DECOMPOSITION OF GASEOUS MIXTURE INTO BALLISTIC AND COLLISION PART: MATHEMATICAL FORMULATION AND APPLICATION WITH DSMC METHOD

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KEY WORDS

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ABSTRACT

In this work, the method of decomposition of a gaseous flow refers to the process of investigating the flow by separating the gas particles into two groups, namely the "ballistic" one, composed of particles that have arrived at a defined space having performed free movement, with their last collision to be with a boundary wall and the "collision" one, for the particles group that arrived at the same space having previously experienced at least one intermolecular collision. The mathematical formulation of the decomposition method for gas mixtures is presented. Next, the method is incorporated into the Direct Simulation Monte Carlo method and used to model and simulate the flow and the process of gas mixing of two gases inside a simple two-dimensional configuration of a micro-mixer.

INTRODUCTION

In general, a kinetic solution at some point in a flow domain consists of two parts, namely the ballistic and the collision parts. The former one is due to particles arriving at this point from the boundaries with no collisions, while the latter one is due to particles arriving at this point after an arbitrary number of collisions (at least one). From the Boltzmann equation, the dimensionless velocity distribution function $g = g(x, y, \zeta)$ at a local point (x, y) is decomposed as $g(x, y, \zeta) = g^{(b)}(x, y, \zeta) + g^{(c)}(x, y, \zeta)$, where $g^{(b)}$ and $g^{(c)}$ denote the ballistic and collision parts of the distribution function respectively. It is noted that particles contributing to the ballistic part of the solution at point (x, y) may collide other particles in their movement after that point. This novel approach of modeling a gas flow was conceptualized and presented by the group of Vargas, Tatsios, Valougeorgis and Stefanov in order to investigate a thermally induced rarefied single gas flow in a rectangular enclosure with non-isothermal walls [1]. The same year, the same approach was used to predict the Knudsen minimum and provide a quantitative measurement that verified the previously reported qualitative physical arguments of the Knudsen "paradox" [2]. The readers are referred for a detailed reasoning and the derivation of the equations for the decomposition of a single gas flow in [2,3]. Here, following from the latter works the solution is extended to cover the more general case of gas mixtures. In

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the following sections, the mathematical formulation of the decomposition method for gas mixtures is presented, focusing on the derivation of the macroscopic density, velocity and temperature. Furthermore, the decomposition is implemented in the DSMC method and it is employed to analyze the flow properties of two gases during the mixing process inside a micro-mixer.

MATHEMATICAL FORMULATION

For the general case of gas mixtures, the following variables are defined: the macroscopic density is equal to the sum of the individual species densities

$$\rho = \sum_{p=1}^{Nsp} (m_p n_p) = n\overline{m} \, , \tag{1}$$

where Nsp is the total number of species, m_p and n_p the species mass and number density respectively and n the mixture's number density. The mass average velocity is defined by

$$c_0 = \frac{1}{\rho} \sum_{p=1}^{Nsp} \left(m_p n_p \overline{c_p} \right) = \overline{mc} / \overline{m} \tag{2}$$

The peculiar or thermal velocity c' of each molecule is measured relative to c_0, that is $c' = c - c_0$, and the mean thermal velocity of species p is

$$\overline{c'_p} = \overline{c_p} - c_0 \tag{3}$$

This quantity is called the diffusion velocity and is denoted by C_p. The species translational temperature is calculated as follows

$$\frac{3}{2} k_B T_{tr,p} = \frac{1}{2} m_p \overline{c''^2_p} + \frac{1}{2} m_p C_p^2 \text{ or } T_{tr,p} = \frac{m_p}{3k_B} \left(\overline{c''^2_p} + C_p^2 \right) \tag{4}$$

where k_B is the Boltzmann's constant and c''_p is the single species thermal velocity measured relative to the average velocity $\overline{c_p}$ of the species, that is $c''_p = c_p - \overline{c_p}$ [4]. The total translational temperature is given by

$$T_{tr} = \sum_{p=1}^{Nsp} \frac{n_p}{n} T_{tr,p} \tag{5}$$

The number density the velocity and the temperature of species p are decomposed according to

$$n_p = n_p^{(b)} + n_p^{(c)} \, , \tag{6}$$

$$u_{\alpha,p} = u_{\alpha,p}^{(b)} + u_{\alpha,p}^{(c)}, \tag{7}$$

$$T_{tr,\alpha,p} = T_{tr,\alpha,p}^{(b)} + T_{tr,\alpha,p}^{(c)}, \tag{8}$$

where the superscripts (b) and (c) denote the ballistic and collision parts respectively and $\alpha = x, y, z$ for the three spatial dimensions. Note that $T_{tr,p} = T_{tr,x,p} + T_{tr,y,p} + T_{tr,z,p}$.

