

Effect of Adsorbed Layer on Methane Flow in Silicon Nano Slits for Different Channel Heights

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1. Introduction

There are intrinsically mono or several fluid molecule layers physically adsorbed to the solid channel wall when the fluid flows through the channel [1-4]. In macro-scale flows, the effect of the adsorbed layer is often negligible. However, in microscale or nanoscale flows, it should often be considered [5]. In the classical modeling of multiscale flows in micro/nano channels, the flow of the adsorbed layer was simulated by molecular dynamics simulation (MDS), while the flow of the intermediate fluid between the two adsorbed layers was simulated by using the Newtonian or non-Newtonian continuum fluid model [5-8]. Although this approach much saves the computational time and the computer storage than full MDS, it still suffers from being incapable of modeling big channel size such as occurring in engineering owing to the unaffordable computational sources. For reducing the computational difficulty, other simulation methods for micro/nano channel flows were also proposed, such as the quasi-continuum model [9, 10], the modified Navier-Stokes equation model [11], and the dissipative particle dynamics method [12]. These methods have their own imperfections like the huge computational time requirement for big channel size or the computational inaccuracy.

In recent years, Zhang proposed a new multiscale scheme for simulating the multiscale flow in micro/nano slit channels [13]. He treated the adsorbed layer flow by the equivalent non-continuum model and described the flow of the intermediate continuum fluid by the Newtonian fluid model. He derived the closed-form explicit flow equations respectively for the adsorbed layer flow and the intermediate continuum fluid flow. By comparison with full MDS results, it was shown that the flow velocity pro-

files across the micro/nano channel height calculated from his approach approximate those calculated from full MDS, while the flow rates through the channel calculated from his approach and full MDS are close to one another [14]. His approach is valid for the very wide channel heights covering from the 1nm scale to the macro size scale [14]. The advantage of his approach is to give fast solution for engineering micro/nano channel flows with normal computers.

The present study aims to investigate the effect of the adsorbed layer on the flow velocity profile and the flow rate in multiscale micro/nano channel flows for widely varying channel heights by using Zhang's multiscale flow model. The values of the characteristic parameters of the adsorbed layer required by Zhang's model were extracted from full MDS results. The flow velocities and the flow rates were calculated from his model and compared with those calculated from the classical Hagen-Poiseuille equation for different channel heights. The influence of the channel height on the nanochannel flow is explored. The mechanism of the narrow nanochannel flow is revealed. The effect of the adsorbed layer on the Poiseuille flow is shown by the present study to be the main cause of the improvement of the load-carrying capacity of micro/nano bearings with very low clearances and no wall slippage.

2. Modeled Multiscale Poiseuille Flow in Silicon Nano Slit

Jiang and Zhang [14] carried out full molecular dynamics simulation for the pressure-driven flow of methane in the silicon nano slits respectively with the channel heights 5.79 nm, 11.57 nm and 17.36 nm. They showed that for these channel heights the number (n) of the fluid

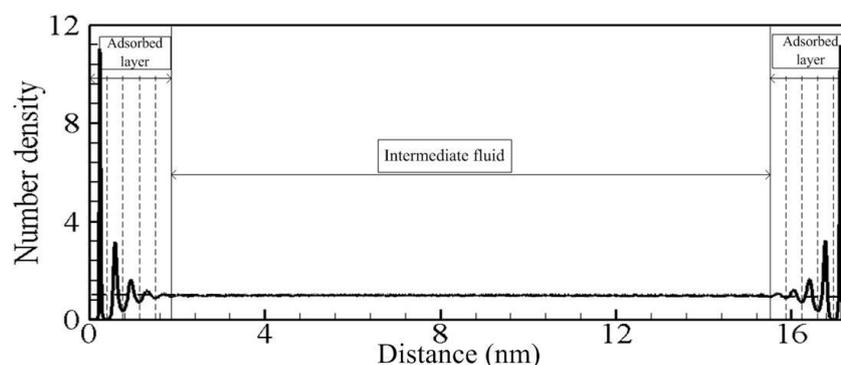


Fig. 1 The number density distributions across the whole channel height obtained by MDS for the channel height equal to 17.36 nm [14]

molecule layers adsorbed to the solid wall is 5. It appears that the value of n is independent on the channel height. Also, it was shown by them that the values of the characteristic parameters of the adsorbed layer are weakly influenced by the channel height [14]. Fig. 1 shows the distinguished adsorbed layer zone and the intermediate fluid zone in their simulation when the channel height is 17.36 nm.

