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SIMULATION OF LONG MICROCHANNEL FLOW IN TRANSITIONAL REGIME USING LATTICE BOLTZMANN METHOD

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ABSTRACT

Microscale flow simulation is considered in this paper for a microchannel flow geometry. Lattice Boltzmann Model (LBM) was used as the numerical method for flow simulation, in which an effective mean free path was used in relaxation time appeared in LBM. The effective mean-free-path makes it possible to investigate flow characteristics in transition flow regime, for which Knudsen number varies from 0.1 to 10. Such implementation does not change the computational efficiency of LBM significantly. Results are obtained for flow configuration in a long microchannel. The slip velocity was predicted in this flow configuration with good accuracy. Good correspondence with Direct Simulation Monte Carlo (DSMC) method was observed.

INTRODUCTION

Microscale gas flows have received much attention particularly due to the rapidly emerging technology of Micro-Electronic-Mechanical-System (MEMS) [1] and the need of studying flow through them. Two main characteristics of the flow in MEMS are low Mach number and nonzero Knudsen number, $Kn = \lambda / H$, a parameter defined as the ratio of mean-free-path, λ, to the characteristic length of the domain, H. Low-speed gaseous flows in micro-devices have large Knudsen numbers in the range of slip ($0.001 < Kn < 0.1$) or transition flow ($0.1 < Kn < 10$) which are far from thermodynamic equilibrium. The Navier-Stokes equations with no-slip boundary condition are only appropriate when $Kn < 0.001$ while Boltzmann Equation (BE) is valid for flows with arbitrary Knudsen number. On the other hand, numerical solution of BE is very time expensive especially for the most accurate one which is called Direct Simulation Monte Carlo (DSMC) method [2]. Moreover, this method is suitable for high-speed transition flow, a situation never exist in microchannels.

Gas microflow experiences some non-equilibrium phenomena, among them are velocity slip and temperature jump at the solid walls and a nonlinear stress-strain relationship within the Knudsen layer which is a region near a solid wall with a thickness of a few mean free path. Lattice Boltzmann Model (LBM) which is a numerical method derived from BE, is a relatively new and effective numerical approach in simulating fluid flows [**3**,**4**]. LBM has greater potential to model non-equilibrium flows with non-zero Knudsen number due to its origin which is BE. Moreover, LBM has some major advantages as compared to other methods in fluid flow simulations: implementation of fully parallel algorithms, computationally efficient and accurate method. It was shown that LBM is able to simulate flows in microchannels for a range of Knudsen numbers up to the transition flow regime [5, 6]. Although transition flow regime was investigated by some authors [7,8], prediction of flow characteristic in this regime still remains a challenge in modeling such flow regimes.

Various authors studies microchannel flows through LBM. Verhaeghe et al. [6] presented the lattice Boltzmann equation (LBE) with a multiple relaxation times (MRT) to simulate pressure-driven gaseous flow in a long micro channel. Zhang et al. [7] proposed an effective mean-free path to address the Knudsen layer effect. Guo et al.[5] studied the physical symmetry, spatial accuracy, and relaxation time of the lattice Boltzmann equation (LBE) for microgas flows in both the slip and transition regimes. They indicated that for a microgas flow, the channel wall confinement exerts a nonlinear effect on the relaxation time, which should be considered in the LBE for modeling microgas flows. Such treatment can improve the accuracy of the LBE for simulating microgas flows with a relative large Knudsen number. Niu et al. [8] provided a systematic description of the kinetic LBM, including the lattice Boltzmann equation and definition of the relaxation time to capture the nonlinear effects due to the high-order moments and wall boundaries. They used an effective relaxation time and a modified regularization procedure of the non-equilibrium part of the distribution function based on previous works.

The present study focused on the application of an effective mean free path (EMFP) and diffuse scattering boundary condition (DSBC) for slip and transition flow regimes in microchannel flow. A common flow configuration in microchannels, namely long microchannel flow, is discussed with the application of the EMFP and DSBC.

