INVESTIGATING THE ENHANCED MASS FLOW RATES IN PRESSURE-DRIVEN LIQUID FLOW THROUGH NANOPORES

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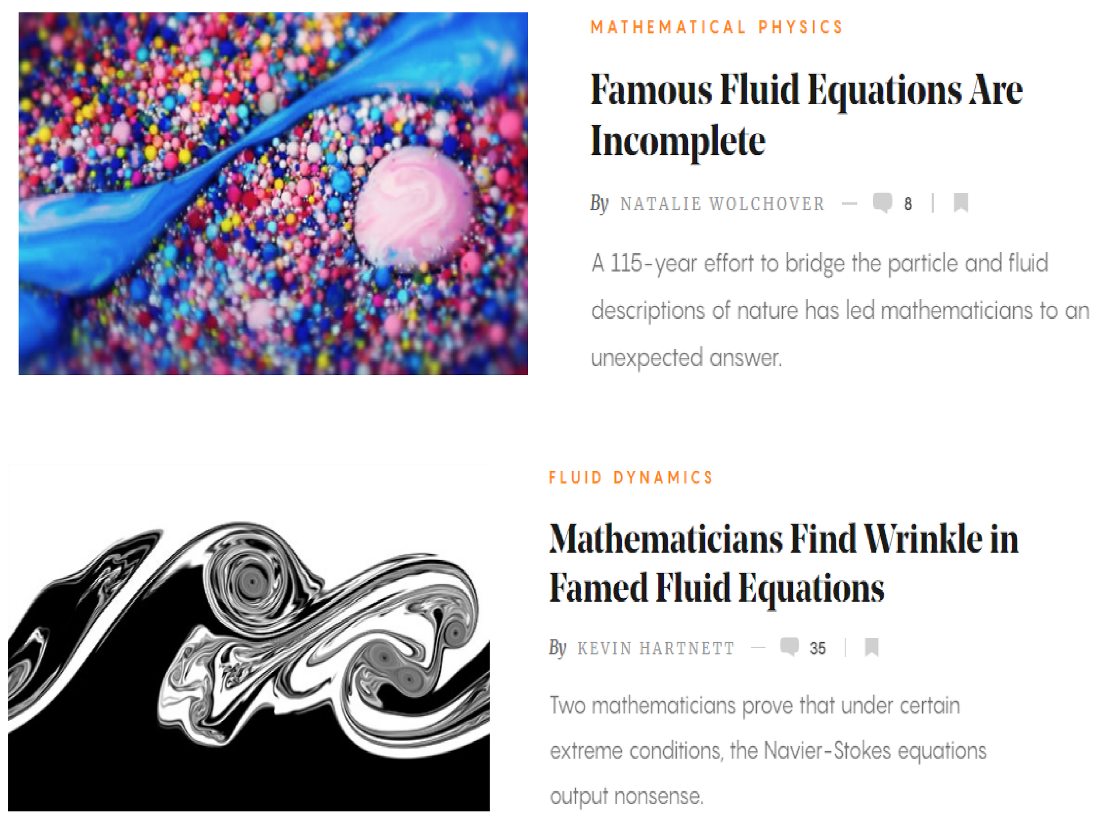
Introduction

■ Experiments have shown that mass flow rates in pressure-driven liquid flow through nano-tubes hugely exceed those predicted by the Navier-Stokes equations.

■ The current work investigates a possible explanation of this phenomenon based on a new continuum model: the Recasted Navier-Stokes equations



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Navier-Stokes Equations

■ Assume isothermal liquid flow, with constant fluid density ρ and viscosity μ

■ Mass balance equation:

$$\nabla \cdot \mathbf{u}_m = 0 \tag{1}$$

■ Momentum balance equation:

$$\rho \frac{\partial \mathbf{u}_m}{\partial t} + \rho \mathbf{u}_m \cdot \nabla \mathbf{u}_m = -\nabla p + \mu \nabla^2 \mathbf{u}_m \tag{2}$$

Poiseuille Flow Law

■ Navier-Stokes-predicted mass flow rate in long ducts at low Reynolds number:

$$\dot{M}_{NS} = \frac{\pi \rho R^4}{8\mu} \frac{\Delta P}{L} \ , \quad \Delta P = P_{in} - P_{out} \tag{3}$$

■ Problem: at the nano-scale, predicted rates are several orders of magnitude lower than measured rates

■ Conventional explanation: wall-slip flow, leading to very large slip-length parameters

New Continuum Approach

■ Methodology is based on a technique which is similar in nature to that of a Lorentz transformation.