DIRECT SIMULATION MONTE CARLO IMPLEMENTATION

The prescribed decomposition of the particle distribution in a given cell of the computational grid with center point (x, y) can be implemented in the basic DSMC algorithm by making some additions in the indexing stage. More specifically, all model particles $j = 1, \ldots, N_T$ taking place in the simulation are tagged by introducing the indicator I_j, which has the value of 0 or 1 indicating if a particle contributes to the ballistic or the collision part of the distribution respectively. A particle passes into the ballistic part when it is

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reflected from a wall and goes into the collision part when interacts with another particle. The indicator is set to 0 each time that a particle is reflected from the bounding walls, while in the stage of particle free motion the indicators are not changed. In the stage of binary collisions the indicators (I_j, I_i) of any pair of particles (j,i) involved in a collision are set to 1. During the simulation process the particle indicators may change their values all the time. In the sampling stage of the macroscopic properties at given time t_k all particles with indicators $I_j = 0$, are considered belonging to the ballistic part of the particle distribution and all particles with indicators $I_j = 1$ to the collision part. As a result, the total number of all particles accumulated in a cell is divided into two groups $N_T = N^{(b)} + N^{(c)}$ and the macroscopic quantities are sampled into the two corresponding parts. From equations (7), (8) and (9) the corresponding number densities, velocities and translational temperatures per species are formed as

$$n_p^{(b)} = \frac{N_p^{(b)}}{SV_c}, \; n_p^{(c)} = \frac{N_p^{(c)}}{SV_c} \tag{9}$$

$$u_{\alpha,p}^{(b)} = \frac{1}{N_T}\sum_{k=1}^{S}\sum_{i=1}^{N(t_k)}\left[1-I_i(t_k)\right]\zeta_{\alpha,i}(t_k), \; u_{\alpha,p}^{(c)} = \frac{1}{N_T}\sum_{k=1}^{S}\sum_{i=1}^{N(t_k)}I_i(t_k)\zeta_{\alpha,i}(t_k) \tag{10}$$

and

$$T_{p\alpha}^{(b)} = \frac{1}{N_{Tp}}\sum_{k=1}^{S}\sum_{i=1}^{N(t_k)}\left[1-I_{pi}(t_k)\right]\left[\left(\zeta_{p\alpha,i}-u_{p\alpha}\right)^2+\left(u_{p\alpha}-c_{0\alpha}\right)^2\right],$$

$$T_{p\alpha}^{(c)} = \frac{1}{N_{Tp}}\sum_{k=1}^{S}\sum_{i=1}^{N(t_k)}I_{pi}(t_k)\left[\left(\zeta_{p\alpha,i}-u_{p\alpha}\right)^2+\left(u_{p\alpha}-c_{0\alpha}\right)^2\right] \tag{11}$$

where S is the total number of samples, V_c is the volume of the current cell, $N(t_k)$ is the total number of particles inside the cell at time t_k and $\zeta_{p\alpha,i}$ and $u_{p\alpha}$ are the molecular velocity and the averaged molecular velocity of species p respectively. The terms $\left(\zeta_{p\alpha,i}-u_{p\alpha}\right)^2$ and $\left(u_{p\alpha}-c_{0\alpha}\right)^2$ correspond to the squared single species thermal velocity and to the squared diffusion velocity respectively, as shown in Eq.(5).

TEST CASE: Application of the decomposition method to a gas micro-mixer

The decomposition method was implemented as described above in an in-house developed DSMC code. The test case is based on one of our previous published work [5] and refers to a simple 2-dimensional configuration composed by two parallel plates of length L, positioned in $y=0$ and $y=H$ respectively. A splitter plate with length equal to $L/4$ is positioned at $y=H/2$ and in parallel with the other two, forming in that way two inlets. Two pure gases enter the domain from the upper and lower inlet respectively and they start mixing after the end of the splitter plate and the area defined at $L/4 < x \le L$ is considered as the main mixing zone. The flow is induced by a pressure difference. A fixed pressure is applied equally at both inlets at $x=0$, while at $x=L$ vacuum condition is set in order to prevent backflow. In [5] the value relative density difference $\xi_{p,j}$ is defined per species p at a column of cells j, and it provides a homogeneity index, in the ideal case where $\xi_{p,j} \to 0$ the species p at column j is considered perfectly homogeneous. In this work $\xi_{p,j}^{(b)}$ and $\xi_{p,j}^{(c)}$ are calculated as well, corresponding to the relative density differences of the fraction of particles p that belong to ballistic and collision part respectively. A simple test to validate the implementation of decomposition is to investigate the two extreme cases in terms of inlet pressure. For very small inlet pressures, where $Kn \gg 1$ it is expected that the evolution of $\xi_{p,j}$ across the length of the mixer

