Numerical modeling of Stokes flows over a superhydrophobic surface containing gas bubbles

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Abstract. This paper continues the numerical modeling of Stokes flows near cavities of a superhydrophobic surface, occupied by gas bubbles, based on the Boundary Element Method (BEM). The aim of the present study is to estimate the friction reduction (pressure drop) in a microchannel with a bottom superhydrophobic surface, the texture of which is formed by a periodic system of striped rectangular microcavities containing compressible gas bubbles. The model proposed takes into account the streamwise variation of the bubble shift into the cavities, caused by the longitudinal pressure gradient in the channel flow. The solution for the macroscopic (averaged) flow in the microchannel, constructed using an effective slip boundary condition on the superhydrophobic bottom wall, is matched with the solution of the Stokes problem at the microscale of a single cavity containing a gas bubble. The 2D Stokes problems of fluid flow over single cavities containing curved phase interfaces with the condition of zero shear stress are reduced to the boundary integral equations which are solved using the BEM method.

1. Introduction
In the production and use of superhydrophobic surfaces (SHS), it is necessary to determine the hydrodynamic characteristics of viscous-fluid slip on the SHS, caused by the heterogeneous structure of the SHS containing gas bubbles on whose surfaces the shear stress can be neglected. The main parameter characterizing the averaged velocity slip is the effective slip length tensor [1]. This tensor is used in the effective slip boundary condition of Navier type, specified on SHS for macroscopic problems of viscous-fluid flows [2, 3]. In addition, the principal values of the effective slip length tensor (averaged slip lengths) are used for estimating the friction reduction in microchannels with superhydrophobic walls [4]. In most publications, the texture of SHS is assumed to be periodic, consisting of the alternating areas of a solid wall with the no-slip condition and gas bubbles with the condition of partial or complete velocity slip of the fluid on their surfaces [5, 6]. The need in the calculation of the slip length tensor components (averaged slip lengths) leads to the formulation of a broad class of problems of microhydrodynamics, dealing with viscous-fluid flows over a periodic system of microcavities containing gas bubbles. The goals of solving such problems are to optimize the SHS texture and maximize the values of the principal averaged slip lengths, which can allow to reduce the friction (or to decrease the pressure drop in a microchannel flow). For practical applications [7, 8], it is necessary to develop efficient numerical methods which could make it possible to easily perform parametric studies.
of the dependence of the averaged slip lengths on the shape of the gas bubble surface and/or the position of the meniscus relative to the microcavity walls.

In our previous work [9], in which we first applied the BEM to solving the Stokes flow problem on the scale of a single cavity and a group of cavities, the position of the meniscus relative to the microcavity walls was fixed. However, if the initial static positions of the bubbles of a superhydrophobic surface are uniform (the masses of all bubbles are the same), in a pressure-driven microchannel flow the actual positions of the meniscus in the cavities should depend on the local pressure over the chosen microcavity. The static pressure in the fluid changes along the channel and, accordingly, due to the compressibility of the gas, the position of the meniscus changes from cavity to cavity. In [9], it was shown that both the gas bubble shape and the shift of the meniscus into the cavity significantly affect the value the averaged slip length. Below, a mathematical model is proposed which takes into account the variation of the bubble surface shift into the cavities with the development of viscous flow in a microchannel having a superhydrophobic bottom wall. The model proposed makes it possible to study the friction reduction in the microchannel by matching the solutions of the problem on the macroscale (channel length) with the solution of the Stokes problem on the scale of single cavities.

2. Pressure-driven flow in a microchannel with a superhydrophobic bottom wall

In this section, we consider a steady-state viscous fluid flow at a constant volume flow rate $Q^*$ in a microchannel with a superhydrophobic bottom wall (figure 1(a)). The bottom wall is a periodic striped superhydrophobic surface with period length $L$, containing rectangular microcavities of depth $H_c$ and width $d$, partially filled with a compressible gas (figure 1(b)).