It was examined by them that Zhang's multiscale flow model [13] approximates full MDS in both the flow velocity profile and the total volume flow rate through the channel for very wide channel heights [14]. The present study succeeds their research and explores the flow behavior of methane in the silicon nano slits with widely varying channel heights by using Zhang's multiscale flow equations [13]. This research sheds light on the effect of the adsorbed layer for different nanochannel heights. It helps to reveal the mechanism of the hydrodynamic flow in very small surface clearances such as in micro bearings and give us the proper understanding on the physical background of the operation of such small devices.

According to Zhang's multiscale flow model [13], the pressure-driven flow of methane in the silicon nano slit is equivalently treated as Fig. 2 shows. Zhang equivalently treated the adsorbed layer in Fig. 1 as the several fluid molecules (with the number n) across the adsorbed layer thickness regularly positioned normal to the solid wall. He considered the discontinuity and inhomogeneity across the adsorbed layer thickness as found by MDS (for the varia-

tions of the local density and the local viscosity within the adsorbed layer). This leads to the behavior of the adsorbed layer flow essentially in the non-continuum. Between the two adsorbed layers is the continuum fluid film the rheological behavior of which obeys the Newtonian or non-Newtonian fluid models.

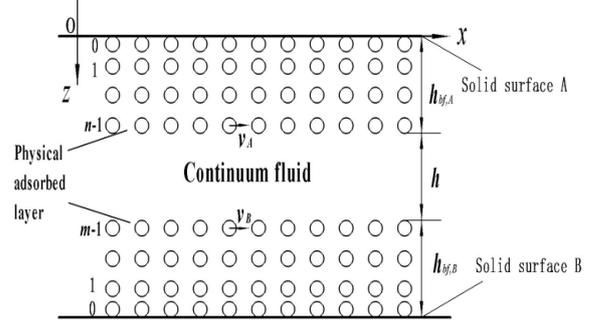


Fig. 2 The multiscale fluid flow in a very small surface clearance according to Zhang's model [13]

By assuming the fluid as Newtonian and the two solid channel surfaces as identical and using the condition of the continuity of both the flow velocity and the shear stress on the boundary between the fluid and the adsorbed layer, Zhang gave the flow velocity of the i^{th} fluid molecule in both the upper and lower adsorbed layers as [13]:

$$u_i = \bar{u}_a + \frac{(\bar{u}_b - \bar{u}_a)\eta}{2\eta \sum_{j=1}^{n-1} \frac{\Delta_{j-1}}{\eta_{line,j-1}} + h} \left[i(\Delta_i / \eta_{line,i})_{avr,i} \right] - \frac{\partial p}{\partial x} \left(\frac{h}{2} + Dn \right) \left[i(\Delta_i / \eta_{line,i})_{avr,i} \right] + \frac{\partial p}{\partial x} D \left[i(\Delta_{i-1} / \eta_{line,i-1})_{avr,i} \right], \quad (1)$$

for $i = 1, 2, \dots, (n-1)$.

where D is the fluid molecule diameter, n is the equivalent number of the fluid molecules across the adsorbed layer thickness, h is the thickness of the intermediate continuum fluid, p is the pressure driving the flow, x is the coordinate along the flow direction (Fig. 2), η is the fluid bulk viscosity, \bar{u}_a and \bar{u}_b are respectively the velocities of the fluid molecules on the upper and lower channel walls, i is the order number of the fluid molecules across the adsorbed layer thickness shown in Fig. 2, $\eta_{line,j-1}$ and Δ_{j-1} are respectively the local viscosity and the separation between the j^{th} and $(j-1)^{\text{th}}$ fluid molecules across the adsorbed layer thickness, $i(\Delta_i / \eta_{line,i})_{avr,i} = \sum_{j=1}^i \Delta_{j-1} / \eta_{line,j-1}$, and

$i(\Delta_{i-1} / \eta_{line,i-1})_{avr,i} = \sum_{j=1}^i j \Delta_{j-1} / \eta_{line,j-1}$. The Newtonian

fluid should often be true for small shear strain rates. In some micro devices, it is actually the case. For high shear strain rates, the fluid is normally non-Newtonian shear thinning. For the non-Newtonian fluid, the fluid bulk viscosity η in Zhang's model should be the fluid effective viscosity. The two identical channel surfaces can be ob-

tained by using the same (coating) materials for the two surfaces.

