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Effect of Obstacles Location and Flow Injection on the Mixing of Two-Gaseous Flow in a Microchannel

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ABSTRACT: In the present study, the direct simulation Monte Carlo method is utilized to investigate the effect of obstacles number, location, and also flow injection on the mixing in a channel with 16 µm length and 1 µm height. A mixing length is defined which is the length at which two species are mixed completely. Eight cases with different blockage ratios are considered to study the obstacle effect on the mixing. The blockage ratio shows the reduced flow cross-section due to the addition of obstacles. In All cases, CO2 and N2 gases enter the domain and are separated by a splitter plate that extends up to 1/3 of the channel. The blockage ratio increasing decreases mixing length up to 10%. Whereas the mass flow rate decreased significantly. Flow injection into the channel is also studied. Four cases are considered: the first case is a simple channel without injection, the second case has cross injection, the third case has inverse injection, and flow is injected vertically through an obstacle in the fourth case. Mixing length is increased by 17% and 5% for cases 2 and 3, respectively. In case 4, the mixing length is decreased 2% due to the obstacle.

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1- Introduction

Progresses in the fabrication of Micro-Electro-Mechanical-Systems and their superiority to their macro-counterparts, led to more utilization of such devices, especially in mixing applications [1]. The mixing process is slow in micro scale and is mostly due to the diffusion of particles. Gaseous micromixing is almost a non-touching area and is a field of interest. Yan and Farouk [2] investigated the mixing of Oxygen and Hydrogen in a channel. They showed that mixing length is increased by increasing of channel inlet-outlet pressure difference. Wang and Li [3] investigated the mixing of Nitrogen and Carbon-monoxide in a microchannel. Their results show that mixing length is proportional to gas temperature and inverse of the Knudsen number. Le and Hassan [4] simulate the mixing of the two above-mentioned gases in a T-shape micromixer and concluded that higher Knudsen number regimes have smaller mixing lengths. Darbandi and Lekzian [5] also showed that the mixing of Nitrogen and Carbon-monoxide in a straight microchannel is enhanced when inlet pressure ratios are increased. Huang et al. [6] investigated the micromixing of Nitrogen and Oxygen experimentally. They observed that mixing length is increased by the promotion of Reynolds number.

In the present paper, gas mixing in a microchannel with obstacle and flow injection is simulated using the direct simulation Monte Carlo method. The main aims of this research are to find the effects of obstacles location and number, blockage ratio, and flow injection on the mixing length.

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2- Methodology

2- 1- Basic equations

In micro scales, the continuity assumptions of flow are not applicable, therefore classical Navier-Stokes equations are invalid. Thus, Boltzmann equations are utilized and the direct simulation Monte Carlo method is used to solve these equations numerically. The Boltzmann equation is as follows:

$$\frac{\partial}{\partial t}(nf)+c.\frac{\partial}{\partial r}(nf)+F.\frac{\partial}{\partial c}(nf)=\int_{-\infty}^{+\infty}\int_{0}^{4\pi}n^2\left(f^* f_1^* - f f_1\right)c_r \sigma d\Omega dc_1 \quad (1)$$

which f is the velocity distribution function, F is the force between two particles, c is the particle speed, n is particle density, σ is collision cross-section, and c_r is particle relative velocity. For a gas mixture which has s species, a separate distribution function is considered for each species. At such conditions, the Boltzmann equation is a set of s equations and each species is shown by p or q index. For species p, the Boltzmann equation is as follows:

$$\frac{\partial}{\partial t}\left(n_p f_p\right)+c_p.\frac{\partial}{\partial r}\left(n_p f_p\right)+F.\frac{\partial}{\partial c}\left(n_p f_p\right)= \sum_{q=1}^{s}\int_{-\infty}^{\infty}\int_{0}^{4\pi} n_p n_q\left(f_p^* f_{1q}^* - f_p f_{1q}\right)c_{rpq}\sigma_{pq} d\Omega dc_{1q} \quad (2)$$

