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2D-DSMC SIMULATION OF NON-REACTIVE GAS MIXING INSIDE DIFFERENT TYPES OF MICRO MIXERS

Stavros Meskos*[1], Stefan Stefanov[2]
[1]stameskos@imbm.bas.bg, [2]stefanov@imbm.bas.bg
[12]Institute of Mechanics - Bulgaria Academy of Sciences

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ABSTRACT

While a lot of scientific work is done considering single gas flows at micro scale much less is done for mixtures and especially for simulation of mixing processes in various type mixers. Some of the very early works are published by Yan & Farouk [1], later by Wang &Li [2] and Hassan & Le [3], and most recently by Darbandi & Sabouri [4].
In the present work we contribute to the later studies by examining various cases of gas mixture flows in micro-mixer configurations. The first part involves mixers composed of two inlet channels and a mixing chamber. Two different gases enter the mixing chamber separately through two inlet channels which are placed either in parallel or in Y-shape setup. Within the mixing chamber the mixing length is measured, which is defined as the point in the chamber in longitudinal direction after which the two gases are found to be fully mixed. Different geometrical parameters as well as boundary conditions have as a result different mixing lengths, which lead to determine the mixing efficiency for different mixer types. It is observed that the efficiency is improved by increasing the angle of the inlet channels, by reducing the pressure at the inlets (Knudsen number is increased) and finally by increasing the temperature at the walls. The last part of this work suggests a new configuration of gas mixer by adding a second splitter plate, which is positioned inside the mixing chamber in parallel with its upper and lower walls. The aim is to separate the mixture into two different streams that have different concentrations at the outlet. Since the mixing length is now known from the previous setup the exact position of the splitter could be arranged in order to give mixtures with specific gas ratio at the outlet.

Computational considerations

A DSMC algorithm is built, using No-Time-Counter (NTC) collision model [5, 6]. The results presented at this abstract correspond to the VHS molecular model. The Knudsen number (Kn) and the mean free path (MFP) are calculated at the beginning of the mixing chamber. Velocity reference is the most probable velocity (MPV) of the first species. The time step is chosen to be less than 1/3 of the mean free time (MFT), i.e. the time for a molecule to travel a MFP at MPV. At inlets and outlet pressures and temperatures are given. At inlet particles enter with Maxwellian velocities and exclusively for the presented cases below, an average bulk velocity is enforced upon, corresponding to 0.3 Mach. The reason for this was to validate initial results with that of Wang &Li [2]. Microscopic

* Corresponding author, 2nd e-mail: stameskos@gmail.com; Tel.:(GR) +30 69 79 774 773; (BG) +35 98 84 942 197

properties are sampled and averaged every ten kinetic steps. Sampling steps are set to 500. Ensemble averaging is also applied upon time averaging and results are therefore averaged over 100 independent simulations. To calculate the mixing length the relative density difference (RDD) method is used as described in [2,3].

$$RDD_j = \frac{\rho_1 - \rho_2}{\rho_1} \tag{1}$$

where RDD_j denotes the relative density difference of species j, ρ_1 and ρ_2 denote the densities of that species measured at the denser and diluter side of the configuration respectively. Denser and diluter sides correspond to the row of cells adjacent to the upper and lower walls for the species that enters from the upper channel and the opposite for the species that enters from the lower channel. The gases are considered fully mixed when evolutions of RDD for each of them reach 0.5%. This method captures the two extremes by considering only the number densities near the two walls. While it gives reliable results for isothermal cases or in general for cases where the density distribution along the vertical axes is expected to not greatly vary, that may not be the case for not isothermal cases. For that reason another approach is introduced here:

$$RDD_j = \frac{1}{Ny}\sum_{i=1}^{Ny}\left|\frac{\rho_i - ColumnAvg}{ColumnAvg}\right| \tag{2}$$

Where RDD_j here again denotes the relative density difference (for species j) but defined as the average of the deviations of the number density ρ_i at each cell i from the column's average (Ny is the total number of cells at this column).

Results

In all presented cases below, the temperatures at walls and at inlets are set initially and kept constant. Note: if a reference temperature is provided it is assumed that the same temperature is applied to all the other boundaries. Furthermore all walls reflect particles fully diffusely i.e. accommodation coefficients are equal to unity. Finally vacuum is imposed at the outlet.
Concerning the first part of this work in Fig 1,2 and 3 is depicted the evolution of mixing length over different parameters. It is observed that the mixing length is decreased by increasing the angle between the inlet channels, by increasing the temperature at walls and finally by reducing the inlet pressure which is depicted in terms of Knudsen number.
The second part of this work corresponds to the implementation of a splitter at the outlet and studies the resulting outlet mixtures' consistency and how these results are influenced by the positioning of this splitter. The positioning is not random, but based on the former knowledge of the dependence of the mixing length, of a particular geometrical configuration, on the wall temperature. For example in Fig 4 (a) and (b) are the depicted the contours of the mixture's (CO-N_2) density and the CO concentration respectively. At the inlets the pressure is 0.45 [bar], temperature at 300 [K] and for both species at the inlet the velocities are Maxwellian with an average bulk velocity corresponding to 0.3 Mach. The depicted results corresponds to the steady state solution. From the previous micro-mixer simulations it is known that for a similar set up, see Fig. 1 (phi=0° and T = 300 [K]), and for those species it is expected a mixing length of about 2.5 [μm] therefore by placing a splitter plate at a shorter length it is expected two resulting mixtures with different concentrations. Here the splitter is placed at 1[μm] length after the inlet channels and at 0.5 [μm] height over the lower wall. As the results depict at the upper outlet the mixture is composed of an average 57% CO and 43% N_2 while at the lower outlet the reverse is received i.e. 43% CO and 57% N_2. In Fig. 5 (a) and (b) is depicted the same case with the only difference that the splitter height is now at 0.1 [μm]. For this case the resulting output mixtures have average concentrations of 50% CO – 50% N_2 at the upper outlet and 25% CO – 75% N_2 at the lower.
In a future detailed study, results will be presented for many different boundary parameters over the position of the splitter in order to draw conclusions on the correlation with the outlets' concentrations.

