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Lattice Boltzmann Method for Simulation of Microfluidic Mixing in Modified T-shape Micromixer

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Abstract

This paper presents the 2D simulation of modified microfluidic T-shape micromixer with the lattice Boltzmann method (LBM) using the palabos library for simulation, that runs on multi-core CPUs and GPUs. T-micromixer is modified with obstacles in the form of circles. The walls of micromixer are modified to triangular shape. This modifications allows to achieve better mixing of fluids in microchannels. The modeling was performed by using the palabos library for D2Q9 LBM lattice.

Keywords: lattice Boltzmann method, T-micromixer, D2Q9 LBM lattice, modeling, microchannel.

1. Introduction

The main practical application of the microflows is development of microflow MEMS devices or lab-on-chips(LOC). LOC devices are used for various needs in the field of enzymatic analysis, DNA analysis, immunological analysis, monitoring of toxicity, biochemical diagnostics, regenerative medicine [D. Erickson, D.Q. Li, 2004].

Challenges in modeling of microfluidic MEMS can be classified into:

1. Simulation of microflows
2. Simulation of microchannels
3. Simulation of microenvironment
4. Modeling microflow effects:
    - Mixing;
    - Droplet;
    - Separation;
    - Filtration.

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Microfluidic devices include many operations, such as sample pre-treatment and sample preparation, mixing, pumping, analysis, DNA sequencing, cell separation and detection. Mixing is one of the most important part in the realization of labs-on-chip (LOC) or micro-total-analysis systems (µTAS) because microfluidic handling and operations carried out in these chips require rapid mixing of reagents and samples. Rapid mixing of two or more components or analytes is important for many microfluidic systems used in biochemical analysis or DNA analysis or microreactors with complex chemical synthesis. Mixing in the microscale is very difficult process, because it occurs by diffusion, which is very slow in microscale (mass diffusion coefficient $D \sim 10^{-10}$ m^2/s). In most microfluidic devices the flow is laminar with very low Reynolds number and diffusion dominates the mixing process.

2. Discretized 2D Boltzmann equation

Before simulating the dynamics of the continuous Boltzmann equation on the computer we should discretise it. To do this end, we introduce first a uniform grid spatial coordinates - grid spacing shall be the same for all axes. We will determinate the behavior of the liquid exactin the grid. In fact, allow the molecules to be only in certain spatial nodes. In addition, we will discretise the time, let's define the condition of the fluid in equidistant from each other moments. Molecules will have only certain values of speed – such that making one step in the time they went into any neighbor node. These allowed directions will be the same for all spatial nodes. Obviously the velocity of particles which move in the diagonal direction will be larger than ones which move nondiagonal.

We assume that this discrete system switches to the classic Boltzmann equation in case of an very small interval of time and lattice step, which, goes in it's turn to the Navier-Stokes equation in the macroscopic scale.

In next step it's assumed that the system of units is such that one step of lattice is the unit of length and step of time - a unit of time. We assume below that external forces are absent for simplicity. Let's number the permitted directions of speed from 1 to Q with index i. Now, if we mark the mass of particles that fly out of the node in the direction i at time step as f_i, then the equation can be written like:

$$f_i(r + v_i, t + 1) - f_i(r, t) = -\frac{(f_i - f_i^{eq})}{T} \qquad (1)$$

It is taken into consideration that the time step is equal to one, and all dt per unit are replaced. f_i^{eq} denotes the discrete equilibrium density distribution that depends on the macroscopic mass and velocity in a given node. We do not specify the node from which f_i^{eq} from r + V_i t will be used at the moment of time t + 1 or from r at the moment of time t. It is more convenient for computational scheme to use a node r + V_i t at time t + 1.

Then the equation above can be decomposed into two components: streaming step and collision step [S. Chen, G. D. Doolen, 2008].

Streaming step:

$$f_i(r + v_i, t + 1) - f_i(r, t) = -\frac{(f_i - f_i^{eq})}{T} \tag{2}$$

Collision step:

$$f_i(r, t) = \tilde{f}_i(r, t) - \frac{(\tilde{f}_i - f_i^{eq})}{T} \tag{3}$$

Here $\tilde{f}_i$ - denotes the mass of particles that come in a node in the direction i, but has not faced the rest of the particles, which also came into this node.

The following figure (Fig.1) shows one iteration of a pair of "streaming- collision". Colored arrows represent the flow of molecules. The intensity of the color reflects the mass of molecules flying in this thread, the length of the arrows nearly corresponds to the path traversed by the flow for the time step.

