International Communications in Heat and Mass Transfer 38 (2011) 1443–1448

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

DSMC simulation of subsonic flow through nanochannels and micro/nano backward-facing steps ☆

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ARTICLE INFO

Available online 16 August 2011

Keywords:
DSMC
Nanoflow
Microflow
Nanochannel
Backward-facing step
Subsonic flow

ABSTRACT

In this study, we use direct simulation Monte Carlo method to simulate subsonic flow in nanochannels and micro/nanoscale backward-facing (BF) step considering a wide range of Knudsen number regimes. The nanochannel flow simulation indicates that the nanoscale flow through the nanochannel resembles unique features such as encountering negative pressure deviation behavior and observing flat velocity profiles at higher Knudsen number regimes. On the other hand, the micro/nano BF step flow simulations demonstrate that the length of separation region considerably decreases as the flow becomes more rarefied and approaches the transition regime. Meanwhile, the variations in the flow properties are much slower in the mid-transition and free-molecular regimes compared with the slip and early transition regime cases.

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1. Introduction

Fast progress in micro/nanoscale devices has drawn the attention of many workers to extend suitable numerical tools to analyze nanoscale flows through basic geometries, e.g., channels, backward-facing (BF) steps, and nozzles, more accurately. However, the flow in such scales can be rarefied. Indeed, Knudsen number is known as a key parameter to measure the gas rarefaction in micro/nano scales. It is defined as the ratio of mean free path of gas molecules, λ, to one characteristic dimension of flow, L, i.e., $Kn=\lambda/L$. Using this definition, the non-rarefaction and rarefaction regimes can be categorized as no-slip ($Kn<0.01$), slip ($0.01<Kn<0.1$), transition ($0.1<Kn<10$), and free-molecular ($Kn>10$) ones. Based on the past experiences, the Navier–Stokes (NS) equations have been largely used to simulate the non-rarefied flows through basic macro-scale geometries subject to the classical no-slip boundary conditions [1–3] and the rarefied flows through basic micro/nano-scale geometries subject to the velocity slip and temperature jump boundary conditions [4–10]. However, the resulting inaccuracies in the latter cases are high enough to promote the researchers to use the kinetic-based approaches such as the direct simulation Monte Carlo (DSMC) method [11] in treating highly rarefied flows. As is known, DSMC is capable of solving flow for a wide range of rarefaction regimes with sufficient accuracies [12]. Bao and Lin [13] used the continuum-based Burnett equations and simulated the microscale BF step flows at transition regime. Their results were in good agreement with the DSMC solution; however, if $Kn<0.5$.

Literature shows that DSMC has been widely applied to simulate rarefied flows through the aforementioned basic geometries since many years ago. Beskok [14] used the DSMC solution to validate the accuracy of high order slip velocity boundary conditions in predicting BF step flows. Xue and Chen [15] and Xue et al. [16] used DSMC and simulated micro BF step flows in slip and transition regimes. Their results showed that the flow separation and recirculation, which are two main characteristics of the BF step flow in macroscales, would disappear if $Kn>0.1$. Agrawal et al. [17] simulated the rarefied slip flow regime in microchannels with sudden expansion or contraction using the Lattice Boltzmann method. Zhen et al. [18] used 2D and 3D DSMC calculations to evaluate heat transfer in short microchannels. Wang et al. [19,20] used DSMC and studied the flow and heat transfer behavior in microchannels with constant wall heat flux boundary condition. Roohi et al. [21] used DSMC and simulated the subsonic flow through micro/nanoscale channels. They studied the effects of different wall thermal boundary conditions on the flow field behavior. Gatsonis et al. [22] used an unstructured DSMC solver to study supersonic flow in 3D nanochannels. Hsieh et al. [23] used the DSMC and solved the flow through 3D microscale BF step. They indicated that the approaching level of 3D flows to 2D simplifications would be over 98% for the flow with a inlet Knudsen number of 0.041. The approaching level decreased as Kn increased. They also reported that the flow separation, recirculation, and reattachment would disappear as the cross-section aspect ratio became less than unity. Darbandi and Roohi [24] used an unstructured DSMC solver and studied the subsonic and supersonic flows in micro/nanoscale converging–diverging nozzles. They reported that the mixed impacts of rarefaction,

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☆ Communicated by W.J. Minkowycz.

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0735-1933/$ – see front matter © 2011 Elsevier Ltd. All rights reserved.
doi:10.1016/j.icheatmasstransfer.2011.08.002