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Effect of wall surface roughness on mass transfer in a nano channel

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ABSTRACT

The effect of wall surface roughness on the fluid mass flow rate through a nano slit pore in the Poiseuille flow was analytically studied by using the flow factor approach model. One wall surface was perfectly smooth and the other coupled wall surface was periodically distributed with rectangular protrusions or dents. Weak, medium-level and strong fluid–wall interactions were respectively considered. It was shown that even the wall surface protrusion with a small height significantly reduces the mass flow rate through the channel in spite of the fluid–wall interaction; this effect is especially significant for a strong fluid–wall interaction. The increase of the width of the wall surface protrusion also significantly reduces the mass flow rate through the channel. The effect of the wall surface protrusion is weakened with the increase of the channel height. The wall surface dent was found to increase the mass flow rate through the channel and the mass flow rate is enhanced with the increases of both the depth and the width of the dent. This effect is more significant for a stronger fluid–wall interaction. However, for deep dents, the effect of the wall surface dent on the mass flow rate is almost independent on both the depth of the dent and the fluid–wall interaction. While for narrow dents, the effect of the wall surface dent is negligible in spite of the fluid–wall interaction. The effect of the wall surface dent is also weakened with the increase of the channel height.

1. Introduction

Nano channel flows for perfectly smooth wall surfaces have been studied plentifully by molecular dynamics simulation (MDS) or other powerful approaches [1–11]. It has been known that a nano channel flow is different from conventional continuum theory description because of the fluid–wall interaction and the local density variation of the fluid across the channel height. The velocity profiles across the channel height for both the Couette and Poiseuille flows are significantly distorted compared to conventional theory description. This is due to the non-continuum effect of the confined fluid. As a result, the average flow velocity across the channel height in the Couette flow is equal to the continuum theory calculation, while the magnitude of the velocity in the Poiseuille flow is considerably or even much lower than the continuum theory calculation. The solidification of the fluid across the channel height makes the values of the local density and viscosity of the fluid both significantly greater than the bulk values of the fluid [1–4,12]; while, the frequently occurring fluid slippage at the wall surface makes the flow inside a nano channel deviate from conventional hydrodynamic theory, which neglected the fluid–wall interfacial slippage [5]. The nano channel flow for smooth wall surfaces may depend on the combined dynamic, non-continuum and interfacial slippage effects of the confined fluid.

The wall surfaces may be unlike to be ideally smooth in an actual nano channel. There may be unavoidably existing the molecular scale wall surface protrusion or dent, which would have an unnegligible influence on the nano channel flow. The wall surface roughness effect in a nano channel flow has been studied a lot by MDS or other approaches.

Kasiteropoulou et al. [13] studied the influence of the height of the wall surface protrusion on nano channel flows by using the dissipative particle dynamics method. They showed that the wall surface protrusion considerably influenced the density, velocity and pressure inside the channel. They found that the increase of the protrusion height significantly reduced the fluid flow velocity across the channel height. They also found that the slipping velocities on both the upper and lower wall surfaces were reduced with the increase of the protrusion height. This indicates that when the protrusion height was increased, the interfacial slippage at the wall surface was alleviated but the frictional impedance to the fluid flow was increased. These agreed with the friction factors for different protrusion heights obtained by them.

The effect of wall surface roughness in a nano channel flow was mainly studied by MDS in the past, as reviewed in the following. Sofos et al. [14] showed that the shear viscosity of the fluid

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confined in a nano channel was increased in the region of the wall surface protrusion. They showed that the wall surface protrusion overall reduced the magnitudes of the velocity across the channel height [15]. They also showed that the interfacial slippage was reduced at the rough wall surface and ascribed it to the reduction of the magnitude of the flow velocity at the rough wall surface [15]. Kasiteropoulou et al. also obtained the similar results by the dissipative particle dynamics method [10]. Sofos et al. [16] showed that groove orientation on the wall surface has an important influence on a nano channel flow and the transport properties of the fluid are significantly influenced by the fluid–wall interaction. Noorian et al. [17] studied the influences of both the surface roughness height and surface roughness geometry on a nano channel flow. They found that the increase of the height of the wall surface roughness significantly reduced the magnitudes of the velocity across the channel height whenever the wall surface roughness was spherical or cubical. They also found that the cubic surface roughness more reduced the magnitude of the flow velocity than the spherical surface roughness for the same operating condition. Cao et al. [18] studied the effect of the wall surface roughness in a nano channel flow by using triangular surface ridges. They found that the increase of the height of the surface ridge not only increased the contact angle of the fluid and then reduced the wettability of the fluid, but also significantly reduced the magnitude of the flow velocity across the channel height. Liu et al. [19] showed that with the increase of the height of the wall surface protrusion, the fluid volume flow rate through a nano channel in a Poiseuille flow was significantly reduced even when the protrusion height was small compared to the channel height. They also showed that with the increase of the protrusion width, the fluid volume flow rate was considerably reduced. Yang [20] showed that with the increase of the width of the wall surface protrusion, the fluid volume flow rate through a nano channel in a Poiseuille flow was significantly reduced. They showed that the wall surface roughness alleviated the interfacial slippage at the wall surface. Sun et al. [21] studied the wall surface roughness effect in a nanochannel flow by molecular dynamics–continuum hybrid simulation. They found that when the channel height was sufficiently small, the wall surface roughness effect was significant and it equivalently narrowed the channel so that the flow was slowed.