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will coincide to $\xi_{p,j}^{(b)}$ since the majority of the particles will perform ballistic movement. In contrast, for large inlet pressures, where $Kn < 0.001$, the evolution of $\xi_{p,j}$ across the length of the mixer will coincide to $\xi_{p,j}^{(c)}$ since the majority of the particles will perform collisional movement. The evolutions of relative density differences for two cases corresponding to inlet pressures $P_{in} = 1 \times 10^{-3}$ atm and $P_{in} = 2$ atm are depicted in Fig. 1(a) and (b) respectively. The working gases are CO entering from the upper inlet and N_2 entering from the lower inlet. The relative density differences[5] "rdd 1", "rdd 2", "rddfm 1", "rddfm 2", "rddc 1" and "rddc 2" correspond to $\xi_{CO,j}$, $\xi_{N_2,j}$, $\xi_{CO,j}^{(b)}$, $\xi_{N_2,j}^{(b)}$, $\xi_{CO,j}^{(c)}$ and $\xi_{N_2,j}^{(c)}$ respectively. In both cases the expected outcome is retrieved. It is worth noting the collision part of $\xi_{CO,j}^{(c)}$, $\xi_{N_2,j}^{(c)}$ in (a) and the ballistic part of $\xi_{CO,j}^{(b)}$, $\xi_{N_2,j}^{(b)}$ in (b), are both evolving separately and do not coincide with the rest. This behavior is expected, since in DSMC there is a probability that a very small number of particles will perform intermolecular collisions in a highly rarefied flow (a) and similarly a number of particles will perform ballistic movement, most probably only at the cells adjacent to the wall boundaries, in near continuum flow (b). However, since in both cases this number is very small, their contribution to the mixture's macroscopic flow values is equivalently very small. For demonstration purposes, in Fig. 3(a), (b) and (c) are presented the dimensionless contours of mixture's density, collision density and ballistic density corresponding to case for $P_{in} = 2$ atm.
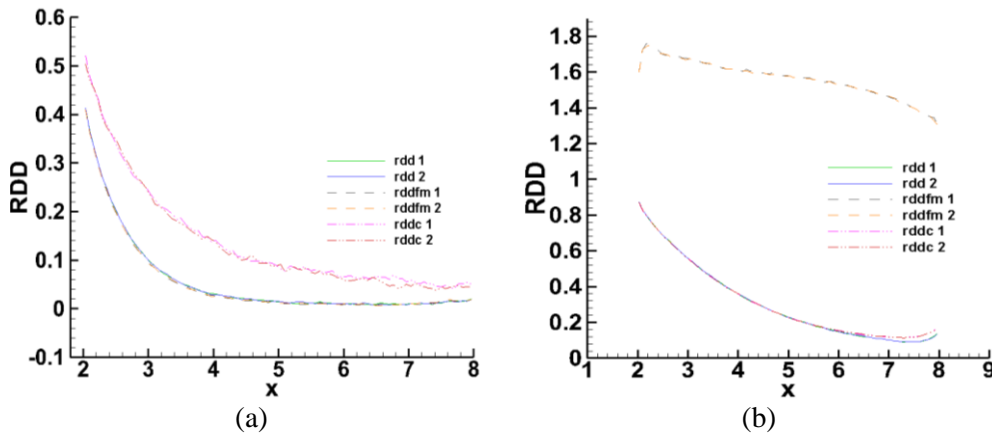

Figure 1. Relative density difference evolutions over the main mixing zone for the cases: (a) inlet pressure equal to 0.001 atm and (b) inlet pressure equal to 2 atm.

CONCLUSION

The decomposition method has been applied to gaseous mixtures. The derivation of the mathematical formulas of ballistic and collision parts as well as the extraction of macroscopic values have been presented. A test case of mixing two gases in a simple micro-mixer is presented in order to validate the implementation in a DSMC code and illustrate the analysis of a mixture problem. The decomposition of the flow at a micro scale into ballistic and collision part could be interpreted as a result of transport process due to diffusion and advection respectively in macro-physics and -engineering. For the case of a slip flow regime, the final result is provided by simple addition of ballistic and collision part in micro-scale corresponding to a convection in macro-scale which is the combination of advective and diffusive transport.
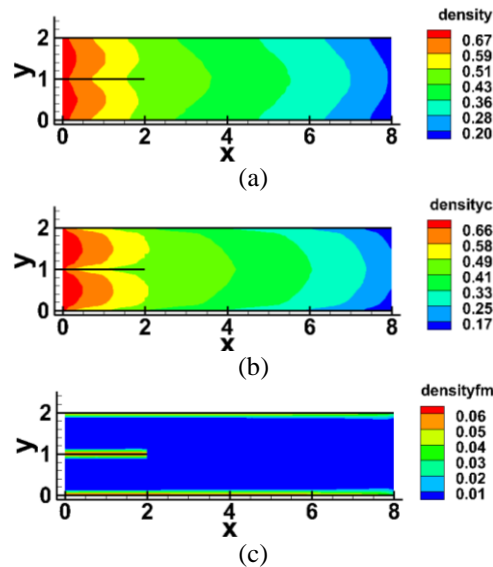
(a)

(b)

(c)

Figure 2. Density contours of (a) mixture's total, (b) collision part and (c) ballistic part for the case with inlet pressure equal to 2 atm.

Acknowledgementsa

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