International Journal of Heat and Mass Transfer 125 (2018) 681–685

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

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

Size effect on nanochannel flow explored by the flow factor approach model

Yongbin Zhang

College of Mechanical Engineering, Changzhou University, Changzhou, Jiangsu Province, China

ARTICLE INFO

Article history:
Received 9 December 2017
Received in revised form 10 April 2018
Accepted 15 April 2018

Keywords:
Nanochannel flow
Poiseuille flow
Solidified layer
Molecular dynamics
Model

ABSTRACT

The flow factor approach model (FFAM) was newly compared with molecular dynamics simulation (MDS) when simulating the Poiseuille flow in a nano slit pore where the effect of the solidified layer on the confining wall may be considerable. For direct comparisons, the MDS results were for no fluid-wall interfacial slippage under a relatively strong fluid-wall interaction; In this case, certain solidified layers may occur on both the confining walls. The comparisons show that these two approaches match well not only in the flow velocity profiles across the channel height but also in the volume flow rates through the channel. The study shows that when the total thickness of the solidified layers on the walls is comparable to the channel height, the effective channel height which is the nominal channel height minus the total thickness of the solidified layers on the walls, may need to be incorporated by FFAM for simulating a nanochannel flow; Otherwise, the effect of the solidified layer on the wall is negligible.

1. Introduction

Nanochannel flows show their special phenomenon unable to be described by continuum flow theories, because of the effect of the fluid-wall interaction [1–4]. In a nanochannel, the density of the confined fluid may be varied across the channel height and the confined fluid may have somewhat solidification [5–7]; Very close to the wall, the solidification can be strong. Consequently, the viscosity across the channel height may also be varied [8,9]; Closer to the wall, the local viscosity may be larger. These two size-dependent rheological characteristics may be the important factors that govern a nanochannel flow. The third factor resulting in a special nanochannel flow may be the fluid-wall interfacial slippage, which was omitted by conventional continuum flow theories [10–13]. The charged fluid molecule i.e. the electrokinetic effect can also significantly influence the flow rate through the nanochannel under external electric fields [14–17]. Even molecular-scale wall surface roughness can greatly influence a nanochannel flow [18]. Chan and Horn experimentally showed that when the separation between two solid surfaces was on the nanometer scale, the drainage force of a confined fluid was not predictable from conventional Reynolds equation [19]. Vincent et al. [20] suggested by experiment the monomolecular immobile layer adsorbing to the wall surface for explaining the reduced flow rate through a narrow nanochannel. Gruener et al. [21] suggested two immobile molecular layers of water adsorbing to the wall surface to explain the experimentally observed reduced flow rate when water flowed through hydrophilic silica pores with 3.5 nm and 5 nm mean radii. Koklu et al. [22] experimentally studied the pressure-driven flow of water in hydrophilic alumina nanoporous membranes, and proposed the sticking layer adsorbing to the pore surface which did not participate in the mass transfer and reduced the flow rate through the membrane.

Molecular dynamics simulation (MDS) has been widely used in studying nanochannel flows [23–29]. It belongs to a direct simulation and has the advantage of giving more accurate results. However, this approach is more suitable for simple fluid flows with small sizes [23–29]. It is difficult to carry out on normal computers for complex fluid flows with big sizes, because of the huge consumptions in both the computational time and the computer storage. For overcoming this shortcoming, other approaches have been proposed for simulating nanochannel flows, such as the quasi-continuum model [30], the modified Navier-Stokes equation model [31], the dissipative particle dynamics method [32], the lattice Boltzman method [33], the multiscale hybrid model [34] and the flow factor approach model (FFAM)[35]. Although most of these approaches can treat simple fluid flows in more enlarged nanochannels with tolerable computation, concerns are on their accuracy and efficiency.

The flow factor approach model is very efficient for simulating non-electrokinetic nanochannel flows with big channel lengths and even thick channel walls such as in nanoporous filtering mem-

E-mail address: engmech1@sina.com

https://doi.org/10.1016/j.ijheatmasstransfer.2018.04.064
0017-9310/

branes and nano bearings [36,37]. This model has been shown to well match the MDS results not only in the flow velocity profiles across the nanochannel height but also in the flow rates through the nanochannel when the effect of the solidified layer on the wall was negligible [38–41]. The present paper presents a new comparison between FFAM and MDS in simulating the nanochannel flow when the effect of the solidified layer on the wall may be considerable. Although the MDS results for nanochannel flows are plentiful [5–10,23–29], in this comparison the MDS results are from Liu and Li [42] for no fluid-wall interfacial slippage. Both the flow velocity profiles across the channel height and the volume flow rates through the channel respectively calculated from FFAM and MDS are compared for two channel heights. The comparisons show that these two approaches are correlated well. Important conclusions are drawn concerning the effect of the solidified layer on the confining wall in nanochannel flows. It is shown that FFAM can be used for simulating nanochannel flows by incorporating the effective channel height which is the nominal channel height minus the total thickness of the solidified layers on both the walls, when the effect of the solidified layer is considerable.

