# Three-dimensional simulation of flows in microchannels with deterministic lateral displacement system using the boundary element method

© A.Z. Bulatova, D.M. Tuigunova, O.A. Solnyshkina

Ufa University of Science and Technology, Ufa, Russia
E-mail: dianatgnv@gmail.com

Received May 3, 2024
Revised July 4, 2024
Accepted October 30, 2024

Microfluidic systems with deterministic lateral displacement (DLD) are one of the most effective technologies for particle control in the flow. In this paper, the influence of the geometry features of microchannels with DLD on the hydrodynamic features of fluid flows is investigated. Numerical modelling was performed for the three-dimensional case using the Boundary Element Method, accelerated by the Fast Multipole Method on heterogeneous computing architectures. The effect of the DLD structures shape and row displacement on the velocity distribution in the channel has been studied. Additionally, the variation of the velocity gradient between rows of structures and in the gaps between two neighbouring columns has also been examined.

**Keywords:** deterministic lateral displacement, hydrodynamics, Stokes flows, boundary element method, microfluidic systems.

DOI: 10.61011/TPL.2024.12.60347.6504k

A wide variety of practical applications and promising technological opportunities necessitate the study of flows in microfluidic systems. Such systems are used to control fluid flows, mix reagents, separate particles, and implement other processes at the micro level [1]. In biomedical diagnostics, microfluidic systems may serve as instruments for analysis of biomedical samples of cells, proteins, blood, and other biological fluids. An insight into the specifics of flows in such systems is important for the development of new diagnostic, screening, and therapeutic methods [2]. Microfluidic systems offer a number of advantages. Their size allows for the construction of compact devices and chips, which translates into a reduction in the size of laboratory equipment. Owing to their typical small size, microdevices require a minimum amount of reagents and samples, which makes them very efficient in experiments with expensive reagents or enzymes. Microfluidic devices offer a high spatiotemporal resolution, which is a significant advantage in the study of individual cells. Automation of microfluidic systems simplifies the process of analysis and eliminates the possibility of human errors, and portability allows for multiple functions (separation, micromixing, reacting, and detection) to be combined in a single device [3].

The isolation and sorting of cells from complex heterogeneous mixtures are one of the most important tasks in various fields of biology, biotechnology, and medicine. Several techniques for particle manipulation in microchannels are known at present. They may be divided tentatively into active (utilizing external physical fields) and passive ones [4]. Passive techniques rely on such properties of sorted particles as their size, density, shape, and deformability, as well as on the geometry of a microfluidic device and its hydrodynamic characteristics. One of the best known approaches is deterministic lateral displacement (DLD) [5], which uses a specific order of pillars or posts in a channel to control precisely the trajectory of particles and separate them. Each row in such a channel is shifted by a certain distance from the previous one, forming several flow lines in the gaps between the pillars or posts. These flow lines are separated by stagnation flow lines that begin and end at the pillars or posts (Fig. 1). Depending on their size, particles either move along a specific route in a zig-zag pattern or move to the next flow line each time it passes through an obstacle. However, certain difficulties arise in DLD sorting of deformable particles, since they may be deformed under the action of forces and alter their apparent size. Since the degree of deformation of all deformable particles (macromolecules, droplets, and cells) depends on viscous and inertial forces, the separation efficiency varies with flow velocity [6]. The use of optimized DLD pillars or posts geometries reduces the velocity gradient, prevents clogging of the microfluidic device, and increases the sorting efficiency [7]. Thus, the aim of the present study is to investigate the influence of geometric features of microchannels with deterministic lateral displacement on the parameters of hydrodynamic flows. The work is focused on improving the design characteristics of microfluidic systems for the purpose of enhancing the accuracy and efficiency of particle sorting and separation processes.

