Viscous fluid flow in a microchannel with hydrodynamic traps

O A Solnyshkina and N B Fatkullina
Center for Micro and Nanoscale Dynamics of Dispersed Systems, Bashkir State University, Ufa, Russia
E-mail: olgasolnyshkina@gmail.com

Abstract. Simulation of creeping flows in complex three-dimensional domains is crucial for microfluidics applications, creating multipurpose microfluidic devices, which are used, for example, to study multistage chemical reactions and as analytical devices in medicine. In this work we study the features of the incompressible viscous fluid flow in a flat microchannel with a nontrivial internal structure (the hydrodynamic traps of various configurations) under the constant pressure drop. The three-dimensional boundary element method, improved by utilization high-efficient fast multipole method and heterogeneous computational workstation, was used in numerical simulation. We studied the flow pattern around C-shaped hydrodynamic traps distributed in a flat microchannel and consisting of five cylindrical elements of the same size. Such geometry is widely used in microfluidic devices for fixing particles in the flow, for example, biological objects during tests in medicine. The influence of the distance between the rows of traps on the flow pattern and distribution of the longitudinal and transverse components of the flow velocity was considered.

1. Motivation

Recent developments in microelectronics, genetic engineering, production of micromechanical devices have led to the creation of a scientific direction called "microfluidics" aimed at studying the behavior of liquid systems on a microscopic scale (from 1 µm to 100 µm). Nowadays, the application of new effective technologies based on fundamental research in the field of microfluidics is an urgent problem in many fields of science and industry. Three-dimensional modeling of Stokes flows of a viscous fluid in microchannels with hydrodynamic traps is important for microfluidics. For example, for choosing more suitable geometry parameters in the manufacturing of Lab-on-a-Chip devices actively used in biochemistry, and pharmacology to study multi-stage biochemical processes, where one of the controlling mechanisms is the mixing of reagents. Microfluidic devices (MFD) are also widely employed in biophysics and medicine to control the movement of micro-particles and, for example, to separate and sort them by size, density, and elasticity. The main advantage of such systems is the small amounts of reagents or samples required for reactions and analytical processes. The integration of special functional elements into MFD enables the creation of new analytical systems, platforms, and instruments with unique technical and operational characteristics for biological sample analysis. Thus, one of the critical tasks in this area is the selection of optimal parameters for the design of different types of MFD for the study of biological objects and particle sorting (separation), particle fixation, cultivation of biological objects (cells, bacteria), sample preparation and processing. The influence of the structure geometry in microchannels is being actively studied both from experimental and theoretical points of view.
The paper [1] provides a review of the methods for sorting cells/particles by using hydrodynamic effects in microchannels. Details of the fundamental hydrodynamic mechanisms that cause cross-migration of objects in shear and vortex flows are considered. Also, in [2] the review of the experimental study of trapping particles and cells in microfluidic devices is represented. Different technical features of MFD are considered.

Mechanical and hydrodynamic traps are used in the channel of the microfluidic chip to capture the objects. The main idea of such traps is the stable fixing or holding of a particle in a specific region of the microfluidic chip due to the fluid flow. Currently, many different types and configurations of hydrodynamic traps are known. Several authors have proposed the construction of a two-layer microfluidic platform for capturing single cells using U-shaped hydrodynamic traps, which allow fluid to flow into the lower layer, where the particles are trapped [3]. The microparticles are fixed when the fluid flows through channels whose width is less than the characteristic sizes of the particles. A U-shaped hydrodynamic trap is presented in the form of a cell with nanoscale channels, and two microchannels on either side, the width of which exceeds the characteristic particle size.

Trapezoidal traps, consisting of several elements with narrow channels between them, are also used. The paper [4] presents an experimental and numerical study of the particle dynamics and hydrodynamic flows in MFD with this type of traps. The two-dimensional finite element method is used as a numerical method due to the high computational complexity of three-dimensional modeling.

