THE BERNOULLI EQUATION IN NANOCHANNELS

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Abstract

The Hagen-Poiseuille equation of fluid mechanics based in classical physics that assumes a no-slip condition at the channel wall cannot explain the dramatic increase in flow found in nanochannels. Even if slip is assumed at the wall, the calculated slip-lengths necessary to explain the flow enhancement exceed the typical slip on non-wetting surfaces by 2 to 3 orders of magnitude. QM differs from classical physics. QM stands for quantum mechanics. Enhanced flow at the nanoscale is proposed to be the consequence of the size effect of QM that causes the viscosity of the fluid to vanish that otherwise does not occur in flow at the macroscale. In nanochannels, the fluid atoms are placed under EM confinement that by QM requires their heat capacity to vanish thereby precluding the conservation of viscous heating by the usual increase in temperature. Instead, conservation proceeds by QED inducing the viscous heat to create EM radiation that charges the atoms or is lost to the surroundings. EM stands for electromagnetic and QED for quantum electrodynamics. To explain the flow enhancement, MD finding basis in classical physics that assumes the atoms always have heat capacity is no longer valid by QM. MD stands for molecular dynamics. Therefore, MD algorithms were modified to assure the viscous heating does not increase the temperature of the fluid atoms by constraining temperatures near absolute zero to avoid temperature dependent atomic velocities. Conservation of viscous heat then proceeds by QED inducing EM radiation that charges the atoms thereby producing Coulomb repulsion allowing the viscosity to vanish as the atoms separate. The MD simulations suggest the flow in nanochannels should be frictionless given by the Bernoulli equation. Indeed, flow experiments on various fluids reported in the literature are shown to be reasonably upper bound by the Bernoulli equation.

Keywords: Hagen-Poiseuille, Bernoulli, molecular dynamics, quantum mechanics

1 Introduction

Water flow observed [1 - 3] through nanochannels in membranes of CNTs is found to be 2-5 orders-of-magnitude greater than those predicted by the no-slip Hagen-Poiseuille equation of classical physics. CNT stands for carbon nanotube. To explain this surprising flow enhancement, slip at the wall of the nanotube is assumed because of the non-wetting nature of CNTs. For bulk water viscosity, the Hagen-Poiseuille relation [1] requires slip lengths of 50 microns to reproduce the measured flow in 7 nm CNT membranes. Since MD simulations [4] indicate that the water/graphene slip length is on the order of 50 nm, the required slip-length is 1000 times larger than that of non-wetting boundaries. Because of this, slip cannot be the mechanism for the significant flow enhancement in nanochannels. Another mechanism is at play.

In this regard, flow enhancement is more likely caused by the size effect of QM causing the viscosity of the fluid to vanish in nanochannels that otherwise does not occur at the macroscale. How QM causes the viscosity to vanish is an important purpose of this paper. Vanishing viscosity as the explanation of enhanced flow allows the Hagen-Poiseuille equation to be replaced by the frictionless Bernoulli equation to explain the observations of enhanced flow in nanochannels.

1.1 Heat Capacity of the Atom

Vanishing viscosity is the consequence of QM denying [5] the atom the heat capacity to conserve viscous heating by an increase in temperature. Figure 1 compares classical physics with QM based on the Planck energy E of the atom in terms of its *kT* energy given by the Einstein-Hopf relation [6] for the atom as a harmonic oscillator.

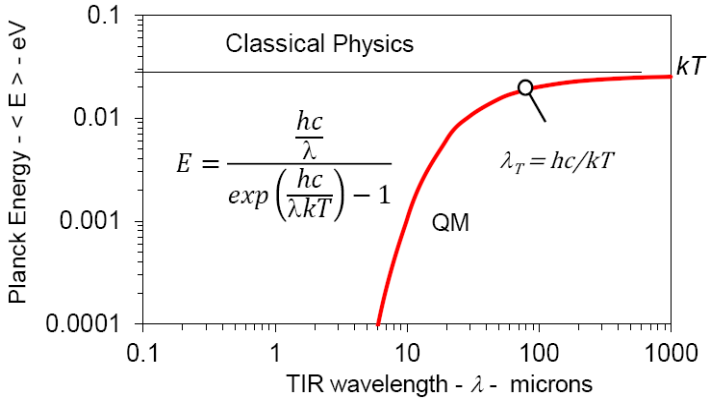

Figure 1: Heat Capacity of the Atom at 300K.
In the inset, *h* is Planck's constant, *c* is the speed of light, and λ is wavelength, *k* is Boltzmann's constant and *T* absolute temperature