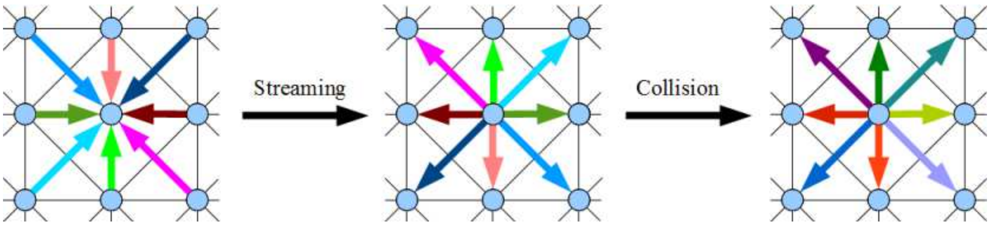
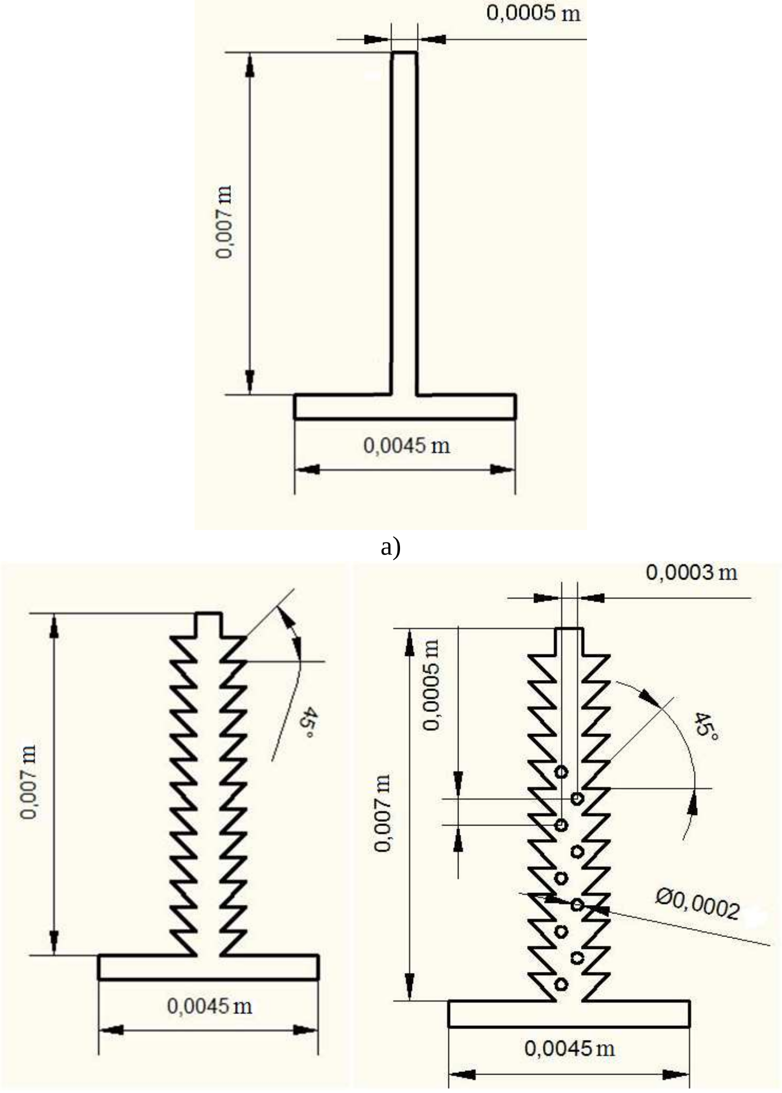


Fig. 1. Iteration “streaming - collision”

3. Modification of T - shape micromixer

Basic T-micromixer needs microchannels tens of centimeters long for complete mixing. This makes it very impractical for use in microfluidic labs on a chip or total analysis microsystems (mTAS). As in the passive micromixers no external forces are applied and mixing occurs only by diffusion, the only solution is to change the geometry of the microchannels, so that mixing was faster at shorter distances [N. Nguyen, Z. Wu, 2005, V. Hessel et al., 2005].

The aim of the research is to improve the mixing in a projected micromixer. To achieve this, let’s change the geometric shape of the micromixer first. Standard form of T - micromixer changes by giving the walls a triangle form and introducing obstacles in the form of circles into the channel. Than introduce the obstacles in the form of circles with the radius of 0.0002 m, distance between the centers of which is 0.0003 m horizontally and 0.0005m vertically. The dimensions of the model and subsequent modifications are shown in Fig. 2.



a)

b) c)

Fig. 2. Basic T-micromixer (a), T-micromixer with modified microchannel walls (b) T-micromixer with modified microchannel walls and obstacles in the form of circles (c).