One of the methods for fixing microparticles is the use of hydrodynamic traps, in which immobilization is achieved due to the pressure of the incoming flow in one direction and the reaction of the microstructure in another. An important role is played by ensuring both the capture of particles in the traps and the possibility of their removal to prevent clogging of the device. There are also C- or Π-shaped traps. The first is a vertical hollow half-cylinder. The second is a box with a vertical rectangular cavity. In all types, there are two narrow channels in the traps to reduce hydrodynamic drag.

Among the numerical methods of three-dimensional modeling of continuum mechanics problems, the finite-difference methods, finite element method, finite volume method (FVM), and boundary element method (BEM) [5] are the most popular. These approaches differ in the way of the computational domain representation and the mathematical basis. The first method is based on the implementation of the differential operator of the initial differential equation, it does not require any complicated mathematical calculations, as compared with the BEM, and discretize all considered domain by uniform mesh. In the second approach, the computational domain is divided into a number of subdomains, called finite elements. Since the finite elements can be of different shapes and sizes, it allows the better boundary approximation and discretization of the domains with the flow features. The computational part is based on the minimization of the functional variational problem on the set of functions defined on each particular subdomain. Despite several advantages, the control volume method also requires the sampling of all considerable domain (which is quite expensive for the three-dimensional modeling). It describes the boundaries of the objects less accurate than the BEM.

Low Reynolds number flows, which can be described by simplified Navier-Stokes or Stokes equations typical of microfluidics. The specifics of the Stokes equations is that they are linear and can be solved using the BEM. It is interesting to note that most analytical and numerical studies of Stokes flow of single-phase liquids or emulsions are dedicated to plane and axisymmetric channels. One reason for that is that the mesh of channel surface for the solution of three-dimensional problems even for relatively simple shapes should be large enough (tens of thousands boundary elements), and such problems were not efficiently solvable about 20 years ago. The current emerging techniques based on algorithmic and hardware accelerations are capable of handling such flows.

Despite the significant interest in the use of microfluidic devices, there are a very limited number of comprehensive studies of single-phase and multiphase flows in similar domains, including laboratory experiments and three-dimensional direct numerical simulation, especially based on the boundary element method. The present work is dedicated to the numerical simulation of hydrodynamic flows around the C-shaped traps distributed in a flat microchannel using an effective
numerical approach based on the 3D boundary element method accelerated heterogeneous fast multipole method. The main goal of this part of the research is to select the optimal parameters of the trap distribution for further conduction of the numerical and laboratory experiments to study the particle fixation in multiphase flows.

2. Problem statement and numerical approach

In this paper, we consider the features of hydrodynamic flows around traps inside a flat microchannel with a rectangular cross-section that arises when the viscous incompressible fluid flows under the constant pressure drop. All processes were considered at small Reynolds numbers (Re < 1) and under isothermal conditions. Such flows are governed by steady Stokes equations. The non-slip condition is specified on the surface of all fixed elements. A high-quality triangulation of micro-structures with flat smooth walls of complex geometry, including hydrodynamic traps of various configurations, has been developed (Figure 1).

Figure 1. Schematic representation of the considered domain in y = 0 plane.

In this work the boundary element method was chosen as a numerical basis of the approach. Despite the advantages of using the BEM for solving three-dimensional problems, the utilization of the conventional BEM is very limited by the size of the considered problem. It is due to the time, and memory costs of the BEM that has the $O(N^3)$ complexity.

Achievements in computing practice and the emergence of new methods of calculations based on studies of large systems consisting of millions or billions of discrete components would be impossible if they only depend on the hardware. However, new needs generate new approaches to the solution of such problems. Thus, the development and improvement of scalable algorithms and effective methods with low computational complexity and low memory cost represent an integral part of computing progress.