Classical physics always allows the atom to have *kT* energy. QM differs in that *kT* energy depends on the wavelength λ of TIR confinement. By QM, *kT* energy is only available for atoms at the macroscale, i.e., for $\lambda > \lambda_T$ and otherwise is << *kT*. Because of QM, the atom cannot conserve viscous heat in the nanochannel.

1.2 QED induced EM radiation

The QM requirement that the heat capacity of the atom vanishes under TIR confinement in nanochannels precludes conservation of viscous heat by the usual increase in temperature. Instead, QED conserves the viscous heat produced as the fluid molecules flow through the nanochannel by inducing the creation of EM radiation that charges the atoms in the molecules or is lost to the surroundings. At the TIR confinement wavelength λ of the nanochannel, the Planck energy of QED radiation is sufficiently high to ionize the fluid molecules and charge the atoms to produce Coulomb repulsion between the atoms that causes the viscosity to vanish. Here, $\lambda = 2\ nd$, where *n* is the refractive index of the fluid and *d* the tube diameter or channel thickness. For $d < 100$ nm, the EM radiation has wavelengths λ in the UV and beyond, i.e., $\lambda < 300$ nm. In nanochannels, QED induced EM radiation has sufficient Planck energy to ionize most fluid molecules having ionization potentials of ~ 10 eV, i.e., wavelength $\lambda < 125$ nm that for $n = 1.5$ requires nanochannels having d < 45 nm. What this means is the fluid viscosity in nanochannels vanishes as the fluid is highly charged with Coulomb repulsion producing a loosely bound frictionless state of flowing atoms.

2 Purpose

Perform MD simulations valid by QM to show the viscosity of liquid argon vanishes in nanochannels.

3 Analysis and Results

3.1 Validity of MD

To show fluid viscosity vanishes in nanochannels, MD simulations would seem especially suited. However, MD computer programs, e.g., [7] finding basis in classical physics allow the atom the heat capacity at the nanoscale that is forbidden by QM. What this means is the MD simulations of nanochannel flow, e.g. [8, 9], that abound the literature are invalid [10] by QM. Because of this, standard MD computer programs are modified to simulate the QM effect of vanishing heat capacity on fluid viscosity.

3.2 Lennard-Jones Potentials

The reduction in viscosity may be understood by considering the L-J potential between fluid-fluid and fluid-wall atoms. L-J stands for Lennard-Jones. Here, the L-J parameter σ is the repulsive atom core and ε the attractive potential. Figure 2 shows QED induced charge offsetting the ε attractive potential of the atom giving a zero net (atom + charge) attractive potential.

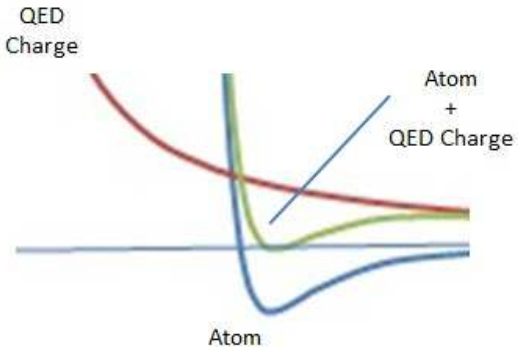

Figure 2: QED charging of Fluid Atoms producing Zero Net Attractive Potential

3.3 MD Simulation

MD simulations that are valid by QM require the viscous heat is not conserved by an increase in temperature and instead conserved by charging the atoms. MD solutions are therefore made near absolute zero temperature, say 0.001 K to avoid temperature dependent atom velocities. Usually, MD solutions of nanochannel flow are performed with Lees-Edwards [11] periodic boundary conditions. However, charging the atoms requires long range corrections that may be avoided by using a discrete MD model and considering all atoms without invoking a cut-off in force computations. On this basis, a discrete 2D model comprising 100 atoms in a BCC configuration of liquid argon was selected as shown in Fig. 3.

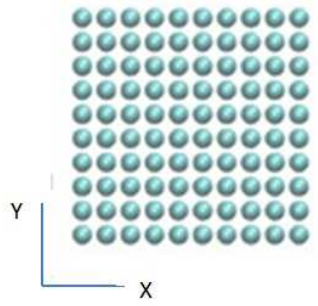

Figure 3: Nanochannel 2D MD Model

The BCC configuration assumed liquid argon at a density of 1407 kg/m^3. The atomic spacing was 3.62 Å. The L-J potential for argon has σ = 3.45 Å and ε = 120·k. The MD computation box is a 32.6 Å square. Time steps were < 2 fs. The MD loading imposed a velocity gradient of 3.06 x10^{10} s^{-1} normal to the flow direction having velocity of 100 m/s over the height of the MD box. Unlike Lees-Edwards, the MD computation box became highly distorted after 150000 iterations. The distortion after 25000 iterations is shown in Fig. 4.

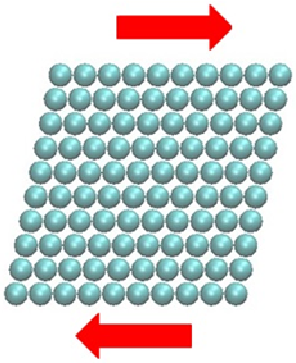

Figure 4: MD Solutions – Distorted Computation Box

In the MD solution for liquid argon having ε = 120·k, the L-J viscosity converged to ~ 144 μPa·s. Experimentally, the viscosity [12] of liquid argon at -130 C is 54 μPa·s, but 175 μPa·s has been [11] reported. Instead of performing MD for repulsive Coulomb forces between atoms including the attractive L-J potential ε = 120·k·, the Coulomb repulsion was first simulated by neglecting Coulomb repulsion and simply reducing the attractive L-J potential by 100 times to ε = 1.2·k that gave viscosity of ~ 1 μPa·s. The MD solutions of L-J viscosity for ε = 120·k and 1.2·k shown in Fig. 5.

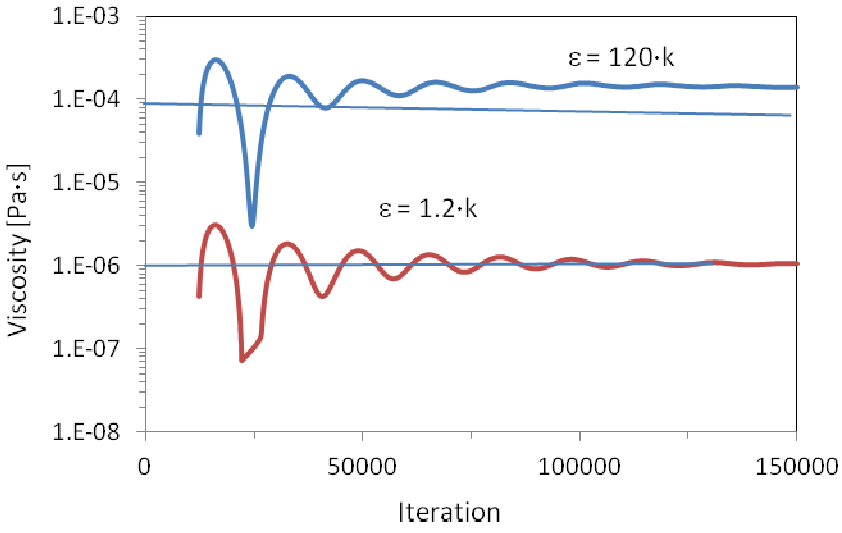

Figure 5: Argon Viscosity at ε = 120·k and 1.2·k

In an alternative MD solution, the Coulomb repulsion between all atoms is directly simulated by QED inducing the creation of charge from conserving viscous friction heat instead of increasing temperature. The electrostatic potential U_{ES}, for atoms separated by distance R having electron charge e is,