We consider the steady periodic flow of a viscous incompressible fluid in a flat microchannel with deterministic lateral displacement of elements of different shapes and displacement of each row relative to the previous one. It is assumed that the flows are sufficiently slow for inertial forces to be insignificant compared to the viscous ones. Thus, the Navier−Stokes equations for an incompressible fluid are reduced to the Stokes equations and may be used to characterize the dynamics of the system under

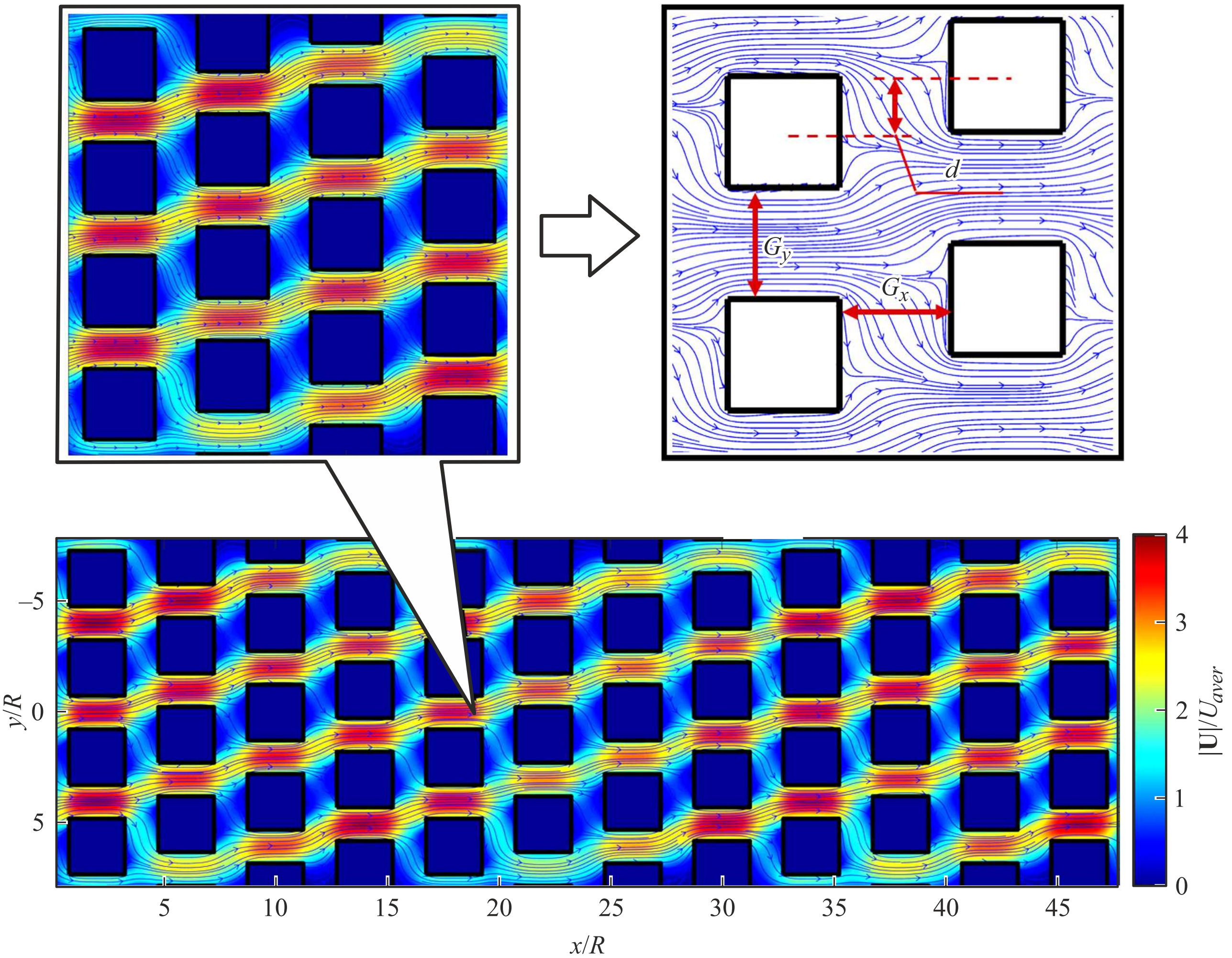


**Figure 1.** Distribution of velocity modulus $|\mathbf{U}|/U_{aver}$ and streamlines in a microchannel with DLD at $d = 10\,\mu$m.

