CAPILLARY NEGATIVE PRESSURE AND CAVITATION IN RECTANGULAR NANOCHANNELS

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Introduction

Nanofluidics has attracted much attention in recent years due to the rise of the newly nanoscience and nanotechnology. A ubiquitous example is the capillarity-induced transport phenomena of fluids in nanochannels due to the large surface-to-volume ratios. Capillary action as a driving force to control liquids has been studied to explore the principle of nanofluidics. The Young-Laplace equation has been proven experimentally to be still valid on nanoscale [1]. Negative pressure as an interesting phenomenon has been observed during capillary two-phase flow in a planar nanochannel [2]. However, there are few reports about negative pressure in nanochannels with varying sizes since its direct experimental measurement is very difficult. Negative pressure in liquids often promotes cavitation possibility in liquids. The occurrence of cavitation depends on multiple factors that can be temperature, fluid properties, roughness of channel inner surface, channel geometry, etc.

In the present study, we examine the pressure field of water flow in three dimensional (3D) hydrophilic nanochannels with widths ranging from 500 nm down to 20 nm under constant room temperature by using the finite element method (FEM). The channel height is kept constant at 110 nm. The contact angle of water/air interface to all inner surfaces is constant as the surface roughness of channel walls is neglected. The density and viscosity of water and air are assumed constant during the dynamic filling process. The cavitation probability is analyzed quantitatively for channels with uniform and nonuniform cross section.

Model Equations

Fig.1 shows the top view of a geometrical sketch of 3D channels with rectangular cross section.

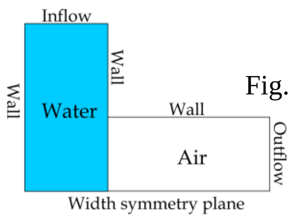

Fig.1 Top view of symmetric geometry description of 3D rectangular channels.

The capillary flow in nanochannels is described by the Navier-Stokes equations for incompressible fluids of constant density and viscosity:

$$\rho\left(\frac{\partial u}{\partial t}+u\cdot\nabla u\right)-\nabla\cdot\left(\mu\left(\nabla u+\nabla u^{T}\right)\right)+\nabla p=F, \qquad (1)$$

$$\nabla\cdot u=0, \qquad (2)$$

Where ρ, u, μ, p, F, and t represent density, velocity, viscosity, pressure, body force, and time, respectively. The body force acting on the flow is the gravity. The capillary pressure in a rectangular channel can be described by the classical Young-Laplace equation:

$$P_{cap}=P_{liq}-P_{vap}=-2\sigma\cos\theta\left(\frac{1}{w}+\frac{1}{h}\right), \qquad (3)$$

where σ is the surface tension, θ is the contact angle, w and h are the channel width and height, respectively.

Results and Discussion

The pressure field is calculated based on the Navier-Stokes equations. Fig.2 presents a snapshot of 3D pressure profile in a 100 nm wide channel at the moment of 150 nanoseconds. There is a pressure jump of roughly -24 bars across the interface. It implies that the water front just behind the interface is at a significant negative pressure of -23 bars, since the reference pressure of air is 1 bar. Obviously, the tension force induced by negative pressure gets more relaxed for the water flow further away from the interface.

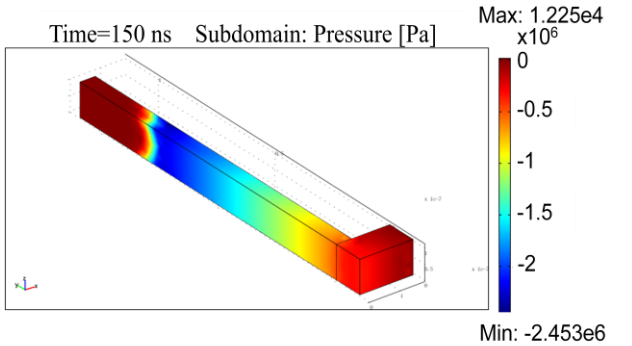

Fig.2 3D pressure profile in a channel with a width of 100 nm and a height of 110 nm at t=150 ns.

