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GAS MIXING IN SIMPLE GEOMETRICAL CONFIGURATIONS

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KEY WORDS

DSMC, cavity, thermal relaxation, channel flow, mixing length

ABSTRACT

The aim of this work is to simulate the process of gas mixing inside micro - configurations. At this stage of the work the Direct Simulation Monte Carlo (DSMC) method was employed. Two basic problems were studied. The first studies the thermal relaxation of binary and ternary gas mixtures enclosed in an orthogonal cavity with stationary walls see Fig.1(a). The second problem measures the mixing length inside a channel where two gases enter separated by a middle plate see Fig.1(b). Regarding the first problem it was investigated how the physical properties of different species influence the mixing process. To achieve this, the infinity space area was considered , therefore all boundaries of the finite size domain were set to specular reflection walls, consequently all particles after colliding with walls maintain the same energy as before and the problem is reduced to zero-dimensional. The final temperature that the gases will relax was calculated analytically as

$$T_{mix} = \sum_{p}^{M} C_p T_p \tag{1}$$

where C_p, T_p are the initial concentration and temperature of species p and M is the total number of species. It is obvious here that the final temperature is only influenced by the initial concentrations and temperatures and is easily calculated. This was the motivation to investigate where and how the different species are influencing the mixing process and how it evaluates in relaxation time. Different combinations of species reach the same relaxation temperature but the relaxation time are different. Several cases were tested at different concentrations, temperatures, and Knudsen numbers. A representative example is depicted at Fig. 2 (a) and (b).

The second problem investigates the mixing length of binary gas mixture flow in a 2d-channel configuration shown in Fig. 1b and it is considered as the distance from the end of the separation plate until the point at which both species are found fully mixed. When the gases are fully mixed at a specific length, it is expected that their particles will be equally distributed over vertical distance of the channel and then their individual number densities near the two channel walls will be equal and therefore their relative density difference will approach to zero, Fig.3. This method is used and validated in Ref. [1]. Let ρ_1 refers always to the denser side and ρ_2 to the diluter ($\rho_1 > \rho_2$), by side is meant upper and lower wall, then relative density difference of species i is

$$\xi_i = \frac{\rho_{1,i} - \rho_{2,i}}{\rho_{1,i}} \tag{2}$$

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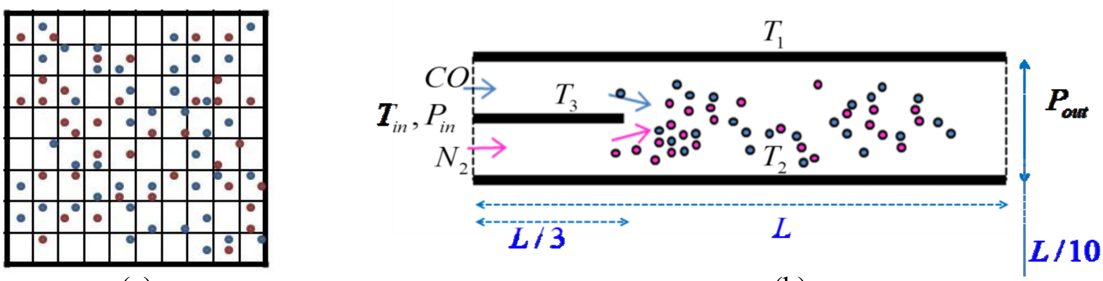
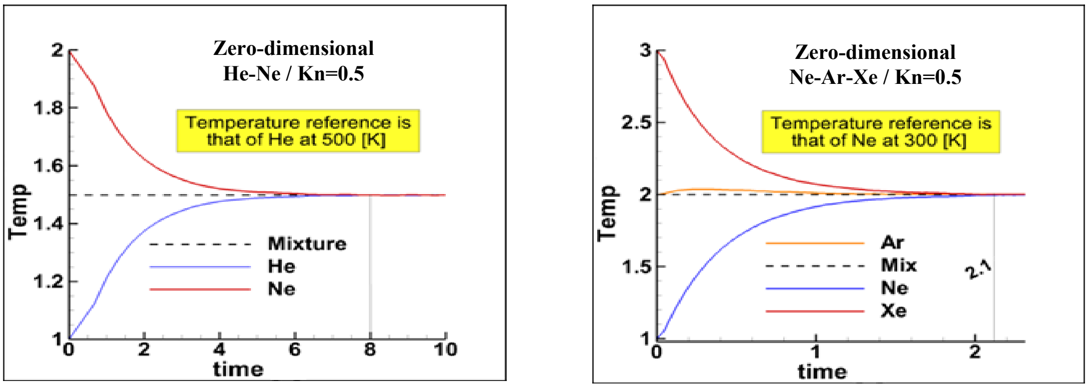


(a) (b)

Figure 1: Graphical representation of the computational domains where (a) is for the case of cavity and (b) is for a channel configuration.



(a) (b)

Figure 2 : Evolution of Temperature until steady state. Walls are reflecting specularly thus zero-dimensional case. Time is in dimensionless form (time reference = MostProbableVelocity / MeanFreePath), $Kn = l_{mfp} / L,\ l_{mfp} = 1/\left(\sqrt{2}\pi d^2 den\right),\ d = diameter, den = density$

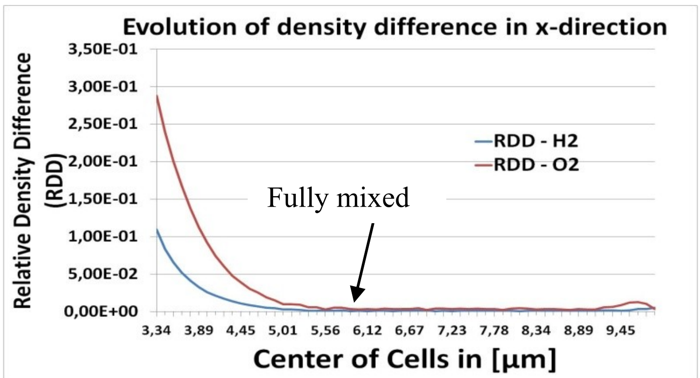


Figure 3 : Evolution of relative density difference for H2 and O2. They are fully mixed when $\xi_{H_2} = \xi_{O_2} = 0$ and this is measured approximately at 5,8µm. Total length of the channel is 10µm and the splitter plate has a length of 3,33µm.

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References and Citations

[1] Moran Wang, Zhixin Li (2006). *Gas mixing in microchannels using the direct simulation monte carlo method*. International Journal of Heat and Mass Transfer 49 1696–1702. Elsevier Ltd.