CHARGE MANIPULATION OF FLOW IN NANOCHANNELS

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Abstract

The manipulation of flow in nanochannels by charge is thought confirmed by numerous MD simulations of flow by a single file of molecules interacting with the interior of CNTs through L-J potentials. MD stands for molecular dynamics, CNT for carbon nanotubes, and L-J for Lennard-Jones. MD simulations give unusual findings: The flow can be stopped by placing a static positive charge near the outside of the CNT while a vibrating charge can increase the flow. Vibrating charge gives maximum flow at NIR frequencies suggesting the breakage of hydrogen bonds with the CNT walls. NIR stands for near infrared. However, the questionable MD model of a string of molecules suspended on hydrogen bonds has not been confirmed by experiment. A different MD model is therefore proposed. Since nanochannel cross-sections have at least one dimension < 100 nm, the molecules upon entering the nanochannel are irradiated by the EM radiation produced as QM precludes the heat from the surroundings from being conseved by raising the temperature of the nanochannel. QM stands for quantum mechanics. Instead, standing EM radiation is created across the < 1 nm dimension of the CNT having Planck energy at X-ray levels > 300 eV which is sufficient to ionize including the inside surface of the CNT wall. What this means is the hydrogen bonds do not break by the flow, but are broken by EM radiation, the electrons removed leaving a flow of positive charged atoms in the CNT with the inside surface also charged postive. EM stands for electromagnetic. Nanochannel flow is therefore significantly enhanced above classical theory because Coulomb repulsion between atoms and with the CNT wall precludes frictional contact producing a flow of positive charged atoms approaching a frictionless condition bounded by the Bernoulli equation. MD simulations are performed for a single-file flow of positive charged atoms that show water flow in CNTs can be manipulated with static and vibrational charge.

Keywords: nanochannel flow, charge, quantum mechanics

1 Introduction

Flow through nanochannels is of importance in understanding water permeation through biological membranes. In retrospect, the author presented a paper [1] at Topical Problems in Fluid Mechanics 2015 that showed nanochannel flow may be upper bound by the frictionless Bernoulli equation, the frictionless flow being the consequence of the charging of fluid molecules from the EM radiation produced upon entering the nanochannel. Unlike Hagen-Poiseuille flow that follows classical physics, nanochannels obey the rules of QM that require the heat capacity of atoms in fluid molecules to vanish under the high EM confinement provided by the nanoscale dimensions of nanochannels. What this means is QM precludes heat flowing into the nanochannel from being conserved by increasing fluid temperatures. Instead, conservation proceeds by creating low level intensity high frequency EM radiation inside the nanochannel that by removing electrons from fluid molecules produces positively charged atoms. And since the EM radiation is emitted at the inside surface of the nanochannel, the surface charge of the nanochannel is also charged positive. But under EM confinement, the free electrons recombine to create a flow of fluctuating positive and neutral charges that by Coulomb repulsion reduces frictional contact between atoms and between atoms and the inside nanochannel surface. Hence, the Bernoulli equation for frictionless flow may be used in biological membranes to upper bound water permeation.

2 Background

Water transport through nanochannels does not follow classical physics. Indeed, MD simulations[2] and experiments[3] demonstrated that the flow rate through CNTs is three to five orders of magnitude faster than that predicted from the Hagen-Poiseuille equation. But as explained by QM in [1] that at the nanoscale heat is not conserved by increasing temperature, but rather by creating EM radiation. Electrons

from atoms in fluid molecules are then removed by the photoelectric effect to produce a momentary flow of positive charged atoms. Coulomb repulsion then reduces frictional contact until the electrons recombine with the atoms, the process repeating as long as the atoms remain in the nanochannel. The creation of charge at the nanoscale is supported by experiments. Charged potassium K+ ions in protein channels are found [4] to enhance water permeation in single file of K+ ions rather than the traditional alternating ion and water configuration. Coulomb repulsion between adjacent ions is the key to high-efficiency K+ conduction. Similarly, a pH-sensitive fluorescent probe to monitor proton H_3O^+ diffusion in water found [5] a 4-fold enhancement if the size of the EM confinement channel is 180 nm, but the questionable Grotthuss mechanism was proposed to explain enhanced proton mobility. Of direct interest to this paper, MD showed water permeation through a nanochannel was altered by placing a stationary or vibrating positive charge close to a single file flow of water molecules in a CNT. More fundamentally, experiments are not known to describe how nanochannels charge fluids.

