Proceedings of the 4th International Conference on Nanostructures (ICNS4)
12-14 March, 2012, Kish Island, I.R. Iran

DSMC Simulation of Shear Driven Flow in Nano Gap Structures

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Abstract: In the present work, argon flow confined within a gap at nanoscale between two moving parallel plates and maintained at the same uniform temperature is simulated using direct simulation Monte Carlo (DSMC) method. Simulations are performed to investigate rarefaction effects on velocity, temperature, heat flux, shear stress and entropy profiles. The specific contribution of this work is detailed discussion on heat flux and shear stress behavior of the gas besides calculation of entropy as a thermodynamics property which shows the molecular chaos. The results show that, as the flow rarifies the bulk velocity of the domain decreases, however the absolute amount of non-dimensional temperature, heat fluxes, and shear stresses increases. Investigation of entropy profiles shows that by increasing the Knudsen number entropy tends to a finite value in the domain.

Keywords: DSMC; Nano-Couette Flow; Heat Flux; Shear Stress; Entropy

Introduction

In recent years, prediction of rarefied gas flow and heat transfer behaviour of micro/nano-flows attracted attention of researchers due to the wide application of micro/nanoelectromechanical system (MEMS/NEMS) devices such as micro-valve, micro-turbine, micro-pump and micro-nozzle. To measure the degree of rarefaction the Knudsen number (Kn) is defined as the ratio of mean free path of the gas molecules to the characteristic length of the geometry ($Kn = \lambda / L$). Flow regimes are also classified on the basis of the Knudsen number into: continuum (Kn $\leq$ 0.01), slip flow (0.01 < Kn < 0.1), transition flow (0.1 < Kn < 10) and free molecular (Kn $\geq$ 10) [1]. When there is a continuum breakdown, the conventional method to describe gas flows, i.e., the Navier-Stokes (NS) equations fails to predict the flow and the solutions are to be established based on the kinetic principles such as those in treating the Boltzmann equation. Direct simulation Monte Carlo (DSMC) is shown to be the most accurate numerical tool to handle the complexity of the Boltzmann equation. However, the computational cost is larger than the traditional CFD approaches.

Shear driven nano-scale confined gas flows are encountered in the components of micro- and nano-electromechanical systems such as micro/nano-motor, comb mechanism, and micro/nano-bearing, and in magnetic disc drive units. For the latter, distance between the head and media is on the order of 10 nm, and the next generation disc drives strive to reduce this distance to enhance the magnetic storage capacity. The advantage of studying Couette flow is that it includes many features found in more complex rarefied gas dynamics problems. Micro- and nano-Couette flow has been widely studied in the literature: Beskok et al. [2] reported a detailed analysis of the effects of compressibility and rarefaction on pressure-driven and shear-driven microflows. They found that compressibility and rarefaction are competing phenomena and both require consideration in microfluidic analysis. During the last decade many scientists compared different numerical tools in the Couette flow [3-6] and many implemented new meodels to solve this type of flow [7-9]. Chen and Tian [10] analyzed the characteristics of entropy generation due to heat transfer and friction for thermal micro-Couette flows in slip regime using the lattice Boltzmann method. They showed that less entropy generates within more rarefied flow. In the present work we investigate rarefaction effects on velocity, temperature, heat flux, shear stress and entropy profiles. The specific contribution of this work is detailed discussion on heat flux and shear stress behavior of the gas besides calculation of entropy as a thermodynamics property using microscopic formulation, to show the molecular disorder in the channel. A schematic of the problem is shown in Fig. 1.

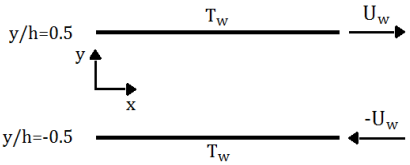

Figure 1- Schematic of the problem.

Modelling

The DSMC method is proved to be the most accurate numerical tool to solve the Boltzmann equation based on direct statistical simulation of the molecular processes described by the kinetic theory [1]. In fact, DSMC simulates particle behavior in a manner consistent with what is described by the Boltzmann equation. The algorithm includes four primary steps: moving the particles, indexing them, collision simulation, and sampling the flow-field. The primary principle of DSMC is to decouple the motion and collision of particles during

one time step. The implementation of DSMC needs breaking down the computational domain into a collection of grid cells. After fulfilling all molecular movements, the collision between molecules are simulated in each cell separately in a statistical manner. The decoupling between the particles movement and collisions is correct if the time step is a small fraction of the mean collision time. The following procedure is used to solve a stationary problem with DSMC. In the entire computational domain, an arbitrary initial state of gas particles is specified and the desired boundary conditions are imposed at time zero. After achieving steady flow condition, sampling of molecular properties within each cell is fulfilled during sufficient time period to avoid statistical scattering. All thermodynamic parameters such as temperature, velocity, density and pressure are then determined from this time-averaged data. In the current study, variable hard sphere (VHS) collision model is used and the collision pair is chosen based on the no time counter (NTC) method.

