A Review on the Effect of Surface Roughness and Liquid Slip on fluid flow in PDMS Microchannels

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Abstract: Microfluidics is about studying flows with characteristic length scales of the orders of microns (typically sub millimeters). The fluid dynamics at the microscale can vary from “macro fluidic” behavior in those factors such as surface tension and energy dissipation. The fluidic resistance will keep on developing to dominate the system. Polydimethylsiloxane (PDMS) is a polymer commonly used for microfluidic chip manufacture and prototyping. PDMS becomes a hydrophobic elastomer after cross linking. Small dimensions make it impossible to produce a microchannel with smooth surface. Hence entrance effect, surface roughness, turbulence and viscous effects have a reasonable effect on fluid flow. This paper aims to look into characterization techniques of surface roughness in a channel and liquid slip phenomenon considering changes in elementary geometry, flow conditions and different roughness elements.

Keywords: Surface Roughness, LBM, Microchannel.

1. Introduction

Microfluidics has been an essential part in “lab on chip” device. The complications of micro-hydrodynamics were considered in different conditions. As length scale becomes smaller, surface effects tend to dominate. PDMS polymer can be used for the fabrication of microchannels using soft lithography technique developed by Whitesides.. Soft lithography has the constraints of fabricating different geometries of the channel. This method could only create a cross section in rectangles. Theoretically, circular channel is the best shape for fluid flow mechanism. The reasons are, First of all, channels of circular geometry offer least surface area exhibited to the fluid that could limit the friction between the fluid and the wall surface. So, the energy required to pump the water for a given flow rate is less. Secondly, internal pressure of the fluid is efficient to handle in circular shape. Pressure distribution is uniform around the entire circumference of the channel. PDMS formula is (C2H6OSi)n and its fragmented formula is CH3[Si(CH3)2O]nSi(CH3)3, n is the number of monomers repetitions. PDMS is optically transparent within the range of optical frequencies (240 – 1100), which helps to visualize the flow using a microscope. Using a simple plasma treatment PDMS can be adhered thoroughly to glass or another PDMS layer. Hence the production of multilayers PDMS devices is more advantageous than that of a glass substrate. A wide range of patterns and channel dimensions can be easily prepared, including straight, T-shapes, X-, Y-, and S-curve which may replicate the vascular network.
The rudimentary flow behavior in microchannels has been broadly studied and phenomenal advancements are achieved in experimental and theoretical investigations. Therefore, for liquid flows in microchannels Navier-Stokes equations and use of the continuum assumption are generally assumed to be valid and, in many studies, are experimentally in good agreement. Rigid microchannels have reported exceptionally higher values of friction constant (f_Re). Reduction of aspect ratio (α) and the ratio of channel height to width in rectangular geometry microchannels increased the friction factor considerably. Huge deviation is observed in the forecasted values with respect to the friction factor (f) due to experimental variability, channel geometry, and surface roughness. Among these the roughness of the surface should be carefully examined. Lattice Boltzmann method (LBM) [1] has emerged as productive alternative simulations for fluid flow.

2. Evaluation of Flow and Theory
These are with respect to Rectangular microchannels
Mean hydraulic diameter was calculated as follows:

\[ D_h = \frac{4A}{P} \]
\[ D_h = \frac{4Wch}{Hch^2 Wch} + \frac{1}{Hch} \]

The numerator is volume of microchannels. Denominator is the surface area of rectangular microchannels.
Reynolds number for the laminar flow in microchannel should be less than 2000, which is achieved here [2]. Expression for Reynolds number is,

\[ \text{Re} = \frac{\rho V D_h}{\mu} \]

Reynolds number is directly proportional to the velocity of water through the microchannel, ass the Density, hydraulic diameter and dynamic viscosity of water remains constant,

The cumulative drop in pressure in the microfluidic system, Psys, is calculated using the equation.

\[ \text{Psys} = \Delta P_{\text{tube}} + \Delta P_{\text{pent}} + \Delta P_{\text{needle}} + \Delta P_{\text{interference}} + \Delta P_{\text{capillary}} + \Delta P_{\text{exit}} \]

Across the microchannel length L in steady-state laminar flow the pressure drop is defined as

\[ \Delta p = Q \frac{(12\mu L)}{(h^3 w)} = v \frac{(12\mu L^2)}{h^3} \]

To understand the flow phenomenon Normalized friction constant (C*) is used widely to observe a deviation from the laminar theory. This value of C* is a non dimensional number.

\[ C^* = \frac{f_{\text{Re}}_{\text{experiment}}}{f_{\text{Re}}_{\text{theory}}} \]

A measure of the departure from the continuum is introduced through the Knudsen number, Kn, defined as,

\[ k_n = \frac{\alpha}{D_h} \]
In liquid flow Knudsen number is much less than unity in the channels with hydraulic diameter ranging from $10^{-6}$ m to $10^{-3}$ m. Occurrence of deviation between the results are due to specific flow characteristics which are unaccounted in conventional theory.

