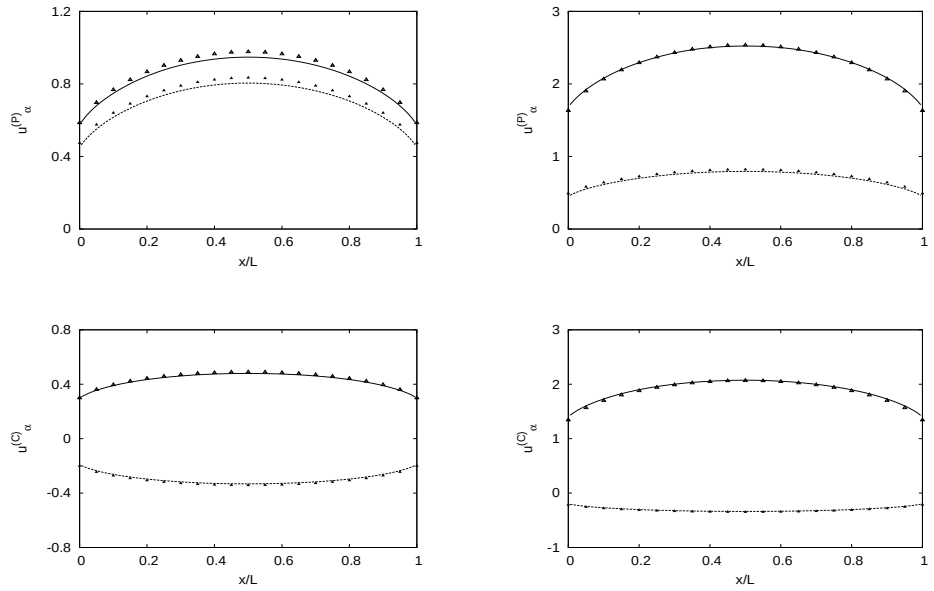

FIGURE 1. Velocity profiles obtained from the DSMC and McCormack approaches at $\delta = 1$. Pressure driven flow for Ne/Ar and He/Xe mixtures: top left and right. Concentration driven flow for Ne/Ar and He/Xe mixtures: bottom left and right. The solid and dashed lines stand for the results of the DSMC simulations for the first and second components, while $\triangle, \blacktriangle$ stand for the corresponding McCormack results.

CONCLUSION

In this paper, a DSMC method has been developed for modelling and calculating pressure and concentration driven binary rarefied gas flows between two parallel plates. The feasibility of the DSMC to solve the linearized Boltzmann equation for hard-sphere molecules is confirmed by benchmarking the DSMC results to the ones provided by the LBE for slow flows. It is concluded that the DSMC is a viable approach for solving the Boltzmann equation for binary hard-spheres. Furthermore, the DSMC results (LBE hard-sphere) are compared against the McCormack kinetic model. It has been found that the agreement between the two approaches is relatively good. This can be an important outcome for modeling binary rarefied gas flows. The present DSMC approach will be applied to other flow configurations in the near future.

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REFERENCES

1. L. Szalmas, *Physica A* **379**, 401–408 (2007).
2. G. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon Press, Oxford, 1994.
3. W. Wagner, *J. Stat. Phys.* **66**, 1011–1044 (1992).
4. S. Dietrich, and I. D. Boyd, *J. Comput. Phys.* **126**, 328–342 (1996).
5. G. A. Bird, *AIP Conf. Proc.* **762**, 541–546 (2005).
6. G. Strang, *SIAM J. Numer. Anal.* **5**, 506–517 (1968).
7. R. D. M. Garcia, and C. E. Siewert, *SIAM J. Appl. Math.* **67**, 1041–1063 (2007).
8. C. E. Siewert, and D. Valougeorgis, *Eur. J. Mech. B/Fluids*, **23**, 645–664 (2004).
9. C. L. Pekeris, and Z. Alterman, *Proc. Natl. Acad. Sci.* **43**, 998–1007, (1957).
10. L. Szalmas, J. Pitakarnnop, S. Geoffroy, S. Colin, and D. Valougeorgis, *Microfluid. Nanofluid.* DOI : 10.1007/s10404-010-0631-2 (2010).