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EFFECT OF TEMPERATURE ON WATER TRANSPORTATION IN NANOCHANNEL

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ABSTRACT

The flow factor approach model was used to study the effect of temperature on water transportation in a nano slit pore flow driven by the pressure. The influences of the temperature on the density and viscosity of water and on the water-wall interaction were considered. The results show that enhancing the temperature of water significantly improves water transportation in nanochannel, especially when the channel height is so low that the water non-continuum effect is significant. The mechanism of this temperature effect is that the temperature increase not only appreciably reduces the water viscosity but also considerably alleviates the water non-continuum effect, in these circumstances the water flow rate through the channel owing to the Poiseuille flow is significantly increased.

Keywords: *Water transportation; Nanochannel; Flow; Temperature; Model*

1. INTRODUCTION

The super-purification of water is important to the life of human beings. It needs to filter out very small substances such as bacteria, virus, tiny pollutants, organic contaminants and ions. It often relies on the use of nanoporous filtration membrane, which prevents the going-through of big size molecules but permit water to flow through (Das, et al., 2014; Han et al., 2013; Jackson and Hillmyer, 2010; Surwade, et al., 2015; Wei, et al., 2014). The flow of water in a nanoporous membrane is driven by the pressure, and this flow rate is very small because of the confinement of water in the nanoscale channel (Gordillo and Marti, 2007; Marti, et al., 2010; Marti, et al.,2006; Mamontov, et al., 2005; Nagy, et al., 2007; Su and Guo, 2012; Zangi, 2004; Zhang, 2015). It is a research task that how to improve the flow of water through a nanochannel. This research is definitely of significant interest to the treatment of water by nanofluidics.

For improving the transportation, the concept of the nanotube tree with branches was proposed (Zhang, 2017). It was suggested that the transportation capacity of the nanotube tree is equivalent to that of a conventional tube the inner radius of which is on the millimeter scale even when the fluid-wall interaction is strong (Zhang, 2017).

On the other hand, from the principle of the Poiseuille flow in a nanochannel, we can explore the way to improve the transportation capacity of a single nanochannel. According to the flow factor approach model for nanochannel flow (Zhang, 2016), it was found that the mass flow rate through the nanochannel owing to the Poiseuille flow is largely influenced by the effective viscosity of the confined fluid and the fluid non-continuum effect, both of which are enhanced with the reduction of the channel height and actually strongly impedes the fluid flow through the channel. These two factors are however strongly influenced by the fluid temperature, the increase of which remarkably reduces the fluid viscosity, the interaction strength between the fluid and the wall and thus the fluid non-continuum effect. The enhancement of the fluid temperature thus should have a significant positive effect on mass transportation through a nanochannel.

The present paper carries out an analysis for the effect of water temperature on the transportation of water through the nanochannel owing to the Poiseuille flow, by using the flow factor approach model. The water temperature varies from $5\,^oC$ to $90\,^oC$. The temperature effect for different channel heights was investigated. The calculation results show that enhancing the water temperature greatly improves the transportation capacity of water through the nanochannel, especially when the channel height is low.

2. ANALYSIS

The mass flow rate of water through a nano slit pore driven by the pressure is analytically investigated by using the flow factor approach model. The influences of the pressure of the confined water on the density and viscosity of water in the channel are neglected, as the pressure in nanofluidics is normally not so high. For convenience, the water film slippage at the wall surface is also neglected; This should not alter the obtained conclusions.

For no interfacial slippage, the mass flow rate per unit channel length through a nano slit pore owing to the Poiseuille flow is (Zhang, 2016):

$$q_{m,bf} = \frac{S\rho_{bf}^{eff} h^3}{12\eta_{bf}^{eff}} \frac{dp}{dx} \tag{1}$$

where h is the channel height, p is the pressure of the confined fluid, x is the coordinate along the flow direction, ρ_{bf}^{eff}, η_{bf}^{eff} and S are respectively the average density of the fluid across the channel height, the effective viscosity of the fluid and the parameter accounting for the discontinuity and inhomogeneity effects of the fluid across the channel height i.e. the non-continuum effect of the fluid ($-1 \le S < 0$). It is defined that:

$$r = \left| \frac{12\eta_1 q_{m,bf}}{\rho_1 h^3 dp/dx} \right| \tag{2}$$

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where ρ_1 and η_1 are respectively the bulk density and bulk viscosity of the fluid for a reference high temperature T_1 under ambient pressure. The parameter r represents the ratio of $q_{m,bf}$ to the mass flow rate per unit channel length through the channel at the high temperature T_1 based on the continuum fluid assumption. It can be used to measure the mass transportation ability of the channel at different temperatures.