For no wall slippage, $\bar{u}_a = \bar{u}_b = 0$, and the flow expressed by Eq. (1) is simply the Poiseuille flow term. Eq. (1) obviously shows that the pressure-driven flow of the adsorbed layer is largely different from the description by the classical Hagen-Poiseuille equation and it is influenced by both the local density and the local viscosity in the adsorbed layer which are determined by the interaction between the fluid and the channel wall.

The flow velocity of the intermediate fluid film is:

$$u = \frac{z^2}{2\eta} \frac{\partial p}{\partial x} + c_1 z + c_2, \quad \text{for } z_{min} \leq z \leq z_{max}, \quad (2)$$

where z is the coordinate across the channel height shown in Fig. 2, and the formulations for the parameters c_1 , c_2 , z_{min} and z_{max} have been shown in [14].

For the current nanochannel flow, Zhang gave the volume flow rate per unit channel length of both the upper and lower adsorbed layers as [13]:

$$q_{v,bf,A} = q_{v,bf,B} = \bar{u}_a h_{bf} + \frac{\bar{u}_b - \bar{u}_a}{2} h_{bf} \frac{\varepsilon \lambda_{bf}}{2\lambda_{bf} + C_y \left(1 + \frac{\Delta x}{D} \right)} + \frac{F_1 h_{bf}^3}{12\eta_{bf}^{eff}} \frac{\partial p}{\partial x} - \frac{h_{bf}^3}{2\eta_{bf}^{eff}} \frac{\partial p}{\partial x} \left(1 + \frac{1}{2\lambda_{bf}} - \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n} \frac{\Delta_{n-2}}{h_{bf}} \right) \frac{\varepsilon}{1 + \frac{\Delta x}{D}}. \quad (3)$$

where:

$$\begin{aligned}\lambda_{bf} &= h_{bf} / h, \quad F_1 = \eta_{bf}^{eff} (12D^2\psi + 6D\phi) / h_{bf}^3, \\ \eta_{bf}^{eff} &= Dh_{bf} / \left[(n-1)(D + \Delta_x)(\Delta_l / \eta_{line,l})_{avr,n-1} \right], \\ \varepsilon &= (2DI + II) / \left[h_{bf} (n-1)(\Delta_l / \eta_{line,l})_{avr,n-1} \right], \\ I &= \sum_{i=1}^{n-1} i (\Delta_l / \eta_{line,l})_{avr,i}, \\ II &= \sum_{i=0}^{n-2} \left[i (\Delta_l / \eta_{line,l})_{avr,i} + (i+1) (\Delta_l / \eta_{line,l})_{avr,i+1} \right] \Delta_l, \\ \psi &= \sum_{i=1}^{n-1} i (l\Delta_{l-1} / \eta_{line,l-1})_{avr,i}, \\ \phi &= \sum_{i=0}^{n-2} \left[i (l\Delta_{l-1} / \eta_{line,l-1})_{avr,i} + (i+1) (l\Delta_{l-1} / \eta_{line,l-1})_{avr,i+1} \right] \Delta_l.\end{aligned}$$

h_{bf} is the thickness of the adsorbed layer, and Δ_x is the separation between the neighboring fluid molecules in the flow direction in the adsorbed layer. The total volume flow rate per unit channel length through the channel is:

$$q_{v,tot} = q_{v,bf,A} + q_{v,bf,B} + q_{v,bf}.$$

For no wall slippage, the Hagen-Poiseuille equation gives the flow velocity in the present nanochannel as:

$$v = \frac{1}{2\eta} \frac{\partial p}{\partial x} \left[z^2 - z(2h_{bf} + h) \right]. \quad (4)$$

It gives the total volume flow rate per unit channel length through the channel as:

$$q_{v,conv} = -\frac{(2h_{bf} + h)^3}{12\eta} \frac{\partial p}{\partial x}. \quad (5)$$

3. Calculation Results

In all the calculations, the fixed parameter values are shown in Table 1.