consideration:

$$-\nabla p + \mu \nabla^2 \mathbf{U} = 0, \qquad \nabla \cdot \mathbf{U} = 0, \tag{1}$$

where $\mathbf{U}$ is velocity, $p$ is pressure, and $\mu$ is viscosity. The no-slip condition is set on the lateral surface of the channel and on the surface of non-deformable structures, and the flow periodicity condition is set at the inlet and outlet channel sections:

$$\mathbf{U}|_{x=0} = \mathbf{U}|_{x=L} = \mathbf{U}_S, \qquad \mathbf{f} = \boldsymbol{\sigma} \cdot \mathbf{n},$$

$$\mathbf{f}|_{x=L} = -\mathbf{f}|_{x=0} + \mathbf{f}_p, \qquad \mathbf{f}_p = \mathbf{i}_x \Delta p, \tag{2}$$

where $\boldsymbol{\sigma}$ is the stress tensor; $\mathbf{n}$ is the surface normal; $\Delta p$ is the pressure difference; $\mathbf{f}$ is the stress vector in a fluid; $L$ is the length of a fragment of the computational domain or the periodicity scale in direction $x$; $S$ is the channel inlet section subscript; and $p$ denotes the addition to the stress vector corresponding to a given pressure difference. Modeling was performed with the use of the pre-developed 3D boundary element method accelerated by the fast multipole method on heterogeneous computing architectures [8–10]. The correctness of the chosen mathematical model and numerical approach was verified by comparison with the analytical solution of the problem of a viscous fluid flow in a flat rectangular channel. This comparison was discussed in detail in [10].

The flow in channels with a rectangular cross section and an array of columns with deterministic lateral displacement of elements was considered (Fig. 1). The shape of elements and row displacement $d$ were varied at fixed channel width $W = 160\,\mu$m and height $H = 20\,\mu$m, lateral gap $G_y = 20\,\mu$m between columns, and distance $G_x = 20\,\mu$m between rows. Channel length $L$ depends on the row positioning periodicity along axis $y$ and varied from 160 to 320 $\mu$m. Calculations were performed at $\mathrm{Re} = 0.15$. A constant pressure difference $\Delta p$ within fragment length $L$ was set at the channel inlet.

Figures 2, $a$ and $b$ present the distribution of velocity modulus $|\mathbf{U}|$ values, which were normalized at each calculation point by dividing them by the average velocity in the cross section (plane $yOz$) between rows of elements

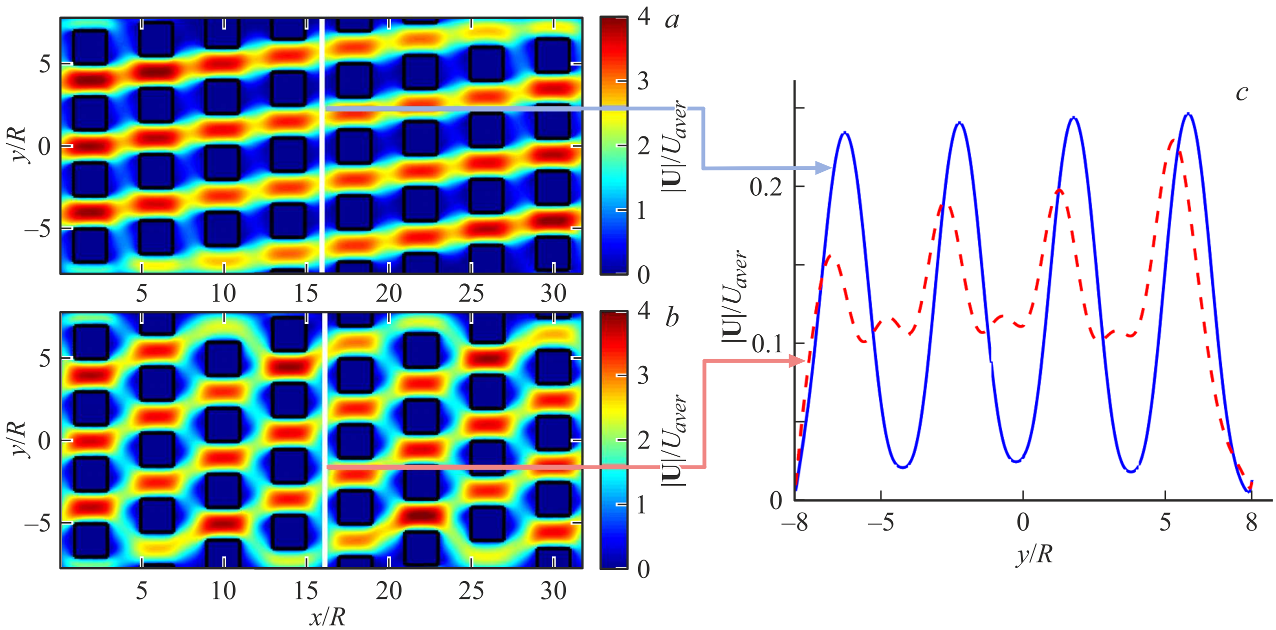


**Figure 2.** Distribution of velocity modulus $|\mathbf{U}|/U_{aver}$ at row displacement $d = 5$ ($a$) and $15\,\mu$m ($b$). $c$ — Velocity profile between the rows.

