Mixing Length in a Micro Channel

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Abstract. Having a very good mixture is a problem in MEMS devices because of their miniaturized dimensions for which the flows are always laminar. The gas flows in micro-channels are rarefied and characterized by Knudsen numbers in the range of transition flows. In the present paper, Direct Simulation of Monte Carlo method is used to analyze some factors affecting the gas mixture within a micro-channel with a splitter plate. Our purpose is to numerically simulate the flow of a gas mixture in a micro channel, in order to analyse the evolution of the mixing length in several configurations.

Key words: rarefied gases, direct simulation of Monte Carlo (DSMC), mixing length
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INTRODUCTION

The study of gas or liquid flows in micro systems is developing extremely rapidly because of their many applications in various fields. Today, these devices are used in industrial manufacturing processes (micro filters…), medical tools (micro pumps…) and in measuring instruments (micro sensors…). Because of their small size, they can be produced in very great number and thus having a low cost of manufacture. In addition, their miniaturized size enables them to respond quickly to excitations, enabling the fabrication of actuators [1].

Gas mixing is a basic problem for the design of propulsion devices in Power-MEMS and in a variety of these devices, the inside mixing process determines the efficiency of the whole system [2,3]. For these reasons, the study of the gas mixing and the identification of the factors allowing to decrease the mixing length in a micro channel, has been intensely studied [2,3,4]. In micro channels, the continuum assumption is not valid any more because the Knudsen number is not very small. Therefore these flows are usually analyzed with kinetic methods like, for instance the Direct Simulation Monte Carlo method (DSMC).

Yan and Farouk [4] simulate gas mixing in micro channels using the DSMC method. They investigated the mixing of the H_2 and O_2 parallel gas streams driven by inlet-outlet pressure differences, which were separated by a splitter plate in a micro channel. In their work, the gases are considered to be mixed when the mass density contours are symmetric with respect to the centerline of the channel. They showed that the mixing length increases with the increasing of the inlet-outlet pressure difference. Otherwise, the mixing process was very sensitive to the wall boundary condition. It is showed that the mixing length is shorter in the case with fully diffuse reflection than in the case with the specular reflection [2,3,4]. Wang and Li [2], simulated the mixing process of CO and N_2 in the same type of micro channel than in paper [4]. In their study, the gases are considered to be mixed when the gas mixture density near the upper and lower walls are equal. In their work, it was emphasized that the main flow velocity and the temperature are the most important factors affecting on the gas mixing performance. Le and Hassan [3], studied the gas mixing, taking the same gases CO and N_2 but in a T-shape micro mixer with the inlet-outlet pressure boundary condition when the flow is driven in the channel by the pressure gradient. They showed that increasing Knudsen number decreases the mixing length and enhanced the mixing process.

In our paper, the mixing of two parallel gas streams of CO and N_2 with the same inlet boundary conditions (for the velocity, the pressure and the temperature) is analyzed from DSMC simulations, in the same channel as in [4] with additional bumps (see figure 1). Our purpose is to obtain the numerical references which could be compared with the analytical results in the slightly rarefied regime based on the Navier-Stokes equations with slip. The influence on the mixing length of some parameters related to the bumps and the inlet velocity is studied.

NUMERICAL METHODS

DSMC method

DSMC is a statistical method consisting of numerical experiments which simulate a limited number of test molecules while each of them is representative of a large number of real molecules. During each time step, the code carries out two uncoupled stages: one of displacement and one of collision. This decoupling requires that the time step is smaller than the average time of the flight of the molecules. During the first step, the molecules undergo a displacement without any collision; the molecules which leave the field of calculation are eliminated and the collisions with the walls are treated. For the interaction of the molecules with the walls, the model of diffuse reflection with perfect accommodation is used. In the second step, the collisions between molecules are treating in a probabilistic way (method NTC [5]). The flow field is subdivided in several cells whose characteristic dimension is smaller or equal to the mean free path of the molecules and where are evaluated the macroscopic quantities. The mean free path depends on the characteristics of the mixture; in this study it is approximately $4\ 10^{-2}$ μm. Consequently the number of Knudsen built with the height of the micro channel (1 μm) is equal to 0.04.