NOMENCLATURE

f_α	Particle density distribution functions
e_α	Particle velocity direction
ρ	Density
u	Macroscopic velocity
T	Temperature
x	Location
t	Time
λ	Mean free path of the molecules
Kn	Knudsen number
H	Characteristic length
μ	Viscosity
P	Pressure
R	Ideal gas constant
τ	Dimensionless relaxation time
λ^*	Effective mean free path
τ^*	Effective relaxation time
δ_t	Time step
α	Discretized direction
eq	Equilibrium condition
ξ	Particle velocity

Lattice Boltzmann method

LBM approximates kinetic equation for the single particle distribution function $f(x,\xi,t)$ on the mesoscopic level. BE with BGK approximation using single relaxation time is written as:

$$\partial_t f + \xi.\nabla f = -\frac{1}{\lambda}[f - f^{(0)}] \quad (1)$$

Where ξ is the particle velocity, $f^{(0)}$ is the equilibrium distribution function (the Maxwell-Boltzmann distribution function), and λ is the relaxation time. The velocity space ξ can be discretized into a finite set of points, ξ_α. In the discretized velocity space the Boltzmann Eq. (1) becomes:

$$\partial_t f_\alpha + \xi_\alpha.\nabla f = -\frac{1}{\lambda}[f_\alpha - f_\alpha^{(eq)}] \quad (\alpha = 0,1,...,8 \ for\, 2-D) \quad (2)$$

$f_\alpha^{(eq)}$ is the equilibrium distribution function in discretized velocity space. A two-dimensional nine-velocity component (D2Q9) square lattice is used in the present computations which is shown in Fig. 1.

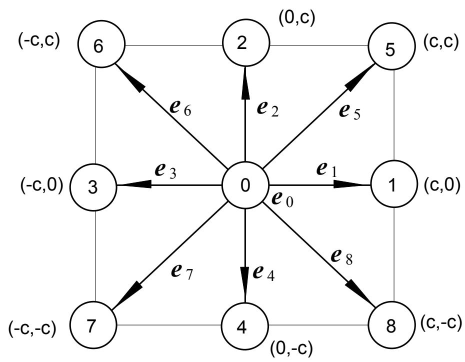

Fig. 1 Velocities in the D2Q9 lattice Boltzmann model

Here e_α is used to denote the discrete velocity set, which can be written as

$$e_\alpha = \begin{cases} (0,0) & \alpha = 0 \\ (\cos[(\alpha-1)\pi/4], \sin[(\alpha-1)\pi/4])c & \alpha = 1,3,5,7 \\ (\cos[(\alpha-1)\pi/4], \sin[(\alpha-1)\pi/4])\sqrt{2}c & \alpha = 2,4,6,8 \end{cases} \quad (3)$$

Where $c = \delta_x / \delta_t$ is the lattice constant (δ_t, and δ_x are the time step and lattice spacing respectively). The equilibrium distribution function, $f_\alpha^{(eq)}$, is a function of density and macroscopic velocity of the fluid as follows: [9]

$$f_\alpha^{(eq)} = \omega_\alpha \rho [1 + \frac{3}{c^2} e_\alpha . \vec{u} + \frac{9}{2c^4} (e_\alpha . \vec{u})^2 - \frac{3}{2c^2} \vec{u} . \vec{u}] \qquad (4)$$

Where

$$\omega_\alpha = \begin{cases} \frac{4}{9}, & \alpha = 0 \\ \frac{1}{9}, & \alpha = 1,3,5,7 \\ \frac{1}{36}, & \alpha = 2,4,6,8 \end{cases} \qquad (5)$$

With the discretized velocity space, the hydrodynamic moments, which show density and macroscopic velocity, are given by:

$$\rho = \sum_\alpha f_\alpha \qquad (6a)$$

$$\rho \vec{u} = \sum_\alpha e_\alpha f_\alpha \qquad (6b)$$

Proceeding with the Chapman-Enskog analysis, it can be shown the NS equations are recovered in the near incompressible limit from the BE [10]. Eq. (2) can be further discretized in space and time. The completely discretized form of Eq. (2), with time step δ_t and space step $e_\alpha \delta_t$, is:

$$f_\alpha (x_i + e_\alpha \delta_t, t + \delta_t) - f_\alpha (x_i, t) = -\frac{1}{\tau} [f_\alpha (x_i, t) - f_\alpha^{(eq)} (x_i, t)] \qquad (7)$$

Where $\tau = \lambda / \delta_t$ is the nondimensional relaxation time, and x_i is a point in the discretized physical space. The above equation is called LBE with Bhatnagar-Gross-Krook (BGK) approximation. The left-hand side of Eq. (7) is physically a streaming process for particles while the right-hand side models collision through relaxation time.