2. Poiseuille flow in nanochannel by FFAM

The flow in nanochannel may be significantly different from the description by conventional continuum flow theory because of the channel confinement [5–10]. Due to the physical adsorption of the confined fluid to the wall surfaces, the fluid may be ordered to the wall surface and the fluid rheological properties such as the fluid density and viscosity may be varied across the channel height [5–10]. For a one-dimensional flow, the flow factor approach model (FFAM) equivalently treats an ensemble averaged nanochannel flow as shown in Fig. 1 [35,43].

In Fig. 1, for the Poiseuille flow i.e. $u_a = u_b = 0$, for the absence of the fluid-wall interfacial slippage (i.e. $\bar{u}_a = \bar{u}_b = 0$), the dimensional velocity of the i^{th} fluid molecule across the channel height calculated from FFAM is [35,43]:

$$u_i = Di\frac{dp}{dx}(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i}\left[1-\frac{(\Delta_l/\eta_{line,l})_{avr,i}(l\Delta_{l-1}/\eta_{line,l-1})_{avr,n-1}}{(\Delta_l/\eta_{line,l})_{avr,n-1}(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i}}\right] \tag{1}$$

where D is the fluid molecule diameter, p is the fluid pressure, x is the coordinate shown in Fig. 1, i is the order number of the fluid molecule across the channel height ($i = 1, 2, \ldots, (n-1)$), n is the equivalent number of the fluid molecules across the channel height and assumed as an odd number, $\bar{u}_a$ is the velocity of the $(n-1)^{\text{th}}$ fluid molecule across the channel height which is on the upper solid wall, $\bar{u}_b$ is the velocity of the 0th fluid molecule across the channel height which is on the lower solid wall,

$$(\Delta_l/\eta_{line,l})_{avr,i} = \frac{\sum_{l=0}^{i-1}\Delta_l/\eta_{line,l}}{i} \tag{2}$$

and

$$(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i} = \frac{\sum_{l=1}^{i} l\Delta_{l-1}/\eta_{line,l-1}}{i} \tag{3}$$

Here, Δ_l and $\eta_{line,l}$ are respectively the local separation and the local viscosity between the l^{th} and $(l+1)^{\text{th}}$ fluid molecules across the channel height.

According to Eq. (1), the volume flow rate per unit channel width through the channel calculated from FFAM is [39]:

$$q_{v,bf} = \sum_{i=0}^{n-1} u_i[(\Delta_{i-1}+\Delta_i)/2 + D] = \frac{Sh^3}{12\eta_{bf}^{eff}}\frac{dp}{dx} \tag{4}$$

where h is the channel height, η_{bf}^{eff} is the effective viscosity of the confined fluid across the channel height, and S is the parameter describing the fluid discontinuity and inhomogeneity effects i.e. the fluid non-continuum effect across the channel height.

It is assumed that [35,43]:

$$\Delta_{i+1}/\Delta_i = q_0 > 1 \tag{5}$$

and

$$\eta_{line,i}/\eta_{line,i+1} = q_0^m > 1 \tag{6}$$

where q_0 and m are respectively constant, and $i = 0, 1, \ldots, (n-1)/2 - 2$. The normalized channel height h/D is expressed as [35,43]:

$$\frac{h}{D} = n + \frac{\Delta_{im}}{D}\left[\frac{q_0^{im}-1}{q_0^{im}-q_0^{im-1}} + \frac{q_0^{-im}-1}{q_0^{-1}-1}\right] \tag{7}$$

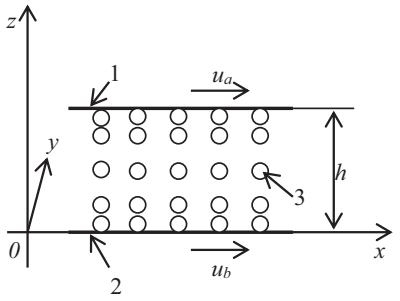
where

$$im = \frac{n-1}{2} \tag{8}$$

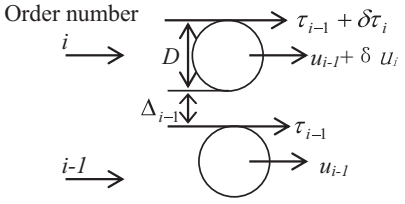
Here, im is the order number of the fluid molecule on the median plane of the confined film, and Δ_{im} is the local separation between the neighboring fluid molecules across the channel height on the median plane of the confined film.

The parameter S ranges between −1 and 0 and it is expressed as [35,43]:

$$S = F_1 - F_2 \tag{9}$$



(a)



(b)

Fig. 1. The flow of a fluid confined in a nano slit pore on ensemble average [35,43]. (a) Magnified low channel height, ordered (non-continuum) fluids across the channel height. (b) Two exemplary magnified fluid molecules across the channel height. 1-upper wall surface, 2-lower wall surface, 3-ordered fluids. u_a and u_b are respectively the speeds of the upper and lower wall surfaces.