There are various models of potentials of collision but most usually used in simulations DSMC, are VHS (Variable Hardware Sphere) and VSS (Variable Software Sphere) models [6], based on the model "Inverse Power Law"(IPL). In these models the cross section of collision depends only on the relative velocity of the two colliding molecules. Moreover, they allow to obtain models which lead to a realistic viscosity power law and to a simple calculation of the collisions [7]. To study a mixture, it is preferable to use VSS model [6].

In this paper, to compute numerical simulations, we have used the DS2V code developed by G. Bird [5]. This program is based on the DSMC method which allows to simulate the solution of the Boltzmann equation and to obtain a reference solution for the transition regime.

Position of the problem

We consider two gases, Nitrogen (N_2) and Carbon Monoxide (CO) which are separated at the upstream by a splitter plate in a micro channel of height 1 μm and of length 10 μm. The Carbon Monoxide is on the upper side of the plate. The length of the micro channel is considered long enough for mixing the gases and the plate is placed in a symmetrical way in the middle of the micro channel. The thickness of the plate is 0.1 μm and its length is 3 μm. At the channel entrance, the volume rates of each gas are equal, and they flow through the micro channel under the effect of a pressure gradient set between the inlet and the outlet (Fig. 1). The initial boundary conditions for the two gases at the inlet are identical, with a velocity equal to 300 m/s and a pressure equal to $5\ 10^4$ Pa. The problem is isothermal and the constant temperature is 300 K. We set diffuse reflection on the channel walls. At the outlet of the micro channel we set a vacuum boundary condition to have the lower outlet pressure to prevent a backflow. This allow to speed up the mixing process and thus to enhance its performance.

The first calculation has been done in the micro channel without the bumps. As it will be shown in the next section, the results are qualitatively comparable to Wang and Li results [2], but not quantitatively because of some geometry differences. In our study, the goal is to improve the mixing. For this purpose, we add two symmetrical bumps (Fig. 1) at the top and at the bottom of the micro channel to compare the results with the first calculation without the bumps. The bumps are placed after the end of the splitter plate at x_p = - 1.7 μm and b, the height of the bumps, is equal to 0.2 μm (orthonormal axes are shown In Fig.1). In all the simulations the bump width c is equal to 0.1 μm which is almost three times larger than the mean free path. The gases start to mix after the plate and they are completely mixed after the length *l*, which we call the mixing length. We consider the mixture as a perfect gas.

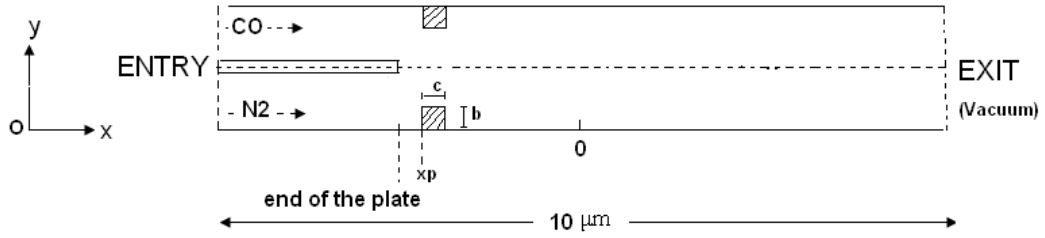

FIGURE 1. Scheme of the studied geometry

As in [3], we use a quantitative determination of the mixing length. We introduce the mixing parameter ζ :

$$\varsigma = 1 - \frac{\rho_{diluter}}{\rho_{denser}} \qquad (1)$$

where ρ is defined as the density of CO which is calculated in each section near the upper and the lower channel walls. In each section the larger CO density value is denoted by ρ_{denser} and the smaller value by $\rho_{diluter}$. Along the channel, ζ should change asymptotically from 1 to 0. In order to take into account the statistical errors of DSMC simulations, we shall say that the gases are fully mixed when $\zeta \leq 2\%$,.