Results and Discussion

Argon with molecular mass of m=6.63×10−26 kg, viscosity-temperature index of ω=0.81, variable hard-sphere diameter of d_{vhs}=4.17×10−10 m and specific heat ratio of γ=1.667 is considered as the simulated gas. In figures, the ordinate is normalized by the distance between the parallel plates h. Flow velocity and temperature are normalized by the relative velocity of the plates U_w and the temperature of the wall T_w, respectively. Also heat flux and shear stress are normalized by the parameters $\rho_\infty U_w C_p T_w$, and $1/2\rho_\infty U_w^2$, respectively. Here, ρ_∞ and C_p are the free stream density and the specific heat capacity of argon, respectively. The normalized heat flux and shear stress are referred to as the heat flux coefficient (C_h) and the friction coefficient (C_f), respectively with a second subscript indicating its direction, in the figures. Also because of the symmetry in the domain results are reported just for half of the channel.

Rarefaction effects gain importance with the reduction in the geometry size, since the sizes of the geometries become comparable to the mean free path of the gas molecules. It is observed in Fig. 2 that the slope of velocity profile decreases as Knudsen number increases. This means decrease of velocity in the domain. Analytical solution of the linearized Boltzmann equation indicates that the bulk flow velocity profile is essentially linear for all Knudsen numbers. However, a kinetic boundary layer named *Knudsen layer* on the order of one to a few mean free paths starts to become dominant between the bulk flow and solid surfaces in the transition flow regime. The velocity profile and other physical variables are subject to appreciable changes within the Knudsen layer.

Figure 2 illustrates the temperature profiles at different Knudsen numbers. As the Knudsen number increases, temperature in the domain and also temperature jump at the plates becomes more significant, but the curvature of temperature profiles reduces. In a constant wall Mach number flow, the amount of wall kinetic energy is constant. As the flow becomes more rarefied, this constant kinetic energy will be saved in smaller number of the molecules and shows itself in term of temperature rise.

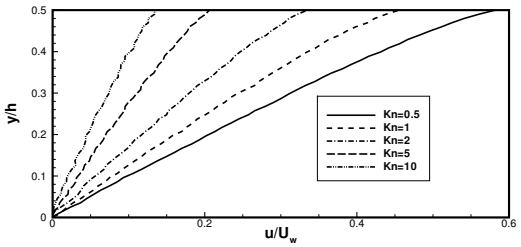

Figure 2- Velocity Profile.

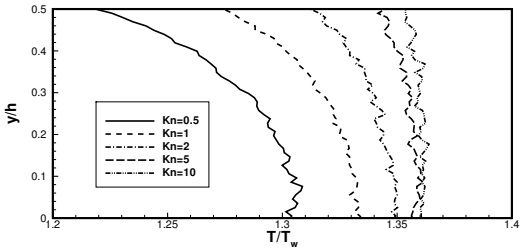

Figure 3- Temperature Profile

Figure 3 shows the non-dimensional heat flux variation in x and y direction. An interesting non-equilibrium phenomenon that occurs in planar Couette flow is the appearance of a heat flux without the presence of a temperature gradient, i.e. in x direction, and this is called non-gradient transport. It is observed in Fig. 4 that by increasing the Knudsen number, the magnitude of heat flux in both directions in the domain increases. This is because of increase of the surface-molecular collisions due to increase of the mean free path of the molecules. As a result, not only the molecules near the surface but also molecules in the center of channel can collide with the surfaces. It is also observed that the amount of non-gradient transport is greater than the gradient transport.

Our simulations show that as the gas becomes more rarefied, it would experience less shear stress due to smaller amount of intermolecular collisions. However, the magnitude of non-dimensional shear stress would still increase as observed in Fig. 5 for all components of shear stress tensor.

In contrast to the macro-state, which characterizes plainly observable average quantities, a microstate specifies all molecular details about the system including the position and velocity of every molecule. The more such states available to the system with appreciable probability, the greater the entropy. More specifically, entropy is a logarithmic measure of the density of states. It is observed in Fig. 6 that the maximum amount of entropy which is an indicator of molecular disorder is in the center of the channel. This is because of the molecular

chaos in the center which is caused by the great amounts of intermolecular collisions in the center of the channel. By comparing entropy profiles with the DSMC temperature profiles it is observed that this two quantities follow a same trend, i.e., a parabolic profile with the maximum value at the center of the channel. This is because the heat is a disordered form of energy and the entropy flows with heat. Consequently entropy or molecular chaos increases in the regions of higher temperature. It is also observed that the curvature in the entropy diagrams decreases as the Knudsen number increases and the magnitude of entropy in the near wall regions increases as Knudsen increases, however the amount of entropy in the central parts of the channel is smaller in high Knudsen simulations. Therefore, a general conclusion is: the more rarefied flow, more uniform entropy profiles is observed. The justification for this conclusion is the more uniform distribution of the molecules in the domain for rarefied flows rather than dense gases.

