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TRANSPORT PROPERTY OF CELLULAR MEMBRANE

Wei Lin[a] and Yongbin Zhang[b, *]

[a] *School of Mechanics Technology, Wuxi Institute of Technology, Wuxi, Jiangsu Province, China*
[b] *College of Mechanical Engineering, Changzhou University, Changzhou, Jiangsu Province, China*

ABSTRACT

The cellular membrane of animal has the thickness normally between 5nm and 10nm and has the filtration nanopores with the diameters normally between 0.4nm and 1.2nm. The pressure drop and the critical power loss on the single nanopore for starting the wall slippage have been obtained. The wall slippage is sensitively raised with the pore radius reduction and has a linear dependence on the power loss on the pore. Without wall slippage, the water flow in the pore is much slower than the classical theory calculation; However it is far faster than the classical theory calculation for the wall slippage occurrence.

Keywords: *Cell; Flow; Membrane; Pressure; Slippage; Water*

1. INTRODUCTION

There have been fast progresses on the modeling and simulation of liquid flows in human bodies including the blood flows in large arteries, small arterioles and blood capillaries (Moore et al., 1999; Perdikaris et al., 2016; Taylor et al., 1998). The main constituent of an animal body is water and the fundamental flow in an animal body is the water flow, which carries the metabolites like carbon dioxide and the nutrients like oxygen, protein, sugar, grease and ions etc. Levitt (1974) derived the relation between the macroscopic permeability constant of the cell membrane and the pore structure without any assumptions about the pore shape or about the interactions of the water molecules with each other or with the pore walls. However, it has been widely shown by molecular dynamics simulation that the water flow in a narrow nanopore is essentially microscopic and intimately related to the interactions among the water molecules and the interactions between the water molecules and the pore wall (Borg et al., 2017; Holt et al., 2006; Majumder et al., 2005). It was found that the water flow rates through the carbon nanotubes with the diameters no more than 7nm are far greater than the classical hydrodynamic flow theory calculation (Borg et al., 2017; Holt et al., 2006; Majumder et al., 2005). Chen et al. (2008) studied the water transport property through the mouse dendritic cell membrane by using a microfluidic perfusion system and monitoring the kinetics of the cell volume changes under various extracellular conditions. Lyu et al. (2014) used a polydime-thylsiloxane (PDMS) microfluidic device with hydrodynamic switching to measure the water transport properties of cell membranes by changing the extracellular solution at controllable rates.

Modeling the water flow in the nanopores such as in the blood capillary wall can be very challenging owing to the relatively large pore radius and pore axial length. Such water flows may be multiscale, contributed by both the flow of the adsorbed layer on the pore wall and the intermediate continuum water flow (Wang and Zhang, 2022). Molecular dynamics simulation is hard to implement for such water flows. Wang and Zhang (2022) studied the water permeability through the wall of the human blood capillary based on the developed multiscale flow equations. For the water flow in narrow nanopores such as in the cell membrane, molecular dynamics simulation may be applicable because of the small size of the pore. Wang and Zhang (2021) also analytically studied the water transport through the nanopores of the intracellular connexon of human bodies based on the nanoscale flow equation.

There are densely disturbed very small nanopores in an animal cell membrane, which play important roles in transporting the water. The thickness of the cell membrane is usually between 5nm and 10nm, and the radii of the nanopores usually range between 0.2nm and 0.6nm only allowing several water molecules to pass through the pore simultaneously. Molecular dynamics simulation may be capable to model the water flow in these small nanopores. However, in the present study, we used the nanoscale flow equation to calculate the water flow rate through these nanopores by considering the dynamic, non-continuum and interfacial slippage effects of the water film. The obtained results are interesting for us to understand the water permeation through the animal cell membrane.

2. NANOPORE OF THE CELL MEMBRANE

Figures 1(a)-(c) show the typical nanopore on the animal cell membrane, which is filled with water. The pore radius R is so small that across the pore diameter can only be contained 1-3 water molecules. The pore should be a "deep" pore as the ratio of the pore axial length l to the pore diameter is over 7. In these circumstances, according to the classical hydrodynamic flow knowledge, there should be a large flow resistance in the pore and the water flow through the pore should require great pressure drop and power loss on the pore. However, this contradicts to the actual case, for which water easily passes through the pore with a considerable flow rate.