Different from the previous researches, the present study used the flow factor approach model to study the influences of the rectangular-shaped wall surface protrusion or dent on the fluid mass flow rate through a nano slit pore. The used model has been validated for a nanoscale fluid flow [11,22–25]. This model has the advantage of much less consumption in computational time and storage compared to MDS, and can successfully simulate a nanoscale fluid flow even in a much longer channel. This makes the mentioned model particularly suitable for studying the wall surface roughness effect in a nanochannel flow. In the present study, the effective density and viscosity of the fluid were considered as dependent on the channel height and the fluid non-continuum effect i.e. the fluid discontinuity and inhomogeneity effects across the channel height were also considered; The influences of the wall surface roughness on the fluid–wall interfacial slippage and subsequently on the mass flow rate through the channel were also evaluated. The effect of the wall surface roughness was investigated respectively for weak, medium-level and strong fluid–wall interactions and for widely varying channel heights and geometrical parameter values of the surface protrusion or dent. The obtained results are qualitatively in agreement with the previous ones. New insights were gained into the wall surface roughness effect in a nano channel flow.

2. Channel description

Fig. 1(a) shows the nano channel flow studied in the present paper. One plane wall surface is perfectly smooth and stationary, while the other coupled plane wall surface is stationary and periodically distributed with rectangular surface protrusions or dents. When the width (l_2) of the surface projection is relatively small ($l_2 \leqslant l_1$), it can be considered that surface protrusions are distributed on the wall surface; Otherwise, it is regarded that surface dents with the width l_1 are distributed on the wall surface. The

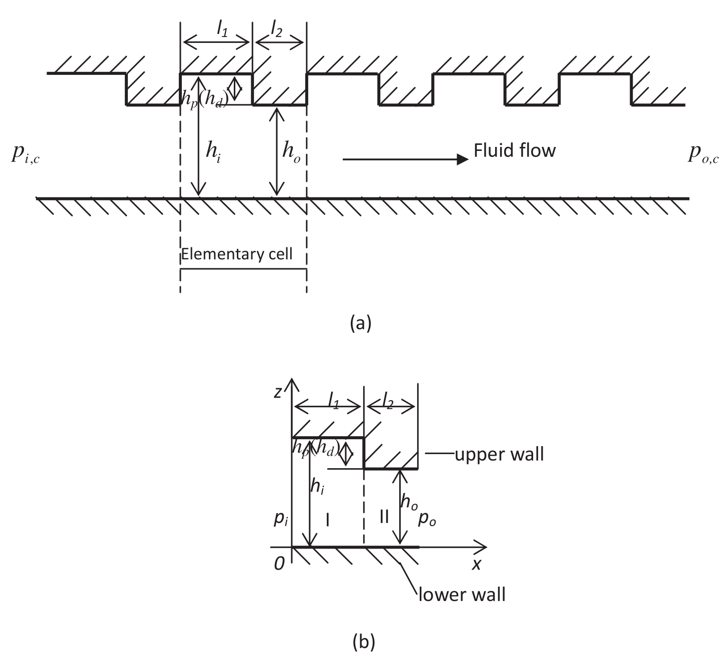

Fig. 1. The studied nano channel flow. (a) A nano channel flow driven by the pressure difference ($p_{i,c} - p_{o,c}$) (>0) with periodically distributed wall surface protrusions or dents on one wall. For wall surface protrusions, $l_2/l_1 \leqslant 1$; for wall surface dents, $l_2/l_1 > 1$. h_p is the height of the wall surface protrusion, or h_d is the depth of the wall surface dent. (b) An elementary cell of the channel in (a). p_i is the pressure at the inlet and p_o is the pressure at the outlet. $p_i - p_o = (p_{i,c} - p_{o,c})/N$, N is the number of the elementary cells in the whole channel.