RESULTS AND DISCUSSION

In Fig. 2, we show the evolution of the mixing parameter ζ along the channel from the simulation results for two cases: With and without the bumps. The splitter plate ends at x_p = - 1.7 μm . The mixing point, that is the abscissa x where the gases are fully mixed, in the DSMC simulation result, after smoothing the curves, is shown in the figure. As expected, the change in ζ along the channel was asymptotically from 1 to 0. In the case without the bumps, the mixing length is about 1.8 μm and the main flow velocity leaving the splitter plate is about 70 m.s^{-1}; these results are qualitatively comparable with the results of Wang and Li [2], but not quantitatively because of some geometry differences.

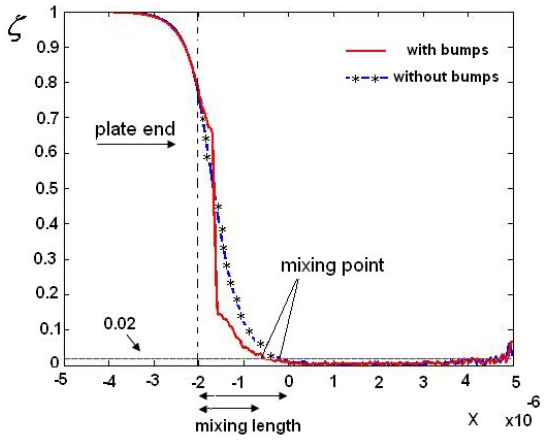

FIGURE 2. Evolution of the mixing parameter ζ along the channel

Moreover we observed two discontinuities at the places of the bumps because they disturb the flow by decreasing the channel width and by changing the points at the top and at the bottom of the channel where the values of ζ are calculated. As it is shown in the figure 2, the bumps allow to decreases the mixing length. In this case, the mixing length is decreased to 1.5 μm.

The figure 3 shows the flow stream lines along the micro channel in the gas mixture velocity field. We observe the flow at the right angles beside the bumps is almost at rest. Because of the pressure drop, the gas mixture velocity increases along the channel. First we observe that the fluid velocity is increased by the bumps. After the bumps, the velocity decreases and increases again because of the vacuum boundary conditions.

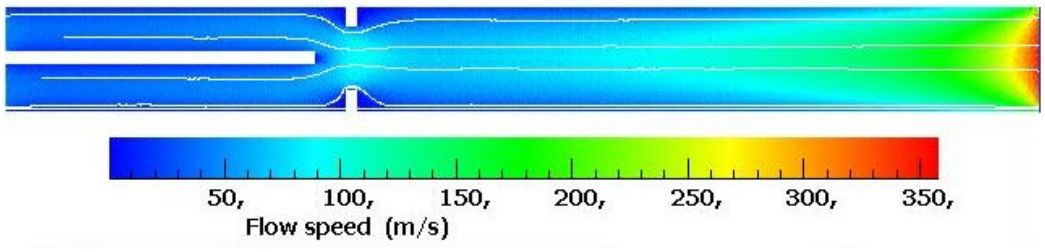

FIGURE 3. Velocity field and stream lines along the micro channel.

In the following, in order to improve the mixing process and to decrease the mixing length, we change the bump height and the gas inlet initial velocities separately.

Bump height variation

In order to study the effects of the bump height, b increases from 0 (without bumps) to 0.3 µm while the position of the bumps is fixed at x_p = - 1.7 µm . In Fig. 4, we show the evolution of the mixing length regarding to the bump height. The length and the thickness of splitter plate are fixed at 3 µm and 0.1 µm.

