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The flow equation for a nanoscale fluid flow

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ABSTRACT

The flow equation for a fluid confined in a nano channel proposed previously was re-examined by comparison with the molecular dynamics simulation (MDS) results. In themselves, this equation as well as the flow factor for the confined nano fluid flow were finely proven. The comparisons showed good agreements between the calculation results from this equation and the MDS results for both the Couette and Poiseuille flows.

1. Introduction

The understanding on the flow of a fluid confined in a nano channel is important for the design of a micro fluidic device. Molecular dynamic simulations (MDS) as well as experiments have been carried out plentifully on the rheology and flowing properties of such fluids [1–11]. It was however still a pity that in MDS there lacked a closed-form equation governing a nanoscale fluid flow. This indeed makes the modeling of a nanoscale fluid flow by MDS in engineering quite time-consuming and often unaffordable.

In recent years, there were some attempts to develop quasi-continuum models for a fluid flow in a nano channel to capture the MDS calculated fluid ordering across the channel [12,13]. Also, for improving computational efficiency, the multiscale computation scheme as well as the dissipative particle dynamics method were proposed for simulating a nanochannel flow [14–16]. These approaches showed efforts towards realizing an efficient simulation of a nanoscale fluid flow in engineering.

In 2006, the author and his colleague ever proposed the flow factor approach model for the fluid flow in a nano channel, considering both the fluid inhomogeneity and discontinuity across the film thickness [17,18]. This model gave a closed-form equation for describing a nanoscale fluid flow. It can capture the main characteristics of a nanoscale fluid flow as obtained in MDS, and effectively describe the fluid non-continuum effect. It is efficiently applicable for a multiscale simulation of a fluid flow covering from nano to macro [19,20].

Recent researches [21,22] showed that the flow factor approach model agrees well with the MDS results for both the Couette and Poiseuille flows of a confined nano fluid. This leads me to further look at this model by comparing the flow rates through the nano gap calculated from this model with the MDS results. The present paper presents the results obtained in this study.

2. The flow factor approach model

For clarifying the subject, the flow factor approach model for describing the fluid flow in a nano channel is repeated here.

Fig. 1 shows a fluid flow in a nano slit pore, modeled by the flow factor approach model [17]. By an equivalent transformation method, a flowing fluid confined between two parallel solid plane walls can be treated as Fig. 1 shows [23]. In Fig. 1, the confined fluid is ordered to the wall in the normal direction because of the fluid-wall interaction, and the momentum transfer mainly occurs in the direction normal to the wall when the coupled walls slide against one another.

Both the local viscosity and the separation between the neighboring fluid molecules across the film thickness are varied dependent on the distance from the wall [24]; they play important roles in the momentum transfer across the film thickness.

According to the model, the velocity of the ith fluid molecule across the film thickness in Fig. 1 (for $i = 1,2,\ldots,(n-1)$, n is the number of the fluid molecules across the film thickness) is [17]:

$$u_i = \bar{u}_b + \frac{i(\bar{u}_a - \bar{u}_b)(\Delta_l/\eta_{line,l})_{avr,i}}{(n-1)(\Delta_l/\eta_{line,l})_{avr,n-1}} + Di\frac{\partial p}{\partial x}(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i} \times \left[1 - \frac{(\Delta_l/\eta_{line,l})_{avr,i}(l\Delta_{l-1}/\eta_{line,l-1})_{avr,n-1}}{(\Delta_l/\eta_{line,l})_{avr,n-1}(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i}}\right] \quad (1)$$

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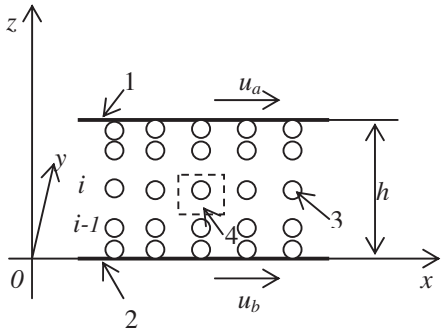