■ It involves transforming the fluid velocity field variable $\mathbf{u}_m$ within the standard fluid flow hydrodynamic equations

■ The form of the transformation depends on the main driving-mechanism. For the pressure-driven, isothermal liquid flow we suggest the following transformation:

$$\boxed{\mathbf{u}_m = \mathbf{u}_p - \kappa_p \nabla \ln p} \tag{4}$$

■ The pressure diffusivity constant κ_p is thought to be of the form

$$\boxed{\kappa_p = \alpha^* \frac{\mu}{\rho}} \tag{5}$$

Recasted Navier-Stokes

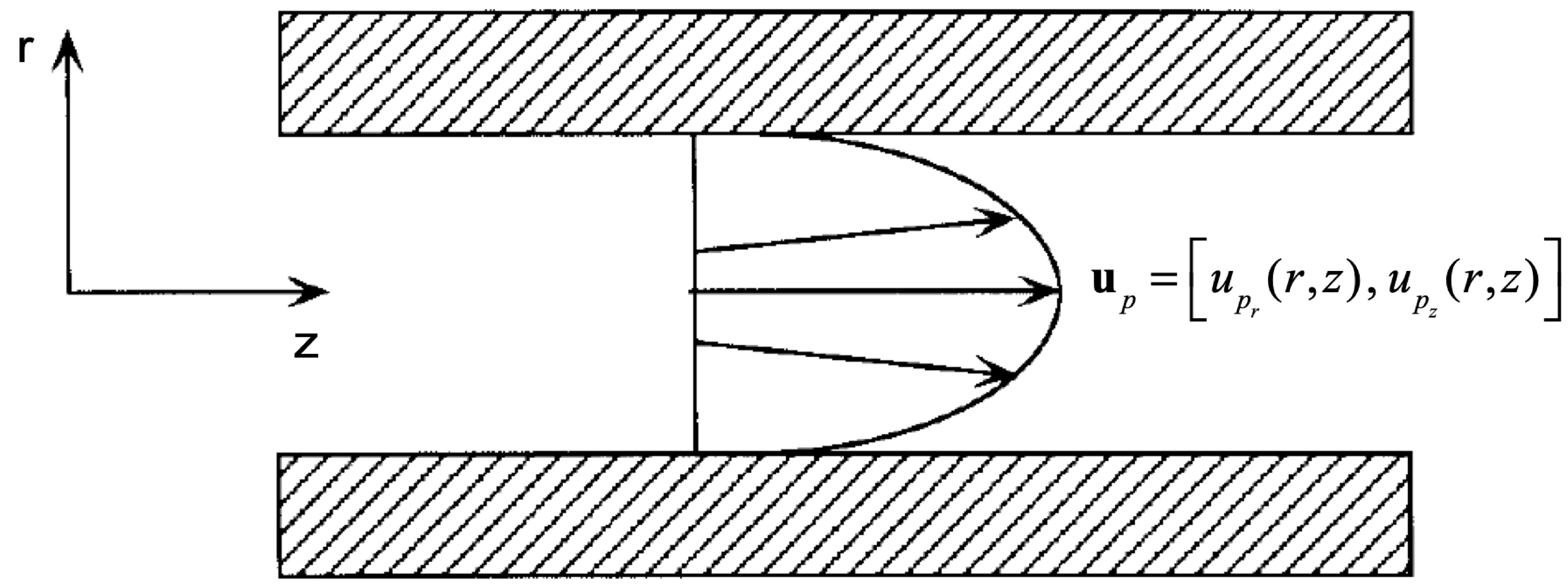
■ Re-casted mass balance equation:

$$\nabla \cdot \mathbf{u}_p - \kappa_p \nabla^2 \ln p = 0 \tag{6}$$

■ Re-casted momentum balance equation:

$$\begin{aligned} &\rho \mathbf{u}_p \cdot \nabla \mathbf{u}_p - \rho \kappa_p \nabla \ln p \cdot \nabla \mathbf{u}_p \\ &- \rho \kappa_p \mathbf{u}_p \cdot \nabla (\nabla \ln p) + \rho {\kappa_p}^2 \nabla \ln p \cdot \nabla (\nabla \ln p) \\ &+ \nabla p - \mu \nabla^2 \mathbf{u}_p + \kappa_p \mu \nabla^2 (\nabla \ln p) = 0 \end{aligned} \tag{7}$$

Analysis of Nanotube Flow



■ Transform the Recasted Navier-Stokes equations (6)-(7) to cylindrical polars (r, θ, z)

■ Tube symmetry implies independence of θ

■ Introduce non-dimensional variables:

$$\tilde{r} = \frac{r}{R}, \ \tilde{z} = \frac{z}{L}, \ \tilde{u}_{p_r} = \frac{u_{p_r}}{U_p}, \ \tilde{u}_{p_z} = \frac{u_{p_z}}{U_p}, \ \tilde{p} = \frac{p U_p \mu L}{R^2}$$