3. Effect of Surface Roughness

The presence of wall roughness leads to increase in the friction between the fluid and channel due to decrease in the value of the critical Reynolds number, during which the flow transition takes place from laminar to turbulent. In laminar flow the drag coefficient on the Reynolds number remains the same for both smooth and rough micro-channels. More surface roughness leads to increase in surface area resulting in adsorption effect and possibility of trapped air bubbles during the flow. Effect of Surface roughness is crucial with respect to fluid flow because of four reasons: (i) Controlling surface roughness at micro scale in a realistic manner is not easy, (ii) Roughness of the surface causes interfacial properties such as interfacial forces, wettability and trapped air, (iii) Rough surface generates swollen boundaries that make accurate interpretations of specific boundary positions more complicated, and (iv) No theoretical characterization for the inherent randomness and nonperiodic roughness of the surface. A good approach for rough contours or surfaces and their random behavior is very important in some engineering problems. Fractal modeling [2] can provide an alternative to generate rough geometries based on statistically self-similar geometries. Table 1 shows the important parameters to be studied and investigated to understand the flow of fluid in microscale.

The following are the best analytical characterization techniques to understand the effect of surface roughness in a PDMS microchannel.

3.1 Fast Fourier Transform (FFT) method:

Fast Fourier Transform (FFT) [3] can be used to simulate the surface roughness. In this method the roughness can be measured as a function which represents the height of surface at each point in xy plane.

$$f(x) = \sum_{k=0}^{M-1} \sum_{l=0}^{N-1} \sqrt{S_{m,n}} \exp\left(i2\pi[\varnothing_{m,n} + \frac{mx}{M} + \frac{ny}{N}]\right)$$

Where $x = 0, 1, \ldots, (M-1)$, and $y = 0, 1, 2, \ldots, (N-1)$ are the coordinate of the base plane are taken as integer, $\varnothing_{m,n}$ is the phase angles ranging over 0 and 2\pi. $S_{m,n}$ is spectral density used to generate surface and $m$ and $n$ are integers with $m = 0, 1, 2, \ldots, M/2$ and $n = 0, 1, 2, \ldots, N/2$. Autocorrelation function is used for plotting the surface.

Spectral density is calculated by following equation:

$$S(m,n) = \frac{1}{MN} \sum_{l=0}^{N-1} \sum_{k=0}^{M-1} R_{rs} \exp\left(-i2\pi[\frac{mr}{M} + \frac{ns}{N}]\right)$$
3.2 Mandelbrot–Weierstrass function:

Fractal dimension (D) can quantitatively describe surface microscopic roughness[4]. Mandelbrot–Weierstrass function is used to model the rough surface represented by following equation.

\[
f(x) = \sum_{l=0}^{N-1} p^{-n(2^{-l})} (1 - k \cos(p^{n}x + \phi))
\]

f(x) is the rough profile, f is a non integer value known as fractal dimension, varies between 1 and 2, P is the multiplier frequency value, which usually ranges between 1.1 which 3.0. and \(\phi\) is a randomly generated phase. k can be used to alter the profile. For regular surfaces usually these values will be fixed \(k = 1\) and \(p = 2\). Routine measurements used in fabrication can detect highly irregular surfaces. In fractal models, surface roughness can thus be described by fractal dimension f. The major advantage of fractal modelling is it is scale independent. Once the topography is generated we can find all the parameters such as RMS (Root Mean Square Error) values. Since some of the experimental results are reported in terms of RMS or any other parameters, we can change the model parameters. Any profile can be developed and fine-tuned by setting the parameter D and k. Fig.2[3] shows the Mandelbrot – Weierstrass equation generated surfaces and plotted using wire-mesh models.