$$U_{ES} = \frac{e^2}{4\pi\varepsilon_o R} \tag{1}$$

where, ε_o is the permittivity of the vacuum. The L-J potential U_{LJ} between an atom pair,

$$U_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6}\right] \tag{2}$$

The L-J potential minimum occurs at $R = 2^{1/6}\sigma$ giving $U_{LJ} = -\varepsilon$. The fraction η_c of the available electrostatic energy U_{ES} to counter the attractive potential ε is,

$$\eta_c = \frac{U_{LJ}}{U_{ES}} = \frac{4\pi 2^{1/6}\sigma\varepsilon_o\varepsilon}{e^2}$$

Taking $\varepsilon = 120\cdot k$ for argon, the fraction $\eta_c = 0.0027$. The remaining $(1-\eta_c)$ U_{ES} energy is radiated as EM radiation to the surroundings. However, Coulomb repulsion is collectively enhanced above that for a single atom pair, and therefore $\eta < \eta_c$. MD solutions were obtained for various η to determine the optimum at which the viscosity vanished. By trial and error, $\eta = 0.0006 < \eta_c$ was found optimum as shown in Fig. 6.

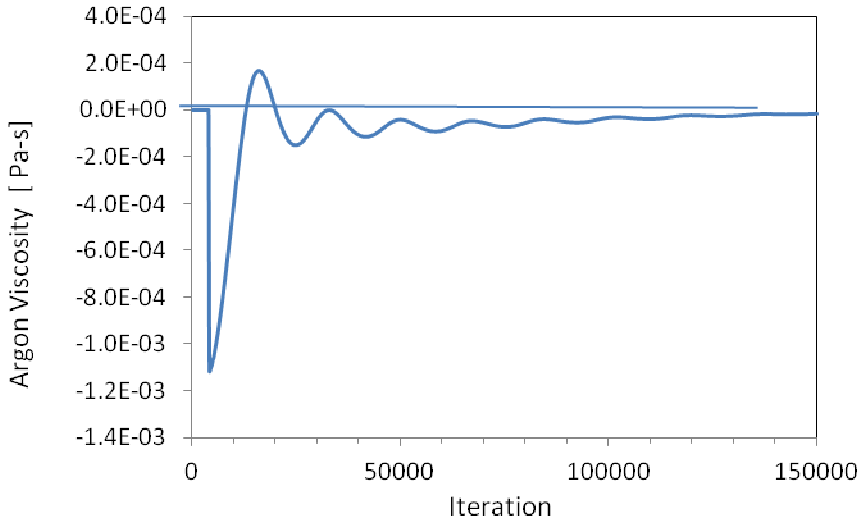

Figure 6: MD with Coulomb Repulsion $\varepsilon = 120\cdot k$ and $\eta = 0.0006$

The MD solution with Coulomb repulsion for Argon at $\varepsilon = 120\cdot k$ is observed to vanish. However, $\eta = 0.0006 < \eta_c = 0.0027$ means the collective effect of about 5 atom interactions is occurring. Flow enhancement above Hagen-Poiseuille at bulk viscosity is indeed frictionless and represented by the Bernoulli equation.

4 Discussion

4.1 Modified Hagen-Poiseuille Equation

The Hagen-Poiseuille equation modified [13] for slip gives the flow Q through a circular nanochannel of radius r under the pressure drop ΔP,

$$Q = \frac{\pi r^3 (r + 4b)}{8\mu L} \Delta P \tag{4}$$

where, μ is the viscosity, L the channel length, and b the slip length.

The QED induced reduction in viscosity μ is observed to inversely enhance the flow Q. However, the flow Q is even further enhanced by slip b. Regardless, the QED induced reduction in viscosity is the dominant factor in flow enhancement.

4.2 Exit Losses

Unbounded flow in nanochannels [13] is consistent with QED induced vanishing viscosity. As long as the fluid is under TIR confinement by the channel walls, the flow is indeed frictionless. However, the fluid must eventually leave the nanochannel at which time there is no TIR confinement whereupon the atom regains it classical behavior and the flow velocity is diminished by viscous friction. Nevertheless, flow within the nanochannel is indeed frictionless.