3 Theory

Molecules upon entering the nanochannel are irradiated by the EM radiation produced as the Planck law of QM [7] denies the atoms of fluid molecules the heat capacity to conserve heat by raising the temperature of the nanochannel. Conservation then proceeds by creating EM radiation inside the nanochannel by simple QED. QED stands for quantum electrodynamics, but is far simpler than the relatavistic theory advanced by Feynman [8] and others.

3.1 Heat Capacity

The Planck law of QM at 300 K is illustrated in Figure 1. By classical physics, the kT heat capacity of the atom is independent of the EM confinement wavelength λ, where k is the Boltzmann constant and T absolute temperature. QM differs as the heat capacity of the atom decreases under EM confinement λ < 100 microns, but at the nanoscale for λ < 100 nm, the heat capacity may be said to vanish.

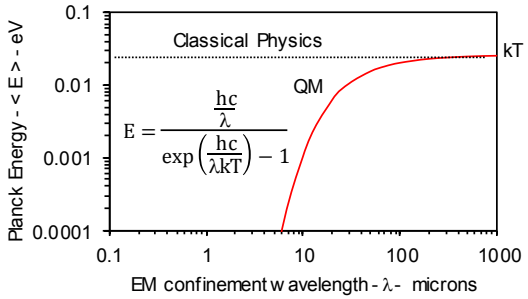

Figure 1: Planck law of the Atom at 300 K
In the inset, E is Planck energy, h Planck's constant, c light speed,
k Boltzmann's constant, T temperature, and λ EM confinement wavelength

3.2 Simple QED

The simple QED of light-matter interaction in a circular nanochannel cross-section converting heat Q into standing EM radiation is illustrated in Figure 2.

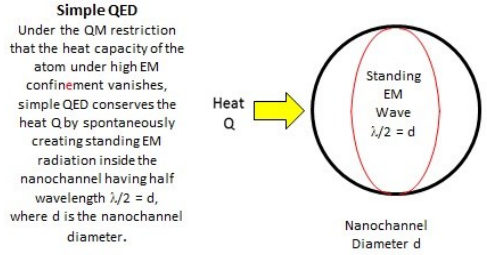

Figure 2: Simple QED

The Planck energy E of the standing EM radiation is,

$$E = \frac{h\left(c/n\right)}{\lambda} = \frac{hc}{2nd} \quad (1)$$

where, the velocity of light c is corrected for the slower speed in the fluid by the refractive index n of the fluid. The EM radiation in single-file flow of water molecules in CNTs reaches X-ray levels. For CNTs having diameters d ~ 0.84 nm in water with index n ~ 1.30, the EM radiation at X-ray levels has wavelength λ = 2.18 nm with Planck energy E = 0.57 keV.

Heat Q required to create the X-ray energy E comes from the water bath as turbulence recycles molecules having kT energy from the macroscopic surroundings. At the CNT surface, QM precludes each oxygen and 2 hydrogens of 3 atoms of a water molecule from having kT energy, the thermal energy U of each molecule having U = 1.5 kT = 6.21 x10^{-21} J of energy at ambient temperature T = 300 K. Upon creating the X-ray photon, the thermal energy U of water molecules at the CNT surface is replenished by turbulence in the bath. Hence, the X-ray photon energy E is, E = 3NU, where N is the number of water molecules. For E = 0.57 keV, N = 4895. The number N of molecules in a cylindrical slice of width S in a diameter D through the CNT is , $N = \pi(D/S)^2/4$. Here, S is the cubical dimension of the water molecule, i.e., S^3 = Amu/Avogadro/ρ, where ρ is water density, S = 3.1 x10^{-10} m giving D ~ 25 nm. Standing X-rays are likely to penetrate the CNT wall and lower E < 0.57 keV, but still far more than the 5 eV sufficient to ionize the water molecules in the string inside the CNT.

4 MD Simulation

The MD model selected to simulate a single file of water molecules flowing at velocity V interacting with a static and vibrating charge is illustrated in Figure 3. The nanochannel is not modelled because the flow is upper bound [1] by the frictionless Bernoulli equation. Hydrogen bonds do not break by the flow [6] but are broken by the EM radiation produced by simple QED. The MD program modified the algorithms [10] for QM. The L-J parameters for water were, σ = 0.315 x10^{-9} m and ε = 73.3 k. But consistent with [1] the value of ε was reduced by a factor of 100 to simulate frictionless flow.

