The numerical study of the fluid flow along a superhydrophobic textured surface

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Abstract. A superhydrophobic phenomenon during fluids flow through microchannel due to the presence of the textures on the walls of the channels was considered. A numerical study of fluids flow and mixing in the microchannel at different Reynolds numbers and average roughness sizes has been carried out. The shift in the critical Reynolds number of the transition from the vortex symmetric flow regime to the vortex asymmetric (engulfment) regime towards lower values in the T-shaped microchannels with textured walls was found. The substantially unsteady structures in the straight microchannels with textured walls at Reynolds numbers of about 1000 were obtained.

1. Introduction

Energy efficiency and energy saving are becoming very important in various fields of science nowadays. The miniaturization of devices and technological processes is actively promoted in various fields of science and technology, e.g., the aerospace industry, transport, and energy. In this regard, as well as the rapid development of electronics and medicine, there is a significant increase in interest in capillary hydrodynamics in microsystems. As the micro- and nanotechnologies are developed and introduced into various branches of human activity (electronics, chemical, biological, and food industries), the problems concerning the fluid flow in micro- and nanochannels appear more and more often. Microchannels (the channels with a characteristic hydraulic diameter of about 100 microns) are now very widespread in various applications. They are used for the transport of nanoparticles, bacteria, DNA molecules, cooling microelectronic devices, as chemical reactors for microscopic quantities of matter, and much more. However, the main advantage of microsystem technology, which consists in its miniature size, at the same time, is its main disadvantage, since as the average characteristic size of the channel decreases, the energy costs for pumping fluids through such channels significantly increase too due to a significant increase in the channel hydraulic resistance. Therefore, for example, the water flow velocity in a microchannel with an average hydraulic diameter of 100 μm at a Reynolds number equal to one will be equal to 10 m/s, while the pressure drop in the channel of such a transverse dimension and 10 cm long will be about 6.32 atm.

One of the possible solutions to this problem is to use the phenomenon of velocity slip on the wall, which consists in the fact that, due to certain surface properties, the fluid velocity at the walls becomes nonzero. Such surface properties can be hydrophobicity of the surface, the presence of gas in the cavities of superhydrophobic surface textures, surface charge, a combination of these effects, etc. The superhydrophobic surfaces have a rather complex relief that differs from the plane. They can stabilize
the gas phase bubbles inside the cavities of this relief. When using such surfaces, the fluid moves most of its way over the gas phase rather than over a solid surface of the wall. At the liquid-gas interface the friction is very small, which leads to a sharp increase in the slip length at such surfaces, and, as a result, the hydraulic resistance of such a channel is significantly reduced. Usually, superhydrophobic surfaces are fabricated using special texturing techniques.

One of the interesting research directions is studying surfaces with deposited microtextured layers with extremely high or extremely low wettability and further control of the wettability of these nanostructures. It is well known that wettability is controlled by both the chemical composition and the morphology of a solid surface. High wettability corresponds to a surface condition where the contact angle formed by a drop of liquid on a given solid surface (wetting angle) is less than 90°. This condition is called hydrophilic. At the same time, the wettability of the material, as well as its ability to repel water or retain the droplet due to its strong adhesion to the surface of a solid, play a decisive role in micro- and nanoelectronics technologies, such as immersion lithography, dip-coating and ink-jet printing [1]. If the contact angle exceeds 90°, then the surface of the solid is called hydrophobic, and the water on such a surface forms drops. In recent years, it has become possible to fabricate microtextured materials with contact angles of about 120° and 150°, which were called highly hydrophobic and superhydrophobic, respectively. They are characterized by the effects of self-cleaning, water repellent, anti-icing, and anti-fogging, and can be used in many types of electronic and optical devices [2].

Also, various microfluidic devices, such as the micro-scale thermophysical devices, biological microelectromechanical systems (bio-MEMS), and lab-on-chip [3–5] using superhydrophobic properties, are still being developed. Certainly, the ever-growing need for such materials and devices based on such materials has generated an ever-increasing interest in this topic in the scientific community. In the next few years, a more significant increase in interest is expected, which, therefore, is extremely relevant. Therefore, in recent years, great interest has been shown in the study of highly and superhydrophobic microtextured surfaces, as well as in the development of methods for their manufacture [1–11]. Two approximations in the state of a droplet are used to describe theoretically the contact of a liquid droplet with a microstructured solid surface: the Wenzel state and the Cassie–Baxter state. If water penetrates the voids of microtexture and fills them, then Wenzel’s state takes place [10]. If a drop of liquid comes into contact only with a small part of the surface of a solid, and wetting occurs involving atmospheric air trapped by irregularities of the surface, then the Cassi-Baxter state takes place.