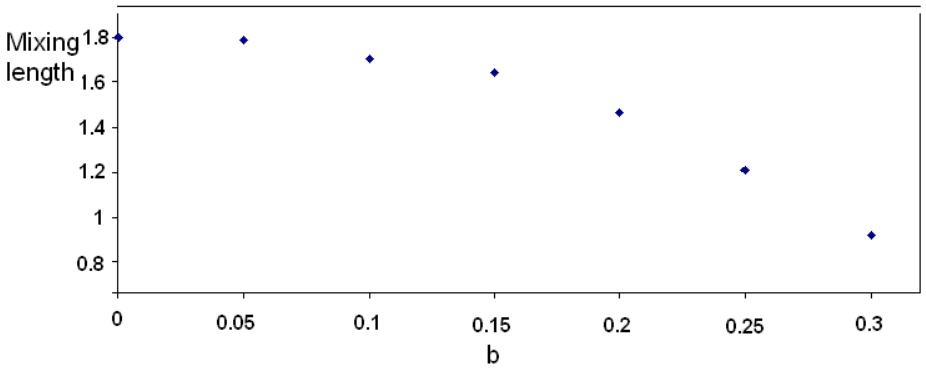

FIGURE 4. Mixing length evolution along the channel (x in µm) regarding to the bump height (b in µm)

The increasing of the bump height decreases the mixing length. As the figure 4 shows, between the two cases respectively without the bumps and with the bump height equal to 0.3 µm, there is about 0.92 µm for the mixing length difference; that is that the mixing length is reduced by 51 %.

Inlet velocity variation

To study the effects of initial boundary conditions on the mixing process, the initial inlet velocities are increased from 200 m.s^{-1} to 400 m.s^{-1}. As in the previous calculations, the two gases have the same initial inlet velocity. The bump height is equal to 0.3 µm. The results are shown in Fig. 5. As this figure indicates, the mixing length increases linearly when the inlet velocity increases while the other calculation parameters are fixed (of course in the considered parameter domain). These calculations show that the inlet velocity is one of the most important factors affecting the micro gas mixing. The mixing length is reduced by 71% when the initial inlet velocity is decreased from 400 m.s^{-1} to 200 m.s^{-1}.

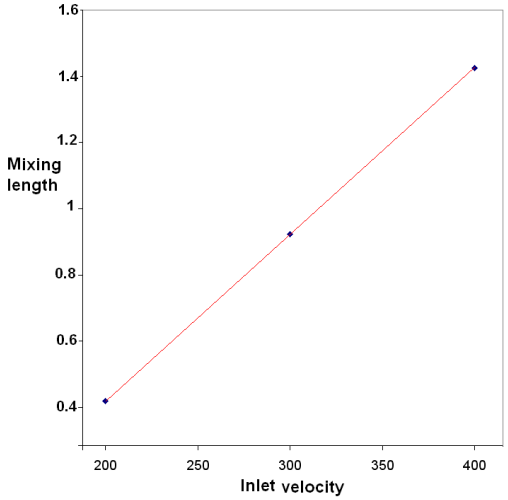

FIGURE 5. Mixing length evolution along the channel (x in µm) compared to the entering velocity (in m.s^{-1})

Bump effect on the gas mixture pressure

In this part, the bump effect on the gas mixture pressure is studied. Fig. 6 shows the pressure comparison between the result obtained by the DSMC simulation and an analytical calculation along the channel. To obtain the analytical curve, the theoretical continuum approach based on the compressible Navier-Stokes equations with first order slip boundary condition, is taken [8,9,10]. This approach gives the pressure along the micro channel with the length L in function of ξ which is the X-coordinate measured from the entry of the channel.

As in [9], by considering the diffuse reflection boundary condition for the channel walls, in dimensioned form, we obtain:

$$\gamma_1 p^2 + p = \gamma_2 \xi + \gamma_3 \qquad (2)$$

with:

$$\gamma_1 = 1/(12 Kn_o p_o)$$
$$\gamma_2 = \left[p_o^2 - p_i^2 + 12 Kn_o (p_o^2 - p_o p_i)\right]/(12 Kn_o p_o L)$$
$$\gamma_3 = (p_i^2 + 12 Kn_o p_o p_i)/(12 Kn_o p_o)$$