Jiang and Zhang [14] showed by MDS that under the fixed pressure gradient $\delta p / \delta x = -1.18332 \times 10^{14}$ Pa/m, the values of q_0 are respectively 1.1783, 1.2066 and 1.2347 when the channel height is 5.79 nm, 11.57 nm and

17.36 nm. These channel heights are for full molecular dynamics simulation, but over greater channel heights make the burden of full MDS heavily increased. Nevertheless, the values of the characteristic parameters obtained for these channel heights can be applied for much higher channel heights such as occurring in micro bearings. The value of q_0 might slightly varies with the channel height. However, once q_0 is fixed, the value of Δ_{n-2} / D should be corrected according to the following equation to satisfy the thickness of the adsorbed layer:

$$h_{bf} = nD + \Delta_{n-2} \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n}. \quad (6)$$

The average value of $\eta_{line,j-1} / \eta_{line,j}$ in the adsorbed layer was calculated by MDS to be 1.1, independent on the channel height [14]. In the present calculation, for all the channel heights $\eta_{line,j-1} / \eta_{line,j} = 1.1$, and the value of m is calculated according to the equation $q_0^m = 1.1$. The values of the other characteristic parameters required by Zhang's model can be calculated once q_0 is given. Table 2 shows the calculated characteristic parameter values for the three values of q_0 .

In the present calculation, the pressure gradient is set as $\delta p / \delta x = -1.18332 \times 10^{14}$ Pa/m, and no wall slippage occurs i.e. $\bar{u}_a = \bar{u}_b = 0$. For $h = 5$ nm, Fig. 3 shows the flow velocity profiles across the whole channel height calculated when the value of q_0 is different. It is shown that for the three values of q_0 in Table 2, the calculated flow velocity profiles across the channel height are overlaid. This indicates that the calculated flow velocity from Zhang's model is very weakly influenced by the variation of q_0 . Table 3 shows that the calculated values of the flow rates $q_{v,bf,A}$, $q_{v,bf,B}$, $q_{v,bf}$ and particularly the total volume flow rate $q_{v,tot}$ by Zhang's model are very weakly varied with q_0 . Owing to these calculation results, in the following calculations for varying channel heights, it is taken that $q_0 = 1.2347$ i.e. the parameter values for Case 1 in Table 2 are used.

Table 1

Values of the characteristic parameters obtained from MDS [14]

Parameter	D , nm	h_{bf} , nm	n	Δ_x / D	$\eta_{line,j-2}$, Pa s	η , Pa s
Value	0.312279	1.80848	5	0.38755	6.7348×10^{-5}	6.52×10^{-5}

Table 2

Values of the other characteristic parameters in Zhang's model calculated for different q_0

Parameter	q_0	Δ_{n-2} / D	m	η_{bf}^{eff} , Pa s	F_1	F_2	ε
Case 1	1.2347	0.264	0.4478	3.97251×10^{-4}	1.494186	2.144310	1.171049
Case 2	1.2066	0.2565	0.5283	3.95562×10^{-4}	1.479462	2.110479	1.160517
Case 3	1.1783	0.2488	0.5308	3.96794×10^{-4}	1.507244	2.119007	1.141226

Table 3

Comparisons among the volume flow rates calculated from Zhang's model when $h = 5$ nm

Volume flow rate	$q_{v,bf,A}$, m ² /s	$q_{v,bf,B}$, m ² /s	$q_{v,bf}$, m ² /s	$q_{v,tot}$, m ² /s
Case 1	1.450×10^{-9}	1.450×10^{-9}	2.505×10^{-8}	2.795×10^{-8}
Case 2	1.444×10^{-9}	1.444×10^{-9}	2.501×10^{-8}	2.790×10^{-8}
Case 3	1.407×10^{-9}	1.407×10^{-9}	2.511×10^{-8}	2.792×10^{-8}