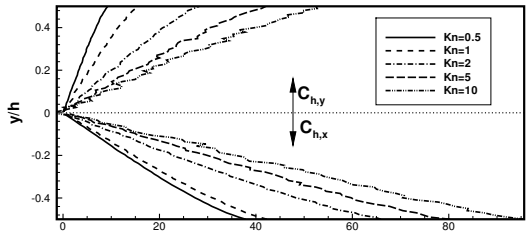

Figure 4- Heat Flux Profiles.

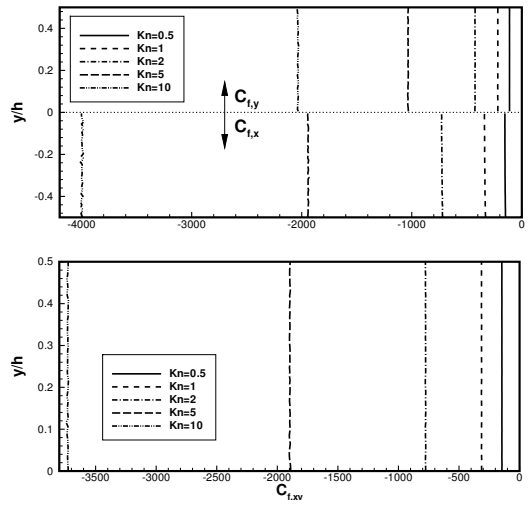

Figure 5- Shear Stress Profiles

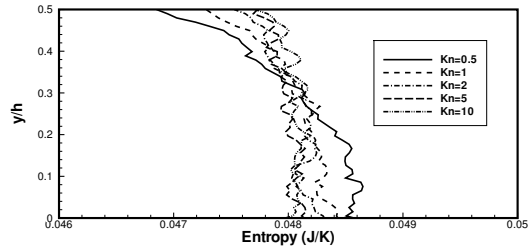

Figure 6- Entropy Profile.

Conclusions

In the present work the problem of nano-Couette flow is simulated using DSMC. The flow behavior due to variation of Knudsen number is justified and important non-equilibrium characteristics like the nonlinear velocity profiles and non-gradient transport in heat flux are shown. Also entropy as a criterion for molecular disorder is calculated using microscopic formulation. It is shown that as the flow becomes rarefied, entropy distribution tends to uniform profiles.

References

[1] G.A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Clarendon Press, Oxford, United Kingdom, 1994.

[2] A. Beskok, G.E. Karniadakis, W. Trimmer, "Rarefaction and Compressibility Effects in Gas Microflows", Journal of Fluids Engineering, 118(3) (1996) 448-456.

[3] L. Popken, P.W. Cleary, "Comparison of Kinetic Theory and Discrete Element Schemes for Modelling Granular Couette Flows", Journal of Computational Physics, 155(1) (1999) 1-25.

[4] D. Reitebuch, W. Weiss, "Application of High Moment Theory to the Plane Couette Flow", Continuum Mechanics and Thermodynamics, 11(4) (1999) 217-225.

[5] H. Xue, H.M. Ji, C. Shu, "Analysis of micro-Couette flow using the Burnett equations", International Journal of Heat and Mass Transfer, 44(21) (2001) 4139-4146.

[6] Kumar, Rakesh, Titov, E. V., Levin, D. A., "Reconsideration of Planar Couette Flows Using the Statistical Bhatnagar-Gross-Krook Approach", Anglais, 24 (2010) 9.

[7] W. Marques Jr, G.M. Kremer, F.M. Sharipov, "Couette flow with slip and jump boundary conditions", Continuum Mechanics and Thermodynamics, 12(6) (2000) 379-386.

[8] M.J. McNenly, M.A. Gallis, I.D. Boyd, "Empirical slip and viscosity model performance for microscale gas flow", International Journal for Numerical Methods in Fluids, 49(11) (2005) 1169-1191.

[9] A. Frezzotti, L. Gibelli, "A kinetic model for fluid-wall interaction", Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, 222(5) (2008) 787-795.

[10] S. Chen, Z. Tian, "Entropy generation analysis of thermal micro-Couette flows in slip regime", International Journal of Thermal Sciences, 49(11) (2010) 2211-2221.