Application of LBM in microchannel flow simulation needs special attention duo to the phenomena of Knudsen layer, determination of the effective relaxation time τ and boundary conditions. A brief discussion of each of these phenomena is presented here along with their computational procedure.

MICROCHANNEL FLOW SIMULATION BY LATTICE BOLTZMANN

A key non-dimensional parameter for gas microflow is Knudsen number, which is defined as the ratio of the mean free path λ to the characteristic length, H, of the flow configuration:

$$Kn \equiv \frac{\lambda}{H} \qquad (8)$$

Rarefaction effect becomes more important as the Knudsen number increases. A fluid flow can be considered as continuum for $Kn \le 10^{-3}$ and free-molecular flow for $Kn \ge O(10)$. A rarefied gas can be considered neither an absolutely continuous medium nor a free-molecular flow. It covers a range of Knudsen numbers between 10^{-3} to 10. This region is divided into two parts, i.e slip flow $(10^{-3} < Kn < 0.1)$ and transition flow regimes $(0.1 < Kn < 10)$, see Fig. 2.

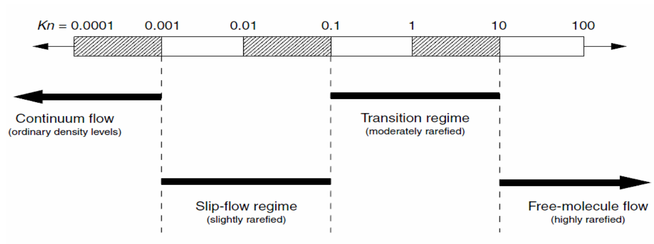

Fig. 2 Knudsen number regimes.

The Knudsen number defined in Eq. 8 is called oulet Knudsen number, Kn_{out}, in microchannel flows. There is a local Knudsen number in such flows which is not constant and changes with location. For isothermal flow in microchannel, the relation between Kn_{out} and local Knudsen number, Kn, is: $Kn_{out}=Kn \times P$. The parameter “P” is the local pressure.

Knudsen layer (or kinetic boundary layer) is a region near a solid wall with a thickness of a few mean free paths where the usual linear relationship between the stress and rate of strain is no longer valid [**7**]. Fig. 3 shows schematically the Knudsen layer. Solid line in this figure shows the structure of the Knudsen layer within a shear flow bounded by a planar wall.

In this region the gas is far from a state of local thermodynamic equilibrium. For many flow situations, the scale of the Knudsen layer is negligible in comparison to the macroscopic length scale of interest. However, for Knudsen numbers greater than about 0.01, Knudsen layer starts to impact on the entire flow field. A slip-boundary condition is used in Navier-Stokes equations for simulating Knudsen-layer effects [2]. However the slip velocity obtained from this boundary condition is not the actual velocity slip that occurs at the gas surface interface as is observed in Fig. 3. Knudsen layer becomes a significant proportion of the flow field for high Knudsen numbers, where the Navier-Stokes equations would not be appropriate.

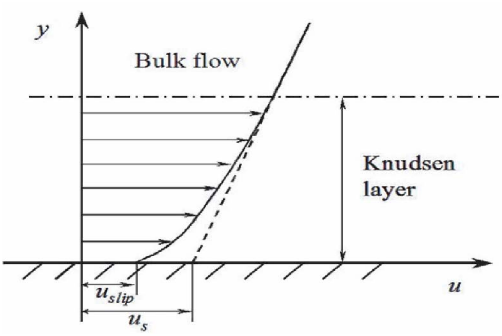

Fig. **3** Schematic diagram showing the Knudsen layer. real velocity profile(solid line), velocity profile obtained by Navier-Stokes (dashed line).