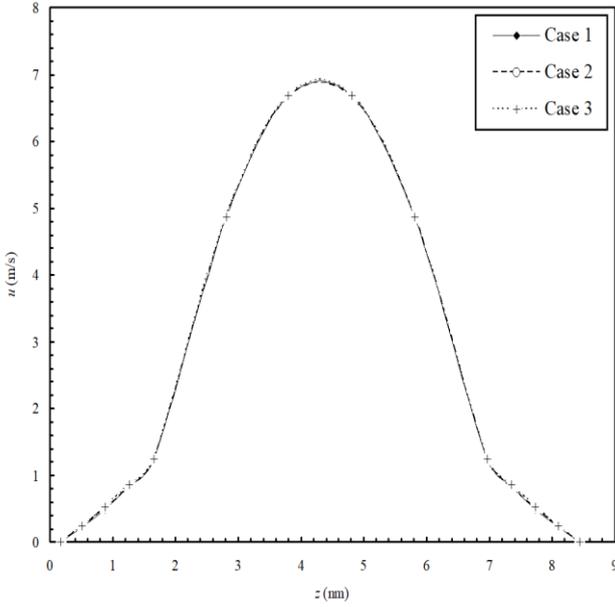


Fig. 3 The flow velocity profiles across the whole channel height calculated from Zhang's model respectively for the three cases in Table 2 when $h = 5$ nm

Fig. 4, a shows that when h is no more than 20nm, the flow velocity calculated from Zhang's multiscale flow model is significantly or much lower than that calculated from the classical Hagen-Poiseuille equation. The flow velocity of the adsorbed layer is particularly lower than classically calculated, and it encumbers the flow velocity of the intermediate continuum fluid. As a result, the total flow rate through the channel calculated from Zhang's model is significantly smaller than that calculated from the classical equation. Since Zhang's model approximates full MDS in both the flow velocity profile and the total volume flow rate through the channel, it means that for the small channel heights the flow rate of the Poiseuille flow through the nanochannel is significantly smaller than that calculated from the classical Hagen-Poiseuille equation owing to the effect of the adsorbed layer. This provides the physical explanation for the significantly increased load-carrying capacities of the hydrodynamic micro thrust bearing with very low clearances as compared to the classical hydrodynamic lubrication theory calculation when the effect of the adsorbed layer is incorporated. The reason is that for the same operating condition when the effect of the adsorbed layer is involved, the hydrodynamic pressures in the micro thrust bearing must be higher than those calculated from the classical equation to generate the greater magnitudes of the Poiseuille flow rate to maintain the flow continuity in the whole bearing.

Fig. 4, b shows the comparisons between the flow velocity profiles calculated from Zhang's model and those calculated from the Hagen-Poiseuille equation when h is respectively 50 nm, 100 nm and 180 nm. The difference between these two calculated flow velocity profiles is much reduced compared to those in Fig. 4, a owing to the increase of the channel height. This indicates that with the increase of the channel height the effect of the adsorbed layer is reduced. Although there are still some differences between the two calculated flow velocities for $h=50$ nm~180 nm, the flow velocities calculated from these two approaches are well close. It means that the effect of the