Fig. 1. The flow of a fluid confined in a nano slit pore, with equivalently treated ordered films across the film thickness [17,23]. 1-upper solid wall, 2-lower solid wall, 3-ordered films, 4-flowing volume of a molecule. u_a and u_b are respectively the speeds of the upper and lower confining walls.

where i is the order number of the fluid molecule across the film thickness, $\eta_{line,l-1}$ and Δ_{l-1} are respectively the local viscosity and the separation between the lth and $(l-1)$th fluid molecules across the film thickness, D is the fluid molecule diameter, p is the fluid pressure, x is the coordinate in the direction of the fluid flow, $\bar{u}_a$ is the velocity of the $(n-1)$th fluid molecule across the film thickness which is on the upper wall, $\bar{u}_b$ is the velocity of the 0th fluid molecule across the film thickness which is on the lower wall,

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

and

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

In the flow factor approach model [17], it was assumed that the separation between the neighboring fluid molecules across the film thickness is symmetrical with respect to the median plane of the confined fluid film [17]. This assumption agrees with the MDS results [10]. According to the model [17], it is here taken that $\Delta_{i+1}/\Delta_i = q_0 > 1$ and $\eta_{line,i}/\eta_{line,i+1} = q_0^m > 1$ (for $i = 0,1,\ldots,(n-1)/2-2$). Here, q_0 and m are respectively constant, and n is the number of the fluid molecules across the film thickness and is an odd number ($n \geqslant 5$). Nevertheless, the values of Δ_{i+1}/Δ_i and $\eta_{line,i}/\eta_{line,i+1}$ both may be varied across the film thickness, the model takes q_0 as the average value of Δ_{i+1}/Δ_i (for $i = 0,1,\ldots,(n-1)/2-2$).

It has been widely examined that equation (1) agrees well with the MDS results [21,22]. By using Eq. (1), the flow equation for the fluid flow in a nano slit pore is here further proven as follows.

3. Flow rate of the confined fluid

Fig. 1 shows the flowing volume of a molecule across the film thickness defined by a dashed box. The volume flow rate per unit contact length of the ith molecule across the film thickness is $u_i[(\Delta_{i-1}+\Delta_i)/2+D]$. The volume flow rate through the wall separation per unit contact length is thus $\sum_{i=0}^{n-1} u_i[(\Delta_{i-1}+\Delta_i)/2+D]$ (where $\Delta_{-1}=0$ and $\Delta_{n-1}=0$). This volume flow rate is exactly equal to $\int_0^h u_{cf,q}(z)dz$ $(=(u_0+u_{n-1})D/2+\sum_{i=0}^{n-2}(u_i+u_{i+1})(\Delta_i+D)/2))$, where $u_{cf,q}(z_i)=u_i$, z_i is the z coordinate of the ith molecule across the film thickness, and between the ith and $(i+1)$th molecules across the film thickness the value of $u_{cf,q}$ is linearly interpolated according to u_i and u_{i+1}. Here, the interpolation for $u_{cf,q}$ across the film thickness is accurate and the number of the confined molecule layers across the film thickness has no influence on the accuracy of this interpolation. Fig. 2 shows the distribution of the value of $u_{cf,q}$ across the film thickness. In the figure, the calculated area of the shadowed zone is the volume flow rate through the wall separation per unit contact length (i.e. $\int_0^h u_{cf,q}(z)dz$). This proves that the treatment of the function $u_{cf,q}(z)$ in the development of the flow factor approach model as shown in Ref. [17] was correct. The velocities u_0 and u_{n-1} of the fluid molecules on the confining walls as shown in Fig. 2 can respectively be equal to or different from the moving speeds of the corresponding walls depending on the fluid-wall interaction and the operating condition [4,10]. The slippage of the fluid on the wall is allowed in the present model.