The parameter ρ_{bf}^{eff} at low pressures is formulated as dependent on the fluid temperature and the channel height and it is (Zhang, 2017) :

$$\rho_{bf}^{eff}(T,h) = \rho_1[1 - k_\rho(T - T_1)]Cq(T,h) \tag{3}$$

where T is the fluid temperature in ^oC, T_1 is a reference high temperature, ρ_1 is the bulk density of the fluid at the temperature T_1 under low pressure, k_ρ is constant, and Cq is the parameter accounting for the fluid solidification due to the confinement of the wall.

The parameter η_{bf}^{eff} at low pressures is also formulated as dependent on the fluid temperature and the channel height and it is (Zhang, 2017):

$$\eta_{bf}^{eff}(T,h) = \eta_1 e^{-\lambda(T-T_1)} Cy(T,h) \tag{4}$$

where λ is constant, η_1 is the bulk viscosity of the fluid at the temperature T_1 under low pressure, Cy is the parameter accounting for the wall confinement effect on the fluid viscosity.

Substituting Eq. (3) and (4) into Eq. (1) and further substituting Eq. (1) into Eq. (2) yields:

$$r = \frac{|S|\, Cq(T,h) e^{\lambda(T-T_1)}[1 - k_\rho(T - T_1)]}{Cy(T,h)} \tag{5}$$

3. CALCULATION

Here, exemplary calculations were made. In the calculation, $Cq(T, h)$ is interpolated according to the values of $Cq(T_1, h)$ and $Cq(T_0, h)$ and expressed as:

$$Cq(T,h) = \frac{Cq(T_1,h) - Cq(T_0,h)}{T_1 - T_0}(T - T_0) + Cq(T_0,h) \tag{6}$$

where $Cq(T_1, h)$ and $Cq(T_0, h)$ are respectively the values of $Cq(T, h)$ at the temperatures T_1 and T_0 which respectively correspond to weak and medium-level fluid-wall interactions. $Cq(T_1, h)$ and $Cq(T_0, h)$ are generally expressed as (Zhang, 2017):

$$Cq(H) = \begin{cases} 1 & , \quad \text{for} \quad H \ge 1 \\ m_0 + m_1 H + m_2 H^2 + m_3 H^3 & , \ \text{for}\ 0 < H < 1 \end{cases} \tag{7}$$

where $H = h/h_{cr,bf}$, $h_{cr,bf}$ is the critical channel height for the confined fluid to be continuum, and the values of m_0, m_1, m_2, and m_3 respectively for T_1 and T_0 are shown in Table 1(a).

$Cy(T, h)$ is interpolated as:

$$Cy(T,h) = \frac{Cy(T_1,h) - Cy(T_0,h)}{T_1 - T_0}(T - T_0) + Cy(T_0,h) \tag{8}$$

where $Cy(T_1, h)$ and $Cy(T_0, h)$ are respectively the values of $Cy(T, h)$ at the temperatures T_1 and T_0 which respectively correspond to weak and medium-level fluid-wall interactions. $Cy(T_1, h)$ and $Cy(T_0, h)$ are generally expressed as (Zhang, 2017):

$$Cy(H) = \begin{cases} 1 & , \quad \text{for} \quad H \ge 1 \\ a_0 + \dfrac{a_1}{H} + \dfrac{a_2}{H^2} & , \quad \text{for}\ 0 < H < 1 \end{cases} \tag{9}$$

where a_0, a_1 and a_2 are respectively constants. The values of a_0, a_1 and a_2 respectively for T_1 and T_0 are shown in Table 1(b).

The value of S is interpolated as:

$$S(T,h) = \frac{S(T_1,h) - S(T_0,h)}{T_1 - T_0}(T - T_0) + S(T_0,h) \tag{10}$$

where $S(T_1, h)$ and $S(T_0, h)$ are respectively the values of $S(T, h)$ at the temperatures T_1 and T_0 which respectively correspond to weak and medium-level fluid-wall interactions. $S(T_1, h)$ and $S(T_0, h)$ are generally expressed as (Zhang, 2017):

$$S(H) = \begin{cases} -1 & , \quad \text{for} \quad H \ge 1 \\ [n_0 + n_1(H - n_3)^{n_2}]^{-1} & , \ \text{for}\ n_3 < H < 1 \end{cases} \tag{11}$$

where n_0, n_1, n_2 and n_3 are respectively constants. The values of n_0, n_1, n_2 and n_3 respectively for T_1 and T_0 are shown in Table 1(c).

