International Journal of Heat and Mass Transfer 71 (2014) 633–638

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

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

Technical Note

Investigation of convective heat transfer through constant wall heat flux micro/nano channels using DSMC

Mojtaba Balaj [a], Ehsan Roohi [a,*], Hassan Akhlaghi [a], Rho Shin Myong [b]

[a] High Performance Computing (HPC) Laboratory, Department of Mechanical Engineering, Ferdowsi University of Mashhad, P.O. Box 91775-1111, Mashhad, Iran
[b] Department of Aerospace and System Engineering, Research Center for Aircraft Parts Technology, Gyeongsang National University, Jinju, Gyeongnam 660-701, South Korea

ARTICLE INFO

Article history:
Received 9 December 2013
Accepted 20 December 2013

Keywords:
Nusselt number
Micro/nano channel
DSMC
Wall heat flux
Iterative technique
Rarefaction
Brinkman number

ABSTRACT

In this research, convective heat transfer of the argon gas flow through a micro/nano channel with uniform heat flux wall boundary condition is investigated using the direct simulation Monte Carlo (DSMC) method. Both of the hot wall ($q_w > 0$) and the cold wall ($q_w < 0$) cases are considered. Implementation of wall heat flux in the DSMC method is performed using the recently developed "iterative" technique. Our investigation considers heat transfer behavior in both of slip and transition flow regimes. We investigate the influence of rarefaction, i.e., Knudsen number, and viscous dissipation, i.e., Brinkman number, on the Nusselt number behavior. We use the generalized hard sphere (GHS) collision model to consider accurate variation of the heat conductivity with the temperature. The DSMC solutions for the Nusselt number are compared with different analytical expressions reported in the literature with suitable accuracy through the slip regime. We observe that the dependency of the Nusselt number on the Knudsen number decreases in nanochannels as Knudsen number increases into the transition regime, i.e., Nusselt number approaches nearly a constant value as Knudsen number goes beyond 1. Additionally, it is shown that the Nusselt number is a weak function of the Brinkman number.

1. Introduction

During the past decades, direct simulation Monte Carlo (DSMC) method has been widely used to investigate flow fields ranging from hypersonic spacecrafts to small scale micro/nano systems [1]. Rapid development in high temperature power, propulsion and high density power electronics has introduced new opportunities and challenges in developing high temperature heat exchangers (HTHE) which are expected to exceed 2500 K [2]. An important issue in future development in micro/nano systems is applying efficient techniques to control thermal condition within allowable operating limits due to high power densities which are expected to exceed 25 W/cm^2 [3]. Because of decreasing in medium's density in small size geometries, flow rarefaction, i.e., Knudsen number, has a significant impact on the heat transfer. *Kn* number is defined as the ratio of the gas mean free path to the characteristic length of the geometry,

$$Kn = \lambda/H \tag{1}$$

Based on the generalized hard sphere (GHS) model, the mean free path of the gas is defined as follows

$$\lambda = \sqrt{\frac{\pi m}{2kT}}\left(\frac{\mu}{\rho}\right) \tag{2}$$

Small geometry size makes it important to take into account viscous dissipation. Viscous dissipation is usually considered in the Brinkman number (*Br*), which is the ratio of the viscous heat generation to the external heating:

$$Br_q = \frac{\mu u_b^2}{q_w 2H} \tag{3}$$

Both of *Kn* and *Br* numbers depends on the gas viscosity, which is a function of the gas temperature. This dependency will be further discussed in Section 2.

A key characteristic of the heat transfer behavior of a system is the Nusselt number (*Nu*), defined as follows:

$$Nu = \frac{2q_w H}{k(T_w - T_b)} \tag{4}$$

where the bulk temperature (T_b) is defined as

$$T_b = \frac{\int_A \rho u_x T dA}{\int_A \rho u_x dA} \tag{5}$$

There are a wide set of studies considering micro/nano channel flows in the slip flow range and beyond, i.e., Refs. [4–6]. Also there are theoretical and numerical investigations around the topic of

---

* Corresponding author. Tel.: +98 511 8805136; fax: +98 511 8763304.
E-mail address: e.roohi@ferdowsi.um.ac.ir (E. Roohi).

