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THERMAL GAS MIXING IN MICROSCALE

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KEY WORDS

Project presentation; Binary gas mixtures; Analytical solutions; Direct Simulation Monte Carlo; No Time Counter Scheme; Simplified Bernoulli Trials Scheme; Discrete Velocity Methods; Time & Thermal relaxation; Different initial states

ABSTRACT

Accurate simulation of gas mixtures in micro-scale is essential to the design of micro-devices. The main purpose of this project targets the development of efficient DSMC and DVM numerical algorithms and the comparison to existing modeling methods in order to improve the process of gas mixing in micro-mixers. A complete study of gas mixing phenomena in the whole range of Knudsen number (Kn) under different flow conditions and initial states is expected. This work will be completed through three phases corresponding to the three different stays, with chronological order, at IMech, UTH and Mitis SA in respect. The researcher will apply analytical solutions where possible and proceed to the formulation of numerical methods - Direct Simulation Monte Carlo and Discrete Velocity Method at the two first stays and compare results with those acquired at Mitis with the use of Navier-Stokes models. The research is twofold: to investigate the basic properties of thermal gas mixing process on simple low-dimension problems and apply the developed numerical codes to gas mixture flow in complex 2D and 3D micro-device configurations.

On the occasion of the first MIGRATE Workshop the early progress of the researcher's work will be presented. Already an analytical solution of 1D planar free molecular flow of a single gas (see Fig.1) is modeled and results are compared to DSMC ones (Table 1). The analytical solution of the established temperature in non-dimensional form reads:

$$T = \frac{\left[\alpha_2(2-\alpha_1)+\alpha_1\left(\frac{T_1}{T_2}\right)^{1/2}(2-\alpha_2)\right]}{\left[\alpha_2(2-\alpha_1)+\alpha_1\left(\frac{T_2}{T_1}\right)^{1/2}(2-\alpha_2)\right]}, \quad (1)$$

where T_1, T_2 (reference temperature) and α_1, α_2 are the temperatures and accommodation coefficients of the two walls, respectively.

Furthermore two cases of binary gas mixture thermal relaxation will be simulated using the DSMC method. While the first refers to two gases already mixed but with different initial temperatures, the second case refers to two gases confined between two walls with temperatures equal

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to the wall ones (Fig. 1) and initially separated from one another, as shown in Fig.2. The first case is a 0-D unsteady state problem. However the second case will be studied by DSMC method as an 1-D or 2-D unsteady state problem. The aim is to simulate the thermal relaxation of both cases in time until the mixtures reach the final equilibrium state and investigate the temporal characteristics of the thermal relaxation process. The results obtained by suing two different collision schemes, namely, the No Time Counter (NTC) and the Simplified Bernoulli Trials (SBT), will be compared in order to investigate the accuracy of both collision schemes.

Finally, a preliminary literature overview [1-6] describing some previous gas mixture investigations and general issues of the DSMC method, which are of interest of the gas mixture simulation, will be presented.

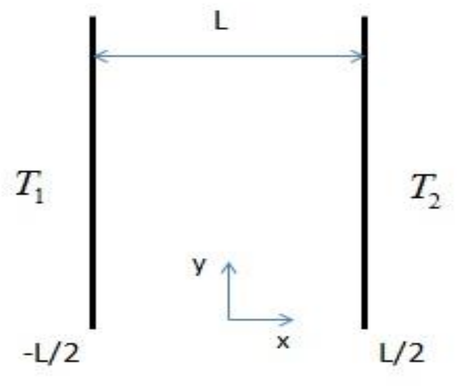

Figure 1: 1D planar flow.

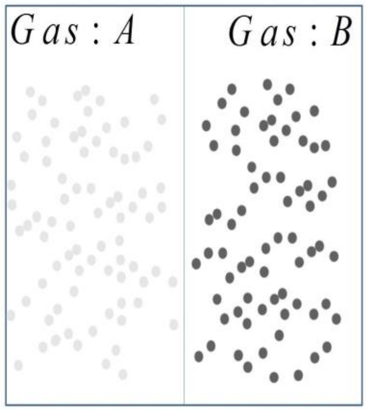

Figure 2: Graphical representation of the initial state of the simulated problem.

Analytical Solution	DSMC - NTC	Error
0.316228	0.316744	0.1632%

Table 1: Temperature results for 1D planar flow when $\alpha_1 = \alpha_2 = 1$(diffuse scattering) and $T_1/T_2 = 0.1$.

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