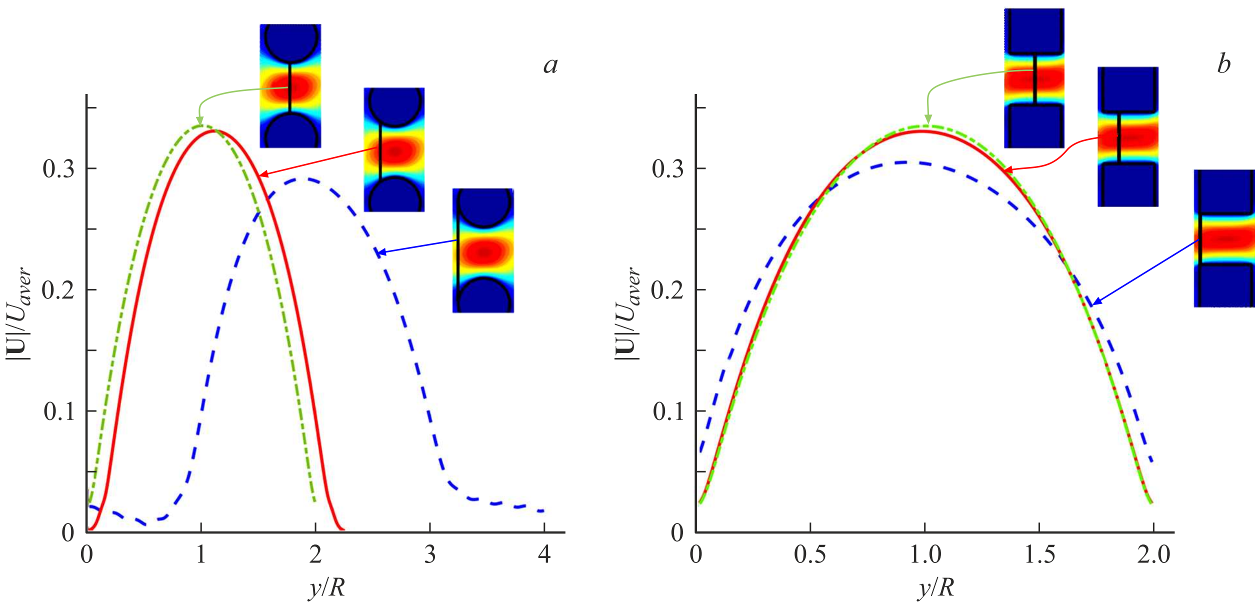


**Figure 3.** $|\mathbf{U}|/U_{aver}$ velocity profiles at different points between two adjacent round ($a$) and square ($b$) pillars or posts.

($U_{aver}$), in channels with square pillars or posts and different row displacements: $d = 5$ and $15\,\mu$m. It is evident that the row displacement has a significant effect on the velocity field in channels. The velocity profile along the $y$ axis between rows of obstacles is uneven and depends significantly on the displacement magnitude (Fig. 2, $c$). A sinusoidal velocity profile with a high amplitude is typical of a microchannel with displacement $d = 5\,\mu$m, while the amplitude of velocity oscillations at displacement $d = 15\,\mu$m is significantly lower. The average difference between maximum and minimum velocities is 90% for the smaller displacement and 48% for the larger one. A microchannel with a strong velocity gradient (with row displacement $d = 5\,\mu$m) may affect strongly the behavior of deformable particles or cells, increasing the probability of their rotation and deformation and eventually altering their trajectory to a significant degree. The study of the velocity field in gaps between DLD structural elements is crucial for practical applications.

Figure 3 shows the velocity profiles formed between a pair of adjacent round and square elements. It can be seen that the flow velocity between columns shapes a parabolic profile. Comparing the presented profiles, one finds that the velocity gradient between round columns is stronger. Specifically, the flow through such shapes is characterized by a 15% change in velocity gradient from the beginning to the middle of the gap. In the case of square structures, the corresponding change is close to 9%. Thus, the non-uniformity of the velocity field between columns may affect significantly the deformation of soft particles or cells, which is an important factor in design of microfluidic devices that utilize the DLD technology.