0017-9310/$ - see front matter © 2014 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ijheatmasstransfer.2013.12.053

Nomenclature

Q	heat flux
Kn	Knudsen number
Br	Brinkman number
H	channel height
T	temperature
m	molecular mass
d	molecular diameter
D_h	hydraulic diameter
k	thermal conductivity
Nu	Nusselt number
Re	Reynolds number
Pr	Prandtl number
RF	relaxation factor
PR	pressure ratio

Greek letters

α_T	thermal accommodation coefficient
α	momentum accommodation coefficient
λ	mean free path
κ	Boltzmann constant
γ	ratio of specific heats
μ	viscosity
ρ	density
σ	collision cross section
Γ	Gamma function
v	relative speed exponent of GHS model

Subscripts

w	wall
b	bulk
q	heat flux
0	reference

heat transfer in micro/nano rectangular channels in low to moderated Knudsen number ranges, i.e., slip flow regime, see Refs. [7–16]. Meanwhile, our literature survey shows that a wide class of the studies considering convective behavior of micro/nano channel is restricted to the analytical solution of the NS equations in the slip regime. The main focus of the current work is to investigate the convective heat transfer of pressure-driven micro/nano channels under specified wall heat flux condition from the slip to high transition flow regimes using the DSMC technique. To the best knowledge of the authors, there are not any archival publications considering the detailed behavior of the Nusselt number through constant wall heat flux (CWH) micro/nano channels using DSMC. Here, we provide a detailed comparison of the existing analytical relations for the Nusselt number in the slip regime with our DSMC solutions. We also discuss the dependency of the Nusselt number on the *Kn* and *Br* numbers under CWH condition from the slip to transition flow regime. In addition, the dependency of Nusselt number on heating/cooling wall heat fluxes magnitudes is investigated. Accurate molecular collision model, i.e., generalized hard sphere (GHS), is employed for considering the dependency of the heat conductivity on the temperature.

2. DSMC method

The DSMC method used in this paper follows the scheme proposed by Bird [17]. DSMC is a particle method based on the kinetic theory for simulation of dilute gases. The method is carried out by modeling the gas flow using many independent simulated particles. These simulated particles are representatives of a large number of real gas molecules in the flow field. The time step in the DSMC method is chosen as small as the positional changes of particles and their collisions could be decoupled for each time step. In order to implement DSMC, flow field must be divided into computational cells. The size of each cell should be small enough to result in small changes in thermodynamic properties across each cell. The cells provide geometric boundaries and volumes, required to sample macroscopic properties. It is also used as a unit where only particles located within the same cell at a given time are allowed for collision. The cells are then typically divided into subcells in each direction. Subcells are utilized to increase the accuracy of the selection of collision pairs.

In the current study, the previous code of Roohi and co-workers [18–23] is extended to simulate rarefied flow in the micro/nano channel geometry. The GHS collision model, introduced by Hassan and Hash [24], is used to consider accurate variation of the viscosity with the temperature. This model is an extension of the variable hard sphere (VHS) model to include terms that allow modeling of molecules with both repulsive and attractive potentials. For the GHS model, the total collision cross section could be written as follows:

$$\sigma = \sigma_0(\phi(g_0/g)^{2\nu_1} + (1-\phi)(g_0/g)^{2\nu_2}) \tag{6}$$

where $\sigma_0(=\pi d_0^2)$ is the reference cross section, $g=\sqrt{4RT}$ and the parameters with subscript zero are calculated at the reference temperature (T_0). The choice of the collision pair is done based on the no time counter (NTC) method. Monatomic argon, $m = 6.63 \times 10^{-26}$ kg and $d_0 = 4.17 \times 10^{-10}$ m, is considered as the working fluid. In order to ensure the satisfaction of the limits on the cell size, the cell dimensions are considered as 0.1λ and are much smaller than that for most cases. 30 molecules are set in each cell to minimize the scattering noise. All walls are treated as diffuse reflectors using the full thermal accommodation coefficient. Half-range Maxwellian distribution is used to determine the velocity of wall-reflected particles. After achieving steady flow condition, sampling of flow properties within each cell is fulfilled during sufficient time period to suppress the statistical scatters of the solution. All thermodynamic parameters such as velocity, density, and temperature are then determined from this time-averaged data. Inlet/outlet pressure boundary conditions are imposed according to the formula suggested by Wang and Li [25]. The wall heat flux is imposed in the DSMC solver using either the iterative technique developed by Akhlaghi et al. [20] or inverse temperature sampling technique suggested by Wang et al. [26]. Our Investigation showed both methods provide almost the same solutions, indicating the independency of the solutions from the method of implication of wall heat flux boundary condition [20].

To calculate the Nusselt number, the thermal conductivity of the gas is related to the gas viscosity as follows:

$$k = (15/4)(\kappa/m)\mu \tag{7}$$

For GHS collision model, gas viscosity is computed according to the following relation [27]:

$$\mu = \frac{15\sqrt{\pi}}{16\Gamma(4-\nu_1)}\frac{(T/T_0)^{0.5+\nu_1}}{(\phi+(1-\phi)S_0(T_0/T)^{\nu_2-\nu_1})}\frac{mg_0}{\sigma_0} \tag{8}$$

For argon gas flows, Macrossan [27] showed that an accurate variation of the viscosity with the temperature could be obtained with $\upsilon_1 = 2/13$, $\phi = 0.61$ and $\upsilon_2 = 14/13$. Macrossan [27] showed that argon viscosity computed by the GHS model agrees well with the experimental data for a wide range of temperature. As the GHS model benefits from a molecular-based model which simulates the collisions correctly, it accurately considers the dependency of the viscosity on the temperature. Therefore, in this work, GHS collision model is employed for Nusselt number calculations.

3. Results and discussion

3.1. Comparison of the Nusselt number with the analytical expressions

There are a wide set of analytical expressions for *Nu* number variations with the Knudsen number. Colin [16] provided a detailed comparison between the analytical expressions for *Nu* number in microchannels with different cross-sections. We compare our DSMC results for *Nu* number with four analytical relations for parallel plate channels with CWH as follows:

(1) Inman correlation [7]

$$Nu = \left[\frac{\xi}{4} + \frac{17 + 84\zeta + 105(\zeta)^2}{140(1+3\zeta)^2}\right]^{-1}, \quad \xi = \frac{2-\alpha_T}{\alpha_T}\frac{8\gamma}{\gamma+1}\frac{1}{\Pr}Kn,$$
$$\zeta = 4Kn\frac{2-\alpha}{\alpha} \tag{9}$$

(2) Miyamoto et al. correlation [9]

Miyamoto et al. [9] analyzed the effect of viscous heating in constant heat flux situation. In the case of full diffusive walls for argon flow, their expression is as follows

$$Nu = \left(\frac{9Br}{(1+6Kn)^2}\left[\frac{3+42Kn+140Kn^2}{35(1+6Kn)} + \frac{4(\frac{2\gamma}{\gamma+1})Kn^2}{\Pr}\right] + \frac{17+168Kn+420Kn^2}{140(1+6Kn)^2} + \frac{\frac{2\gamma}{\gamma+1}Kn}{2\Pr}\right)^{-1} \tag{10}$$

(3) Aydin and Avci [11]

Effects of viscous heating have been considered by Aydin and Avci [11]. In the case of full diffusive walls, they proposed the following correlation.

$$Nu = 4\left[\frac{1}{3}\left(1 + \frac{12\gamma}{\gamma+1}\frac{Kn}{\Pr}\right) + \frac{8Br}{35(1+6Kn)^4} + \frac{44Br}{35(1+6Kn)^3} + \frac{2(1+84Br)}{105(1+6Kn)^2} + \frac{2}{15(1+6Kn)}\right]^{-1} \tag{11}$$