Since superhydrophobic microtextured surfaces are widespread in nature, the effects they cause are called by analogy with natural objects. For example, the “lotus leaf effect” corresponds to a situation where the water drops slide or easily glide over a superhydrophobic solid surface [6]. If well-formed drops are firmly held on a vertical surface or can even be suspended from below a solid surface, then this effect of superhydrophobicity is called “rose petal effect” [7–9]. With the “rose petal effect”, the droplets are pinned or stuck to the surface [8, 11].

In the present paper, a numerical simulation of the fluid flow in a microchannel with structured textures on the wall has been carried out, moreover both with and without taking into account the presence of a two-phase region, when the micro-object was initially empty (filled with air) and then filled with fluid.

2. The computational domain
The paper considers the flow of a single-phase flow moving along a T-microchannel with textured walls, which has two inlets and one outlet. Such a T-shaped microchannel can be characterized by the ratio of channel height/inlet channel width/mixing channel width in a proportion of 1/1/2. The texture height on the channel walls was constant and equal to 100 nm. The texture refers to cones of 100 nm high that are regularly applied to the surface of the channel walls. After a literature review and preliminary studies, it was found that the effect of channel wall textures on the flow of a single-phase fluid is provided when the average roughness size is more than 5% of the characteristic size of the
microchannel. So, the maximum values of the cross-section of the mixing channel were taken equal to 1×2 μm. Geometries and grids of T-shaped microchannels with roughnesses of 5 and 10% of the characteristic size of the mixing channel were constructed. Due to a large number of small cones, the number of cells (polyhedral) in these grids was about 20 million. Besides, the fluid flow in a microchannel with a textured wall was considered taking into account the presence of a two-phase flow, for example, when the micro-object was initially empty (filled with air), and then was filled with fluid. The relative roughness sizes were also equal to 5 and 10%.

3. The mathematical model

The computational fluid dynamics methods based on the numerical solution of the spatial and unsteady Navier-Stokes equations, supplemented by the equations of the energy conservation, transport, and components diffusion are used as a basic theoretical approach when solving the posed problems. At present, there are many techniques for describing micro-flows, however, the hydrodynamic method deserves the most attention. Numerous experiments confirm the validity of such an approach for liquids with no-slip boundary conditions on the walls for channel sizes of the order of 1 μm, and with slip boundary conditions for even smaller channels [12-14]. The difference analog of convective-diffusion equations is found using the finite volume method for structured multiblock grids. The resulting scheme is automatically conservative in this case. The essence of the method consists in dividing the computational domain into control volumes and integrating the initial conservation equations for each control volume to obtain finite-difference relations. The convective terms of the transport equations are approximated using second-order upwind QUICK and TVD schemes, respectively. An implicit second-order scheme is used to approximate unsteady terms of the hydrodynamic equations. Diffusion fluxes and source terms are approximated by finite-volume analogs of central-difference relations with the second order of accuracy. The relations between the velocity and pressure fields, ensuring the continuity equation, are implemented using SIMPLEC procedures on combined grids. The Rhi-Chou approach, which consists in implementing a monotonizer into the equations for pressure correction is used to eliminate the oscillations of the pressure field. Difference equations obtained as a result of the discretization of the original system of differential equations are solved by an iterative method using an algebraic multigrid solver.

To simulate two-phase liquid-gas interactions in microchannels with a textured wall surface a numerical method called «volume of fluid» (VOF) was used [15]. The essence of such a method is that fluids are considered as a single two-component medium and the spatial distribution of phases within the computational domain is determined using a special marker function that specifies the volume fraction of the liquid phase in the computational cell. Special attention should be paid to the phenomenon of surface tension while calculating the flow of two-component flows of immiscible fluids. For its simulation within the VOF method, the CSF algorithm was used, which implies the introduction of an additional force into the motion equation, which is determined on the surface of the fluid through the gradients of the volume fraction of fluid in the computational cell.

