Implementation of molecular reservoirs in 3D micro nozzle gas flows

Nevsan Sengil and Firat O.Edis
Faculty of Aeronautics and Astronautics, Istanbul Technical University
Maslak 34469 Istanbul, Turkiye

ABSTRACT

As their dimensions are between 1 mm and 1 micron, gas flows related with the micro devices have higher Knudsen numbers (Kn) similar to high atmosphere flights. If Kn is higher than 0.1, instead of the classical continuum based Euler or Navier-Stokes (N-S) equations, deterministic or stochastic atomistic models should be used. This is due to the departure from local thermodynamic equilibrium with increasing Kn number. Consequently, both the linear relation between shear stress and velocity gradient, and linear relation between heat conduction and temperature gradient are lost. Direct Simulation Monte Carlo (DSMC) method is a stochastic atomistic simulation method that can be used for high Kn number gas simulations.

In this study two molecule generation method will be analyzed used in direct simulation Monte Carlo method. Volume generation reservoirs are not used as widespread as the surface generators because of the higher calculation time in downstream boundaries, lower number flux than the theoretical number flux and a need for more sophisticated code algorithms. But volume generation reservoirs also has some certain advantages over the surface generation reservoirs. First in high speed flows they are more efficient computationally. Secondly they resemble exact Maxwell-Boltzmann distribution. Next, molecule input rates distribution is a Poisson distribution which can prevent non-equilibrium behavior of the surface generator reservoirs. It will be demonstrated that lower flux numbers problem can be corrected with a new approach in volume generation reservoirs and adopted easily to Pressure Boundary Conditions in 3D micro nozzle simulations.

Figure 1. Volume generation reservoir normalized molecule input flow rate mean values with changing gas flow velocities

Figure 2. Horizontal velocity contours along 3D micro nozzle derived from direct simulation Monte Carlo solver.

REFERENCES: