



## Temperature-tuned transport in biomembrane pores



Chu Rainer Kwang-Hua \*

Transfer Centre, 4/F, No. 16, Lane 21, Kwang-Hui Road, Taipei 116, Taiwan, ROC  
Distribution Centre, Golmud Mansion, 33, Road Yingbin, Golmud 816000, China  
Distribution Centre, No. 120-1, Section 5, Xinhai Road, Taipei 116, Taiwan, ROC

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### ABSTRACT

Fast transport of complex molecular fluids along a biomembrane composed of wavy-rough nanotubes was investigated by using the absolute-reaction approach together with a boundary perturbation method. The critical parameters related to the nearly frictionless transport of molecules were identified to be the possible phase-transition temperature after selecting specific activation energies and activation volumes for confined (cylindrical) geometry considering the dominated role of shear viscosity. Temperature-tuned activation energy as well as activation volume are crucial to the rapid transport of biomolecular fluids. Our numerical results can make the biomembrane composed of aligned wavy-rough nanotubes a promising mimic of protein channels for selective chemical sensing and transdermal drug delivery.

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### 1. Introduction

Fluid transport through a finite length microtube plays an important role in many natural phenomena and industrial processes [1–3]. Biomembranes are highly functional but perhaps sometimes more unstable for engineering use. For instance, voltage dependence and concentration dependence of ion-channel gating leads to possible rectification of current flow, in which specific channels only seem to open when flux is directed in one direction, outward or inward to the cell. Nevertheless, synthetic membranes are stable, but do not have high functionality such as responsiveness to environmental conditions.

Recently carbon nanotubes can be fabricated using self-assembly techniques and they have useful electrical and mechanical properties. The transport of liquids along their central pores is now of considerable interest both for testing classical theories of fluid flow at the nanoscale and for potential nanofluidic device applications. However, the transport properties of fluid in such small confined tubes, usually in the size of ten molecular diameters or less, deviate significantly from its bulk behaviors [4–6]. In order to design nanofluidic devices using nanotubes a much better understanding of the details of fluid flow in cylindrical nanopores is required. Despite some qualitative similarities in fluid behavior in cylindrical and slit-like pores the transport of fluids in these geometries is different in important details, especially for narrow pores [7]. Thus, the boundary conditions in nanodomains must be well prescribed!

To be specific, the discovery of water channel proteins, termed aquaporins, has revealed the molecular basis for understanding fluid

absorption and secretion through cell membranes in response to even very small osmotic gradients created by solute movement [4,8,9]. Aquaporins form water channels that play major roles in a variety of physiological processes so that altered expression or function may underlie pathological conditions [8,9]. Note that water transport across the cell membrane is essential for the maintenance of the intracellular environment. Physiological evidence has shown that water molecules move through a selective pore however water movement across the membrane needs to surmount the energy barrier of water partitioning into hydrophobic lipid phase.

In this paper we shall adopt the verified transition-state or absolute-reaction approach [10,11] which confirmed [12] that this model developed originally by Eyring [10] can be used to describe fluid flows on the nanoscale. To consider the more realistic but complicated boundary conditions in the walls or interfaces of microdomains and nanodomains (which could be a basic element of a bio-membrane), however, we will use the boundary perturbation technique [7,11] to handle the presumed small wavy-roughness along the walls or interfaces of nanotubes. The relevant boundary conditions [13,14] along the wavy-rough surface will be prescribed below after we introduce the Eyring's model [10, 15]. Our numerical results imply that there is rapid transport for some activation energies and volumes around the room-temperature regime.

### 2. Theoretical formulations

In general aquaporins facilitate the movement of water across cell membranes in response to osmotic gradients, functioning in cellular and organismal osmoregulation and solute transport [16]. Recent high-resolution structures (via electron and X-ray crystallography) suggest that selectivity for water is accomplished by a filter that excludes

\* Kwang-Hui Road, Taipei, Taiwan 116, China.  
E-mail address: [2304343144@qq.com](mailto:2304343144@qq.com).

larger molecules and a hydrophobic entrance to the pore that blocks the passage of hydrated ions [17–19]. Electrostatic interactions between highly conserved asparagine residues and water molecules in the pore disrupt the hydrogen bonding pattern that would be formed by the chain of water molecules, thereby preventing the conduction of protons [18]. The unusual combination of a hydrophobic pore and a small number of solute binding sites was proposed to facilitate water transport [19]. With above knowledge, we shall briefly introduce the Eyring's approach.

Eyring derived a hyperbolic sine relation between the shear rate ( $\dot{\gamma}$ ) and the shear stress ( $\tau$ ) [10,11,15] with sound physical foundation from the thermal activation process.

The motion of atoms is represented in the configuration space; on the potential surface the stable molecules are in the valleys, which are connected by a pass that leads through the saddle point. An atom at the saddle point is in the transition (activated) state. Under the action of an applied stress the forward velocity of a flow unit is the net number of times it moves forward, multiplied by the distance it jumps. Eyring proposed a specific molecular model of the amorphous structure and a mechanism of flow (cf. [11,15] for the details).

We consider a steady fully developed flow of the molecular fluid in a wavy-rough nanotube of  $r_1$  in mean-averaged radius and the outer wall being a fixed wavy-rough surface,  $r = r_1 + \epsilon \sin(k\theta)$  where  $(r, \theta)$  is the cylindrical coordinate we adopt,  $\epsilon$  is (peak) amplitude of the (wavy) roughness, and  $k$  is the wave number (cf. Fig. 1).

Firstly, the molecular fluid can be expressed as [10,11,15]

$$\dot{\gamma} = \dot{\gamma}_0 \sinh\left(\psi \frac{r}{r_1}\right), \tag{1}$$

with the forcing parameter

$$\psi = -\left(\frac{r_1}{2\tau_0}\right) \frac{dp}{dz} \tag{2}$$

where

$$\dot{\gamma}_0 = \frac{C_0 k_B T}{h} \exp\left(-\frac{\Delta E}{k_B T}\right), \tag{3}$$

with  $C_0$  : a constant relating rate of strain to the jump frequency, accounting for the interchain co-operation required;  $\Delta E$  is the activation energy,  $h$  is the Planck constant,  $\tau_0 (= 2k_B T/V_h)$  are functions of temperature and have the same dimension as  $\tau$ , and  $dp/dz$  is the pressure-gradient along the nanotube-axis direction ( $z$ ) (for small shear stress  $\tau \ll \tau_0$ ,  $\tau_0/\dot{\gamma}_0$  represents the viscosity of the material). Note that  $V_h = \lambda\lambda_2\lambda_3$  is the activation volume for the molecular event [10,15] with  $\lambda$  being the average distance between equilibrium positions in the direction of motion,  $\lambda_2$  being the distance between neighboring molecules in this same direction (which may or may not equal  $\lambda$ ), and  $\lambda_3$  being the molecule to molecule distance in the plane normal to the direction of motion (cf. Fig. 2) [10].

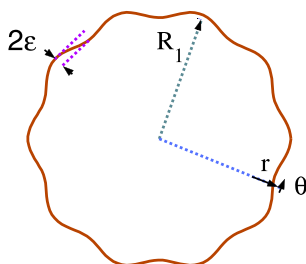


Fig. 1. Schematic of a nanotube with wavy-rough wall.  $\epsilon$  is the amplitude of the wavy-roughness and the wave number of wavy roughness is  $k (= 1/\lambda)$ .

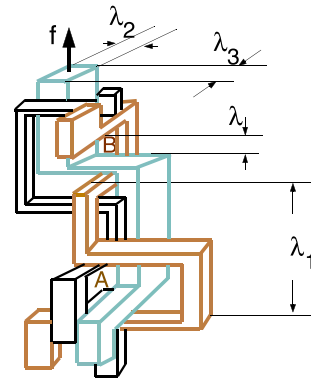


Fig. 2. Schematic model of transport in a molecular fluid (composed of composite molecules) [10,15]. Under an applied force ( $f$ ) of sufficient magnitude a kink in the composite particles will overcome the activation barrier and jump to an available hole (at A or B). We noticed that in Eyring's point of view, flow proceeds by the motion of single (composite) particles into holes left open by neighboring ones [10].

### 2.1. Slip velocity

As  $\dot{\gamma} = -du/dr$  ( $u$  is the velocity of the fluid flow in the longitudinal ( $z$ -) direction of the nanotube), after integration, we obtain

$$u = u_s + \frac{\dot{\gamma} r_1}{\psi} \left[ \cosh\psi - \cosh\left(\frac{\psi r}{r_1}\right) \right]. \tag{4}$$

Here,  $u_s = u_{slip}$  is the velocity over the surface of the nanotube [11,13], which is determined by the boundary condition [13,14]. We noticed that a general slip boundary condition for transport over a solid surface was proposed [14] as

$$\Delta u = L_s^0 \dot{\gamma} \left( 1 - \frac{\dot{\gamma}}{\dot{\gamma}_c} \right)^{-1/2}, \tag{5}$$

where  $\Delta u$  is the velocity jump over the boundary (solid) surface,  $L_s^0$  is a constant slip length,  $\dot{\gamma}_c$  is the critical shear rate at which the slip length diverges. With the general boundary condition from [11,14] we shall derive the velocity field and volume flow rate along the wavy-rough nanotube below using the boundary perturbation technique [7,11].

### 2.2. Boundary perturbation method

We firstly select  $L_s^0$  to be the characteristic length scale and set

$$r' = \frac{r}{L_s^0}, \quad z' = \frac{z}{L_s^0}, \quad R_1 = \frac{r_1}{L_s^0}, \quad \epsilon' = \frac{\epsilon}{L_s^0}.$$

After this, for simplicity, we drop all the primes. It means, from now on,  $r, z, R_1$ , and  $\epsilon$  become dimensionless.

Along the boundary, we have  $\dot{\gamma} = du/dn|_{\text{on surface}}$  and here,  $n$  means the normal.

Let  $u$  be expanded in :

$$u = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \dots, \tag{6}$$

and on the boundary, we expand  $u(R_1 + \epsilon dr, \theta(=\theta_0))$  into

$$u(R_1, \theta) + \epsilon [dr u_r(R_1, \theta)] + \epsilon^2 [dr^2 u_{rr}(R_1, \theta)/2] + \dots = \left\{ u_{slip} + \frac{\dot{\gamma} R_1}{\psi} \left[ \cosh\psi - \cosh\left(\frac{\psi R_1}{R_1}\right) \right] \right\}_{\text{on surface}}, \tag{7}$$

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