![Figure 1. Pressure-driven flow in a microchannel with a superhydrophobic bottom wall on the macroscale (a); flow over rectangular microcavities of a striped SHS containing compressible gas bubbles on the microscale (b)](image)

The microchannel thickness is $H$ and length is $l$. It is assumed that $l$ is of the order of centimeter and $H$ is of the order of tens of microns, so that $H \ll l$. On the macroscale $l$, the bottom SHS can be regarded as an effectively smooth rigid wall with the effective Navier slip boundary condition on this wall for the averaged longitudinal velocity component of the fluid. In dimensional form, the equations of averaged steady fluid motion on the macroscale in the microchannel with the appropriate boundary conditions formulated on the bottom and upper walls can be written as follows:

$$
\mu \frac{\partial^2 u^*}{\partial y^*^2} = \frac{\partial p^*}{\partial x^*}, \quad \frac{\partial p^*}{\partial y^*} = 0, \quad \frac{\partial u^*}{\partial x^*} + \frac{\partial v^*}{\partial y^*} = 0
$$
\[ y^* = 0 : u^* = b^*(x^*) \frac{\partial u^*}{\partial y^*}, \quad y = H : u^* = 0, \quad v^* = 0 \]

Here, the asterisk denotes dimensional variables, \( u^* \) and \( v^* \) are the velocity components of the fluid, \( p^* \) is the pressure, \( b^*(x^*) \) is the effective slip length of the striped superydrophobic surface, and \( \mu \) is the dynamic viscosity of the fluid. The solution of this problem takes the form:

\[ p^* = p^*(x^*), \quad u^*(x^*, y^*) = \frac{1}{\mu} \frac{dp^*}{dx^*} \left( \frac{y^*}{2 - \frac{H^2 y^*}{2(H + b^*(x^*))} - \frac{H^2 b^*(x^*)}{2(H + b^*(x^*))} } \right) \]

The expression for \( v^* \) is omitted. By integrating the expression for the longitudinal velocity component across the channel, we obtain the formula relating the flow rate \( Q^* \) with the pressure gradient in the microchannel:

\[ Q^* = -\frac{dp^*}{dx^*} \left( \frac{H^3}{12\mu} \left( 1 + \frac{3b^*(x^*)}{H + b^*(x^*)} \right) \right) \]

Then, from this expression we obtain the equation for the pressure distribution along the channel:

\[ \frac{dp^*}{dx^*} = -12Q^* \mu \left( 1 + \frac{3b^*(x^*)}{H + b^*(x^*)} \right)^{-1} \quad \text{with} \quad p^*(l) = p^*_a \]

Here, \( p^*_a \) is the atmospheric pressure at the outlet of the microchannel. If the velocity slip length distribution (the function \( b^*(x^*) \)) is known, from the last equation we can find the pressure distribution in the microchannel, supporting the constant flow rate \( Q^* \). If \( b^*(x^*) \) is constant or equals zero, we obtain the standard linear pressure distribution in the microchannel. We note, that the relation between the flow rate and the pressure drop under this assumption is often used for experimental estimates of the mean effective slip length (assumed to be constant) for striped SHS. However, the measured velocity slip length does not coincide with the predictions based on known mathematical models, in which it is usually assumed that on the entire length of the channel the bubble surfaces are flat and the bubbles completely occupy the cavities.

In real flow, the pressure in the fluid decreases along the microchannel and, accordingly, due to the compressibility of gas in the bubbles, the position of the meniscus changes from cavity to cavity. We assume that the texture period \( L \) of the striped SHS is of the same order as the microchannel thickness \( H \). Then, on the macroscale \( l \gg L \) the function \( b^*(x^*) \) can be assumed continuous, and the local value of \( b^*(x^*) \) can be found if we know the local value of the averaged pressure in the channel \( p^*(x^*) \) and hence the corresponding local size of the bubble and the shift of the meniscus into the cavity.

