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Mass flow in nanoporous filtration membrane with small nanopores

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Abstract. The fluid flow in a small cylindrical nanotube such as occurring in the filtration membrane is essentially non-continuum, not predictable from the classical hydrodynamic flow theory. However, it has important practical applications in ultra filtration. It is shown that three factors i.e. the viscosity and density effect, the non-continuum effect and the wall slippage effect control this flow. The present paper shows that all these three effects heavily depend on the fluid-tube wall interaction, the former two effects strongly impede the flow and become more significant with the reduction of the diameter of the nanotube or with the increase of the interaction strength between the fluid and the nanotube wall, while the wall slippage effect speeds up the flow and it is more significant with the reduction of the diameter of the nanotube, with the increase of the power loss on the nanotube, or with the reduction of the interaction strength between the fluid and the nanotube wall. There is the competition between the former two effects and the wall slippage effect, determined by the power loss (POW) on the nanotube driving the flow. If POW is small enough, the viscosity and density effect and the non-continuum effect are dominant, and the mass flow rate through the nanotube is normally much lower than the classical flow theory calculation. If POW is sufficiently great, the wall slippage effect is dominant and the mass flow rate through the nanotube is much higher than the classical flow theory calculation. There are the values of POW which make the former two effects nearly equal to the wall slippage effect.

Keywords: filtration membrane; manotube; mass flow; non continuum; viscosity; wall slippage

1. Introduction

Nanoporous filtration membranes have important application in water purification, hemofiltration, liquid-liquid separation and biological liquid transport etc (Ariono *et al*. 2018, Bottino *et al*. 2011, Conlisk *et al*. 2002, El-ghzizel *et al*. 2019, Harrell *et al*. 2003, Henderson 1996, Kant *et al*. 2014, Levitt 1974, Losic and Simovic 2009, Oka and Murata 1970, Sohi *et al*. 2020, Wang and Zhang 2021). The filtration pores with the ultra small radii on the 1nm scale or less are very important for realizing ultra filtration. However, the understanding on the liquid flow inside these filtration pores is still not well achieved, though the observed flow phenomena are quite special and different from the classical recognition (Borg and Reese 2017, Holt *et al*. 2006, Majumder *et al*. 2005, Qin *et al*. 2011).

Experiments and theoretical studies on nanotube flows have been carried out a lot (Koklu *et al*. 2017, Li *et al*. 2019, Lu *et al*. 2019, Rudyak *et al*. 2018). Different groups may give different findings. But most of them showed that the law of nanotube flows is different from the conventional recognition of the continuum flow. Koklu *et al*. (2017) experimentally measured that the water flow rate in the nanopores with the diameters 10nm, 20nm and 40nm made of hydrophilic alumina was significantly lower than that calculated by the classical Hagen-Poiseuille equation. They proposed the formation of the sticking boundary layer with the thickness about 2.2nm on the nanopore wall. Gruener *et al*. (2009) proposed the formation of two strongly adsorbed boundary layers of water molecules on the wall of the hydrophilic silica pore with the diameters 7nm and 10nm when experimentally studying the water dynamics in the nanopore. Alibakhshi *et al*. (2015) also experimentally observed the similar phenomena when measuring the water flow rate in the silica nano slit pore with the width 7nm. Shadloo-Jahromi *et al*. (2020) found by molecular dynamics simulation (MDS) that the shear viscosity of the water confined in the silicon nano slit pore with the width below 1.85nm was oscillatorily increased with the reduction of the pore width. The increase with the gap reduction of the viscosity of the fluid confined in a nanometer-scale gap has been widely observed (Meyer *et al*. 1998). This viscosity enhancement undoubtedly increases the resistance and reduces the flow rate of the fluid in a nanochannel. The local density of the fluid in a small nanopore was also found by MDS to be oscillatorily increased with the reduction of the distance to the pore wall (Bitsanis *et al*. 1988, Somers and Davis 1992).

In the desalination of seawater by using the reverse osmosis (RO) membrane, the viscous flow model based on the continuum flow was ever used to calculate the water flux (Wijmans and Baker 1995). It was suspected that the stationary water layers would be formed on the nanotube wall, thus significantly reduce the diameter of the nanotube and reject the salt through the membrane. This should be due to the strong interaction between the water molecule and the molecule of the nanotube wall with specific hydrophilic materials as discussed above. However,

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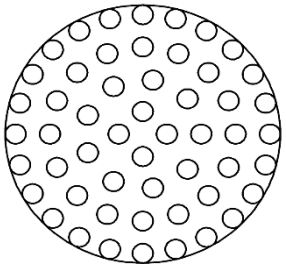


Fig. 1 The studied non-continuum flow in a small nanotube with the inner radius R less than h_{bf} (Li and Zhang 2021)

according to this flow model, the water flux should be greatly reduced owing to the reduction of the diameter of the nanotube. Also, it was suspected that such a flow model may fail for the nanotube with the diameter on the 1nm scale or less because of the non-continuum property of the confined water (Heiranian *et al*. 2023).