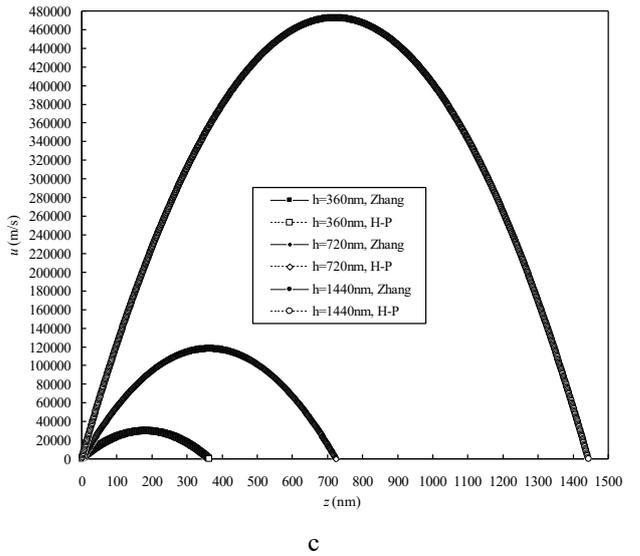
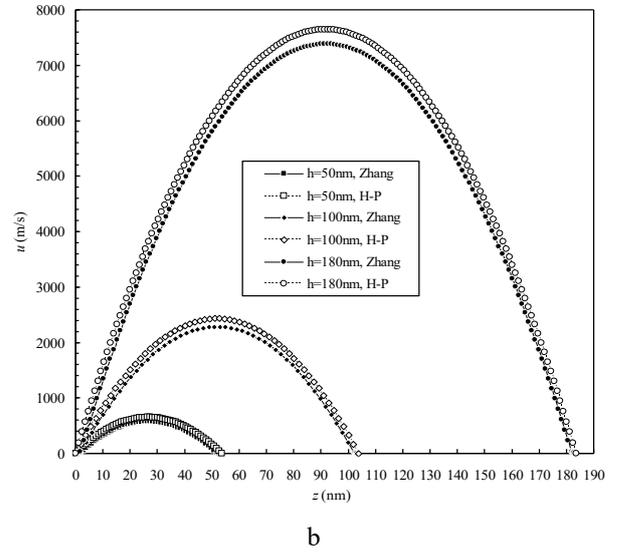
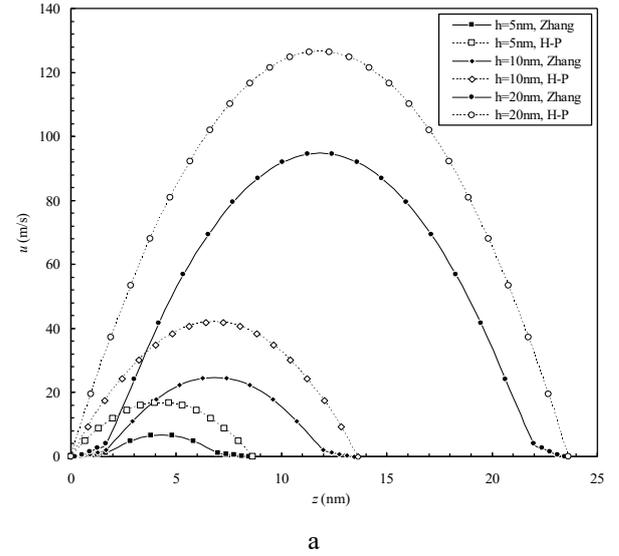


Fig. 4 The flow velocity distributions across the channel height for different channel heights calculated from Zhang's multiscale flow model (for Case 1); H-P denotes the classical Hagen-Poiseuille equation calculation: a - $h = 5 \sim 20$ nm, b - $h = 50 \sim 180$ nm, c - $h = 360 \sim 1440$ nm

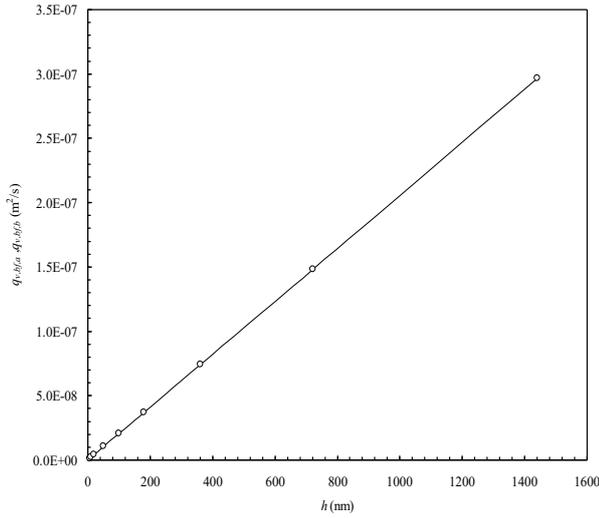


Fig. 5 Variations of the volume flow rates of the two adsorbed layers with the thickness of the intermediate continuum fluid film