(4) Hooman [28]

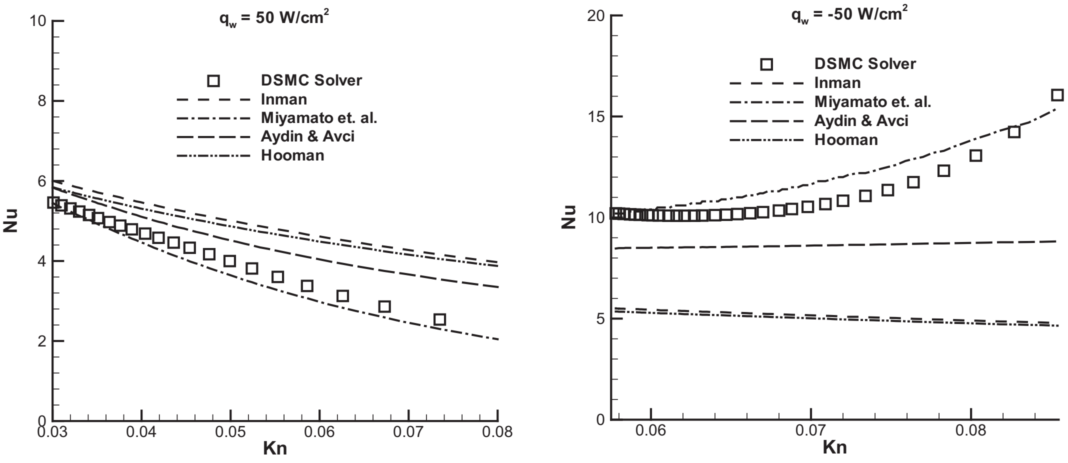
Hooman suggested a correlation using superposition approach. For parallel plate microchannels, the correlation is simplified as below

$$Nu = \left(\frac{2-\alpha_T}{\alpha_T}\frac{2\gamma}{1+\gamma}\frac{0.5Kn}{\Pr} + \frac{17\alpha + 84Kn\alpha + 0.5(24-12\alpha)Kn(14+70Kn)}{140(1+6Kn)(\alpha + (24-12\alpha)0.5Kn)}\right)^{-1} \tag{12}$$

Fig. 1 compares the analytical solutions (Eq. (9) through Eq. (12)) with the current DSMC solution for the Nusselt number variations along a microchannel with a pressure ratio (PR) of 3 for argon gas ($Pr = 2/3$ and $\gamma = 5/3$) subject to CWH equal to 50 and $-50\ \text{W/cm}^2$. We removed the results corresponding to the entrance effects from the DSMC solution because all analytical solution assumed fully developed flow. The analytical solutions do not exactly match each other as they were derived assuming different assumptions. In the case of $q_w = 50\ \text{W/cm}^2$, our DSMC solution is close to Eq. (10) (Miyamoto et al. relation). Fig. 1(b) compares the *Nu* number calculated with the DSMC solver and different analytical solutions for a cold wall subject to $-50\ \text{W/cm}^2$ wall heat flux. In the cooling case, even the trends of analytical solutions are different, i.e., Miyamoto et al. [9] correlation shows that the *Nu* number increases along the channel, Aydin and Avci [11] relation predicts a very slight increase in *Nu* while two other correlations, Inman [7] and Hooman [28] correlations, suggest that *Nu* number slightly decreases with the increase in *Kn* number. Again, our DSMC solution is close to Eq. (10) which considers the viscous dissipation suitably.