Zhang (2015) found that the non-continuum effect of the fluid in a narrow nanochannel greatly reduces the flow rate of the Poiseuille flow for a strong fluid-channel wall interaction, but it has no influence on the Couette flow rate. The non-continuum effect of the fluid is due to the discontinuity and inhomogeneity of the fluid across the channel height.

By experiments or MDS, Majumder *et al*. (2005), Holt *et al*. (2006), Borg and Reese (2017) and Qin *et al*. (2011) found that the water flow rates through the carbon nanotubes with the diameters below 7nm were several orders higher than the classical flow theory calculation. Wang *et al*. (2012) found by MDS that under low pressures the water flow rates through the carbon nanotubes with the diameters between 0.7nm and 1.2nm were far higher than calculated from the Hagen-Poiseuille equation. They found that the velocity profiles across the pore radii were non-parabolic. It was typically regarded that this water flow enhancement should be due to the slippage on the hydrophobic pore wall (Afsharpoor and Javadpour 2016, Mattia *et al*. 2012, Myers 2011).

Molecular dynamics simulation has been widely used in the modeling of nanochannel flows (Fan *et al*. 2002, Lee and Rossky 1994, Morcisno *et al*. 2017, Sofos *et al*. 2010, Stillinger and Rahman 1974). It currently can only simulate a tiny zone because of the computational limit. For overcoming its shortcoming, other models have also been proposed like the quasi-continuum model, the modified Navier-Stokes equation model, the dissipative particle dynamics method, the lattice Boltzman method, and the multiscale hybrid model (Zhang 2017a). Based on the flow factor approach model (Zhang 2006, 2013, 2015), Zhang (2016) derived the closed-form explicit mathematical equation for the non-continuum nanochannel flow. The advantage of his equation is the capability of modeling the engineering nanochannel flow even on the millimeter scale just with very modest computation. His equation was found to well match MDS (Jiang and Zhang 2022).

According to Zhang's nanoscale non-continuum flow equation, the present paper studies the influences of three factors on the flow in the small cylindrical nanotube with the pore radii on the 1nm scale or less by wide computations. These factors are the viscosity and density effect, the non-continuum effect and the wall slippage effect. The weak, medium and strong fluid-tube wall interactions were respectively considered. The value of the power loss ($DPOW$) on the channel for generating the wall slippage ranges between 1.0E-18Watt and 1.0E-12Watt. The new interesting results were found, hard to obtain from other simulation approaches or experiments. They are important for understanding the nanoscale non-continuum flow and the design of nanoporous filtration membrane for improving the flux.

2. Flow in a small nanotube

Here, a small nanotube refers to the nanotube the diameter of which is so small that inside the tube the continuum fluid disappears and there is only the fluid molecule layers physically adsorbed to the tube wall. In such a small nanotube, the flow driven by the pressure is essentially non-continuum. Such a nanotube flow actually popularly occurs and has important applications in people's ordinary lives. Fig. 1 shows the molecules of the fluid like water in a small nanotube; h_{bf} is the thickness of the adsorbed layer potentially fully formed on the tube wall.

As shown in Fig. 1, under the fluid-tube wall interaction, the fluid molecules are adsorbed and orientated in the whole small nanotube. The discontinuity and inhomogeneity in the nanotube are significant. They generate the non-continuum effect of the fluid. Both the average density and effective viscosity of the fluid are also enhanced according to molecular dynamics simulation results (Bitsanis *et al*. 1988, Jabbarzadeh *et al*. 1997). If the adhesive strength of the fluid molecules to the tube wall is not sufficient under the exerted pressure gradient, the fluid molecules will slip on the tube wall i.e. the wall slippage occurs. This is particularly the case for a hydrophobic tube wall. The wall slippage surely alters the velocity profile across the tube radius and consequently the flow rate through the nanotube. All these three factors make the flow behavior in a small nanotube radically deviate from the classical hydrodynamic flow theory (the Hagen-Poiseuille equation).