The capillary pressure for channels with widths ranging from 500 down to 20 nm is shown in Fig.3. As can be seen, it is in accordance with the pressure calculated from the Young-Laplace equation (also shown in Fig.3). The simulated pressure jump across the interface is a significant negative pressure of -75 and -13 bars for a 20 and a 500 nm wide channel, respectively. The pressure jump increases with reducing the channel width. Moreover, it tends to change dramatically for channels with a width less than around 100 nm, and smoothly for channel widths above it. The Young-Laplace equation actually shows an asymptotic relation between the pressure and the geometry of the channel confinement. In fact, it implies the mathematical characteristics of the plot of the pressure change due to the geometrical change as shown in Fig.3. Tas et al. [2] determined a negative pressure of -17 ± 10 bars for water plugs in a silicon oxide nanochannel of 108 nm height and 10 μm width by analyzing the visible meniscus curvature. It appears that this experimental value matches up with the extension of the simulated pressure plot. For thinner channels with width such as below 100 nm, the experimental results of capillarity induced negative pressure are expected.

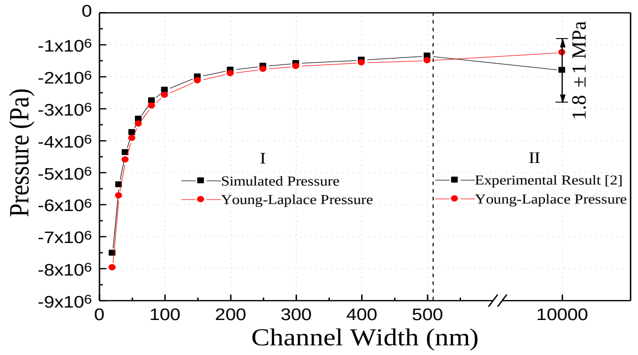

Fig.3 Simulated capillary pressure in 110 nm high nanochannels with variable widths, Young-Laplace pressure, and the available experimental result.

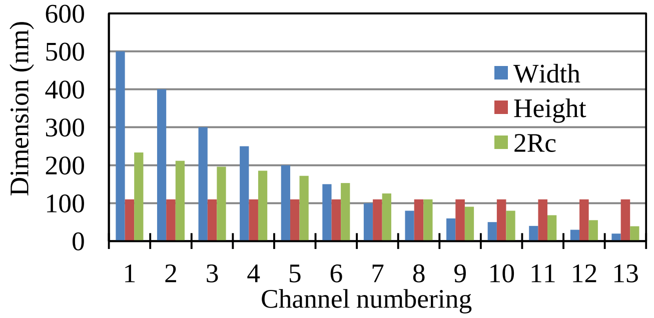

Fig.4 The channel width (blue), height (red), and critical radius (green) for 13 channels.

The behavior of bubble nucleation has been investigated under different solid-liquid interfacial interaction [3] or during heat transfer [4] in micro-nanochannels. Also, the absence of cavitation was explained in nanochannels by the fact that the critical radius is comparable to the height of the channel [2]. The critical cavitation radius R_c in liquid [5] can be expressed as

$$R_c = \frac{2\sigma}{P_{sat} - P_{liq}} \quad , \tag{4}$$

where P_{sat} is the saturated vapor pressure and P_{liq} is the actual liquid pressure. P_{sat} of water is close to zero at room temperature. Fig.4 shows R_c calculated from the simulated pressure for channels in Fig.3. As can be seen, the critical size of cavitation is bigger than the smallest dimensions of geometry (h or w) for each channel. This suggests that bubbles of critical size cannot enter these channels. It agrees with the absence of cavitation observed in reference [2].