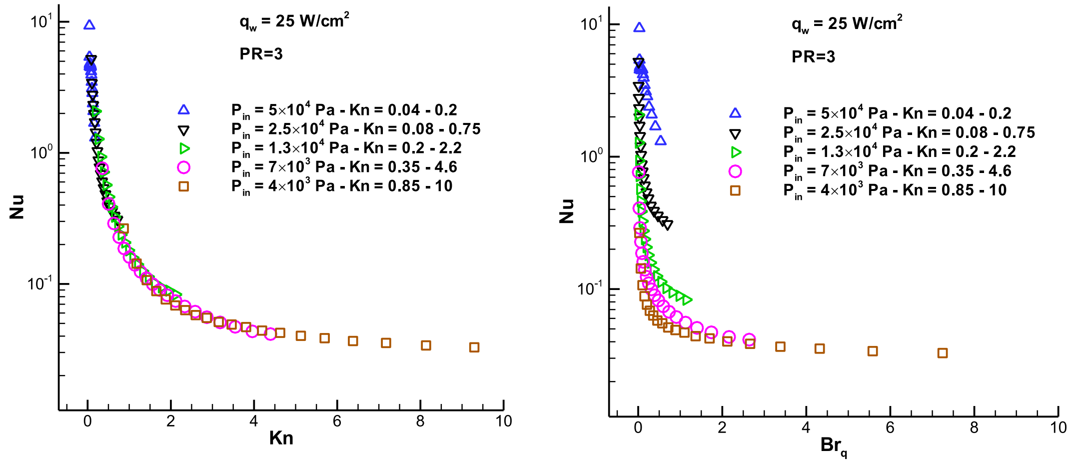
3.2. Dependency of the Nusselt number on Kn and Br

Now we consider the variations of the Nusselt number with *Kn* for slip and transition regimes. Fig. 2(a) shows variations of *Nu* number with *Kn* obtained from five different independent test cases covering a wide range of *Kn* number. As the figure shows, independent solutions overlap each other. Nusselt number decreases monotonically with increasing the Knudsen number at constant wall heat flux condition. Also it shows that the Nusselt number is less dependent on *Kn* at higher Knudsen numbers, i.e.,



(a) Heating condition (b) Cooling condition

Fig. 1. Comparison of *Nu* number from the DSMC with different analytical methods.



(a) (b)

Fig. 2. Variation of Nu number with (a) Kn number and (b) Br_q number for q_w = 25 W/cm^2.

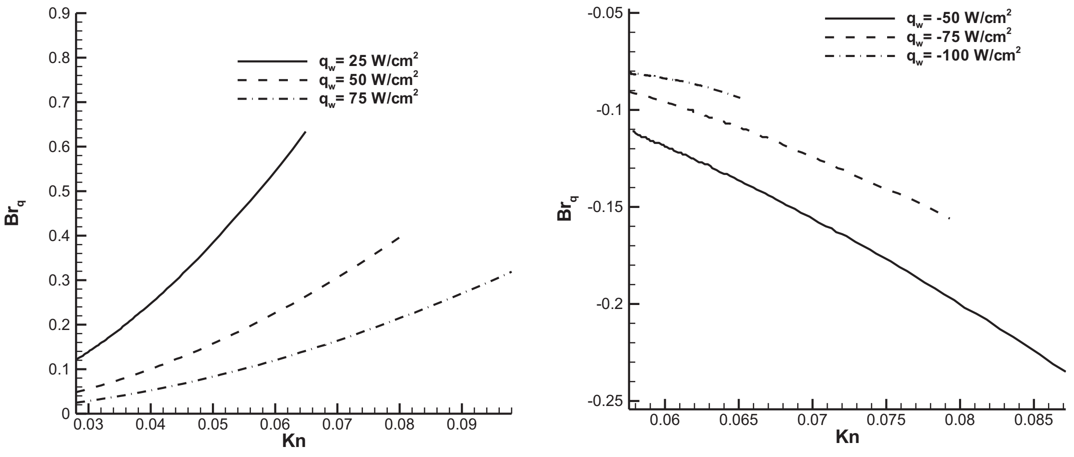
nanochannel flows. The decrease in Nusselt number of nanochannels could be attributed to decrease in inter-molecular collisions at higher Kn flows. As the inter-molecular collisions decrease, the effects of wall heat flux are not transmitted into the bulk region while T_w increase due to the wall heating, therefore, Nu number decreases.