3. Mathematical formulations for the non-continuum flow in a small nanotube

Zhang (2006) showed the physical explanation and mathematical formulation for the non-continuum flow of the fluid confined in the molecular-scale surface gap. The discontinuity of the fluid is characterized by the separation Δ between the neighboring fluid molecules across the surface gap. The inhomogeneity of the fluid is characterized by both the variations of Δ and the local viscosity across the surface gap. These two factors leads to the non-continuum effect of the fluid, which is described by the parameter S $(= F_1 - F_2)$. Zhang (2006) showed the mathematical formulations respectively for F_1 and F_2. Here, the mathematical equation for S was regressed out and fits the molecular dynamics simulation results (Zhang

2004 and 2016). Zhang (2006) also showed the mathematical formulation for the termed effective viscosity η_{bf}^{eff} of the fluid, the value of which is greater than that of the fluid bulk viscosity. Because the local density of the fluid is varied across the molecular-scale surface gap due to the fluid-solid surface interaction, the average density ρ_{bf}^{eff} of the fluid across the surface gap is dependent on both the value of the surface gap and the fluid-solid surface interaction, and it is greater than the fluid bulk density. The present formulations for both η_{bf}^{eff} and ρ_{bf}^{eff} were regressed out and fit the experimental and MDS results (Zhang 2004).

Zhang (2017b) gave the following equation for calculating the mass flow rate through a small nanotube by incorporating the effects of the wall slippage, the fluid non-continuum property and the fluid rheological property enhancement:

$$q_m = \pi\rho_{bf,2}^{eff}u_s R^2 + \frac{\pi\rho_{bf,2}^{eff}SR^4}{4\eta_{bf,2}^{eff}}\frac{\partial p}{\partial x}, \quad \text{for} \quad R \le h_{bf} \tag{1}$$

where u_s is the wall slipping velocity, $\rho_{bf,2}^{eff}$ and $\eta_{bf,2}^{eff}$ are respectively the average density and the effective viscosity of the non-continuum film in the whole tube, and S is the parameter accounting for the non-continuum effect of the film, p is the pressure driving the flow, and x is the coordinate in the axial direction of the tube. Jiang and Zhang (2022) substantiated the correctness of the non-continuum flow model as shown by Eq. (1).

The classical hydrodynamic flow theory gives the mass flow rate through the cylindrical tube as:

$$q_{m,conv} = -\frac{\pi\rho R^4}{4\eta}\frac{\partial p}{\partial x} \tag{2}$$

where ρ and η are respectively the bulk density and bulk viscosity of the fluid.

Based on the interfacial limiting shear strength model (Zhang 2014), which interprets the wall slippage as the result of the wall shear stress exceeding the wall shear stress endurability i.e. the wall shear strength, the following ratio is calculated (Li and Zhang 2021):

$$r_m = \frac{q_m}{q_{m,conv}} = \frac{4C_q\theta_\tau^2\eta(DPOW)}{\pi R^2\tau_s^2 l} - \frac{C_q S}{C_y} \tag{3}$$

where $C_q = \rho_{bf}^{eff}/\rho$, $C_y = \eta_{bf}^{eff}/\eta$, τ_s is the shear strength of the fluid-tube wall interface, l is the axial length of the whole nanotube, θ_τ is the correction factor for the wall shear stress due to the fluid non-continuum effect (Zhang 2006), $DPOW = POW - POW_{cr}$, POW is the externally applied power loss on the whole nanotube for driving the flow in the unit Watt, which is the independent parameter and measures the energy cost and the technical (energy conservation) performance of the realistic membrane with the specific thickness (l), and POW_{cr} is the critical power loss on the whole nanotube for initiating the wall slippage. Both the values of C_q and C_y are dimensionless and greater than unity for the very small nanotube because of the fluid-tube wall interaction (Zhang 2004). They respectively measure the enhancements of the average density and the effective viscosity of the confined fluid in the nanotube (Meyer *et al*. 1998, Zhang 2004).

If neglecting both the non-continuum effect and the wall slippage effect, by only considering the effect of the density and viscosity enhancements in the nanotube, the ratio r_m becomes:

$$r_{m,v-d} = \frac{C_q}{C_y} \tag{4}$$

If neglecting both the wall slippage effect and the effect of the density and viscosity enhancements, by only considering the non-continuum effect, the ratio r_m becomes:

$$r_{m,nc} = -S \tag{5}$$

where $-1 < S < 0$ for the non-continuum fluid and $S = -1$ for the continuum fluid. The value of the dimensionless parameter S measures the non-continuum effect of the fluid in the very small nanotube (Zhang 2006, 2016). Smaller the magnitude of S, stronger the non-continuum effect of the fluid, which reduces the mass flow rate of the Poiseuille flow as shown by Eq. (1). The reduction of the diameter of the small nanotube yields the stronger non-continuum effect and thus the smaller magnitude of S as shown by Eq. (9). This fits the physical nature and the MDS results (Zhang 2016).