Knudsen layer will have a significant impact on the distance a gas molecule can travel between successive collisions through the presence of a solid wall. As a consequence, the mean free path will be smaller than that observed in the bulk flow for near-wall region. Some authors used an effective mean free path [5,6] in their computations, which is defined as the average distance a gas molecule will travel between consecutive collisions with either another gas molecule or the solid wall.

Effective relaxation time (ERT)

In kinetic theory, the relaxation time τ can be defined in term of viscosity μ as [11]:

$$\tau = \frac{\mu}{P} \tag{9}$$

Where P is the pressure and viscosity is proportional to a qualitatively defined molecular mean-free-path λ. For gas molecules considering as hard spheres, it is expressed as:

$$\lambda = \frac{\mu}{P}\sqrt{\frac{\pi}{2RT}} \tag{10}$$

Where R is the Gas Constant and T is the temperature. Consequently, the relaxation time can be written as:

$$\tau = \sqrt{\frac{2}{\pi}}\lambda c_s = \sqrt{\frac{2}{\pi}}Kn\, c_s H \tag{11}$$

Here $c_s = c/\sqrt{3}$ is the speed of sound. The mean free path given by Eq. (10) is valid for unbounded systems. In a micro-scale gas flow system confined by the solid boundaries, some molecules will hit the walls and their flight path may be shorter than the molecular mean free path λ defined in the unbounded systems. Therefore the mean free path in bounded system should be modified to reflect the boundary wall effects. According to the previous investigations for an isothermal, incompressible flow [**7**], an effective mean free path (EMFP) λ^* can be used to denote the property of gas flow in the bounded systems, which can be expressed as:

$$\lambda^* = \frac{\lambda}{1 + 0.7\, e^{-cy/\lambda}} \tag{12}$$

Where y is the distance normal to the wall, and C is a constant. Substituting λ^* as λ in Eq. (11) results in an effective relaxation time as follows:

$$\tau^* = \sqrt{\frac{2}{\pi}}\left(\frac{Kn\, c_s\, H}{1 + 0.7\, e^{-cy/\lambda}}\right) \tag{13}$$

Eq. (13) represents the effective relaxation time (ERT) for a bounded system. This ERT is used in Eq. (7) instead of τ.

Boundary conditions

Capturing slip flow in microchannels is done through appropriate boundary conditions. Several methods were used for capturing slip velocity in microchannel flows among them a commonly used boundary condition, called diffuse-scattering boundary condition (DSBC) [12] was used here. DSBC was used in the present work to capture the slip velocity at the wall. It is expressed a (see Fig. 4):

$$\left|(e_\alpha - u_w)\cdot n\right| f_\alpha = \sum_{(e_{\alpha'} - u_w).n<0} \left|(e_{\alpha'} - u_w)\cdot n\right| R_f(e_{\alpha'} \to e_\alpha) f_{\alpha'} \tag{14}$$

With

$$R_f(e_{\alpha'} \to e_\alpha) = \frac{A_N}{\rho_w}((e_\alpha - u_w)\cdot n) f_\alpha^{(eq)}\Big|_{u=u_w} \tag{15}$$

Where α' and α are directions of the incident and reflected particles, respectively. n is the inward unit normal vector of the wall and w indicates the wall boundary. A_N is a normalization coefficient and can be obtained by satisfying zero normal flux conditions on the wall. It is represented as follow:

$$A_N = \rho_w \frac{\sum_\alpha \left|(e_\alpha - u_w)\cdot n\right| f_\alpha}{\left|(e_\alpha - u_w)\cdot n\right| f_\alpha^{(eq)}\Big|_{u=u_w} \sum_\alpha \left|(e'_\alpha - u_w)\cdot n\right| f_{\alpha'}} \tag{16}$$

A_N depends on the velocity model used in the lattice Boltzmann method. Its value is 6 for D2Q9 model which is based on the fact of zero normal velocity at the wall.

