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RESEARCH PAPER

Geometry effects on rarefied nanochannel flows

Junghan Kim · Arjan J. H. Frijns · Silvia V. Nedea · Anton A. A. van Steenhoven

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Abstract A three dimensional molecular dynamics method was used to study the effect of different geometries for rarefied gas flows in nanochannels. Argon molecules have been used. The velocity profiles in the channel were obtained and analyzed with three different channel geometries: a circular, a rectangular (square), and a slit channel. A channel width of 50 nm was used for the simulation. It was found that when using the same driving force, the maximum velocity of the flow increases when the geometry changes in the order from circular to rectangular to slit geometry, where the latter becomes 2–2.5 times as large compared with either the rectangular or circular channel. For *Kn* larger than 1.0, the rectangular channel showed a similar maximum and slip velocity as the circular channel while the velocity profile was qualitatively similar to the slit channel. The effect of different Knudsen numbers on the velocity profiles was also investigated. We found that for *Kn* larger than 2–3, the Knudsen number has a relatively small influence on the slip velocity for circular channels and rectangular channels. The effect of the accommodation coefficient on the average flow velocity for all three geometries was studied and expressed as an allometric equation model.

Keywords Nanochannel flow · Geometric effect · Rarefied gas dynamics · Molecular dynamics

J. Kim (✉) · A. J. H. Frijns · S. V. Nedea · A. A. A. van Steenhoven
Department of Mechanical Engineering, Eindhoven University of Technology, PO Box 513, 5600 MB Eindhoven, The Netherlands
e-mail: junghan.kim@outlook.com

1 Introduction

Gas flows at micro- and nanoscale have recently gained interest due to the rapid developments in MEMS and NEMS. In the process of miniaturizing these components, surface effects dominate the fluid flows in these devices due to the large surface to volume ratio. On micro- and nanoscale, the viscous forces are of the same order of magnitude as inertial forces contrary to a macroscale vessel, where viscous forces are usually negligible compared to inertial forces (Gravesen et al. 1993; Gad-el-Hak 2001).

The rarefaction effect is one of the most important characteristics of gaseous nanochannel flows, as the molecular mean free path is comparable to the channels characteristic dimension. The effect can be characterized by the Knudsen number, *Kn*, which is defined by the ratio of the molecular mean free path λ to the characteristic length of the duct H. The Knudsen number is very small for continuum flows, $Kn < 0.1$ and is increasing as the gas mean free path λ becomes comparable with the characteristic length of the channels (e.g. in small channels and/or, dilute gases). For $Kn > 10.0$, it is considered to be a free molecular flow. Our interest is in studying the rarefaction effects in the different channel geometries for flows going from transition to the free molecular regime. Important experimental studies of gaseous flows in micro channel for different flow regimes have been performed by many researchers (Ewart et al. 2007; Graur et al. 2009; Colin 2005). However, experimental investigations of nanochannel flows still have many difficulties due to the scale limitation of current experimental devices, and therefore, several numerical methods and simulations have been widely used to study the nanochannel flow behaviours (Markvoort et al. 2005; Maruyama 2004; Yamamoto et al. 2006; Nedea et al. 2009.