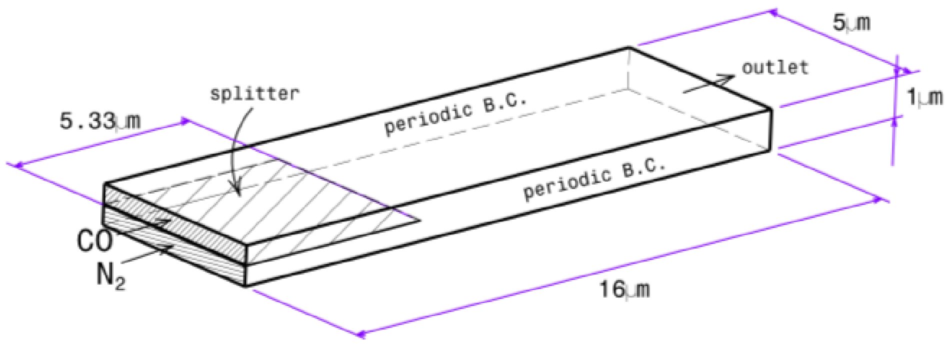

Fig. 1. Domain boundary conditions and dimensions

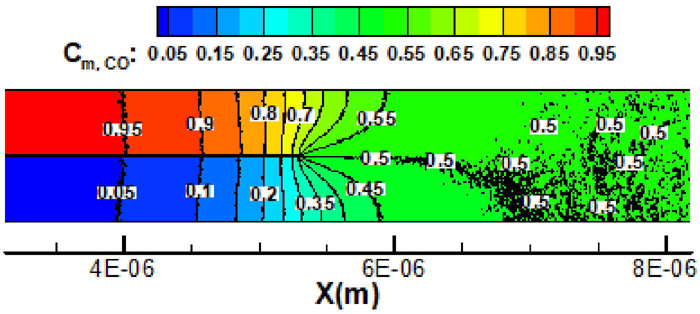

Fig. 2. The mass fraction of CO in the microchannel

In this study, the steady-state condition is considered, and therefore, time derivatives at the left-hand side of Eqs. (1) and (2) are ignored.

2- 2- Boundary conditions

In the present paper, the variable hard sphere model is used to simulate the collision of particles. For all cases, diffuse reflection is considered for upper and lower walls. Side walls are considered periodic which implies a two-dimensional simulation. Inlet boundaries are adapted from Ref. [7] with some modifications:

$$\begin{cases} (u_{in})_j = u_j + \dfrac{P_{in} - P_j}{\rho_j a_j} \\ (v_{in})_j = v_j + \dfrac{P_{in} - P_j}{\rho_j a_j} \\ (w_{in})_j = w_j \end{cases} \tag{3}$$

Outlet boundary conditions are as follows:

$$\begin{cases} (u_e)_j = u_j + \dfrac{P_j - P_e}{\rho_j a_j} \\ (v_{in})_j = v_j \\ (T_e)_j = \dfrac{P_e}{(\rho_e)_j R} \end{cases} \tag{4}$$

3- Results and Discussion

3- 1- Problem definition (benchmark case)

Nitrogen and Carbon Monoxide enters the domain according to Fig. 1.

A splitter plate separates Nitrogen and Oxygen up to 1/3 channel length. The channel length is 16μm. inlet pressure for both species are 100 kPa and the exit pressure is low enough to avoid any reverse flow. Species temperature is 300K. Side walls are periodic. Particle collision to upper and lower walls is a diffuse reflection which is a function of wall temperature. The mass fraction of CO is shown in Fig. 2. When the mass fraction is 0.5, mixing is completed.

For a more precise calculation of mixing, the mixing length is defined as follows:

$$\xi = \frac{\max\left[C_m(i,y) - C_{m,\infty}(i,y)\right]}{C_{m,\infty}(i,y)} \tag{5}$$

Table 1. Mixing length of cases with different blockage ratio

Col. / Case	No. Obstacles 1	2	3	4	ζ (μm)	b
Case 1	---	---	---	---	7.1	0
Case 2	2	---	---	---	6.9	0.43
Case 3	6	---	---	---	6.3	0.85
Case 4	12	---	---	---	6.35	0.83
Case 5	12	---	---	---	6.8	0.5
Case 6	6	---	---	---	6.25	0.95
Case 7	4	5	---	---	6.35	0.83
Case 8	6	6	6	6	6.28	0.93

where $C_{m,\infty}(i,y)$ is the mass fraction of species i at equilibrium and $C_m(i,y)$ is the mass fraction at an arbitrary section from the channel inlet along the y-axis. When $\zeta < 0.01$ mixing is complete. The mixing length for the benchmark case is 7.1μm.

3- 2- Effect of obstacle number and location on mixing

Eight cases with different obstacle numbers and locations are considered. The blockage ratio is defined as follows:

$$b = \sqrt{\frac{\sum_{i=1}^{n} A_i}{l \times H}} \tag{6}$$

where A_i is the wet area of the obstacle, l is the total length of obstacles and H is channel height. According to Table 1, it is observed that when the blockage ratio is increased, the mixing process is promoted.

3- 3- Effect of flow injection on mixing

Four cases are considered: the first case is a simple channel without injection, the second case has cross injection, the third case has inverse injection, and flow is injected vertically through an obstacle in the fourth case. Mixing lengths are presented in Table 2.

According to Table 2, flow injection in cases 2 and 3 led to higher mixing length, while in case 4 mixing enhances due to the obstacle effect in the domain.

Table 2. Mixing length of cases with flow injection

	Mass flow (μg/s) inlet	outlet	ζ (μm)
Case 1	32	32	7.1
Case 2	26.8	32.3	8.3
Case 3	26.8	32.3	7.45
Case 4	18	27.1	6.95

4- Conclusion

In the present study, the effect of obstacle on the mixing of two gaseous flows in a microchannel is studied. It was demonstrated that as the blockage ratio increased, the mixing is enhanced. The injection of flow was also studied. It was concluded that injection behaves similarly to obstacles, but the addition of mass flow due to injection increases mixing length.

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