The characteristics of flow of a viscous incompressible fluid in a microchannel with deterministic lateral displacement of elements of different shape and positioning were investigated. The results revealed that row displacement variations exert a significant influence on the velocity distribution in the channel and the velocity profile between rows. At displacement $d = 5\,\mu$m, the difference between maximum and minimum velocities is 90%; at $d = 15\,\mu$m, this difference drops to 48%. Microchannels with a large row displacement $d$ are better suited for sorting of non-spherical or deformable particles, since they provide a more stable velocity distribution between rows. It was demonstrated that the shape of DLD system elements plays an important role in sorting (especially in studies of soft cells). A comparison of the velocity profiles between a pair of adjacent elements of different shape revealed that the velocity gradient variation from the beginning to the middle of the gap is 15% and approximately 9% for round and square columns, respectively. Thus, the simulation results highlight the importance of careful selection of geometry of elements and their spatial distribution in design of microchannels with DLD. The efficiency of sorting and manipulation of deformable particles, which is especially relevant for biomedical research, may be increased significantly through optimization of the shape and arrangement of elements. For example, a stronger velocity gradient may be used to enhance the separation of hard spherical particles, while a weaker velocity gradient will prevent excessive deformation and damage to soft biological samples. Therefore, a deep understanding of the effect of geometry on sorting opens new opportunities for construction of innovative microfluidic devices.

## Funding

This study was supported by grant No. 24-19-00697 from the Russian Science Foundation (https://rscf.ru/project/24-19-00697/).

## Conflict of interest

The authors declare that they have no conflict of interest.

## References

[1] A.P. Iakovlev, A.S. Erofeev, P.V. Gorelkin, Biosensors, **12** (11), 956 (2022). DOI: 10.3390/bios12110956

[2] O.G. Chavez-Pineda, R. Rodriguez-Moncayo, D.F. Cedillo-Alcantar, P.E. Guevara-Pantoja, J.U. Amador-Hernandez, J.L. Garcia-Cordero, Electrophoresis, **43** (16-17), 1667 (2022). DOI: 10.1002/elps.202200067

[3] A. Wang, A. Abdulla, X. Ding, Proc. Instit. Mech. Eng. H, **233** (7), 683 (2019). DOI: 10.1177/095441191985

[4] M. Sivaramakrishnan, R. Kothandan, D.K. Govindarajan, Y. Meganathan, K. Kandaswamy, Curr. Opin. Biomed. Eng., **13**, 60 (2020). DOI: 10.1016/j.cobme.2019.09.014

[5] J. Zhou, P. Mukherjee, H. Gao, Q. Luan, I. Papautsky, APL Bioeng., **3** (4), 041504 (2019). DOI: 10.1063/1.5120501

[6] A. Hochstetter, R. Vernekar, R.H. Austin, H. Becker, J.P. Beech, D.A. Fedosov, D.W. Inglis, ACS Nano, **14** (9), 10784 (2020). DOI: 10.1021/acsnano.0c05186

[7] A. Zhbanov, Y.S. Lee, S. Yang, Micro and Nano Syst. Lett., **11** (1), 11 (2023). DOI: 10.1186/s40486-023-00175-w

[8] Y.A. Pityuk, O.A. Abramova, N.B. Fatkullina, A.Z. Bulatova, in *Recent research in control engineering and decision making*, ed. by O. Dolinina, A. Brovko, V. Pechenkin, A. Lvov, V. Zhmud, V. Kreinovich. Ser. Studies in Systems Decision and Control (Springer, Cham, 2019), vol. 199, p. 338–352. DOI: 10.1007/978-3-030-12072-6_28

[9] O.A. Abramova, Y.A. Pityuk, N.A. Gumerov, I.S. Akhatov, in *Supercomputing: 4th Russian supercomputing days*, ed. by V. Voevodin, S. Sobolev (Springer, Cham, 2018), vol. 965, p. 427–438. DOI: 10.1007/978-3-030-05807-4_36

[10] O.A. Solnyshkina, N.B. Fatkullina, A.Z. Bulatova, J. Appl. Ind. Math., **17** (2), 396 (2023). DOI: 10.1134/S1990478923020175.

*Translated by D.Safin*