where Kn_o and p_o are the Knudsen number and the pressure at the exit of the channel and p_i is the pressure at the entry. To plot the theoretical curves, we consider the channel in two parts: The first part starts at the entry and finishes at the end of the splitter plate (-5 to -2 μm) and the second part starts from the bumps place and ends at the exit of the micro channel (-1.7 to 5 μm). In these two areas, the numerical simulations show that the pressure depends weakly on the transversal coordinate. The comparison between the theoretical and numerical results are made for a value of the transversal coordinate equal to 1.718 10^{-2} μm and measured from the axis of the channel. The calculated value for Kn_o at the outlet of the first channel part is 0.13 and at the outlet of the second channel part is 0.375. We apply the relation (2) for the two parts of the channel separately. In the first part p_o = 90 kPa and p_i = 143 kPa and in the second part p_o = 10 kPa and p_i = 77 kPa. The results are shown in Fig. 6. We have not plotted the part between the end of the plate and the bumps because (2) is suitable in the case of a channel without the plate or the bumps: In this area the flow is so disturbed that it is not possible to compare it to the theory. In the second part of the channel, the DSMC results and the theoretical results are in a better agreement than in the first part; it can be justified by the usual DSMC errors at the entry although the first points obtained by DSMC at the entry are not taken into account.

In Fig. 6, the pressure profile slope changes between the two channel parts. This is explained by the change of the channel height between the two parts (from 0.45 to 1μm because of the splitter plate) and by the change of the "outlet" pressure (from 90 kPa to 10 kPa) and Knudsen number (from 0.130 to 0.375). This change causes a greater line pressure drop in the first part of the channel.

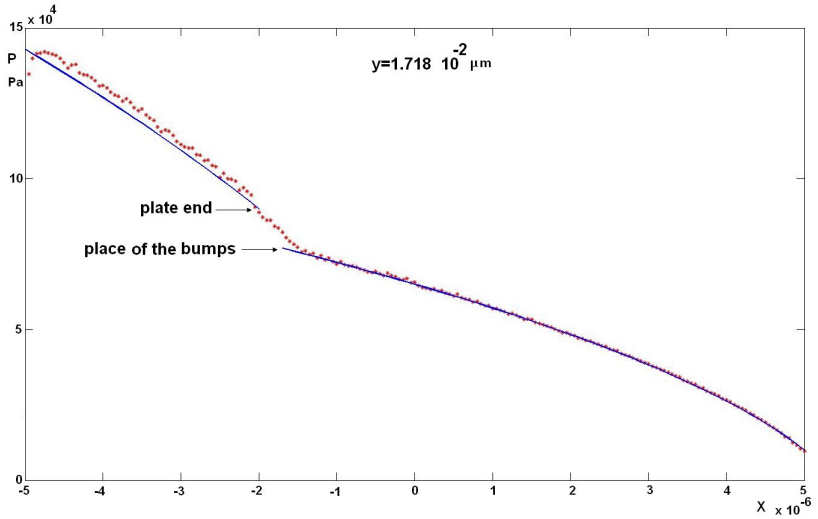

FIGURE 6. Pressure comparison between the results obtained from DSMC simulations (points) and analytical calculations (continuous lines) along the channel at y = 1.718 10^{-2} μm

CONCLUSION

The mixing behavior of two parallel gas streams of CO and N_2 entering in a micro channel with two bumps has been investigated using the DSMC method. The aim of this contribution was to improve the mixing process in terms of some parameters including the geometry and the flow conditions. The two gases are assumed to be mixed when the dimensionless mixing parameter ζ is lower than two percent.

Three factors were introduced to obtain more rapidly a good mixture in a micro channel. First, the results show that the introduction of bumps decreases the mixing length. Second, when the bump height is increased, the mixing performance is enhanced by decreasing more efficiently the mixing length. Finally, the inlet velocity appears as an important factor affecting the mixing process: When the gas inlet velocity decreases, the mixing point is obtained more quickly. Additionally, the pressure profiles in the two parts of the channel have been compared to theoretical results from a Navier-Stokes model with first order slip boundary conditions. The results are in very good agreement, in the second part of the channel after the bumps.

Obviously, these results are suitable in the frame of the numerical experiences which had been done. More numerical calculations and theoretical developments are required to extend these results to more general geometries. Otherwise, other calculations are still in progress in order to study the influence of other parameters like the bump place for instance.

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