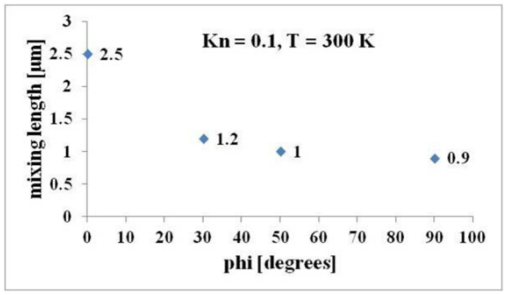


Figure 1: The dependence of the mixing length on the angle between the inlet channels

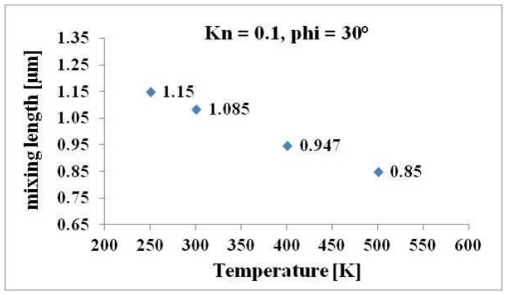


Figure 2: The dependence of the mixing length on the temperature at walls and the Knudsen number**.**

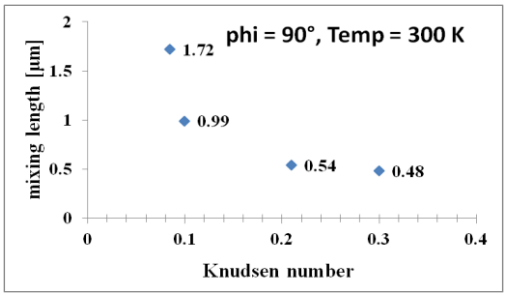
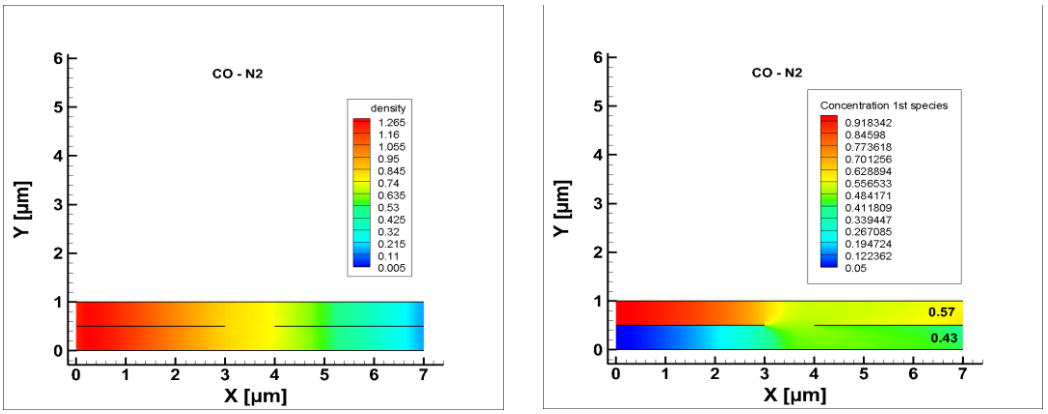
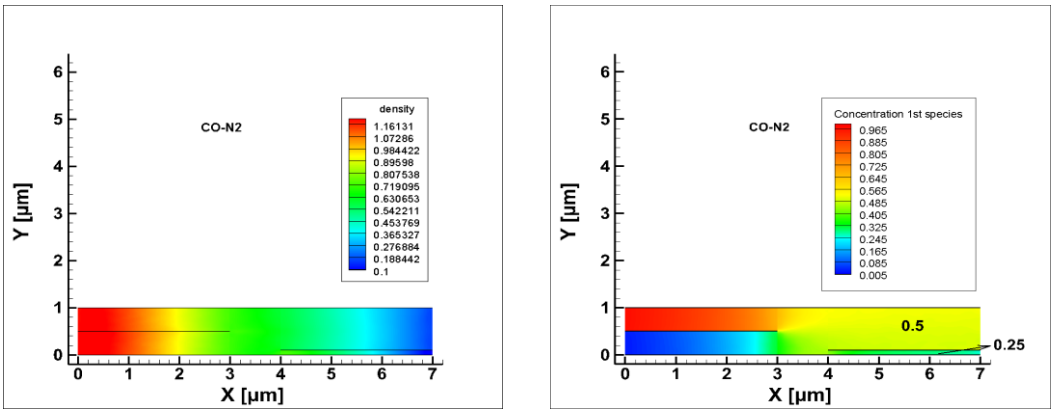


Figure 3: The dependence of the mixing length on the Knudsen number as measured at the mixing chamber



(a) **(b)**

Figure 4: (a) Density contour of the mixture and (b) Concentration of CO, when second splitter at length 1 [µm] and height 0.5 [µm]. All wall temperatures are kept at 300 [K].



(a) **(b)**

Figure 5: (a) Density contour of the mixture and (b) Concentration of CO, when second splitter at length 1 [µm] and height 0.1 [µm]. All wall temperatures are kept at 300 [K].

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References and Citations

References to published literature should be quoted in the text by enclosing between two brackets the number of the reference. Please refer to the following examples:

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