The mass flow rate through the wall separation is thus $\rho_{bf}^{eff}\int_0^h u_{cf,q}(z)dz$, where ρ_{bf}^{eff} is the average density of the confined fluid across the film thickness. If the mass flow rate through the wall separation calculated from the conventional hydrodynamic theory [25] is $\rho_{bf}^{eff}\int_0^h u_{cf,a}(z)dz$, where $u_{cf,a}(z)$ is the distribution function of the fluid flowing velocity across the film thickness derived from the conventional hydrodynamic theory, the flow factor for the confined fluid is thus [17]:

$$\theta_v = \frac{\int_0^h u_{cf,q}(z)dz}{\int_0^h u_{cf,a}(z)dz} \tag{4}$$

By substituting Eq. (1) into Eq. (4), it was finally obtained that [17]:

$$\theta_v = \frac{\frac{2\bar{u}_b}{\bar{u}_a+\bar{u}_b} + \left(\varepsilon - \frac{D}{h}\right)\frac{\bar{u}_a-\bar{u}_b}{\bar{u}_a+\bar{u}_b} + K(F_1-\varepsilon F_2)}{1-K} \tag{5}$$

where $K = (\partial p/\partial x)h^2/\left[6\eta_{bf}^{eff}(\bar{u}_a+\bar{u}_b)\right]$, $\varepsilon = (2DI+II)/[h(n-1)(\Delta_l/\eta_{line,l})_{avr,n-1}]$, $F_1 = \eta_{bf}^{eff}(12D^2\Psi+6D\Phi)/h^3$, and $F_2 = 6\eta_{bf}^{eff}D(n-1)(l\Delta_{l-1}/\eta_{line,l-1})_{avr,n-1}/h^2$. Here, $I = \sum_{i=1}^{n-1} i(\Delta_l/\eta_{line,l})_{avr,i}$, $II = \sum_{i=0}^{n-2}[i(\Delta_l/\eta_{line,l})_{avr,i} + (i+1)(\Delta_l/\eta_{line,l})_{avr,i+1}]\Delta_i$, $\Psi = \sum_{i=1}^{n-1} i(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i}$, $\Phi = \sum_{i=0}^{n-2}[i(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i} + (i+1)(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i+1}]\Delta_i$, and $\eta_{bf}^{eff} = Dh/[(n-1)(D+\Delta_x)(\Delta_l/\eta_{line,l})_{avr,n-1}]$.

It was shown that for the studied condition $\varepsilon = 1$ [17]. According to this result, if $D \ll h$, Eq. (5) is simplified as [17]:

$$\theta_v = \frac{1+K\cdot S}{1-K} \tag{6}$$

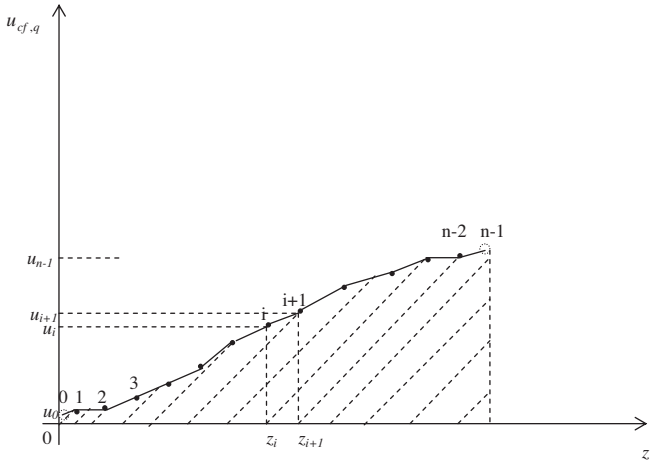

Fig. 2. Plot of the function $u_{cf,q}$ (z). The numerals on the curve are the order numbers of the fluid molecules across the film thickness. The marked points on the curve show the z coordinates and the corresponding moving velocities of the fluid molecules across the film thickness.