Fig. 2(b) shows the variation of the Nu number with the Brinkman number for the five test cases. According to this figure, Nu number decreases as Brinkman number increases. But Fig. 2(b) demonstrates that at constant Brinkman number there are more than one Nu, i.e., it implies that the Nu number is a function of Kn and Br numbers, however, the functionality of Nu number on the Kn number is much stronger than Br number, i.e., once we plotted Nu vs. Kn we obtained one graph for all cases (see Fig. 2(a)). However, once Nu. vs. Br was depicted, it is observed that the solution depends on Kn as well. This fact was observed in analytical solutions. Inman [7] and Hooman [28] did not consider Br number in their analytical solution due to this weak dependency. Miyamoto et al. [9] and Aydin and Avci [11] considered the effect of viscous heating (Br number), while the terms which include Br number in their equations have lower powers compared to the Kn number. Meanwhile, as our comparison in Fig. 1-(b) showed, the effect of viscous dissipation is important in cooling cases and it must be considered during the Nusselt number derivation.

3.3. Dependency of flow parameters on wall heat flux

Nusselt number variation depends on the bulk and wall temperature distributions, rarefaction (Kn number), and viscous dissipation (Br number) along the channel. Shown in Fig. 3 is the variations of the Brinkman number along the channel centerline. Br number increases for heating wall boundary condition and decreases for cooling cases. Additionally, the magnitude of Br number decreases as the magnitude of wall heat flux increases.

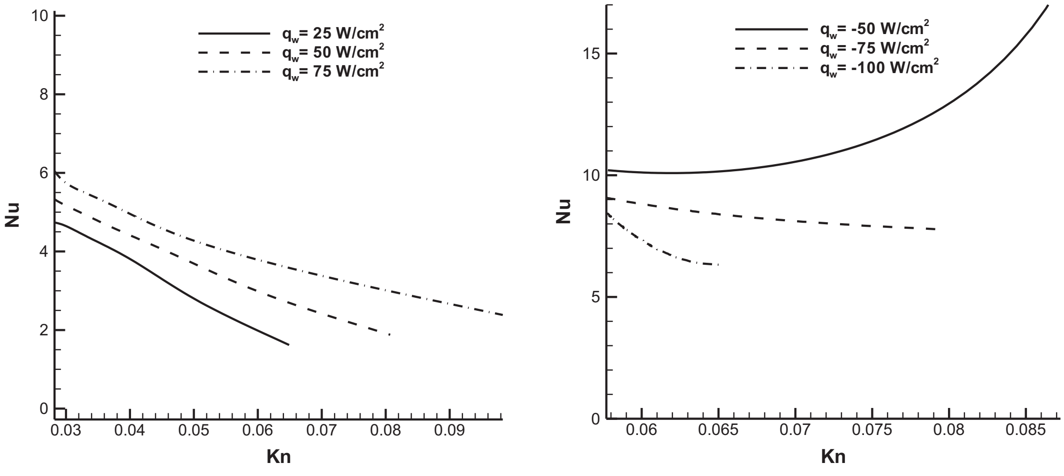
Fig. 4 shows the variations of Nu number with the Kn for different wall heat flux magnitudes. According to Fig. 4(a), in the case of heated wall, higher wall heat flux results in greater Nu number. Meanwhile, Fig. 4(b) shows that as the magnitude of cooling heat flux increases, Nu number decreases. This is expected according to the Nu number definition; however; the effect of increase/decrease in q_w on Nu number is not linear because q_w affects bulk and wall temperature simultaneously. As it is known, the main driving mechanism for the heat transfer from the wall to the fluid is the temperature difference between the wall and the bulk fluid. In



(a) Heating condition

(b) Cooling condition

Fig. 3. Variation of Br_q number with the Kn number at different wall heat flux magnitudes.