Fast multipole method was developed by Greengard and Rokhlin and was first introduced in 1987. It was initially formulated for the summation of gravitational and electrostatic potentials (Green function for the Laplace equation) in two and three dimensions. High-quality interpolation, differentiation and integration of one-dimensional functions defined values at non-uniformly distributed points, which are necessary for the successful implementation of many of the numerical methods, were natural problems to solve with the help of the FMM. So FMM method has been used successfully to speed up calculations in the numerical solution of the Laplace equation, Helmholtz, Stokes, Maxwell, gravitational and electrostatic interactions, and other equations of mathematical physics, as well as to accelerate a variety of methods, which is necessary to calculate the matrix-vector product with matrices of a particular type. Furthermore, the multilevel FMM is effective for the problems with highly non-uniform distribution of mesh nodes.
For higher performance, it is necessary to develop algorithms designed to use high-performance hardware, such as hybrid computing workstations, consisting of central and graphics processors (CPU and the GPU, respectively), or clusters. Nowadays, most of all, the scientific and applied fields in the world begin to use computer systems based on multi-core CPUs and specialized accelerators, such as graphics processors (GPU) and many core systems. The efficient utilization of such systems requires the development of high-performance algorithms. In terms of hardware acceleration the FMM is a very attractive algorithm as it can be efficiently parallelized.

For direct calculations of viscous fluid flow in nontrivial domains with high surface discretization in this study, the boundary element method was accelerated using a scalable algorithm (fast multipole method) implemented on heterogeneous computing architectures (multicore CPUs and GPUs). The details of numerical implementation can be found in [6]. The same approach with appropriate modifications was applied in our previous works for simulation of periodic channel flow, emulsion flow in different geometry, and bubble dynamic in potential flow.

3. Results and discussion

We simulate the flow of incompressible viscous liquid in the channel with the array of hydrodynamic C-shaped traps under constant pressure drop. Such trap geometry is typical for microfluidic devices used for fixing different particles in a flow. The MFD Reynolds number is defined by formula [3]

\[ \text{Re} = \frac{2 \rho Q}{\mu (w + h)} \]

where \( \rho \) is the density and \( \mu \) is the viscosity of the liquid, \( Q \) is the volume flow rate, \( w \) and \( h \) are the width and the height of the channel. Calculations were carried out for C-shaped hydrodynamic traps. Such a trap consists of five cylindrical elements with equal radii \( R \). The width of each trap is \( L_{\text{trap},x} = 9 \cdot R \), the length of each trap is \( L_{\text{trap},z} = 6.25 \cdot R \), and the height of the trap is \( L_{\text{trap},y} = 10 \cdot R \). The configuration with five rows of traps is shown in Figure 1 with the overall number of triangular elements \( N_\Delta = 367800 \). Each subsequent row contains one more trap, and they are staggered to increase the effectiveness of the particle capturing. A similar triangular arrangement of the C-shaped trap rows was used in a microfluidic device in [7] for trapping cells.

Figure 2. Simulation results for longitudinal (left column) and transverse velocity components, streamlines in \( y = 0 \) plane and distribution histogram for the modulus of the velocity vector.
The simulations were conducted for the different distance between the rows in $x$ direction $dx = 0$, $dx = 0.5 \cdot L_{trap \_x}$, $dx = 1 \cdot L_{trap \_x}$, $dx = 1.5 \cdot L_{trap \_x}$, $dx = 2 \cdot L_{trap \_x}$, $dx = 2.5 \cdot L_{trap \_x}$, but for the constant distance between the traps in $z$-direction $dz = 10 \cdot R$. In all cases constant equal pressure was set at the channel inlet, the resulting $Re$ was varied from 0.4 to 0.7. One of the considered configurations for $dx = 0.5 \cdot L_{trap \_x}$ is represented in Figure 1. As it is seen from Figure 1, there are narrow channels between the cylindrical elements in each trap. This design is proposed to solve the problem of reducing the hydrodynamic resistance in the microfluidic device.

