



Investigation of Flow in Microchannels with Superhydrophobic Surfaces Using Hybrid Direct Simulation Monte Carlo-Navier-Stokes Method with Information Preservation Approach

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ABSTRACT: In recent years, superhydrophobic surfaces have received significant attention due to properties such as drag reduction and self-cleaning. A superhydrophobic surface can be made by grooving the wall. In this case, the flow of gas caught in grooves may represent the rarefied flow. Therefore, particle-based approaches such as direct simulation Monte Carlo should be employed to simulate the flow. In this paper, laminar flow in superhydrophobic microchannels with ribs and cavities aligned perpendicular to the channel axis is investigated using a hybrid direct simulation Monte Carlo-Navier-Stokes method. Also, information preservation technique is employed to reduce statistical fluctuations of the direct simulation Monte Carlo method. The effects of the length of the cavity on the flow parameters such as effective slip length, and velocity slip are investigated and the results are compared with the simplified method of using Navier-Stokes equations with shear-free boundary condition as the gas-liquid interface. It is shown that the differences between the hybrid method and shear-free solution increase as the shear-free fraction increases. However, the difference is less than 6% for cases studied in this work. Therefore, it is acceptable to use the shear-free approach to reduce computational costs. Especially for $Fc < 0.2$ where the difference is less than 3%.

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1. INTRODUCTION

Superhydrophobic surfaces can be made by fabricating micro/nano grooves and cavities on hydrophobic surfaces. When a superhydrophobic surface is in contact with liquid, it will not penetrate the cavities due to its surface tension. Therefore, a two-phase flow occurs over these surfaces including the main liquid flow and a gaseous vortex flow in cavities. For simplicity, most of the researches model the gaseous flow with a simple shear-free boundary condition at the gas-liquid interface. Lauga and Stone [1] solved the Stokes flow in circular pipes considering two different configurations of longitudinal and perpendicular ribs on the wall. They modeled the surface by the periodical distribution of shear-free and no-slip regions. Chen et al. [2] applied the shear-free approach to study the effect of phase shift of grooves on the effective slip length. On the other hand, some investigators solve the gaseous flow as well to achieve more accurate results. In this approach, the equality of velocity and shear stress at the interface is used to couple the liquid flow in the microchannel core and the gaseous flow within cavities. Davies et al. [3] explored the flow in Two-Dimensional (2D) microchannels with superhydrophobic engineered surfaces that exhibit microrib/cavities oriented normal to the flow direction. They reported a maximum deviation of 6% between the results of shear-free and hybrid

approaches. Gaddam et al. [4] studied the effects of the shape of cavities over a superhydrophobic surface on the postponing of the Cassie to Wenzel state transition. They showed that the behavior of trapped vortex in the cavity affects the transition remarkably.

In all the available studies, the gaseous flow is considered a continuum. However, based on the dimensions of microcavities it is expected that the gaseous flow lay in the rarefied flow regime. In this case, it is necessary to use particle-based methods such as Direct Simulation Monte Carlo (DSMC) and a hybrid NS-DSMC technique should be utilized [5]. It is worth noting to emphasize that the DSMC method should be accompanied with Information Preservation (IP) technique so that it can demonstrate very low-speed vortex flow in the cavities.

In the present work, flow in microchannels with superhydrophobic walls is simulated using a hybrid NS-DSMC technique. The core liquid flow in the channel is solved using continuum based Navier-Stokes solvers while the trapped rarefied gaseous flow in the cavity is solved using DSMC-IP method. Based on the best knowledge of the authors, hybrid NS-DSMC technique is not performed so far to solve the flow over superhydrophobic surfaces. Using DSMC-IP method, the scheme applied in this study is more accurate rather than the available works which consider the gas medium as a continuum.

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2. METHODOLOGY

The geometry of the problem is shown in Fig. 1. The channel length is prefixed to $L=10\mu\text{m}$, and the cavity aspect ratio $Zc=hc/Wc$ is preset to $Zc=1$.

The constant property incompressible form of Navier-Stokes Equations is solved for water flow in the channel using Comsol Multiphysics 5.2.a software. The pressure drop along the channel is assumed to be 1 kPa for all cases. For gas-liquid interface, the equality of velocities, and shear stresses are applied. The DSMC-IP method is used to simulate gaseous flow in the cavity. The flow Knudsen number is in the range of $0.0058 < Kn < 0.026$. The gas is assumed to be Nitrogen, N_2 at 293K. The hybrid NS-DSMC method algorithm is as follows:

- 1) The procedure starts using an approximate slip length. It can be shown that the solution is independent of the initial guess.
- 2) Liquid flow is solved using NS equations.
- 3) Flow velocity on the gas-liquid interface is calculated.
- 4) Gaseous flow in the cavity is solved using DSMC-IP method with lid velocity from step 3.
- 5) From the DSMC results, the shear stress at the interface, as well as slip length, are calculated.
- 6) Steps 2-5 are repeated until convergence.