(a) Heating condition (b) Cooling condition

Fig. 4. Variation of *Nu* number with the *Kn* number at different wall heat flux.

the case of heating wall, the wall temperature is greater than the bulk temperature. Meanwhile, viscous dissipation increases the bulk fluid temperature. This increase leads to decrease in the wall-bulk flow temperature difference. However, for cooling wall heat flux, the viscous dissipation increases the temperature difference by increasing the fluid bulk temperature while wall temperature is reduced due to the wall cooling. Therefore, from Figs. 3 and 4, it can be concluded that increasing *Br* in the negative direction increases the *Nu* number. When cooling boundary is applied, viscous dissipation decreases along the channel, see Fig. 3(b). As viscous dissipation acts as an internal heating effect for the fluid temperature, decreasing of *Br* may lead to decrease in temperature difference and may lead to an increase in *Nu* number.

4. Conclusions

The convective heat transfer of argon gas flow from the slip to the transition flow through a parallel plate micro/nano channel with the uniform heat flux wall has been investigated using the DSMC technique. The study considered the influence of rarefaction and viscous dissipation on the Nusselt number. We used the GHS collision model to calculate thermal conductivity and viscosity as a function of temperature accurately. Among different analytical Nusselt number relations, we showed that relation developed by Miyamoto et al. is the closest one to our DSMC solution as it suitably considers viscous dissipation effects. It was observed that Nusselt number increases as wall heat flux increases at constant *Kn* number. However, Nusselt number decreases gradually as Knudsen number increases in the slip flow range and beyond. The dependency of Nusselt number on the Knudsen number decreases in the transition flow range and *Nu* number approximately approaches a constant value at high *Kn* number flows. Additionally, we showed that the effects of Knudsen number is stronger than the Brinkman number on the Nusselt number behavior.

Acknowledgment

This work is financially supported by Ferdowsi University of Mashhad under grant No. 24992. This work was also supported partially by the National Research Foundation of Korea funded by the Ministry of Education, Science and Technology (NRF 2012-R1A2A2A02-046270 and NRF 2009-0094104), South Korea. The authors would like to thank Prof. Stefan Stefanov from Institute of Mechanics, Bulgarian Academy of Science and anonymous reviewers for their valuable comments and suggestions for improving the quality of this paper.

References

[1] W. Liou, Y. Fang, Microfluid Mechanics, Principles and Modeling, McGraw-Hill, New York, 2006.

[2] M. Ohadi, G. Buckley, High temperature heat exchangers and microscale combustion systems: applications to thermal system miniaturization, Exp. Therm. Fluid Sci. 25 (2001) 207–217.

[3] G.C. Birur, T.W. Sur, A.D. Paris, P. Shakkottai, A.A. Green, S.I. Haapanen, Micro/nano spacecraft thermal control using MEMS-based pumped liquid cooling system, Proc. SPIE Microflui. BioMEMS 4560 (2001) 196–206.

[4] G.H. Tang, Y.L. He, W.Q. Tao, Comparison of gas slip models with solutions of linearized Boltzmann equation and direct simulation of Monte Carlo method, Int. J. Mod. Phys. C 18 (2007) 203–216.

[5] N. Dongari, A. Agrawal, A. Agrawal, Analytical solution of gaseous slip flow in long microchannels, Int. J. Heat Mass Transfer 50 (2007) 3411–3421.

[6] N. Dongari, A. Agrawal, Modeling of Navier-Stokes equations for high Knudsen number gas flows, Int. J. Heat Mass Transfer 55 (2012) 4352–4358.

[7] R. Inman, Laminar slip flow heat transfer in a parallel plate channel or a round tube with uniform wall heating, NASA Technical Note D-2393, 1964.

[8] C.P. Tso, S.P. Mahulikar, The use of the Brinkman number for single phase forced convective heat transfer in microchannels, Int. J. Heat Mass Transfer 41 (12) (1998) 1759–1769.

[9] M. Miyamoto, W. Shi, Y. Katoh, J. Kurima, Choked flow and heat transfer of low density gas in a narrow parallel-plate channel with uniformly heating walls, Int. J. Heat Mass Transfer 46 (2003) 2685–2693.