In order to obtain a clearer explanation for the absence of cavitation, we derived the analytical relation between R_c and the smallest dimensional geometry for channels with constant cross section and contact angle. By substituting P_{liq} from Eq.(3), Eq.(4) can be rewritten as

$$R_c = \frac{2\sigma}{-P_{cap} - P_{vap}} \tag{5}$$

The aspect ratio ($a = \frac{w}{h}$) of cross section is introduced. Eq.(6) is acquired by combining Eq.(3) and (5).

$$R_c = h \cdot \frac{2\sigma}{2\sigma\cos\theta\left(\frac{1}{a}+1\right) - h \cdot P_{vap}} = w \cdot \frac{2\sigma}{2\sigma\cos\theta(1+a) - w \cdot P_{vap}} \tag{6}$$

Interestingly, in both cases of high aspect ratio ($a \geq 1$, i.e., $w \geq h$) and low aspect ratio ($a \leq 1$, i.e., $w \leq h$), the following relation can be deduced as Eq.(7).

$$\frac{R_c}{h(\text{or } w)} \geq \frac{2\sigma}{4\sigma\cos\theta - h(\text{or } w) \cdot P_{vap}} > \frac{1}{2\cos\theta} \quad , \tag{7}$$

where whether h or w depends on the smaller dimension of geometrical parameters. Therefore, the relation of R_c to the smaller dimensional size of channels can be acquired as

$$R_c > \frac{1}{2} h(\text{or } w) \tag{8}$$

This indicates that bubbles of critical size in diameter are bigger than the channel height or width. It implies that bubbles of critical or larger size will not form in channels with uniform cross section. Besides, the ununiformity of h and w is favorable to the absence of cavitation in the channel. It is worth to mention that this result is suitable not only for nanochannels but also for other channels with uniform cross section and constant contact angle and temperature.

For channels of nonuniform cross section, we suppose the simplest case is the channel with two variable widths (w1>w2) and constant height h. Since R_c scales with channel size, we presume the minimum value R_c' could be obtained in the partial length with the smallest cross section of the channel. This indicates that the bubbles of R_c' might develop in the partial length with bigger cross section of the channel. Eq.(8) explains cavitation will not occur in a planar hydrophilic channel ($w1>w2 \geq h$). Whereas, in the cases of $h \geq w1 > w2$ and $w1>h>w2$, bubbles of size in diameter of $2R_c'$ are larger than the smallest width w2, but they might be smaller than w1 or h. This leads to a possibility for the occurrence of cavitation in the cross section with parameters of h and w1. Additionally, the fluctuation of other factors such as temperature might also lead to the formation of bubbles since the capillary pressure varies accordingly.

Conclusions

FEM simulation has been applied for the investigation of capillary negative pressure of water flow in nanochannels with variable widths. It agrees well with the Young-Laplace pressure. The probability of cavitation has been analyzed quantitatively for channels with uniform cross section and nonuniform cross section or unstable parameters. The cavitation will not occur for the former, yet it might occur in the latter case. The ununiformity of h and w is favorable to the absence of cavitation in the channel. The subject of negative pressure and its adjunct phenomena “cavitation” is very important for future applications in nano science and engineering.

References

1.Sobolev,V.D., Churaev, N.V., Velarde, M.G., Zorin, Z.M. Surface tension and dynamic contact angle of water in thin quartz capillaries. *J.Colloid Interface Sci.*, **222** (2000) 51-54.

2.Tas, N.R., Mela, P., Kramer, T., Berenschot, J.W., van den Berg, A. Capillarity induced negative pressure of water plugs in nanochannels. *Nano Lett.*, **3** (2003) 1537-1540.

3.Nagayama,G., Tsuruta, T., Cheng, P. Molecular dynamics simulation on bubble formation in a nanochannel. *Int.J.Heat Mass Transfer*, **49** (2006) 4437-4443.

4.Li, J., Cheng, P. Bubble cavitation in a microchannel. *Int.J.Heat Mass Transfer*, **47** (2004) 2689-2698.

5.Herbert, E., Caupin, F. The limit of metastability of water under tension: theories and experiments. *J.Phys.: Condens.Mat.*, **17** (2005) S3597-S3602.