4.3 Bernoulli Equation

Vanishing viscosity suggests the flow in nanochannels should approach the frictionless flow given by the Bernoulli equation. The development of the Bernoulli equation from the QED energy equation in nanochannels is illustrated in Table 1.

Table 1:

QED Energy Equation in Nanochannels

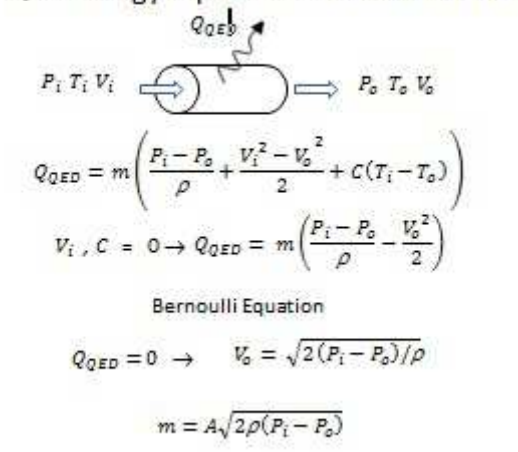

Table 1 describes an incompressible fluid at the channel inlet in the $P_i\ T_i\ V_i$ state leaves the channel in the outlet $P_o\ T_o\ V_o$ state. P stands for pressure T for temperature, V velocity, m mass flow, and ρ density. Classically, viscous friction causes the fluid temperature to increase depending on the heat capacity C. QM differs as temperature changes do not occur because C vanishes. Instead, QED converts the viscous heat into

EM radiation that ionizes the fluid molecules, or is lost to the surroundings. Since the inlet plenum velocity V_i is negligible, and since the ideal fluid is absent viscous heating, Q_{QED} radiation to the surroundings also vanishes, the consequence of which is the nanochannel flow is governed by the Bernoulli equation for frictionless flow.

In nanochannels, the application of the Bernoulli equation to flow measurements [1-4] from experiments on various fluids reported in the literature in Table 1 of [13] is reproduced below in Table 2.

Table 2:

	liquid	μ (cp)	N	L (μm)	Q_M (cm^3/s)	r_M (nm)	$Q_{M,0}$ (cm^3/s)	ϑ	b (μm)
Majunder (2005) et al.	water	1	10^9	34	9.62	<r_M> = 3.5 σ_M = 1.0	1.79	5.37	-
					16.9			9.44	-
	ethanol	1.1	$3.4*10^9$	126	12.4		6.07	2.04	-
	isopropanol	2			5.89		5.06	1.16	-
	hexane	0.3			1.47		3.1	0.47	24.11
	decane	0.9			7.33		20.7	0.35	14.68
					0.877		6.75	0.13	3.99
Majunder (2005) et al.	water	1	$2.4*10^6$	81	$2*10^{-8}$	<r_M> = 3.5 σ_M = 1.0	$8.3*10^{-9}$	2.40	-
Holt et al.	water	1	$2.5*10^{11}$	2	7.47	<r_M> = 0.8 σ_M = 0.15	4.68	1.60	-
				3	2.23			0.48	0.58
				2.8	1.97			0.42	0.43
Du et al.	water	1	$2.4*10^{10}$	$4*10^3$	0.058	<r_M> = 5.0 σ_M = 1.0	0.112	0.52	910
	hexane	0.31			0.154		0.362	0.43	63
	dodecane	1.34			0.082		0.084	0.97	30000

Q_M is the actual flow computed in [13] from published velocities. $Q_{M,0}$ is the total flow rate through a 1 cm^2 membrane comprised of frictionless nanotubes. Here, $\vartheta = Q_M / Q_{M,0}$ is the ratio of actual flow to the frictionless flow given by the Bernoulli equation. As noted in [13] the $\vartheta > 1$ do not comply with known physics of fluid. What this means is $Q_M < Q_{M,0}$ or $\vartheta < 1$ as frictionless Bernoulli flow is the physical upper bound for flow in nanochannels. However, water at CNT radii of 3.5 nm [1, 2] and radii of 0.8 nm [3] shows $\vartheta > 1$. The data [1-3] for flow of water through CNTs is therefore questionable. Nevertheless, the data for ethanol, isopropanol, decane, and hexane, show $\vartheta < 1$ or is reasonably close to 1 to support the argument that Bernoulli flow is indeed a valid estimate of flow in nanochannels.