To make the problem formulation more specific, we assume that the masses of all bubbles are identical, and at the channel outlet (at the atmospheric pressure) the bubble occupies the entire cavity, i.e. the shift of the meniscus is zero. The radius of curvature of the meniscus \( R^* \) is determined by the known properties of the fluid and the wall, i.e. the angle of wettability. Then, at any \( x^* \), the dimensional shift of the meniscus \( \delta \) can be found from the mass conservation condition for the gas trapped in the cavity. The equation of state for perfect gas in the bubble reads: \( p_g^*V_g = m_gRT \), where \( V_g \) is the bubble volume, \( p_g^* \) is the pressure in the bubble, \( R \) is the gas constant, and \( T \) is the temperature. For given bubble curvature radius \( R^* \) and zero shift of the meniscus, the mass of the gas trapped in the cavity is found from the condition \( p_g^* = p_a^* \) at the microchannel outlet. If we know the pressure distribution \( p^*(x^*) \) in the microchannel, using the equation of state and the relation between the pressure in the fluid and in the gas on the phase interface \( p^* - p_g^* = \sigma/R^* \) (where \( \sigma \) is the surface tension), valid at a good accuracy for Stokes flow regime, we can find the shift \( \delta(x^*) \) of the meniscus into the cavity located at any
point $x^*$. Then, from the solution of the microscale problem of Stokes flow over the microcavity located at the point $x^*$, with the given meniscus shift $\delta(x^*)$, we can calculate the local value of the velocity slip length $b^*(x^*)$. By performing this procedure for sufficient number of points $x^*$, we can find the dependence $b^*(p^*)$ on the macroscale.

We will reformulate the problem in dimensionless form. In nondimensionalization, the scales for longitudinal and transverse coordinates are: $l$ and $L$; for pressure: $p^*_{\text{a}}$; and for velocity: $U = Q^*/H$. In dimensionless form, the solution of the macroscale problem reads:

$$
\frac{dp}{dx} = -\frac{12lQ^*\mu}{H^3 p^*_{\text{a}}}
\left(1 + \frac{3b(x)}{H/L + b(x)}\right)^{-1}, \quad p(1) = 1; \quad b(x) = b^*(x^*/l)/L
$$

(1)

3. Stokes problem of viscous fluid flow on the scale of a chosen microcavity

At each value $x^*$, on the microscale there is a rectangular microcavity containing a gas bubble. On the scale of this microcavity, we should solve the problem of 2D Stokes flow over the cavity with the given position of the bubble surface in it. In the Stokes flow regime, when the pressure variation along the phase interface due to the fluid motion is small, the shape of the gas bubble surface, as in statics, can be approximated by a segment of a circle arc. As mentioned above, the radius of the arc is determined by the static angle of wettability at the pinning points of the meniscus. In dimensionless form (here, the length scale is $L$), the equations of fluid motion over a single cavity can be written as follows:

$$
\triangle u = \nabla p, \quad \nabla \cdot u = 0
$$

Here, $u$ is the two-dimensional fluid velocity field and $p$ is the pressure distribution on the microscale $L$. We should specify the boundary conditions at all points of the 2D flow domain boundary containing the curved phase interface shifted into the cavity. On the solid walls, the no-slip condition for the velocity is valid; and on the bubble surface, the kinematic (no-flow) condition and the dynamic condition of zero shear stress are specified. On the inlet and outlet boundaries of the calculation domain, we specify the parabolic velocity profiles. Such velocity profiles satisfies the condition of periodicity for small and moderate values of the gas fraction $d/L$ (see [9]). The formulated mathematical problem of fluid motion over a single rectangular cavity containing a curved phase interface is solved by the Boundary Element Method (BEM). According to the BEM, the original Stokes equations in the domain with a complex boundary are replaced by the equivalent system of boundary integral equations [10]. An original numerical procedure based on the BEM was developed to solve the boundary integral equations by the collocation method. Some aspects of the numerical procedure developed for the similar problem can be found in [9]. As the result of the numerical solution, we calculate the value of $b$ for given channel thickness $H/L$, gas fraction $d/L$, curvature radius $R = R^*/L$, and meniscus position $s = \delta/L$ from the averaged Navier slip boundary condition [9]. For simplicity, below we present the results for $H/L \sim 1$ and $R/c = 8$ (in our notations, $c$ is the half-width of the cavity). This set of parameters provides the maximal value of the averaged slip length for pressure-driven flow with bottom striped SHS [9].