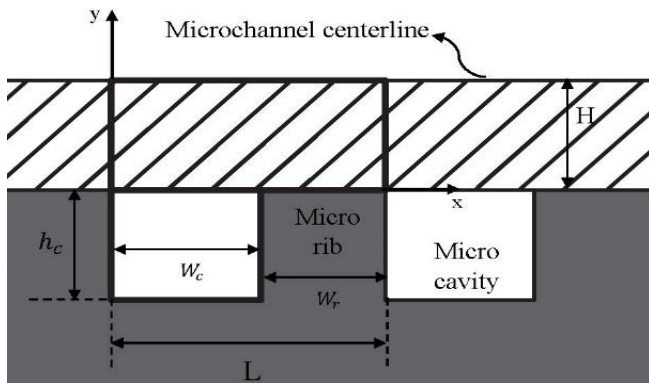


Fig. 1. Microchannel with the superhydrophobic wall

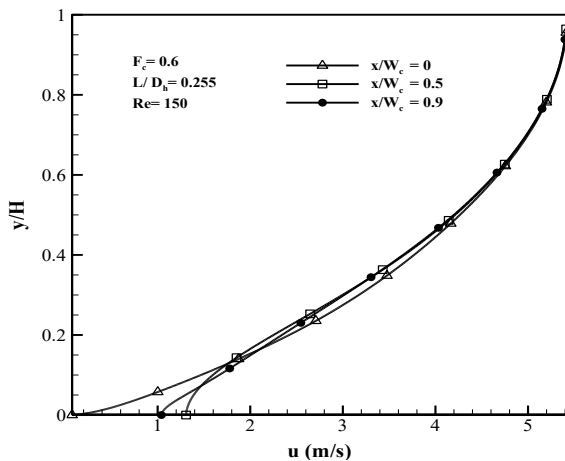


Fig. 2. Variation of streamwise velocity profiles of liquid flow for $Re=150$, $F_c=0.5$ and $L/D_h=0.255$

3. RESULTS AND DISCUSSION

Fig. 2 shows the velocity profile for liquid flow over the gas-liquid interface at three positions of $x/W_c=0$, $x/W_c=0.5$, and $x/W_c=0.9$ along with the channel. The normal velocity gradient at the interface varies significantly along with the flow. However, velocity profiles are nearly the same in the core flow. The slip-velocity increases along the interface to reach its maximum after $x/W_c=0.5$ and then decreases. With the increase of F_c , the position of maximum slip-velocity approaches downstream so that it happens at $x/W_c=0.53$ and 0.7 for $F_c=0.2$ and 0.9 respectively.

This manner is also shown in Fig. 3, where the variation of slip velocity along the interface is shown for various F_c at $Re=150$. For greater F_c , the flow has more time to accelerate along with the interface, which leads to a nearly fourfold increase in the maximum value of slip-velocity with the increase of F_c from 0.2 to 0.9.

Variation of effective slip length versus F_c is shown in Fig. 4 for both the hybrid and the shear-free approaches. The effective slip length increases by increasing F_c . The deviation between approaches is more significant for greater F_c so that it reaches to 5.2% at $F_c=0.9$.

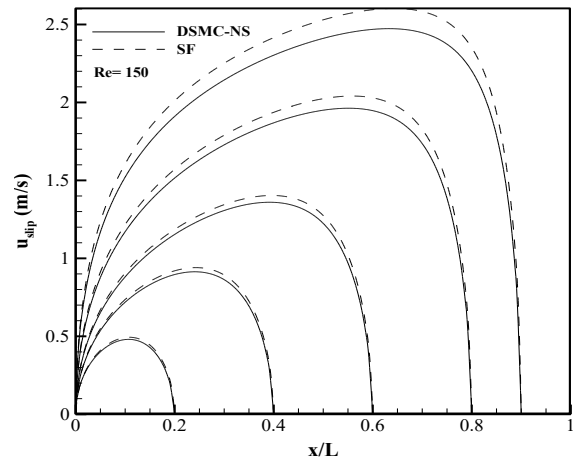


Fig. 3. The effect of the shear-free fraction on the interface velocity distribution at $Re=150$

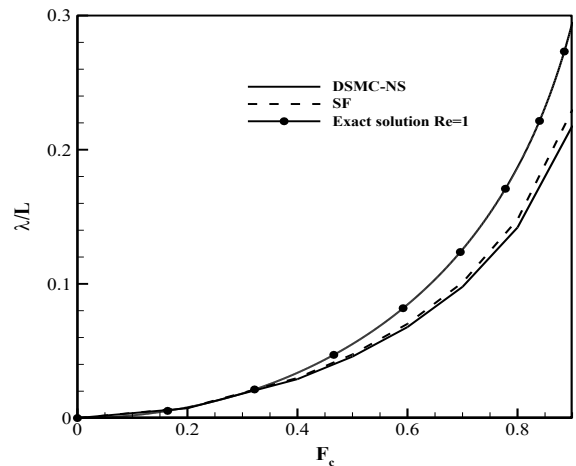


Fig. 4. The effect of the shear-free fraction on the effective slip length at $Re=150$

4. CONCLUSION

In this study, laminar flow in a 2D microchannel with superhydrophobic walls is investigated. Two approaches are used for the simulation of the flow: a) simultaneous solution of the rarified gas flow in the microcavity by the DSMC-IP method and continuum liquid flow in the microchannel by the finite element method; b) simply, applying the shear-free boundary condition as the gas-liquid interface and just solving the liquid flow. The results show that:

1. The slip velocity at the interface is variable, and its maximum happens around the middle of the interface, which moves downstream by increasing the shear-free fraction. So, it shifts from $x/W_c = 0.53$ to $x/W_c = 0.7$ as F_c increases from 0.2 to 0.9.

2. The velocity at the gas-liquid interface increases with increasing the shear-free fraction. A fourfold increase in the maximum slip velocity is seen as the F_c increases from 0.2 to 0.9.

3. The accuracy of the shear-free approach decreases as the shear-free fraction increases; so that a deviation of 5.2% is seen at $F_c=0.9$ in comparison with the hybrid approach.

However, to reduce computational costs, the shear-free approach can be employed for small F_c at the cost of losing some accuracy, say 3% at $F_c = 0.2$.

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