The water flow through the nanopore in Fig.1(a) should be non-continuum. There should also be some increase of the effective viscosity of the flowing water compared to the water bulk viscosity due to the water-pore wall interaction. It should be recognized that these two effects both reduce the water flow rate through the pore (Zhang, 2015). There should be other factors such as the wall slippage effect strongly influencing the water flow through the nanopore (Borg et al., 2017; Holt et al., 2006; Majumder et al., 2005; Zhang, 2015).

* Corresponding Author. Email: yzhang0709@126.com

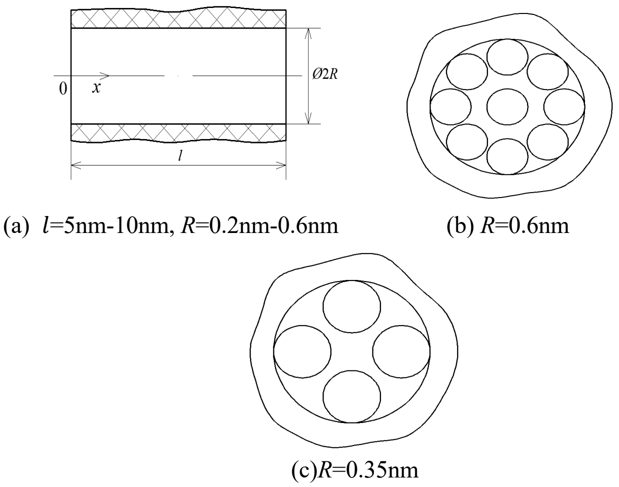

Fig.1 The nanopore on the animal cell membrane.

3. ANALYSIS

Instead of by using molecular dynamics simulation, here we use the nanoscale flow equation (Zhang, 2017) to describe the water flow through the nanopore. The flow is assumed as isothermal and the pressure influences on both the viscosity and density of the water are neglected. When considering the wall slippage, the water mass flow rate through the nanopore in Fig.1(a) reads (Zhang, 2017):

$$q_m = \pi \rho_{bf}^{eff}(\bar{R}) u_s R^2 + \frac{\pi \rho_{bf}^{eff}(\bar{R}) S(\bar{R}) R^4}{4\eta_{bf}^{eff}(\bar{R})} \frac{\partial p}{\partial x} \tag{1}$$

where p is the pressure, x is the coordinate in the flow direction as shown in Fig.1(a), u_s is the wall slipping velocity, ρ_{bf}^{eff} is the average density of the water across the pore radius, η_{bf}^{eff} is the effective viscosity of the water in the pore, and S is the parameter describing the non-continuum effect of the flowing water.On the right hand of Eq.(1), the first term is the Couette flow owing to the wall slippage, the second term is the Poiseuille flow not influenced by the wall slippage but influenced by the non-continuum effect (the parameter S) and the enhanced average density and effective viscosity of the water inside the nanopore. Equation (1) has been physically substantiated (Zhang, 2015).

The pressure drop on the whole single pore for initiating the wall slippage is (Wang and Zhang, 2021):

$$DP = \frac{\tau_s l}{\theta_\tau(R) R} \tag{2}$$

where τ_s is the water-pore wall interfacial shear strength and $\theta_\tau(R)$ is the correction factor for the shear stress on the wall owing to the non-continuum effect of the water.

The critical power loss on the whole single pore for initiating the wall slippage is (Wang and Zhang, 2021):

$$POW_{cr} = -\left(\frac{\tau_s}{\theta_\tau(R)}\right)^2 \frac{\pi S(\bar{R}) R^2 l}{4\eta_{bf}^{eff}(\bar{R})} \tag{3}$$

The wall slipping velocity is equated as (Wang and Zhang, 2021):

$$u_s = \frac{DPOW\theta_\tau(R)}{\pi \tau_s l R} \tag{4}$$

where $DPOW = POW - POW_{cr}$ and POW is the power loss on the whole single pore. Equation (4) shows that the wall slipping velocity is linearly increased with the increase of the power loss on the pore. The power loss on the pore should have the dominant influence on the water flow through the pore if the wall slippage occurs.

The ratio of the water mass flow rate through the pore calculated from Eq.(1) to that calculated from the classical hydrodynamic flow theory is (Wang and Zhang, 2021):

$$r_m = \frac{4Cq(\bar{R})\theta_\tau^2(R)\eta(DPOW)}{\pi R^2 \tau_s^2 l} - \frac{Cq(\bar{R})S(\bar{R})}{Cy(\bar{R})} \tag{5}$$

where $Cy = \eta_{bf}^{eff}/\eta$, $Cq = \rho_{bf}^{eff}/\rho$, η and ρ are respectively the water bulk viscosity and bulk density.

4. CALCULATION

In the calculation, $\eta = 0.001 Pa \cdot s$, $\tau_s = 15kPa$, and the membrane thickness was 8nm. Owing to the relatively weak water-pore wall interaction, it is here taken that $\theta_\tau(R)$=1.0 (Zhang, 2006).

The other parameters are formulated as follows (Zhang, 2004, 2014) :

$$Cy(\bar{R}) = 0.9507 + \frac{0.0492}{\bar{R}} + \frac{1.6447\times10^{-4}}{\bar{R}^2}, \quad \text{for } 0.1 < \bar{R} < 1.0 \tag{6}$$

$$Cq(\bar{R}) = 1.116 - 0.328\bar{R} + 0.253\bar{R}^2 - 0.041\bar{R}^3, \text{ for } 0.1 < \bar{R} < 1.0 \tag{7}$$

and

$$S(\bar{R}) = [-0.1 - 0.892(\bar{R} - 0.1)^{-0.084}]^{-1}, \text{ for } 0.1 < \bar{R} < 1.0 \tag{8}$$

where $\bar{R} = R / R_{cr,bf}$. Here, $R_{cr,bf}$ is the critical radius and chosen as 2.8nm.

5. RESULTS

Figure 2 shows the values of DP for different R. The pressure drops (DP) on the membrane for starting the wall slippage range between 200kPa and 400kPa for R=0.2nm-0.6nm, rapidly increased with the reduction of R. This DP value is 73% of that in the nanopore of the intracellular connexon (Wang and Zhang, 2021). When the pressure difference between intracellular fluids and extracellular fluids is less than the value of DP, no wall slippage occurs and the water flows very slowly through the cell membrane; Otherwise, the wall slippage occurs and it would result in the unexpectedly far faster flow of the water through the cell membrane (Borg et al., 2017; Holt et al., 2006; Majumder et al., 2005). These functions are really required by an animal cell.

Figure 3 shows the critical power loss POW_{cr} on the single nanopore for initiating the wall slippage, which is 1.06 times that in the intracellular connexon (Wang and Zhang, 2021). The value of POW_{cr} for the cell membrane normally ranges between 6×10^{-17} Watt and 4×10^{-16}Watt, rapidly reduced with the reduction of R. It shows that the wall slippage very easily occurs when the water flows through the cell membrane just with a little power loss on the nanopore, and with the reduction of the pore radius R the wall slippage more easily occurs. This is similar with the observation of the water flow through the carbon nanotubes with the diameters less than 2nm (Holt et al., 2006).

Figure 4 shows the wall slipping velocity u_s, which is strongly dependent on the power loss on the nanopore. The value of u_s is also significantly increased with the reduction of R. This indicates that smaller the pore radius, greater the wall slippage. The results follow the experimental observations (Borg et al., 2017; Holt et al., 2006; Majumder et al., 2005). The wall slipping velocity is shown to be in direct proportion to the power loss on the nanopore. In an animal body, for increasing the water flow rate through the cell membrane,the power loss on the cell membrane may just be required to be a little increased for significantly increasing the wall slipping velocity. This is really beneficial for maintaining the normal function of the cell. Figures 3 and

4 show that for keeping the live activity of the cell membrane, the required energy is quite small. It is important for the life of an animal.

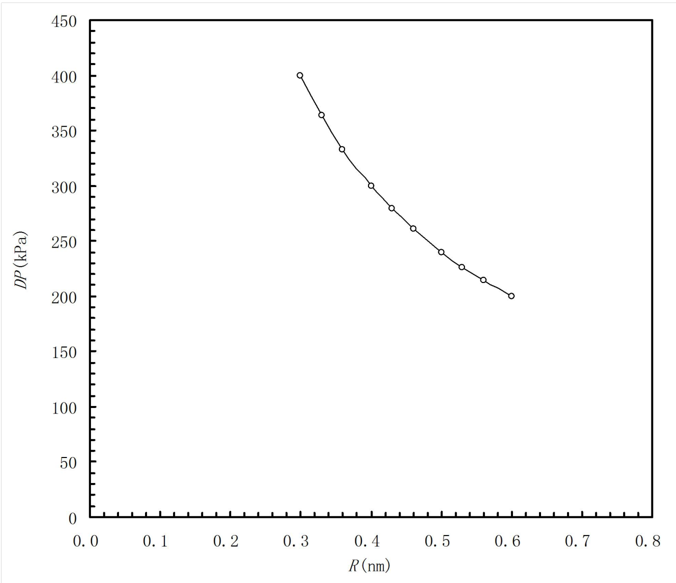

Fig. 2 Values of *DP*.

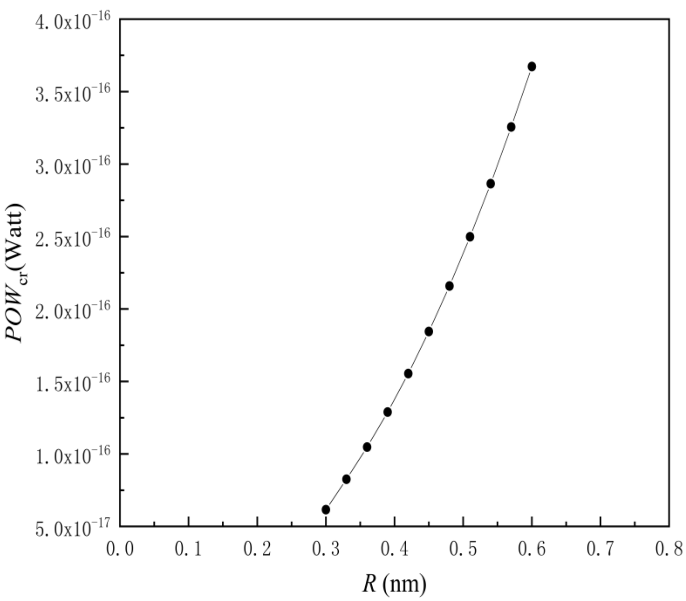

Fig. 3 Values of *POWcr*.

Figures 5(a) and (b) show the values of r_m. For no wall slippage, the value of r_m is considerably lower than unity and significantly reduced with the reduction of R. This indicates that when the wall slippage is absent, the water flow rate through the cell membrane will be significantly smaller than the classical hydrodynamic flow theory calculation, and the smaller pore will result in a much reduced flow rate through the pore. In the absence of the wall slippage, the water flow rate through the cell membrane should be very small. This is the case when there is little difference between the intracellular and extracellular environments. However, these two figures show that when the wall slippage occurs, the value of r_m is usually significantly greater than unity, and it reaches 1×10^5 for *DPOW*= 5×10^{-11}Watt. In the case of the wall slippage, for a given power loss on the pore, the value of r_m is otherwise significantly increased with the reduction of the pore radius R, indicating the increasingly strong effect of the wall slippage; For a given pore radius, the increase of the power loss on the pore results in the flow rate through the pore much higher than the classical hydrodynamic flow theory calculation. These results indicate the important contribution of the wall slippage to the water flow rate through the cell membrane and that the wall slippage plays the vital role in maintaining the ordinary water transport through the cell membrane just with a very small power loss.

