Active solid-state nanopores: Self-driven flows/chaos at liquid-gas nanofluidic interface

SUPPORTING INFORMATION

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## Notations

Table S1: Notations used in the calculations and derivations.

| Symbol | Description |
|--------|-------------|
| $\sigma$ | Position of nanopore from the reference edge |
| $d$ | Diameter of the Nanopore |
| $\gamma$ | Phase volume fraction in the multiphase flow |
| $\rho$ | Phase density |
| $\kappa$ | Phase variable |
| $v$ | Phase velocity |
| $M$ | Mass transport through the nanopore |
| $\overline{\tau}$ | Diffusion term/stress tensor |
| $\dot{m}_{lg}$ | Mass transfer rate from phase $l$ to phase $g$ |
| $\dot{m}_{gl}$ | Mass transfer rate from phase $g$ to phase $l$ |
| $\phi$ | Velocity potential |
| $A$ | Amplitude of the wave |
| $k$ | Wave number |
| $a$ | Acceleration of the molecules |
| $N$ | Number of evaporating particles from the nanopore |
| $W$ | Energy corresponding to work function of evaporation |
| $k_B$ | Boltzmann constant |
| $\Gamma$ | Cross sectional area |
| $P$ | Pressure |
| $\eta$ | Viscosity of liquid |
| $r$ | Radius of nanofluidic pore |
| $L$ | Flow length of instability |
| $\alpha_e$ | Element size in the simulation |
| $N_e$ | Number of elements in simulation |
| $\Phi$ | Area of nanopore |
| $r$ | Position vector |
| $b$ | Distance constant |
| $\beta$ | Constant velocity component in a vortex pair |
| $(u, v, w)$ | Velocity components in $x, y, z$ direction |
| $Re$ | Reynolds number |
| $E$ | Energy |
| $k_{eff}$ | Effective thermal conductivity |
| suffix $g,l$ | Gas phase and liquid phase, respectively |
| suffix $a,s$ | Analytical and simulation, respectively |
| suffix $in$ | Interface |
Governing differential equations

The continuity equation is given by:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0 \]  

(S1)

where \((u, v, w)\) are the velocity components in \((x, y, z)\) direction respectively, \(t\) is the time (usually a large time period is considered for steady state simulation), and \(\rho\) is the density. This is a fundamental equation in fluid dynamics and represents the conservation of mass for a fluid. In this equation:

- \(\frac{\partial \rho}{\partial t}\) represents the rate of change of density \((\rho)\) with respect to time \((t)\).
- \(\frac{\partial \rho u}{\partial x}\) represents the rate of change of the density \((\rho)\) times the velocity component \((u)\) in the \(x\)-direction \((x)\) with respect to \(x\).
- \(\frac{\partial \rho v}{\partial y}\) represents the rate of change of the density \((\rho)\) times the velocity component \((v)\) in the \(y\)-direction \((y)\) with respect to \(y\).
- \(\frac{\partial \rho w}{\partial z}\) represents the rate of change of the density \((\rho)\) times the velocity component \((w)\) in the \(z\)-direction \((z)\) with respect to \(z\).

The equation states that the total rate of change of density within a fluid element is equal to zero, which means that mass is conserved. In simpler terms, it asserts that the change in density at a given point in space and time is equal to the net flow of mass into or out of that point. This equation is a fundamental part of the Navier-Stokes equations, which describe the behaviour of fluid flow. The momentum equation in equation S1 is given by

\[ \frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2)}{\partial x} + \frac{\partial (\rho uv)}{\partial y} + \frac{\partial (\rho uw)}{\partial z} = \]

\[ -\frac{\partial p}{\partial x} + \frac{1}{Re} \left[ \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right] \]  

(S2)
\[ y\text{-component} \]
\[
\frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho uv)}{\partial x} + \frac{\partial (\rho v^2)}{\partial y} + \frac{\partial (\rho vw)}{\partial z} = -\frac{\partial p}{\partial y} + \frac{1}{Re} \left[ \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right] \]  
(S3)

\[ z\text{-component} \]
\[
\frac{\partial (\rho w)}{\partial t} + \frac{\partial (\rho uw)}{\partial x} + \frac{\partial (\rho vw)}{\partial y} + \frac{\partial (\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{Re} \left[ \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right] \]  
(S4)

The energy equation is given by
\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho v (\rho E + P)) = \nabla \cdot (k_{\text{eff}} \Delta T) \]  
(S5)

where \( E \) represents the internal energy, \( P \) is the pressure, and \( T \) is the temperature, which are mass-averaged variables according to the volume fraction model. The phase parameter \( p \) is included to account for multiphase effects, and \( k_{\text{eff}} \) denotes the effective thermal conductivity.\(^1\)
Figure S1: Detailed flow dynamics of 30 nm and 50 nm single nanofluidic pore systems.
Figure S2: Detailed flow dynamics of 70 nm single nanofluidic pore system.
Figure S3: Exemplary cases of local fluidic interactions near the pores (a), (b), (c) Left: Major velocity magnitude distribution patterns and right: velocity streamlines.
Figure S4: 30 nm, 50 nm, and 70 nm nanofluidic pores’ corresponding (a) velocity magnitude distribution patterns and (b) velocity streamline distribution.
Figure S5: Exemplary convergence data of residuals within the nanopore systems. (a) 50 nm pore size single nanopore systems, and (b) 70 nm pore size single nanopore systems.
Figure S6: Flow dynamics through the nanopores at acetone-air interface. (a) 50 nm nanopore systems with varying $\sigma$, (b) 100 nm nanopore systems with varying $\sigma$, (c) 150 nm nanopore systems with varying $\sigma$. 
References

(1) Manual, U. ANSYS FLUENT 12.0. *Theory Guide* 2009,