![Figures 3 and 4 showing simulation results and streamlines.](image)

**Figure 3.** Simulation results for longitudinal (left column) and transverse velocity components, streamlines in $y = 0$ plane and distribution histogram for the modulus of the velocity vector.

**Figure 4.** Streamlines and field of the modulus of the velocity vector in plane $yOz$, $dx = 1 \cdot L_{trap \_x}$. 

In this work, we study the influence of the distance between the trap rows on the flow pattern and distribution of the longitudinal and transverse flow velocity components. The results for all considered $dx$ are represented in Figure 2 and Figure 3. One can see that $U_s$ and $U_z$ fields are significantly changed while the distance increases. It can be assumed that most of the particles in the flow will be trapped by traps located on the sides in the last row in case of a minimum distance $dx$. Such an effect will lead to a significant increase in the hydrodynamic resistance in this area of the device and reduce its effectiveness. The redistribution of the longitudinal and transverse components of the velocity of the carrier fluid will have a significant effect on the particle dynamics in microfluidic devices with similar configuration. The distribution histogram of the velocity vector modulus for all cases is considered (Figure 2, 3). Starting from distance $dx = 1 \cdot L_{trap} \cdot s$, the pattern of the velocity distribution does not change significantly, but only velocity component values increase. With increasing $dx$ the hydrodynamic resistance of the considered area decreases, so the velocity value between the traps increases. It can also be assumed that starting from $dx = 1 \cdot L_{trap} \cdot s$, a more uniform distribution of particles in the traps can be obtained. Furthermore, the values $dx = 1 \cdot L_{trap} \cdot s$ and $dx = 1.5 \cdot L_{trap} \cdot s$ are also suitable for the optimal length of the region with traps rows. It allows placing several similar configurations in the channel with some period. Thus, more effective fixing of the target particles in the flow can be carried out. Then we considered the flow pattern of the velocity between the rows of the traps (Figure 4) in case $dx = 1 \cdot L_{trap} \cdot s$ in plane $yOz$. The calculation results show the separation of the main flow with an increase in the number of traps in each subsequent row.

Conclusions
In the present work, the software developed in Matlab based on the accelerated BEM for the Stokes equations are used. All calculations are performed on the workstation equipped with a graphics card and using CPU/GPU parallelism, which allows one direct 3D simulation of a viscous fluid flow in a flat channel with C-shaped hydrodynamic traps, whose surface is covered by a mesh with tens of thousands of triangular elements in a reasonable time. The features of changing the velocity component distribution inside the channel with the trap array are studied for the different distances between trap rows. It is shown that the proposed approach allows three-dimensional studying of the hydrodynamic flow in the domains corresponding to the geometry of parts of microfluidic devices. It was utilized to select the optimal parameters for the trap row configuration that will be used in the further simulation of the motion of various types of particles in the flow. The results of the detailed studies of hydrodynamic flows in such complex domains can be used in the process of design microfluidic devices for separating or fixing particles in a flow.

Aknowledgements
The reported study was funded by the grant of the President of the Russian Federation MK-549.2019.1.FMM library is provided by Fantalgo, LLC (Maryland, USA).

References
[1] Karimi A, Yazdi S, Ardekan A M 2013 Biomicrofluidics 7(021501) 24
[2] Nilsson J, Evander M, Hammarström B, Laurell T 2009 Analytica chimica acta 649 141–57
[3] Chen H, Sun J, Wolvetang E, Cooper-White J 2015 Lab on a Chip 15 1072–83
[4] Xu X, Li Z, Nehorai A 2013 Biomicrofluidics 7(5) 054108
[5] Pozrikidis C 1992 Cambridge (Cambridge University Press) p 259
[6] Abramova (Solnyshkina) O A, Pityuk Y A, Gumerov N A, Akhatov I S 2017 Communications in Computer and Information Science (CCIS) 753 317–30
[7] Kukhtevich I V, Bukatin A S, Mukhin I S, Evstrapov A A 2011 Nauchnoe Priborostroenie 21(3) 17–22