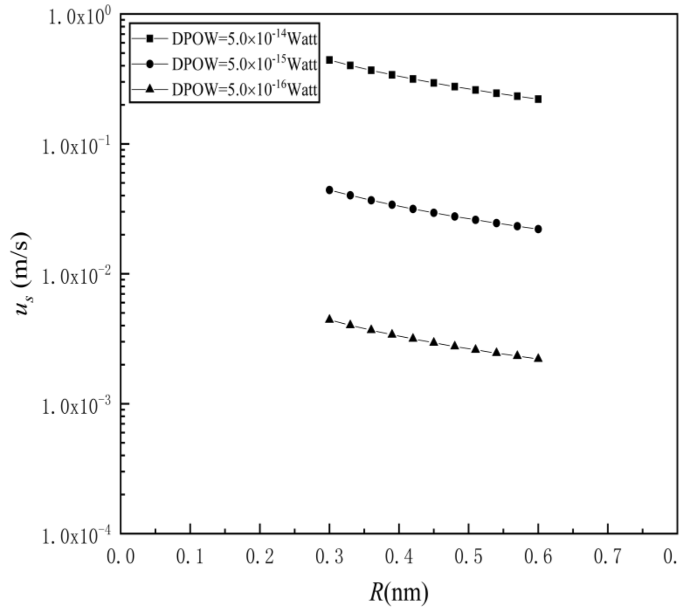

Fig. 4 Values of the wall slipping velocity.

6. CONCLUSIONS

The water permeation through the animal cell membrane was calculated based on the nanoscale flow equation considering the wall slippage. The pressure drop on the cell membrane for starting the wall slippage ranges between 200kPa and 400kPa, significantly increased with the reduction of the radius of the nanopore. The critical power loss on the whole single nanopore for starting the wall slippage ranges between 6×10^{-17}Watt and 4×10^{-16}Watt, rapidly reduced with the reduction of the radius of the nanopore.

It was found that the wall slippage easily occurs when the water flows through the cell membrane just with a very small power loss on the membrane; However the wall slippage has a dominant influence on the water transport through the membrane by increasing the water flow rate by 3 to 5 orders but just with a very small power loss on the membrane; For no wall slippage, the water flows very slowly through the membrane showing the large flow resistance of the membrane. The results obtained by the present study provides an in-depth understanding on the mechanism of the water transport through the animal cell membrane.

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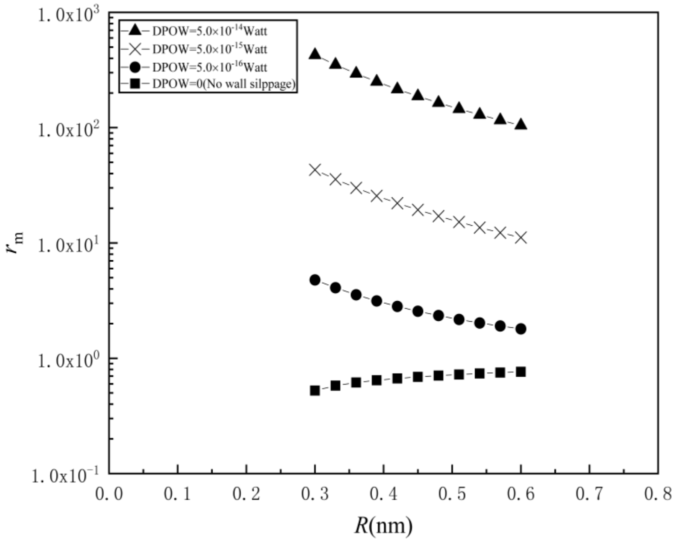
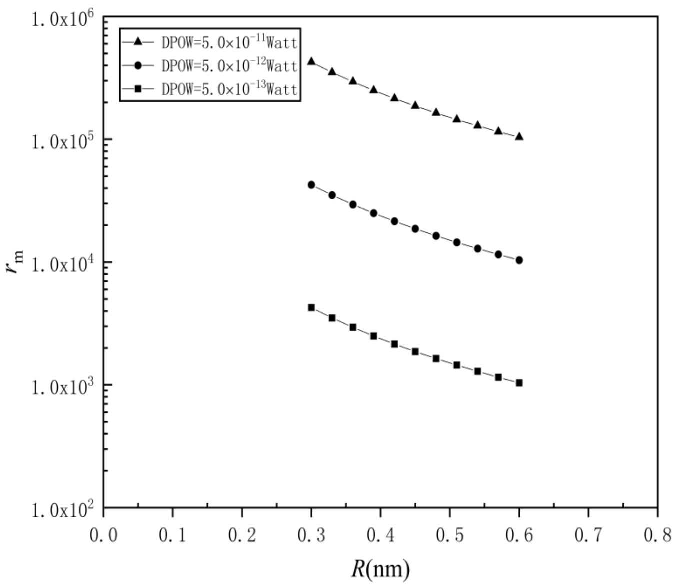


(a)



(b)

Fig. 5 Values of r_m.

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