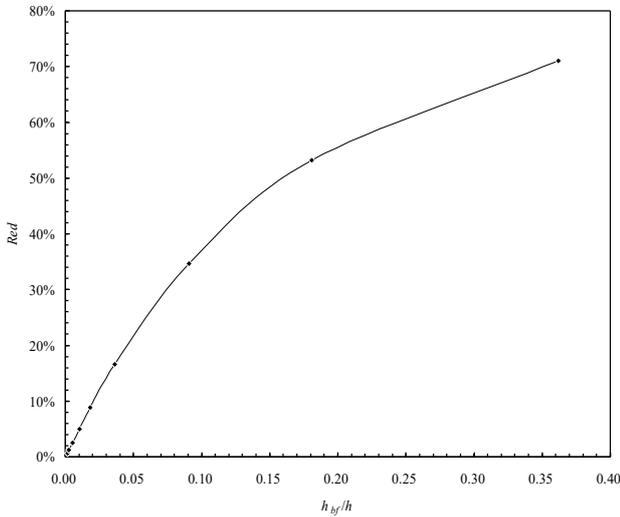


Fig. 6 The percentage reduction of the total volume flow rate per unit contact length through the channel calculated from Zhang's multiscale flow model compared to the calculation from the classical Hagen-Poiseuille equation

adsorbed layer on the load-carrying capacity of the micro hydrodynamic thrust bearing with the surface clearance in the range 50 nm~180 nm is weak. It was shown that when $h_{bf}/h \leq 0.01$, the effect of the adsorbed layer is negligible in the multiscale flow.

Fig. 4, c shows that when $h \geq 360$ nm, the flow velocity profiles calculated from Zhang's model are overlaid with those calculated from the Hagen-Poiseuille equation, indicating the negligible effect of the adsorbed layer. This is owing to the thickness of the adsorbed layer far lower than the channel height. Consequently, the hydrodynamic thrust bearing with the clearance over 360 nm shows no adsorbed layer effect. That is why the conventional macro thrust bearing with the clearance on the 1 μ m or 10 μ m scales can be designed from the continuum hydrodynamic lubrication theory [15], which ignores the adsorbed layer. However, the present results show that when the surface clearance is low enough, the performance of the hydrodynamic bearing must be described by the mul-

tiscale hydrodynamic lubrication theory involving the adsorbed layer flow.

Fig. 5 shows that when the other operational parameter values are given, the magnitudes of the volume flow rates ($q_{v,bf,A}$, and $q_{v,bf,B}$) of the upper and lower adsorbed layers in Fig. 2 are linearly increased with the increase of the thickness (h) of the intermediate continuum fluid film. This result agrees with the full MDS results [14].

Define $Red = (q_{v,con} - q_{v,tot}) / q_{v,con}$. The value of Red shows the effect of the adsorbed layer on the reduction of the rate of the Poiseuille flow. Fig. 6 shows that when $h_{bf}/h \geq 0.01$, the value of Red is greater than 5.5%, indicating the considerable effect of the adsorbed layer. With the increase of h_{bf}/h i.e. with the reduction of h , the value of Red is rapidly increased, showing the significantly increased effect of the adsorbed layer. This may reflect the significantly increased effect of the adsorbed layer on the improvement of the load-carrying capacity of the hydrodynamic micro thrust bearing with the reduction of the bearing clearance. Fig. 6 shows that it is acceptable to set $h_{bf}/h \geq 0.01$ as the condition for which the effect of the adsorbed layer should be considered.

4. Conclusions

The present paper studies the effect of the adsorbed layer on the pressure-driven flow velocity profile and the flow rate of methane in silicon micro/nano slits with the channel height ranging between 8.6 nm and 1444 nm by using Zhang's multiscale flow model. In these multiscale flows, there is the identical physically adsorbed layer on either of the channel wall with the thickness 1.80848 nm, and between the two adsorbed layers is the continuum fluid film which is assumed as Newtonian and with the thickness ranging between 5 nm and 1440 nm. The flow of the adsorbed layer is essentially molecular-scale non-continuum, and the flow of the intermediate fluid obeys the continuum Newtonian fluid model. Because Zhang's multiscale flow model has been verified by full MDS to be valid for the wide channel heights ranging from the 1 nm scale to the macro size scale [14], the present results calculated from this model are reliably convincing.