■ Dimensionless parameters:

$$\varepsilon = \frac{R}{L} \ , \ \mathrm{Re}_p = \frac{\rho U_p R}{\mu} \ , \ \kappa_p = \frac{\kappa_P}{U_p R} = \frac{\alpha^*}{\mathrm{Re}_p}$$

■ Regular perturbation expansion in ε:

$$\tilde{p} = \tilde{p}_0 + \varepsilon \tilde{p}_1 + \varepsilon^2 \tilde{p}_2 + .. \tag{8}$$

$$\tilde{u}_{p_r} = \tilde{u}_{p_r,0} + \varepsilon \tilde{u}_{p_r,1} + \varepsilon^2 \tilde{u}_{p_r,2} + .. \tag{9}$$

$$\tilde{u}_{p_z} = \tilde{u}_{p_z,0} + \varepsilon \tilde{u}_{p_z,1} + \varepsilon^2 \tilde{u}_{p_z,2} + .. \tag{10}$$

■ For a creeping nano-flow regime, it can be shown that

$$\tilde{p}_0 = \tilde{p}_0(\tilde{z}) \ , \ \tilde{p}_1 = \tilde{p}_1(\tilde{z}) \ , \ \tilde{u}_{p_r,0} = 0 \tag{11}$$

■ In dimensional form, the lowest-order non-zero terms in the perturbation expansion satisfy

$$\frac{1}{r}\frac{\partial}{r}(r u_{p_r,1}) + \frac{\partial u_{p_z,0}}{\partial z} = \kappa_p \frac{d^2 \ln p_0}{dz^2} \tag{12}$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial u_{p_z,0}}{\partial r}\right) = \frac{dp_0}{dz} \tag{13}$$

■ These must be solved subject to suitable boundary conditions: e.g. no-slip and no-penetration conditions at wall

Analytical Expression for the Mass Flow Rate

■ Equation (13) is solved to obtain the zeroth-order stream-wise velocity component

$$u_{p_z,0}(r,z) = \frac{1}{4\mu}\left(r^2 - R^2\right)\frac{dp_0}{dz} \tag{14}$$

■ The pressure distribution is then obtained as a *solubility condition* for the small radial velocity in equation (12)

$$-\frac{R^4}{8\mu}\frac{d^2 p_0}{dz^2} = R^2 \kappa_p \frac{d^2 \ln p_0}{dz^2} \quad \Rightarrow \quad \frac{dp_0}{dz} + \gamma \frac{d \ln p_0}{dz} = \beta \ , \ \ \gamma := \frac{8\mu\kappa_p}{R^2} \tag{15}$$

■ The integration constant β is determined using inlet/outlet pressures as

$$\beta = -\frac{1}{L}\left[\Delta P + \gamma \ln \mathcal{P}\right] \ , \ \ \mathcal{P} := \frac{P_{in}}{P_{out}} \tag{16}$$

■ The mass flow rate along the tube in the stream-wise direction is

$$\dot{M}_{RNS} = 2\pi\rho \int_0^R r u_{m_z} dr = 2\pi\rho \int_0^R \left(r u_{p_z} - r\kappa_p \frac{d\ln p}{dz}\right) dr = \frac{\pi\rho R^4 \left(\Delta P + \gamma \ln \mathcal{P}\right)}{8\mu L} \tag{17}$$

Comparison with Experimental Data by Majumder *et al.*(2011)

■ To compare flow-enhancement data with our theory, we consider the ratio of the newly derived mass flow rate and the Poiseuille flow rate:

$$\frac{\dot{M}_{RNS}}{\dot{M}_{NS}} = \frac{(\Delta P + \gamma \ln \mathcal{P})}{\Delta P} \quad \gamma := \alpha^* \frac{8\mu^2}{\rho R^2} \tag{18}$$

■ The value of α^* is found by equating this ratio with the experimental enhancement factor

liquid	membrane thickness L (μm)	viscosity μ (cP)	Poiseuille flow vel. (cm/s)	observed velocity (cm/s)	enhancement factor	α*
hexane	126	0.30	0.000405	5.6	1.38E+04	2.05
decane	126	0.90	0.000135	0.67	4.96E+03	0.91
water (1)	34	1.00	0.00045	25	5.55E+04	11.33
water (2)	34	1.00	0.00045	4.39	9.75E+04	19.91
water (3)	126	1.00	0.000121	9.5	7.82E+04	15.97
EtOH	126	1.10	0.00011	4.5	4.07E+04	5.42
IPA	126	2.00	0.00006	1.12	1.84E+04	0.45

**Flow at 1 bar applied pressure through CNT-membranes with 7nm-diameter pores*

Acknowledgements and References

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