Table 1(a) Fluid viscosity data for different temperatures (Zhang, 2017)

Parameter / Temperature	a_0	a_1	a_2
T_0	1.0822	-0.1758	0.0936
T_1	0.9507	0.0492	1.6447E-4

Table 1(b) Fluid density data for different temperatures (Zhang, 2017)

Parameter / Temperature	m_0	m_1	m_2	m_3
T_0	1.30	-1.065	1.336	-0.571
T_1	1.116	-0.328	0.253	-0.041

Table 1(c) Fluid non-continuum property data for different temperatures (Zhang, 2017)

Parameter / Temperature	n_0	n_1	n_2	n_3
T_0	-0.649	-0.343	-0.665	0.035
T_1	-0.1	-0.892	-0.084	0.1

4. RESULTS

In the calculation, the modeled fluid was water and the following parameter values were taken:

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$T_0 = 3^oC$, $T_1 = 95^oC$, $k_\rho = 0.00053/^oC$, $\lambda = 0.021/^oC$, $h_{cr,bf} = 3nm$ for $T=T_1$, and $h_{cr,bf} = 6nm$ for $T=T_0$

The results were computed for T ranging between T_0 and T_1. In this temperature range, when $h \geq 6nm$, the channel flow is a continuum flow, and Eq. (5) reduces to:

$$r = e^{\lambda(T-T_1)}[1 - k_\rho(T - T_1)] \qquad \text{for a continuum flow} \qquad (12)$$

Figure 1 plots the values of r against the temperature T for different channel heights for which the confined water is in a non-continuum flow. The obtained r values are also compared with those for a continuum flow at different temperatures calculated from Eq. (12). It is shown that whenever the water is in continuum or non-continuum flows, the temperature enhancement significantly increases the value of r and thus significantly increases the mass flow rate through the channel. This effect appears more pronounced for a lower h for which the non-continuum effect of the water is stronger. The calculation results indicate that enhancing the fluid temperature is very helpful for transportation of the fluid through a nanochannel by the pressure driving. This may have an important engineering application value for mass and heat transfer by nanochannel, as the flow rate through a nanochannel driven by the pressure is usually very small, unavoidably limited by the strong non-continuum and viscous effects of the fluid in such a small gap .

If the interfacial slippage at the wall surface is further considered, the drawn conclusion should still stand, as the temperature rise actually stimulates the interfacial slippage and thus further increases the mass flow rate through the channel, by dropping the fluid-wall interfacial shear strength (Zhang, 2015b).

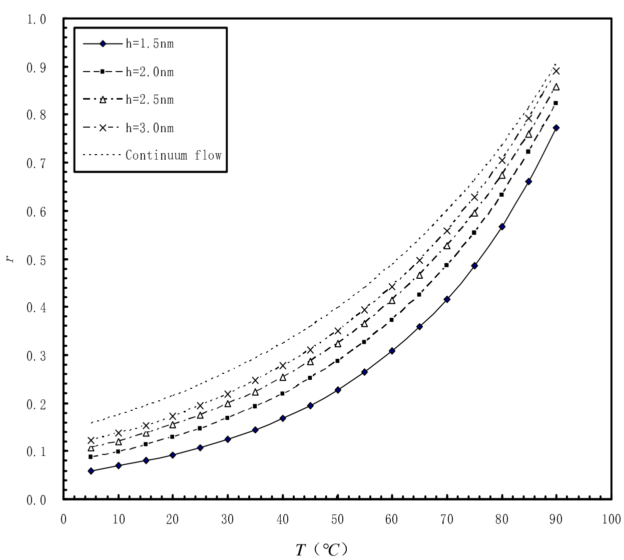

Fig. 1 Plot of the value of r against the temperature T for different channel heights for the confined water flow.

5. CONCLUSIONS

This paper analytically investigates the influence of the water temperature on the mass transportation of water in a nano slit pore driven by the pressure, by using the flow factor approach model. In the analysis, the temperature of water varied from $5\,^oC$ to $90\,^oC$. The dependence of both the density and viscosity of the water on the temperature and the channel height were considered. The influence of the water temperature on the water-wall interaction was also incorporated.

The calculation results show that enhancing the water temperature significantly increases the water mass flow rate through the nanochannel. This effect is due to that the water temperature rise not only significantly reduces the water viscosity, but also considerably alleviates the non-continuum effect of the confined water; The latter two factors are actually harmful for the mass transportation in a nanochannel driven by the pressure.

The obtained results may have an important engineering implication by enhancing the water temperature to improve the water transportation in a nanochannel.

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