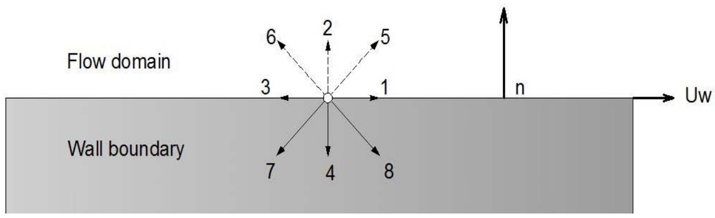

Fig. 4 Schematic diagram of the diffuse-scattering boundary condition based on the D2Q9 model (n is the inward normal vector of the wall boundary; solid arrow lines represent functions of the particles streaming from flow field while dashed arrow lines represent functions of the particles diffused from the boundary).

For the horizontal wall boundary with flow on its upside as shown in Fig. 4, the distribution functions at α = 2, 5 and 6 directions pointing to the flow field from outside the wall are unknown and the distribution functions at α =1, 3, 4, 7 and 8 are known because of the stream from the points inside the flow field. The unknown distribution functions can be determined from the known distribution functions. For the wall boundary shown in Fig. 4, Eqs. (14) to (16) can be simplified to the following explicit forms [12]

$$f_2 = \frac{A_N}{\rho_w} f_2^{eq}(\rho_{w,} u_w)(f_4 + f_7 + f_8) \qquad (17\text{ a})$$

$$f_5 = \frac{A_N}{\rho_w} f_5^{eq}(\rho_{w,} u_w)(f_4 + f_7 + f_8) \qquad (17\text{ b})$$

$$f_6 = \frac{A_N}{\rho_w} f_6^{eq}(\rho_{w,} u_w)(f_4 + f_7 + f_8) \qquad (17\text{ c})$$

RESULTS AND DISCUSSION

To demonstrate advantages of the present LBM approach with ERT introduced above, a long micro channel flow is investigated for a range of Knudsen number in this section. Validate the ERT-LBE was done using the information-preservation direct simulation Monte Carlo (IP-DSMC) and DSMC methods. For comparison, the LBM results of Shen et al. [13] were also included. The ratio of length L to height H of the channel was considered as 100, and the ratio of the pressure at the inlet to the one at the outlet was selected as 1.4 and 2 in our simulations. Three cases were studied according to the Knudsen number at the exit, i.e., $Kn_{out} = 0.0194, 0.194$, and 0.388. This problem has also been used to test the validity of the LBE for microgas flows.
A regular lattice with 2000×20 nodes is used; such number of nodes is required to achieve grid-independent solutionFor two walls, the DSBC and the linear extrapolation method [14] were used to specify the pressure boundary condition at the inlet and outlet.
Figs. 5, 6 and 7 illustrate the normalized streamwise velocity $u/U_{\max}$ at the outlet of the channel for Kn_{out} of 0.0194, 0.194 and 0.388 respectively. As is observed in figure 5, velocity profile obtained from present computation has better correspondence with DSMC for Kn_{out} = 0.0194 as compared to that obtained from LBM. However, LBM computations of Shen et. al. [13] are also in reasonable agreement with DSMC. Velocity profiles computed for Kn_{out} of 0.194 and 0.388 (Figs. 5 and 6) show much discrepancy for those obtained from LBM as compared to the present computation when they are compared to DSMC. Therefore, ERT-LBE is capable of predicting relatively accurate flow for transition flow regimes.
Figures 8, 9 and 10 represent pressure distribution along the channel centerline for the same Kn_{out} mentioned before. As is observed in figure 8, both LBM and present ERT-LBM pressure computations follow the same trend of DSMC for Knout = 0.0194, while ERT-LBM mimics the behavior of DSMC better thatn LBM. Figures 9 and 10 show that pressure distribution obtained from LBM is totally unacceptable for such flow configuration. However, pressure computations obtained from ERT-LBM follow those of DSMC reasonably for Kn_{out} of 0.194 and 0.388.
As expected, using ERT-LBE leads to a significant improvement in the accuracy of the results in contrast to the normal LBM. At $Kn_{out} = 0.0194$, the flow is in the near continuum or the slip flow regime. In this case, the ERT-LBE results agree well with the information-preservation DSMC (IP-DSMC) and the DSMC results of Chen et al. [14]. The difference in maximum $(P - P_{linear})/P_{out}$ obtained by the LBE and IP-DSMC increases as Kn_{out} increases. The difference in $u/U_{\max}$ is relatively small when $Kn_{out} = 0.194$, but becomes larger near the wall when $Kn_{out} = 0.388$.