4. Matching the solutions on the macro- and microscales

We develop the following procedure of matching the solutions on both scales. At the first step, for given flow rate $Q^*$, length $l$, and thickness $H$ of the microchannel, we estimate the maximal possible pressure difference in the channel. For this purpose, we set $b(x) = 0$ and calculate the pressure gradient and find the linear pressure distribution along the channel. At the second step, for sufficiently large number of points from this interval of pressure variation, we solve the corresponding microscale problems (with the corresponding values of the meniscus shift into the
cavity \( s(p) \)) and calculate the function \( b(p) \). Finally, at the third step we integrate numerically the differential equation

\[
\frac{db}{dx} = -\frac{db}{dp} \frac{12lQ^*\mu}{H^3 p_a} \left(1 + \frac{3b}{H/L + b} \right)^{-1}, \quad b(1) = b_{max}
\]

and find the function \( b(x) \). Here, \( b_{max} \) is the value of the effective slip length corresponding to the case when the meniscus is pinned at the cavity corners. From Eq. (1), we find the pressure distribution \( p(x) \).

As a result of this procedure, we obtain \( b(x), p(x), \) and \( s(x) \) in the microchannel. Then, by calculating the pressure at the inlet of the microchannel we find the decrease in the pressure drop, associated with the variation of \( b \) along the microchannel. Some numerical results are presented below.

We selected the following values of the dimensional parameters of the problem (see, Table 1) and consider the striped texture of SHS with \( d/L = 0.8 \) and almost flat phase interface \( R/c = 8 \). For this values of the parameters, we performed calculations of \( p(x), b(p,V_c,H/L,d/L,R/c) \) and \( s(p) \) using the model developed.

Table 1. Characteristic dimensional parameters of the problem.

| \([l]\) cm | \([Q]\) cm²/s | \([U]\) cm/s | \([H]\) µm | \([L]\) µm | \([H_c]\) µm | \([T]\) K |
|---|---|---|---|---|---|---|
| 1.6 | 0.1 | 50 | 20 | 40 | 20 | 293 |
| 1.6 | 0.2 | 50 | 40 | 40 | 20 | 293 |

In figure 2 (a, b), we present the distribution of the pressure \( p(x) \) along the channel for three different cases: linear distribution in the channel with both rigid walls and no-slip condition (— — —), non-linear distribution in the channel with bottom striped SHS wall and varying slip length (——), and linear distribution in the channel with the maximal constant effective slip length corresponding to the meniscus pinned at the cavity corners (- - - -). In figure 2 (c, d), we show the calculated \( b(p) \) and \( s(p) \) for the selected values of the parameters.

As follows from the plots, the bottom SHS results in the decrease of the pressure drop \( p(1) - p(0) \), as compared to the case of the no-slip boundary condition on the channel walls. For the selected values of parameters, the decrease in the pressure drop amounts to 20%. It seems that the maximal decrease in the pressure drop can be attained when \( H/L \) is of the same order as the maximal value of the averaged slip length. From the parametric numerical study, it was found that, for fixed \( H/L, d/L, \) and \( R/c, \) as the depth of the rectangular cavity \( H_c \) or its volume \( V_c \) decreases, the pressure distribution in the channel tends to the curve shown by line (- - - -) in figure 2 (a, b). In this situation, the phase interface is close to the cavity corners and the value of the averaged slip length is almost maximal.

5. Conclusion
The combined solution of (i) macroscale problem of viscous-fluid flow in a channel with a superhydrophobic bottom wall and (ii) microscale problems of Stokes flow over microcavities with gas bubbles made it possible to estimate the variation of the bubble surface shift along the channel length and the corresponding variation of local slip properties of the superhydrophobic surface. The calculations performed for typical microchannel parameters showed that the effect considered may result in a two-fold reduction in the pressure drop, as compared to the case of a superhydrophobic wall with uniform slip properties. The model developed can be used for
Figure 2. Pressure distribution in a channel (a, b); effective slip length $b$ (—I—) and shift of the meniscus $s$ into the cavity (- - - -), (c, d)

optimal design of striped SHS and for estimating the pressure drop reduction in a microchannel with superhydrophobic walls.

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