If neglecting both the non-continuum effect and the effect of the density and viscosity enhancements, by only considering the wall slippage effect, the ratio r_m becomes:

$$r_{m,slip} = \frac{4C_q\theta_\tau^2\eta(DPOW)}{\pi R^2\tau_s^2 l} + 1, \quad \text{for } DPOW > 0 \tag{6}$$

4. Calculation

In the calculation, the fluid was chosen as water. The nanotube material may be various and can be hydrophobic, moderately hydrophilic and strongly hydrophilic. It can be carbon, graphene, silicon, silica, carbonized silicon and alumina etc. The interaction between the fluid and the nanotube wall can be weak, medium-level and strong.

The parameter C_y is formulated as (Zhang 2004):

$$C_y(\bar{R}) = a_0 + \frac{a_1}{\bar{R}} + \frac{a_2}{\bar{R}^2}, \text{ for } 0 < \bar{R} < 1 \tag{7}$$

where $\bar{R} = R / R_{cr}$, R_{cr} is the critical radius for characterizing the rheological property of the fluid in the nanotube, and a_0, a_1 and a_2 are respectively constant.

For $R \ge R_{cr}$ i.e. $\bar{R} \ge 1$, the fluid becomes continuum and the rheological properties like the effective viscosity and the average density of the fluid across the tube diameter are equal to the fluid bulk rheology values, i.e. C_y =1, C_q =1,

Table 1 Fluid viscosity data for different fluid-tube wall interactions (Zhang 2004)

Interaction	Parameter		
	a_0	a_1	a_2
Strong	1.8335	-1.4252	0.5917
Medium	1.0822	-0.1758	0.0936
Weak	0.9507	0.0492	1.6447E-4

Table 2 Fluid density data for different fluid-tube wall interactions (Zhang 2004)

Interaction	Parameter			
	m_0	m_1	m_2	m_3
Strong	1.43	-1.723	2.641	-1.347
Medium	1.30	-1.065	1.336	-0.571
Weak	1.116	-0.328	0.253	-0.041

Table 3 Fluid non-continuum property data for different fluid-tube wall interactions (Zhang 2004)

Interaction	Parameter			
	n_0	n_1	n_2	n_3
Strong	0.4	-1.374	-0.534	0.035
Medium	-0.649	-0.343	-0.665	0.035
Weak	-0.1	-0.892	-0.084	0.1

Table 4 Characteristic parameter values for different fluid-tube wall interactions

Interaction	Parameter		
	τ_s (kPa)	$R_{cr,bf}$ (nm)	l (nm)
Strong	60	10	100
Medium	30	5	100
Weak	10	2.8	8

and $S = -1$ (shown below).

The parameter C_q is formulated as (Zhang 2004):

$$C_q(\bar{R}) = m_0 + m_1 \bar{R} + m_2 \bar{R}^2 + m_3 \bar{R}^3, \quad \text{for } 0 < \bar{R} < 1 \tag{8}$$

where m_0, m_1, m_2 and m_3 are respectively constant.

The parameter S is formulated as (Zhang 2004):

$$S(\bar{R}) = [n_0 + n_1(\bar{R} - n_3)^{n_2}]^{-1}, \quad \text{for } n_3 < \bar{R} < 1 \tag{9}$$

where n_0, n_1, n_2 and n_3 are respectively constant.

The input operational parameter values are as follows: $D = 0.28$ nm, $\eta = 0.001 Pa \cdot s$, $\theta_\tau = 1$. Here, the chosen value of θ_τ gives the overestimation of the wall slippage effect for the medium and strong fluid-tube wall interactions; Stronger the fluid-tube wall interaction, greater this overestimation since $0 < \theta_\tau < 1$ and a stronger fluid-tube wall interaction gives a lower value of θ_τ. However, it can not alter the drawn conclusions. The other operational parameter values are respectively shown in Tables 1-4. For different fluid-tube wall interactions, the variations of C_y, C_q and S with $\bar{R}$ have been shown by Zhang (2004) when based on Tables 1-4. They match the experimental measurements or the MDS results (Jabbarzadeh *et al*. 1997, Meyer *et al*. 1998, Zhang 2016).

