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Lattice Boltzmann Flow Simulation in a Combined Nanochannel

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Abstract. The widely used micro-flow wall-boundary conditions for lattice Boltzmann method (LBM) are evaluated in a force driven combined nanochannel flow. The flow field consists of a two-dimensional nanochannel (mother channel) of an infinite length having flat plates of a finite length inside. The flat plate is set above the bottom wall of the nanochannel with a narrow gap. The flow, thus, develops through this narrow gap (narrower channel) and the other side of the plate (wide gap). The Knudsen number based on the mother channel height is Kn=0.14 whereas the characteristic Knudsen number in the narrower channel is 1.1. To obtain the reference data, the molecular dynamics (MD) simulation is performed with a fully diffusive wall condition. The LBMs are based on the lattice BGK model and with the bounce-back/specular reflection (BSBC) and the diffuse scattering (DSBC) wall boundary conditions. The relaxation time is modified to include sensitivity to Kn. The DSBC shows generally satisfactory results in the test flow cases including fully developed force driven Poiseuille flows, where the BSBC performs worse at Kn>0.5 with a fixed bridge coefficient of b=0.7. This results in its overprediction of the flow rate in the narrower channel region since the characteristic Knudsen number there is 1.1. The MD simulation suggests that the flow develops gradually through the narrower channel region though all the LBM predictions show almost instant flow development. This fact suggests that the relaxation time model needs to have more sensitivity to the locally defined Kn. Further discussions of the BSBC with a different set of models suggest that the regularization process is required for predicting complex nanoscale flows.

AMS subject classifications: 47.61.-k, 47.61.Cb, 47.61.Fg, 47.11.-j, 47.11.Mn, 47.11.Qr

Key words: Lattice Boltzmann method, Knudsen number, molecular dynamics simulation, nanochannel, wall boundary condition, slippage velocity.

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1 Introduction

Due to the recent rapid development of micro flow devices applied in micro-total-analysis-systems (μ-TAS) and micro-electro-mechanical systems (MEMS), modeling and simulation methods for flows in such micro geometries have been of great interest in the society of computational physics [1]. Since the flow geometry in such systems is often in a sub-micron meter scale, those flows are usually distinguished by moderately high Knudsen numbers:

$$\mathrm{Kn} = \frac{\lambda}{H} > 10^{-2},$$

where λ is the molecular mean free path of the fluid and H is the characteristic length of the flow domain. Accordingly, when one considers treating such flows, it is necessary to understand the flows at the molecular level. The continuum Navier-Stokes equations are, however, no longer applicable to such levels of moderately high Knudsen number flows and the flow physics in such flows is described by the Boltzmann equation (BE) of the gas kinetic theory [2,3]. Although several numerical schemes have been proposed for solving micro flows, amongst them, the lattice Boltzmann method (LBM) has been proven as an effective scheme because of its kinetic origin and numerical efficiency. Indeed, the LBMs have been well investigated in micro flows so far [4–13].

At a finite Kn, the statistical fluid dynamics indicates that the fluid in the vicinity of a solid wall should have a net motion relative to the wall. In the LBMs, there have been several schemes to treat this slippage at a wall boundary in micro flows. By the conventional bounce-back wall boundary condition, Nie et al. [4] simulated 2-D microchannel and cavity flows at $0.01<\mathrm{Kn}< 0.4$ introducing Knudsen number dependency into the relaxation parameter of the lattice Boltzmann equation. Shen et al. [9] validated this strategy comparing with the direct simulation Monte Carlo (DSMC) computations of microchannel flows. Succi [5] introduced a mix of bounce-back and specular reflections for the wall boundary condition. Toschi and Succi [10] tested a virtual wall collision concept into the bounce-back and diffuse scattering boundary conditions. The diffuse scattering boundary condition was firstly proposed by Ansumali and Karlin [6]. Zhang et al. [11] applied Maxwellian scattering kernel to the wall conditions with an accommodation coefficient. Verhaeghe et al. [13] proposed a diffuse bounce-back model for fully diffusive stationary walls. The present authors' group [12] also discussed a strategy to simulate such flow topics by the LBM where the diffuse scattering wall boundary condition and the effective relaxation time associated with the Knudsen number are applied. In our LBM, since at least third-order Hermite expansion is required to model the momentum equation at the Burnett level for isothermal and small Mach numbers, the higher order discrete velocity model: D2Q21, model was used. Moreover, to guarantee the nonequilibrium moments of the LBM satisfied in the Hermite space, a modified regularization procedure [14] of the nonequilibrium part of the distribution function was introduced. The results were