In the present calculations, the values of the characteristic parameters of the adsorbed layer are from the molecular dynamics simulation results [14], and they can be considered as independent on the channel height as manifested by MDS and proven by the calculations. For the given pressure gradient $\delta p / \delta x = -1.18332 \times 10^{14}$ Pa/m, there is no wall slippage, and the flow velocity profiles across the whole channel height and the flow rates of the two adsorbed layers, the intermediate fluid and the total flow through the channel have been calculated for widely varying channel heights from Zhang's multiscale flow velocity and flow rate equations. The calculation results are physically rational and agreeing with the earlier calculation results for the multiscale flows in micro/nano channels and in micro bearings.

Based on the obtained results, the conclusions are drawn as follows:

1. The adsorbed layer encumbers the flow in the whole channel and results in the flow velocity and the total flow rate through the channel smaller than those calculated

from the classical Hagen-Poiseuille equation; This effect is particularly significant when the channel height is low; That is the magnitude of the flow rate of the Poiseuille flow in a nanochannel is reduced by the effect of the adsorbed layer especially for small channel heights; It provides the physical explanation for why the load-carrying capacity of the micro hydrodynamic thrust bearing with low clearance is significantly improved compared to the classical calculation when the effect of the adsorbed layer is incorporated.

2. Normally, when the ratio of the thickness (h_{bf}) of the adsorbed layer to the thickness (h) of the intermediate fluid is no less than 0.01, the effect of the adsorbed layer should be considered. For example, when $h_{bf} = 1.80848$ nm, the channel height 183 nm results in the considerable effect of the adsorbed layer owing to the multiscale flow. This indicates that in a hydrodynamic thrust bearing, when the surface clearance is below 100 nm, the effect of the adsorbed layer should often be considerable and the carried load of the bearing should be considerably greater than the classical hydrodynamic lubrication theory calculation.

3. For the sufficiently high channel heights which give $h_{bf}/h < 0.01$, the flow velocity profiles and the total flow rates calculated from Zhang's multiscale flow model are overlaid with those calculated from the Hagen-Poiseuille equation, indicating the negligible effect of the adsorbed layer.

4. Only if the thickness of the adsorbed layer is fixed, the flow velocity and the flow rate calculated from Zhang's multiscale flow model are not sensitive to the variation of the parameter q_0 , provided that the value of A_{n-2}/D is correspondingly corrected according to Eq. (7).

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EFFECT OF ADSORBED LAYER ON METHANE FLOW IN SILICON NANO SLITS FOR DIFFERENT CHANNEL HEIGHTS

S u m m a r y

The pressure-driven flow of methane in silicon nano slits is analytically studied by using Zhang's multiscale scheme (to handle the hybrid continuum and non-continuum flow) for the wide channel heights ranging between 8.6 nm and 1444 nm when there is the intermediate (continuum or quasi-continuum) fluid film between the two non-continuum adsorbed layers and no wall slippage occurs. Zhang's multiscale scheme for nanochannel flow well matches full molecular dynamics simulation with a good accuracy of the calculated total flow rate through the nanochannel. The values of the characteristic parameters of the adsorbed layer required by Zhang's approach were found from molecular dynamics simulation, and they are considered as independent on the channel height. According to the calculation results, the adsorbed layer encumbers the flow in the whole channel especially for the low channel heights which give the ratio of the thickness (h_{bf}) of the

adsorbed layer to the thickness (h) of the intermediate continuum fluid film no less than 0.1, and this makes the total volume flow rate through the channel about 35% smaller than the classical Hagen-Poiseuille equation calculation. The flow is not sensitive to the variation of the value of the ratio (q_0) of the neighboring fluid molecule separations across the adsorbed layer thickness once the thickness of the adsorbed layer is fixed. With the increase of the channel height, the effect of the adsorbed layer is weakened. When $h_{bf}/h < 0.01$, the reduction of the total flow rate through the channel owing to the adsorbed layer is no more than 5.5% and the effect of the adsorbed layer can be considered as negligible. These disciplines of the Poiseuille flow in nanochannels renders the great application values of the adsorbed layer in improving the load-carrying capacity of micro bearings with very low clearances.

Keywords: adsorbed layer, flow rate, multiscale flow, nanochannel, Poiseuille flow, velocity.

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