In Tables 1-4, the strong water-tube wall interaction (or the strongly hydrophilic nanotube wall) may be obtained by using the nanotube made of alumina or silica, the medium water-tube wall interaction (or the moderately hydrophilic nanotube wall) may be obtained by using the nanotube made of silicon, and the weak water-tube wall interaction (or the hydrophobic nanotube wall) may be obtained by using the nanotube made of carbon or graphene.

5. Results

5.1 Effect of the fluid density and viscosity enhancements in the nanotube

Fig. 2 shows the values of $r_{m,v-d}$, which are significantly lower than unity even for the weak fluid-tube wall interaction. In itself, the viscosity enhancement increases the viscous resistance and reduces the mass flow rate through the nanotube. This effect is particularly significant for the strong fluid-tube wall interaction and small nanotube radii as shown in Fig. 2. For the weak interaction, the influence of the nanotube radius R on the value of $r_{m,v-d}$ is modest, and it indicates a slight increase of the fluid effective viscosity (η_{bf}^{eff}) with the reduction of R. However, for the medium and especially for the strong fluid-tube wall interactions, the values of $r_{m,v-d}$ are rapidly reduced with the reduction of R, and it indicates the significant increases of the fluid effective viscosity (η_{bf}^{eff}) with the reduction of R. The effect of the fluid viscosity enhancement on the mass flow in the small nanotube is shown to be very strong for the medium and strong fluid-tube wall interactions (i.e. for the hydrophilic or strongly hydrophilic nanotube walls). It strongly impedes the nanotube flow. For example, for the strong interaction and $R = 0.5$nm, the value of $r_{m,v-d}$ is only about 0.01, and this indicates the almost halting of the nanotube flow suggesting a very large viscous resistance in the flow. Such a result corresponds to the experimental measurements by Koklu *et al*. (2017), Gruener *et al*. (2009) and Alibakhshi *et al*. (2015) for the water flows in strongly hydrophilic alumina nanopores and hydrophilic silica nanopores, which showed that the water flow should be halted in the nanopore due to the formation of the sticking boundary layer on the pore wall when the nanopore radius is less than the thickness of the boundary layer.

5.2 The non-continuum effect in the nanotube

The non-continuum effect of the fluid in a small nanotube essentially exists due to the discontinuity and inhomo-