CONCLUSION

A computational procedure based on Lattice Boltzmann Method with effective relaxation time (ERT) was used for flow computation in a long microchannel with length to height ratio of 200. Such effective relaxation time is capable of predicting flow for higher Knudsen numbers, the ones that occur in transition flow regimes. ERT-LBM results obtained for velocity distribution across the channel show good agreement with those obtained from Direct Simulation Monte Carlo Method (DSMC); LBM results represent remarkable discrepancies especially near walls. Results obtained for pressure distribution along the channel reveal the fact that LBM computations is totally unacceptable for Knudsen numbers greater than 0.1, while those of ERT-LBM are in reasonable agreement with DSMC.

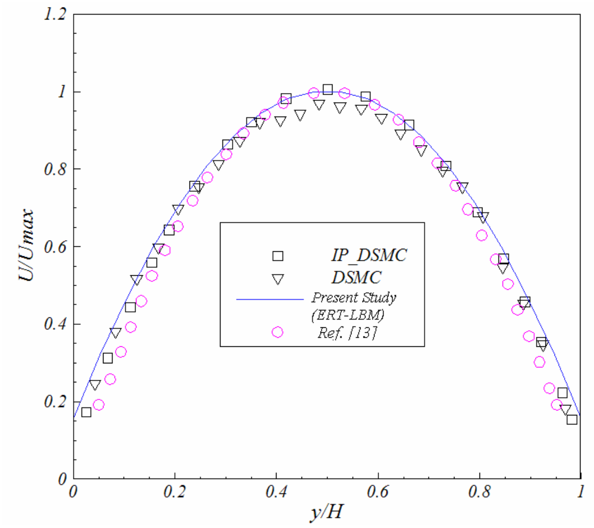

FIG. 5. Streamwise velocity at the exit. Comparison of ERT-LBM (LBM with effective mean free path), normal LBM (without effective mean free path), DSMC, and IP simulations,, Kn_{out} =0.0194, pressure ratio=1.4. DSMC and IP-DSMC data are taken from Ref. [8].

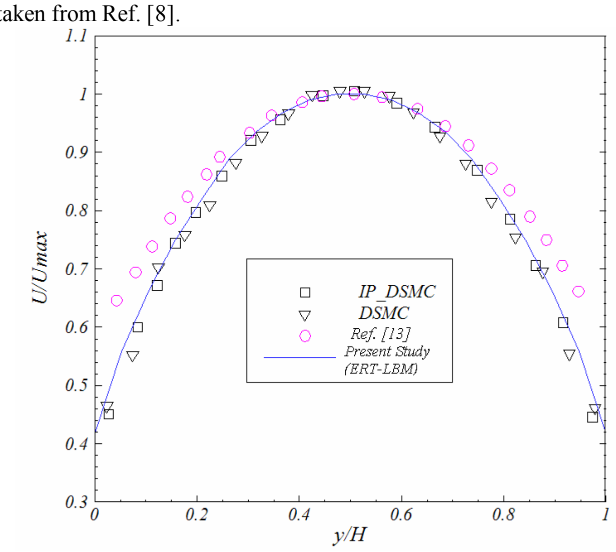

FIG. 6. Streamwise velocity at the exit. Kn_{out} =0.194, pressure ratio=2.0.

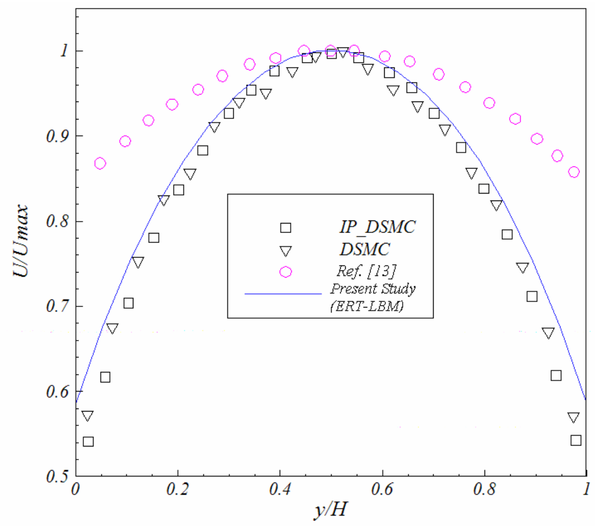

FIG. 7. Streamwise velocity at the exit. Kn_{out} =0.388, pressure ratio=2.0.