5 Conclusions

1. Surprisingly high flow in nanochannels is the consequence of QM that requires the heat capacity of the atom under TIR confinement to vanish and preclude the conservation of viscous heat by an increase in temperature. Instead, the viscous heat is conserved by QED inducing the creation of EM radiation that ionizes the fluid molecules to produce a state of Coulomb repulsion that overcomes the attractive potential of the atom. Hence, nanochannels produce frictionless Bernoulli flow as the fluid viscosity vanishes which is reasonably supported by experiment.

2. For argon, the MD simulation consistent with QM by not conserving viscous heat with an increase in temperature under a constant velocity gradient gave a viscosity of 144 μPa·s compared to an experimental value of 175 μPa·s. By reducing the attractive

L-J potential by a factor of 100, the viscosity was reduced to 1 μPa·s. QED induced flow is enhanced by a factor of 144.

3. MD solutions for argon having an attractive L-J potential ε = 120·k in combination with Coulomb repulsion between atoms do not need to be performed because taking ε = 1.2·k showed a reduction in viscosity by a factor of 144. What this means is others [1-4, 8-9] may readily determine the reduction in viscosity in the MD simulation of their nanochannels by re-running at reduced attractive L-J potentials.

4 MD solutions for argon having a L-J attractive ε = 120·k potential in combination with QED induced Coulomb repulsion between atoms shows the viscosity vanishes for $\eta = 0.0006$. Since $\eta < \eta_c = 0.0027$, the collective action of about 5 atoms appears at play in a vanishing viscosity.

References

[1] Majunder M., Chopra, N., Andrews, R. & Hinds, B.J.: Nanoscale hydrodynamics: Enhanced flow in carbon Nanotubes, *Nature*, vol. 438 (2005) p.44

[2] Holt J.K., Park, H.G., Wang, Y., Stadermann, M., Artyukhin, A.B., Grigoropoulos, C.P., Noy, A. & Bakajin, O.: Fast Mass Transport through Sub–2-Nanometer Carbon Nanotubes, *Science*, vol. 312 (2006) pp. 1034.

[3] Du, F., Xia, Z., Feng, L., & Dai, L.: Membranes of Vertically Aligned Superlong Carbon Nanotubes, *Langmuir*, vol. 27 (2011) pp. 8437-8443.

[4] Verweij, H., Schillo M.C., & Li, J.: Slip flow in graphene nanochannels, *Small*, vol. 3 (2007) pp. 2778-2793.

[5] Prevenslik, T.: See Numerous QED applications at http://www.nanoqed.org , 2009-2014.

[6] Einstein, A. & Hopf, L.: Statistische Untersuchung der Bewegung eines Resonators in einem Strahlungsfeld, *Annalen der Physik*, vol. 33 (1910) pp. 1105-1120.

[7] LAMMPS Molecular Dynamics Simulator, Sandia National Laboratories, October 3, 2010.

[8] Thomas, J. & McGaughey, A.: Reassessing Fast Water Transport through Carbon Nanotubes, *Nano Letters.*, vol. 8 (2008) pp. 2788-2793.

[9] Li, Z.: Surface effects on friction-induced fluid heating in nanochannel flows, *Physical. Review E*, vol. 79 (2009) 026312

[10] Prevenslik, T.: Validity of Molecular Dynamics by Quantum Mechanics, Proceedings of the ASME 2013 4th Micro/Nanoscale Heat and Mass Transfer (MNHMT2013)

[11] Lees, A. & Edwards, S.: The computer study of transport processes under extreme conditions, *Journal of Physics C*: *Solid State Phys.*, vol. 5 (1972) pp. 1921-1929.

[12] Argon Properties, Air Products Co. Ltd.

[13] Sisan, T.B. & Lichter, S.: The end of nanochannels, *Microfluid-Nanofluid*, vol. 11, (2011) pp. 787.