**Figure 2**[3]: Surfaces drawn using M – W for various D values: (a) D = 1.3, (b) D = 1.5 and (c) D = 1.8.

**Figure 3**[3]: Fractal dimensions of surface roughness using LBM.

D is varied between 1 to 2, in order to know the impact of fractal dimension on speed. Velocity is computed at a steady state across the microchannel height from the lowest lattice point to the topmost lattice point, and plotted as shown in Fig. 4. As fractal dimension increases there will be increase in drag coefficient. Corresponding drop in fluid velocity is observed due to this reason near surface. For further more roughness surface (D=2.0), It can also partially block the flow in the channel [4]. Partial channel blockage for the roughest surface is observed up to 28.5 per cent of the total channel height. Remember that only the bottom surface with determined roughness is modelled in simulation. Velocity at the wall tend to oscillate does not remain constant and due to the roughness of the surface.

**Figure 4.**[6]: Effect of surface roughness

**Figure 5.**[6]: experimental and simulation results

Simulation can be performed with and without surface roughness to compare the velocity profile between these two conditional parameters. In Fig. 6 it is clearly visible that the plot is flat and ideal when no roughness is considered, the velocity indicator is consistent throughout the channel. Experimental results however reveal that speed is oscillating and not constant. The
simulation without ruggedness did not notice the velocity oscillatory behaviour. These oscillations occur because of the presence of ruggedness in the channel surface. Implementing a surface roughness model of MW significantly improved the accuracy by capturing the oscillatory behavior in the middle of the tube. This method is thus proven successful in capturing the real phenomenon in the numerical simulations. This model also offered an analysis of the near-surface vorticity behavior. Local oscillations can be seen to be produced because of the Presence of surface ruggedness. It is possible to use this oscillatory activity for microfluidic tasks such as mixing. In addition, by optimizing the manufacturing process one can also improve the mixing by imparting the necessary roughness.

4. Liquid Slip

Knowing basic mechanisms which control liquid slip is still evasive. Without slip velocity, the wall slip length can be perceived as an increase in channel width. The wall slip velocity for liquid flow was first proposed by Navier in 1823, generally expressed as $U_s = \beta \delta u/\delta n$. The parameter $\beta$ is called Slip length ranging from several nanometers to several microns, and has been thought to be a material property parameter and the working fluid. The wall slip velocity is illustrated in following figure.

![Wall slip velocity between wall material and working fluid](image)

**Figure 6.** Wall slip velocity between wall material and working fluid

![Slip length for various slip conditions.](image)

**Figure 7.** [9]: Slip length for various slip conditions.

Lund et al. derived a definition of effective slip length on a surface with periodic roughness in terms of the intrinsic slip length and surface contact area, using the Stokes flow and homogenization method of steady state. Its derived effective slip length [7] reflects the harmonic mean weighted by the surface-to-fluid contact area and is given as follows:

$$L_{eff} = \left[ \frac{1 + \frac{s^2}{L_s}}{L_s} \right]^{-1}$$

Where $L_s$ is intrinsic slip length, $s$ is slope.

The surface wettability of the material is significantly impacted at nanoscale due to liquid slip. Macroscopically, depending on the contact angle produced by a liquid droplet with the surface, the wettability of a surface is defined as wetting, nonwetting, or neutral. Contact angles greater than $90^\circ$ with a liquid is called non-wetting while contact angles smaller than $90^\circ$ with a liquid are considered wetting. A contact angle of $90^\circ$ with a liquid that forms a surface is termed neutral. Nonwetting surfaces are known to be strongly inclined towards liquid slip introduction.
Conclusion

The roughness of the surface depends on the packaging and thus relies directly on the mold packaging. PDMS precisely copies even the tiniest holes and gets the same mold geometry. Soft lithography combined with a thick photoresist reflow phenomenon is a new approach to PDMS microchannel manufacturing to minimize surface roughness. [5]. We could easily change the circular channel diameter and the channel routes. It is much needed to investigate the effect of surface roughness on the microchannel fluid flow for a PDMS-based microfluidic application. The results show that the surface velocity is not constant, but shows oscillating behaviour. This action can be clarified by accounting for ruggedness information on the channel surfaces. Local velocity oscillations in microchannel were recorded because of the ruggedness of the wall. The function of Weierstrass-Mandelbrot was used to develop surface roughness based on a fractal. Fractal dimension of the device constructed can be determined experimentally using AFM (Atomic Force Microscopy) and substituted in model's WM function. Using 3D LBM method the fluid flow can be simulated. The findings demonstrate fluid flow oscillatory behaviour. The result also shows that an increase in the fractal dimension increases the ruggedness and thus the fluid velocity is reduced. Thus, the turbulence in the microchannel can be tuned by synthesizing rough surfaces, and the mixing efficiency can be improved. With respect to liquid slips it affects in terms of nominal scale, but when flow is droplet induced this parameter is very significant.

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