The 10 water molecules (pink) were spaced by S giving the single-file length L = 9 S. Initially, all molecules move at velocity V in the positive X direction. Each water molecules carries a positive charge q to balance the removal of a single electron charge to interact with external charge Q. Points P1 and P2 (blue) are for visual references as the water molecules move back and forth along the X-axis. The time step Δt was 1 x10^{-17} s to resolve contact between molecules. Solutions on a PC comprised 1.5 million iterations took < 1 minute.

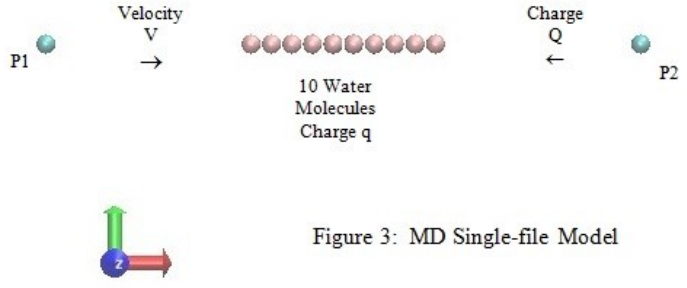

Figure 3: MD Single-file Model

The MD results were obtained for various initial flow velocities V of which the results for V = 1 m/s are shown in Figure 4. The X motion and V velocity are shown in Figures 4 A and B giving the response after the charge Q reacts with charge q of each of the molecules. The molecule nearest point P2 (red) responds immediately to the charge Q while the molecule (blue) nearest P1 responds later. Velocities < 0 show deceleration. The molecule nearest P2 (red) underwent oscillation at 40 GHz. Figure 4 C shows the string length L is disrupted during deceleration, the minimum occurring during compression with the maximum after repulsion.

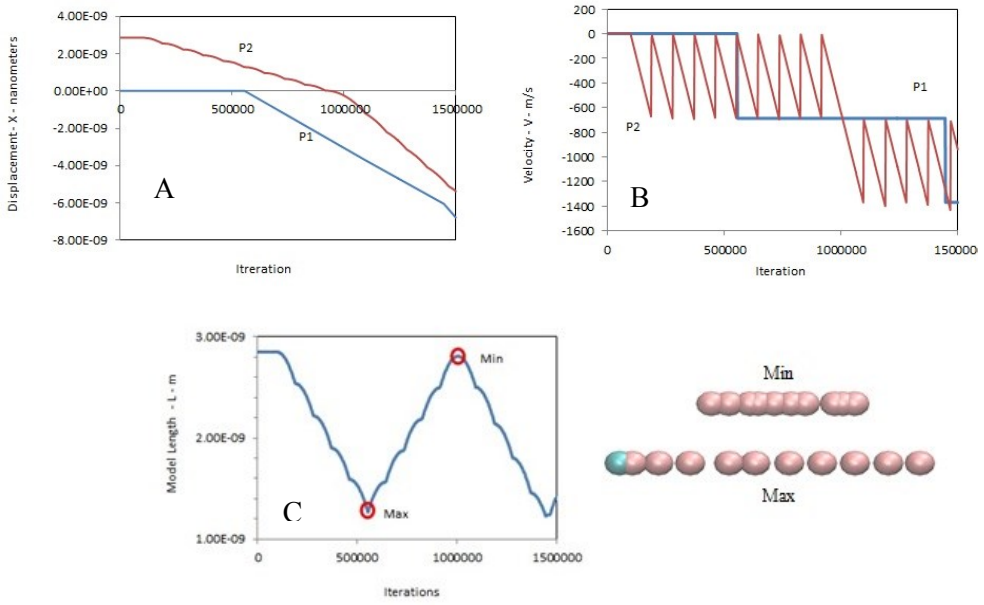

Figure 4 MD Results – Initial Velocity V = 1 m/s

5 CONCLUSIONS

MD simulations of single-file flow of 10 water molecules through a CNT were performed under restrictions imposed by QM that preclude conservation of viscous friction by temperature in classical physics as the heat capacity of the water molecule atoms vanishes under the high EM confinement of the CNT. Instead, heat flow into the CNT is conserved by producing EM radiation that ionizes the water molecules to remove electrons leaving a single-file of positive charged atoms. Coulomb repulsion avoids contacting atoms to produce the well-known frictionless flow given by the Bernoulli equation.

Under high EM confinement, the free electrons recombine with their positive charged counterparts to produce electro-neutrality only to promptly ionize once again, the process repeating until the string of molecules leaves the CNT.

The CNT diameter < 1 nm is small enough to create X-rays as turbulence brings water molecules in the surroundings having thermal kT energy to be expended at the CNT surface. But it is more likely lower energy photons are created because the standing X-ray wave penetrates the CNT wall,

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