[10] R.S. Myong, D.A. Lockerby, J.M. Reese, The effect of gaseous slip on microscale heat transfer: An extended Graetz problem, Int. J. Heat Mass Transfer 49 (2006) 2502–2513.

[11] O. Aydin, M. Avci, Analysis of laminar heat transfer in micro-Poiseuille flow, Int. J. Therm. Sci. 46 (2007) 30–37.

[12] N.P. Gulhane, S.P. Mahulikar, Variations in gas properties in laminar micro-convection with entrance effect, Int. J. Heat Mass Transfer 52 (2009) 1980–1990.

[13] A. Sadeghi, M.H. Saidi, Viscous dissipation and rarefaction effects on laminar forced convection in microchannels, ASME J. Heat Transfer 132 (2010) 072401.

[14] Z. Sun, Y. Jaluria, Convective heat transfer in pressure-driven nitrogen slip flows in long microchannels: the effects of pressure work and viscous dissipation, Int. J. Heat Mass Transfer 55 (2012) 3488–3497.

[15] G. Hadjiconstantinou, O. Simek, Constant-wall-temperature Nusselt number in micro and nano-channels, J. Heat Mass Transfer 124 (2002) 356–364.

[16] S. Colin, Gas microflows in the slip flow regime: a critical review on convective heat transfer, ASME J. Heat Transfer 134 (2012) 020908.

[17] G.A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Oxford Science, Oxford, U.K, 1994.

[18] E. Roohi, M. Darbandi, Extending the Navier-Stokes solutions to transition regime in two-dimensional micro- and nanochannel flows using information preservation scheme, Phys. Fluids 21 (2009) 082001.

[19] O. Ejtehadi, E. Roohi, J. Abolfazli, Investigation of basic molecular gas structure effects on hydrodynamics and thermal behaviors of rarefied shear driven flow using DSMC, Int. Commun. Heat Mass Transfer 39 (2012) 439–448.

[20] H. Akhlaghi, E. Roohi, S. Stefanov, A New iterative wall heat flux specifying technique in dsmc for heating/cooling simulations of MEMS/NEMS, Int. J. Therm. Sci. 59 (2012) 111–125.

[21] H. Akhlaghi, E. Roohi, Mass flow rate prediction of pressure–temperature-driven gas flows through micro-/nanoscale channels, Continuum Mech. Thermodyn. 26 (2014) 67–78.

[22] A. Mohammadzadeh, E. Roohi, H. Niazmand, S. Stefanov, R.S. Myong, Thermal and second-law analysis of a micro- or nanocavity using direct-simulation Monte Carlo, Phys. Rev. E 85 (2012) 056305.

[23] A. Mohammadzadeh, E. Roohi, H. Niazmand, A parallel DSMC investigation of monatomic/diatomic gas flows in micro/nano cavity, Num. Heat Transfer Part A: Applications 63 (2013) 305–325.

[24] H.A. Hassan, D.B. Hash, A generalized hard-sphere model for Monte Carlo simulation, Phys. Fluids A 5 (1993) 738–744.

[25] M. Wang, Z. Li, Simulations for gas flows in microgeometries using the direct simulation Monte Carlo method, Int. J. Heat Fluid Flow 25 (2004) 975–985.

[26] Q.W. Wang, C.L. Zhao, M. Zeng, N.E. Wu, Numerical investigation of rarefied diatomic gas flow and heat transfer in a microchannel using DSMC with uniform heat flux boundary condition part I: numerical method and validation, Num. Heat Transfer Part B: Fundam. 53 (2007) 160–173.

[27] M.N. Macrossan, μ-DSMC: a general viscosity method for rarefied flow, J. Comput. Phys. 185 (2003) 612–627.

[28] K. Hooman, A superposition approach to study slip-flow forced convection in straight microchannels of uniform but arbitrary cross-section, Int. J. Heat Mass Transfer 51 (2008) 3753–3762.