4. The simulation results

Numerical studies of the effect of structured textures on the channel wall were conducted. Calculations of mixing two liquids of the same properties in a T-shaped microchannel with roughness sizes of 5 and 10% at Reynolds numbers of 200, 150, 145, 144, 143, 142, 141, 140, and 120 were carried out. Water and tinted water with the same properties, namely, viscosity (1 mPa·s), density (1000 kg/m³), the diffusion coefficient of paint, which was considered as a passive scalar and did not change the flows of miscible liquids (2.63·10⁻¹⁰ m²/s), were used as working fluids. The Reynolds number was determined by the equivalent diameter of the mixing channel and the flow rate in it. It was found that the presence of the channel textures walls leads to a shift in the critical Reynolds number corresponding to the transition from the vortex symmetric flow regime to the vortex asymmetric (engulfment) regime towards lower values. As was shown in many papers [16–20], for a similar (1/1/2) configuration of a smooth micromixer, the critical Reynolds number was 145. Besides, a correlation was proposed in
[19] to determine the critical Reynolds number depending on geometric dimensions of the mixing channel, according to which, as the width of the mixing channel decreases at its constant height the critical Reynolds number shifts towards the region of large values. It would be logical to assume that textures reduce the width of the mixing channel, thereby causing a shift in the values of the critical Reynolds number, however, as mentioned above, if there are textures on the channel wall, the critical Reynolds number shifts towards a region of lower values. Thus, the presence of textures causes such a shift in the values of the critical Reynolds number due to other mechanisms than just a change in the size of the mixing channel. Fig. 1 shows the concentration profiles of two liquids for Reynolds numbers 200, 150, 145, and 120 in the central longitudinal section of the channel and at the outlet of the mixing channel.

![Concentration profiles of two fluids](image)

**Figure 1.** Concentration profiles of two fluids in the central longitudinal section of the channel and at the outlet of the mixing channel for different Reynolds numbers: a) 200; b) 150; c) 145; d) 120

Besides, a numerical simulation of the fluid flow in a microchannel with structured textures on the wall was carried out, taking into account the presence of a two-phase flow, for example, when the micro object was initially empty (filled with air) and then was filled with fluid. In this case, the retention of air bubbles between conical textures due to capillary effects is quite possible. The fluid will glide over the surface of the air cavities held by these textures. The relative roughness sizes were also equal to 5 and 10%. Reynolds numbers ranged from 1 to 1000. The simulation results in the form of a profile of fluid concentrations for Reynolds numbers 100 and 1000 are presented in Fig. 2. As a result of studies, it was found that when the fluid flows through such channels, the air remains held in the textures cavities. For Reynolds numbers within the range of 1-100, there are practically no differences. When the Reynolds number is 1000, part of the air is carried away by the fluid flow, a flow with a complex structure arises, part of the fluid falls into the region between the roughnesses, and as a result, the friction factor on the wall increases (see Fig. 2b). Such structures are substantially unsteady and require detailed grids in the region of the media interface and high-performance computing. Investigations of the influence of the relative sizes of roughnesses and Reynolds numbers on the slip lengths of the fluid velocity over the surface of the air phase, the pressure drop in the channel, as well as the velocity and pressure profiles in the channel, will be carried out in future.
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Conclusions
A superhydrophobic phenomenon during the fluid flow through microchannel due to the presence of the textures on the walls of the channels was considered. It was found as a result of literature review, that, in recent years, great interest has been shown in the study of highly and superhydrophobic microtextured surfaces, therefore, such investigations is extremely relevant. The geometries and grids of T-shaped microchannels with roughnesses of 5 and 10% of the characteristic size of the mixing channel were constructed. The number of cells (polyhedral) in these grids was about 20 million due to a large number of small cones. The fluid flow in a straight microchannel with the textured wall was considered taking into account the presence of a two-phase flow, for example, when the micro-object was initially empty (filled with air), and then was filling with fluid. The relative roughness sizes were also equal to 5 and 10%. It was found that the presence of the channel textures walls leads to a shift in the critical Reynolds number corresponding to the transition from the vortex symmetric flow regime to the vortex asymmetric (engulfment) regime towards lower values in T-shaped microchannels. Besides, the presence of textures causes such a shift in the values of the critical Reynolds number due to other mechanisms than just a change in the size of the mixing channel. Besides, it was found that during the fluid flows through the straight microchannels with capillary held air in the wall textures, the air remains held in the textures cavities. For Reynolds numbers within the range of 1-100, there were practically no differences, and the interface of the media remained almost flat. On the other hand, when the Reynolds number was 1000, part of the air was carried away by the fluid flow, a flow with a complex structure arise, part of the fluid falls into the region between the roughnesses, and as a result, the friction factor on the wall increases. Future studies will be focused on the effect of the relative sizes of roughnesses and Reynolds numbers on the slip lengths of the fluid velocity over the surface of the air phase, the pressure drop in the channel, as well as the velocity and pressure profiles in the channel.

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