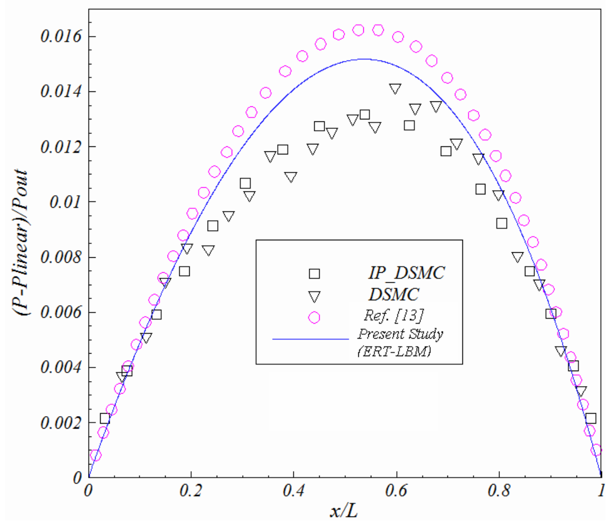

FIG. 8. Pressure along the channel centerline. Comparison of ERT-LBM, normal LBM, DSMC, and IP simulations,, Kn_{out} =0.0194, pressure ratio=1.4.

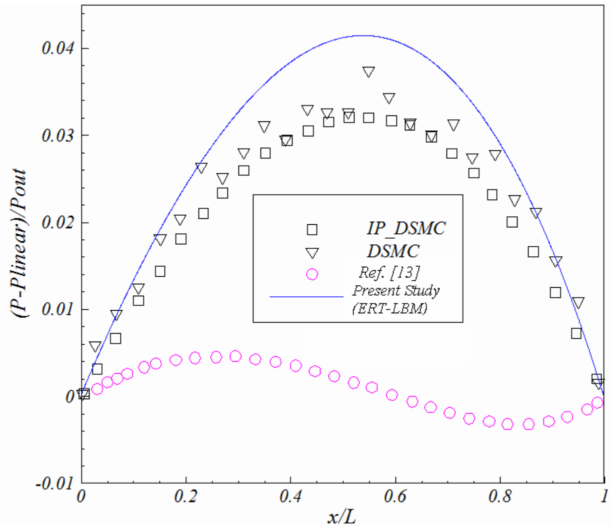

FIG. 9. Pressure along the channel centerline. Kn_{out} =0.194, pressure ratio=2.0.

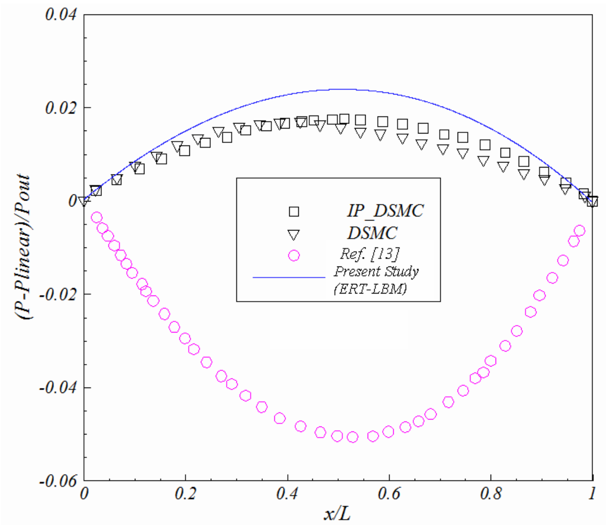

FIG. 10. Pressure along the channel centerline. Kn_{out} =0.388, pressure ratio=2.0.

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