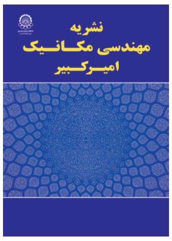

Amirkabir Journal of Mechanical Engineering

Amirkabir Journal of Mechanical Engineering, 49(3) (2017) 215-218
DOI: 10.22060/mej.2016.734

Thermal Lattice Boltzmann Method for Curved Boundaries in the Transition Regime

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ABSTRACT: The three-dimensional thermal lattice Boltzmann-BGK model is developed to simulate the pressure-driven rarefied gaseous flow within a circular channel with constant-temperature-wall in the transition regime (0.1 <Kn<1). The D3Q15 model has been employed for velocity discretization. The captured nonlinear behavior of gas in the Knudsen layer, which dominates the flow characteristics in small-scale gaseous flows by modifying the near-wall correction function along with the variation of properties with density and temperature distributions are implemented in a new formulation. An appropriate combination of advanced straight boundary conditions and a 3D extension of an available curved boundary conditions by identifying the nodes either adjacent to the solid nodes or flow nodes on the computational domain with the structured mesh are employed. The results of small-scale phenomena such as slip-velocity and temperature-jump are reported, which are manifestations of the cases with non-zero Knudsen number. Due to the deficiency of the continuum presumption for high-Knudsen flows, the present study suggests that the TLBM is an efficient tool applicable to the theoretical development of low speed gas flow study, which typically falls within the realm of MEMS/NEMS by virtue of its more straightforward boundary treatments and higher computation capability compared to other atomistic approaches.

Review History:

Received: 27 September 2015
Revised: 27 January 2016
Accepted: 11 April 2016
Available Online: 14 August 2016

Keywords:

Thermal lattice Boltzmann method
Three-Dimensional flow
Curved-boundary
High-Knudsen
Nanoscale

1- Introduction

The Thermal Lattice Boltzmann Method (TLBM) has been increasingly used to simulate the rarified flow and heat transfer in nanofluidics. The use of complex geometries in modern devices necessitates the implementation of curved boundary conditions for high Knudsen numbers. Previous studies showed that the TLBM is capable of correctly modeling the high Knudsen flows for curved boundaries [1-3].

In this paper a universal 3D TLBM algorithm, which concurrently includes all phenomena of nanoscale flows, is developed.

2- Thermal Lattice Boltzmann Method

The discretization of Boltzmann equation with two distinct distribution functions and the BGK model for collision term is as follows.

$$f_i\left(\vec{x}+c_i\delta t, t+\delta t\right)-f_i\left(\vec{x},t\right)= -\frac{1}{\tau_v}\left[f_i\left(\vec{x},t\right)-f_i^{eq}\left(\vec{x},t\right)\right]+F \tag{1}$$

$$g_i\left(\vec{x}+c_i\delta t, t+\delta t\right)-g_i\left(\vec{x},t\right)= -\frac{1}{\tau_c}\left[g_i\left(\vec{x},t\right)-g_i^{eq}\left(\vec{x},t\right)\right] \tag{2}$$

where f and g are density and internal energy distribution functions, respectively. The subscript eq refers to the Maxwell-Boltzmann distribution. The velocity discretization model is D3Q15. The macroscopic parameters, the diffusion coefficients, and the Knudsen number can be calculated based on Eqs. (3-4).

$$\rho=\sum_i f_i,\ \rho\vec{V}=\sum_i f_i c_i,\ \rho\varepsilon=\sum_i g_i$$
$$\nu=\frac{1}{3}(\delta_v-0.5)c^2\delta t,\ k=\frac{5}{9}(\tau_c-0.5)c^2\delta t \tag{3}$$

$$Kn=\sqrt{\frac{8}{3\pi}}\frac{(\tau_v-0.5)}{N_H} \tag{4}$$

In order to capture the Knudsen layer in 3D simulation, the mean-free-path of near-wall particles should be modified based on Eq. (5)

$$\lambda_e=\frac{\lambda}{1+0.7\left(e^{-cy/\lambda}+e^{-c(D-y)/\lambda}+e^{-cz/\lambda}+e^{-c(D-z)/\lambda}\right)} \tag{5}$$

In this relation C=1. So, the modified relaxation time is

$$\tau_v'=(\tau_v-0.5)/[1+\psi\left(\frac{y}{\lambda}\right)+\psi\left(\frac{D-y}{\lambda}\right)+\psi\left(\frac{z}{\lambda}\right)+\psi\left(\frac{D-z}{\lambda}\right)]\times\frac{\rho_{ref}}{\rho}\left(\frac{\varepsilon}{\varepsilon_{ref}}\right)^{\omega-0.5}+0.5 \tag{6}$$

where ω=1. The relation between two relaxation times is expressed in Eq. (7).

$$\tau_c=\frac{\tau_v-0.5}{\Pr}+0.5 \tag{7}$$

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3- Curved Boundary Treatment

Fig. 1 shows the configuration of fluid interior and exterior nodes with respect to the curved boundary. Circles and squares show the nodes located on the wall and in the fluid, respectively. The relation for computing the unknown distribution function involving q<0.5 and q>0.5 are presented in Eqs. (8-9), respectively.

$$f_{14}(x_j,y_j,z_j,t+1)=q(1+2q)f_7^+(x_j,y_j,z_j,t)+ (1-4q^2)f_7^+(x_d,y_d,z_d,t)-q(1-2q)f_7^+(x_e,y_e,z_e,t) \quad (8)$$

$$f_4(x_j,y_j,z_j,t+1)=\frac{1}{q(1+2q)}f_2^+(x_j,y_j,z_j,t)+ \frac{(2q-1)}{q}f_4(x_f,y_f,z_f,t+1)-\frac{(2q-1)}{(2q+1)}f_4(x_g,y_g,z_g,t+1) \quad (9)$$

For other boundary points such as inlet and outlet, the methods presented in references [1-6] were used.