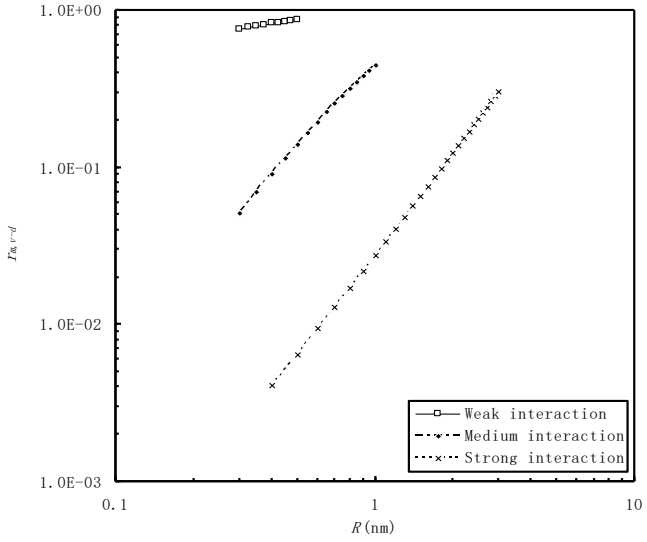


Fig. 2 Values of $r_{m,v-d}$

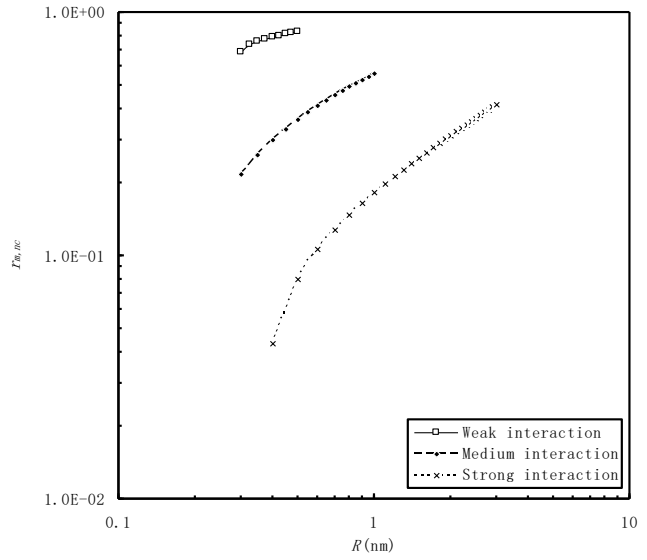


Fig. 3 Values of $r_{m,nc}$

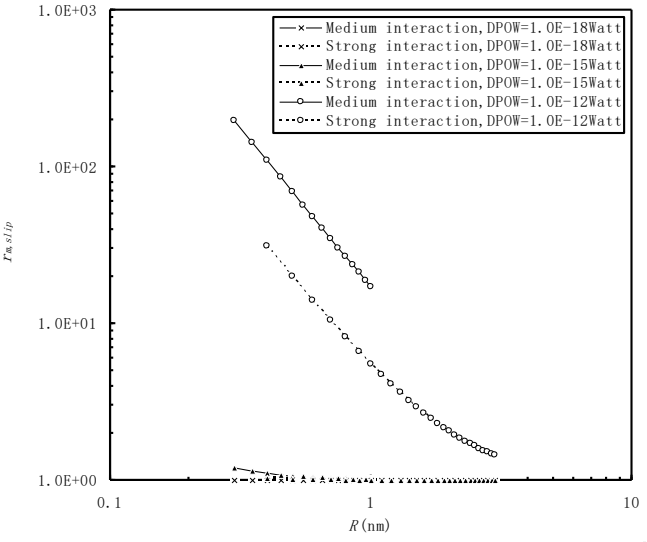


Fig. 4 Values of $r_{m,slip}$

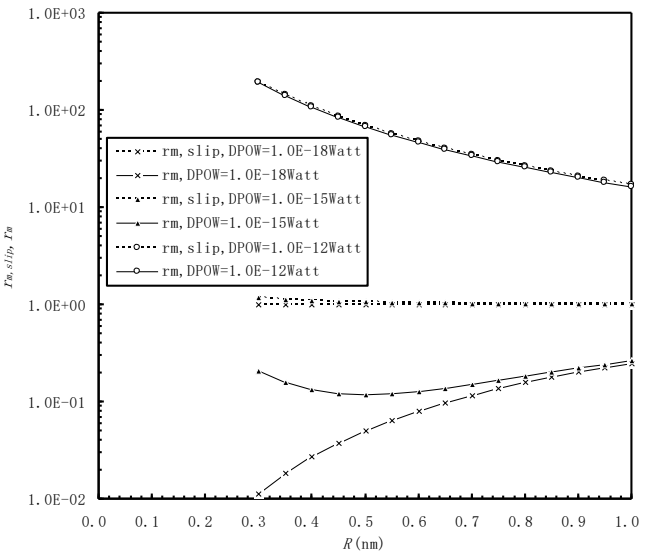
geneity across the tube radius as shown in Fig. 1. It strongly depends on both the fluid-tube wall interaction and the nanotube radius. Zhang (2013, 2016) verified this effect and pointed out that it is only present in the Poiseuille flow. The values of $r_{m,nc}$ shown in Fig. 3 manifest this important effect. For $R \leq 0.5$nm, the non-continuum effect in the nanotube is normally significant even for a weak fluid-tube wall interaction as shown in Fig. 3. It reduces the flow rate through the nanotube. For the strong interaction and $R =$ 0.5nm, Fig. 3 shows that the value of $r_{m,nc}$ is about 0.1; This indicates the huge reduction of the flow rate by the non-continuum effect. As shown by Figs. 2 and 3, for the medium and strong fluid-tube wall interactions, the combined effect of the fluid viscosity enhancement and the non-continuum property should very severely hinder and even almost stop the flow through a very small nanotube. It agrees with the experimental observations (Alibakhshi *et al.* 2015, Gruener *et al*. 2009, Koklu *et al*. 2017).