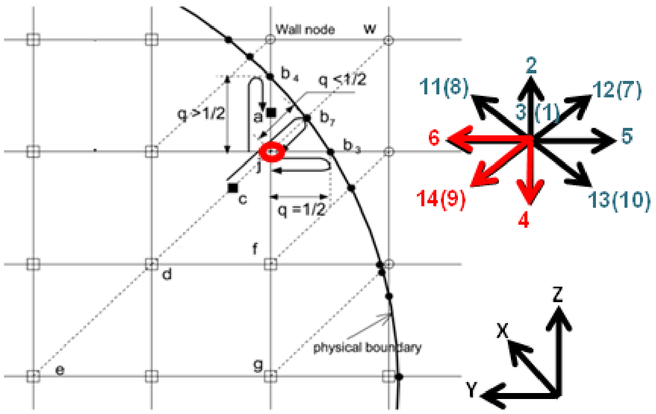


Figure 1. A sample curved boundary treatment and unknown directions for a numerical node adjacent to the boundary

4- Results and Discussion

The numerical results were verified based on the data provided in references [7-9]. Then the mesh-independence test was performed.

Fig. 2 shows the variation of internal energy in radial direction for Kn=0.2 to 1 at x/L=0.01. It demonstrates that by increasing the Kn number the rarification effect of the gas near wall increases, the Kn layer thickens, the minimum temperature is suppressed, and the value of jumped temperature enhances. Fig. 3 illustrates the variation of the CfRe and the Nusselt number with respect to the Knudsen number. The decreasing trend of these figures originates from the slip of flow over walls and the increase of the slip length.

5- Conclusions

The 3D TLBM-BGK simulation of high-Knudsen flows in a nanotube was presented. The formation of the Kn-layer, the dependence of MFP with temperature and location, temperature-jump condition, velocity slip, the compressibility effect, and non-linear axial pressure distribution were captured up to Kn=1. It can be concluded that the TLBM method is an appropriate method for high-Knudsen flow simulations involving curved boundaries.

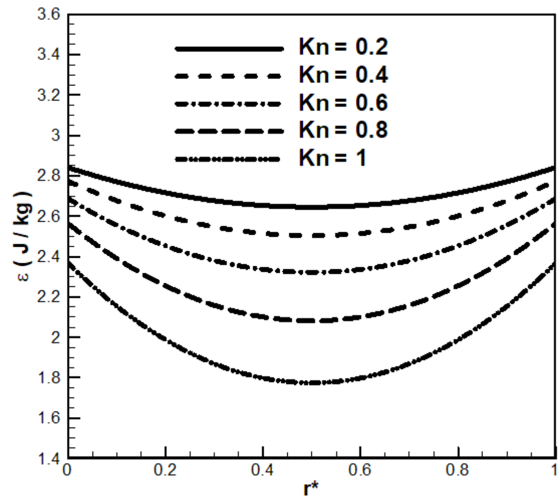
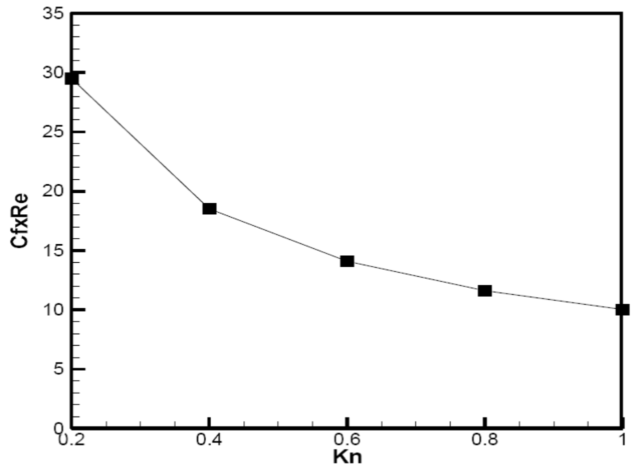
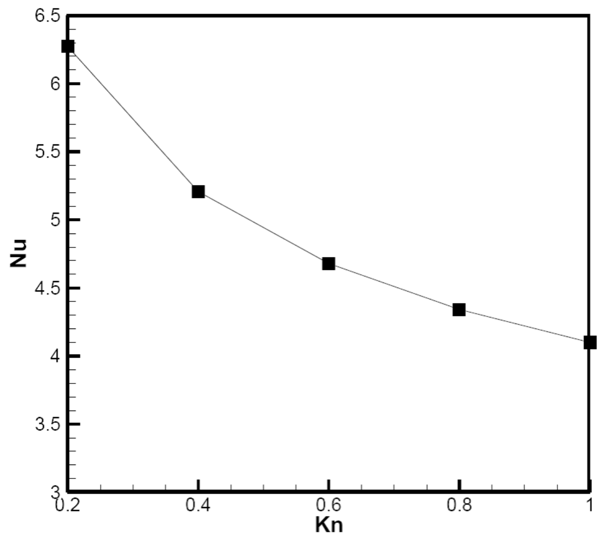


Figure 2. Internal energy distribution in radial direction for various Knudsen numbers in axial position of 0.01



(a)



(b)

Figure 3. Variation of a) $C_f Re$, b) Nusselt number, for nano-tubes at different Knudsen numbers

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Please cite this article using:

J. Ghazanfarian, D. Jamshideasli, A. Abbassi, "Thermal Lattice Boltzmann Method for Curved Boundaries in the Transition Regime" *Amirkabir J. Mech. Eng.*, 49(3) (2017) 617-624.

DOI: 10.22060/mej.2016.734