5.3 Effect of the wall slippage

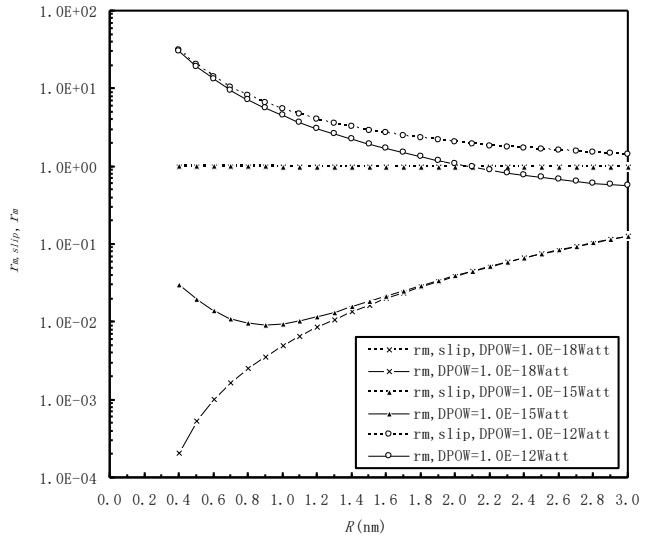
The wall slippage was found to easily occur in the nanotube flow. It frequently occurs in a hydrophobic nanotube (Afsharpoor and Javadpour, 2016, Holt *et al.* 2006, Korg and Reese 2017, Majumder *et al.* 2005, Mattia *et al.* 2012, Myers 2011, Qin *et al.* 2011, Wang *et al.* 2012). It can also occur in a hydrophilic nanotube (Tran-Duc *et al.* 2019). However, in a strongly hydrophilic nanotube, it was much more difficultly observed (Alibakhshi *et al.* 2015, Gruener *et al.* 2009, Koklu *et al.* 2017). The values of $r_{m,slip}$ shown in Fig. 4 indicate that the wall slippage enhances the flow rate through a nanotube. This effect is shown to be mainly decided by the power loss ($DPOW$) on the whole tube for driving the wall slippage. An over small value of $DPOW$ such as $DPOW = 1.0E-18$ Watt or $1.0E-15$ Watt makes the wall slippage effect negligible. However, a sufficiently large value of $DPOW$ such as $DPOW = 1.0E-12$ Watt makes the wall slippage effect very significant even for a strong fluid-tube wall interaction, which increases the flow rate by 1 to 2 orders as shown in Fig. 4. The wall slippage effect is shown to be also strongly dependent on the nanotube radius and the fluid-tube wall interaction. Smaller the nanotube radius or weaker the fluid-tube wall interaction, stronger the wall slippage effect. That may be the reason why the measured water flow rates through the hydrophobic carbon nanotubes with the diameters below 7nm are 3 to 5 orders higher than the classical hydrodynamic flow theory calculation (Holt *et al.* 2006, Korg and Reese 2017, Majumder *et al.* 2005, Qin *et al.* 2011). Fig. 4 shows that the flow enhancement by the wall slippage is huge in a very small hydrophobic nanotube if $DPOW$ is sufficiently large.

5.4 Combined effect of the wall slippage, non-continuum property and viscosity enhancement in a nanotube

The values of r_m shown in Fig. 5 reflects the combined effect of the wall slippage, non-continuum property and viscosity enhancement in a nanotube. They are also



(a) Medium interaction



(b) Strong interaction

Fig. 5 Comparison between the values of $r_{m,slip}$ and r_m

compared with those of $r_{m,slip}$. For a sufficiently high value of $DPOW$ such as $DPOW = 1.0E-12$ Watt, the values of r_m and $r_{m,slip}$ are nearly the same for the medium fluid-tube wall interaction; While they are very close for $R \leq 1$nm and their divergence is obvious for larger R values for the strong fluid-tube wall interaction. This indicates that for a sufficiently high value of $DPOW$, the flow in a small nanotube can be considered to be only influenced by the wall slippage effect, and we should observe the large flow enhancement which is not predictable from the classical flow theory. However, Fig. 5 shows that if $DPOW$ is small such as $DPOW = 1.0E-18$ Watt or $1.0E-15$ Watt, the wall slippage effect is weak and there are great differences between r_m and $r_{m,slip}$. For this case, the combined effect of the viscosity enhancement and non-continuum property is predominant in the nanotube and the flow rate through a small nanotube is much smaller than the classical flow theory calculation especially for the medium and strong fluid-tube wall interactions. These results provide the important indication for the nanoporous membrane filtration that the externally applied power loss on the membrane is the critically important parameter governing the membrane flux. We observe from Figs. 5(a)-(b) that for $DPOW = 1.0E-15$ Watt, there exists the value of the nanotube radius R which results in the lowest value of r_m. This phenomenon is due to the competition between the wall slippage effect and the combined effect of the viscosity enhancement and non-continuum property in the nanotube. It was however still not observed before, and needs to be examined in the following experiment or MDS.

6. Commenting remarks

The present non-continuum flow model has been verified by the MDS results (Jiang and Zhang 2022). The used exemplary values of the operational parameters are fitting the realistic cases (Meyer *et al*. 1998; Zhang 2004). The obtained results of the fast transport of water through the hydrophobic nanotubes (with the weak fluid-tube interaction) with the diameters on the 1nm scale owing to the wall slippage qualitatively fit the experimental observations on the (hydrophobic) carbon and graphene nanotubes with the same diameters (Holt *et al*. 2006; Majumder *et al*. 2005, Qin *et al*. 2011).

Currently, the calibration data required by the present model are lacking from the published experimental source. A direct comparison is difficult to make with those experiments. Once the required data are calibrated, the comparison with the performance of the real nanotube should be successfully made as shown by Jiang and Zhang (2022). Nevertheless, the present results reveal the physical disciplines underlying the liquid flow in the small nanotubes, which are governed by a lot of factors.

7. Conclusions

The mass flow in a small cylindrical nanotube is studied based on the closed-form explicit nanoscale flow equation. It is essentially non-continuum because of the discontinuity and inhomogeneity across the nanotube radius. It has important applications in ultra filtration, cellular membrane transport and biosensors ect and deserves a proper understanding.

The calculations were made for the water flow through the nanotubes with the diameters below 6.0nm respectively for the weak, medium and strong water-tube wall interactions, which respectively correspond to the hydrophobic, modestly hydrophilic and strongly hydrophilic nanotubes.

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

• Both the effects of the fluid viscosity enhancement and the non-continuum property in a small nanotube significantly reduce the flow rate through the nanotube even for a weak fluid-tube wall interaction. Particularly for the medium and

strong fluid-tube wall interactions, they largely reduce the flow rate and even almost halt the flow.

• The wall slippage effect in the nanotube is determined by the power loss POW $(= DPOW + POW_{cr})$ on the whole nanotube for driving the flow. An over small value of POW results in no slippage occurrence or the negligible wall slippage effect. A sufficiently high value of POW generates the wall slippage which greatly enhances the flow rate through the nanotube even by several orders. This flow enhancement heavily depends on the value of POW, the nanotube radius and the fluid-tube wall interaction.

• The combined effect of the wall slippage, non-continuum property and viscosity enhancement in the nanotube is determined by the value of POW. A sufficiently high value of POW makes the wall slippage effect dominant and the flow rate through the nanotube is thus largely enhanced. An over small value of POW makes the effects of the fluid viscosity enhancement and the non-continuum property dominant and thus the flow rate through the nanotube is much lower than the classical hydrodynamic flow theory calculation.

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Nomenclature

$a_0,\ a_1,\ a_2$ constant, Eq. (7)

$$C_q = \rho_{bf}^{eff}/\rho$$
$$C_y = \eta_{bf}^{eff}/\eta$$

D fluid molecule diameter, m

$$DPOW = POW - POW_{cr}$$

h_{bf} thickness of the adsorbed layer potentially fully formed on the nanotube wall, m

l axial length of the whole nanotube, m

$m_0,\ m_1,\ m_2,\ m_3$ constant, Eq. (8)

$n_0,\ n_1,\ n_2,\ n_3$ constant, Eq. (9)

p pressure driving the flow, Pa

POW power loss on the whole nanotube, Watt

POW_{cr} critical power loss on the whole nanotube for initiating the wall slippage, Watt

q_m mass flow rate through the nanotube calculated from the present model, kg/s

$q_{m,conv}$ mass flow rate through the nanotube calculated from the classical Hagen-Poiseuille equation, kg/s

$$r_m = q_m/q_{m,conv}$$
$$r_{m,v-d} = C_q/C_y$$
$$r_{m,nc} = -S$$

$r_{m,slip}$ value of r_m by only considering the wall slippage effect

R inner radius of the nanotube, m

R_{cr} critical radius for characterizing the rheological property of the fluid in the nanotube, m

$\bar{R} = R / R_{cr}$

S parameter accounting for the non-continuum effect of the film in the nanotube

u_s wall slipping velocity, m/s

x coordinate in the axial direction of the nanotube, m

ρ, η bulk density and bulk viscosity of the fluid respectively, kg/m^3, Pa $\cdot\, s$

$\rho_{bf,2}^{eff}$, $\eta_{bf,2}^{eff}$ average density and effective viscosity of the non-continuum film in the whole nanotube respectively, kg/m^3, Pa $\cdot\, s$

τ_s shear strength of the fluid-nanotube wall interface, Pa

θ_τ correction factor for the wall shear stress due to the fluid non-continuum effect (Zhang 2006)