4. Results and discussion of simulation for modified T – micromixer

The physical properties and parameters of fluids are shown in Table 1. The Numerical parameters for LBM simulation are shown in Table 2 [C. Chang, C. A. Lin et al., 2009].

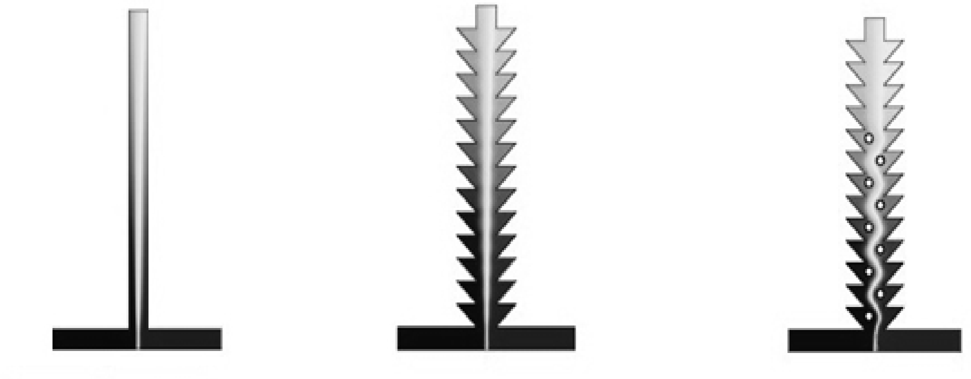
Table 1. Physical properties

Name	Expression	Value
Density	ρ	1000 kg/m^3
Dynamic viscosity	μ	1e-3 kg/m·s
Diffusion coefficient	D	1e-10 m^2/s
Concentration	c0	1 mol/m^3
Velocity	u0	1e-5 m/s
Pressure	P0	1 Pa

Table 2. Numerical parameters for LBM simulation

Name	Value
Density	0.824
Dynamic viscosity	0.0402
Relaxation time (T)	0.62
Lattice spacing	1.1910e-5

Fig. 3 shows the simulation results for D2Q9 lattice Boltzmann method.



a) b) c)

Fig. 3. Distribution of concentration for the lattice Boltzmann method: Basic T-micromixer (a), T-micromixer with modified microchannel walls (b) T-micromixer with modified microchannel walls and obstacles in the form of circles (c)

Diagram of concentration at the outlet of the micromixer for lattice Boltzmann method is shown in Fig. 4.

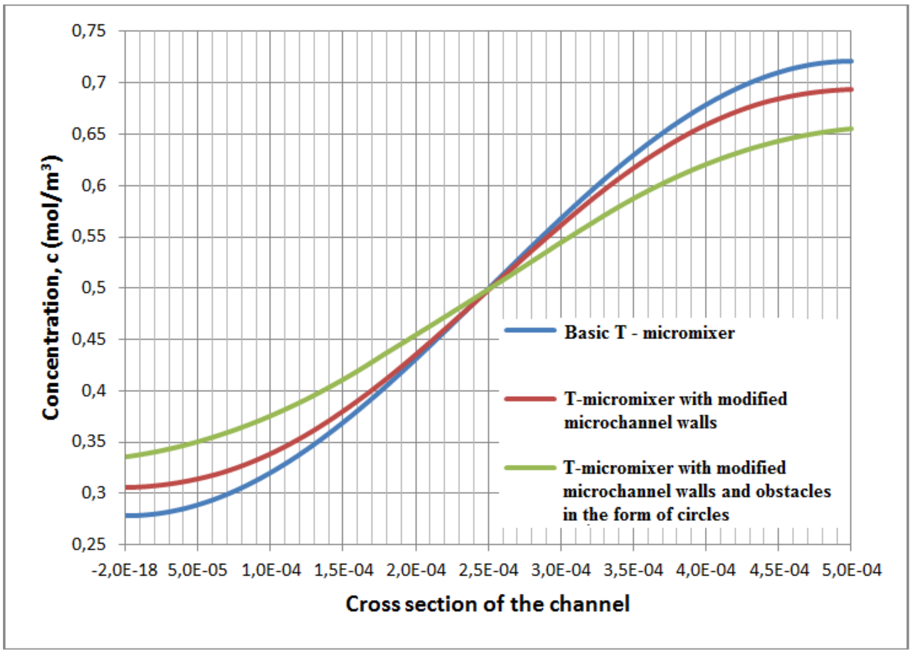


Fig. 4. Diagram of concentration distribution at the outlet of the T-micromixer for lattice Boltzmann method

If to compare the graphs in Fig. 4, we will see that our results of mixing were also improved by changing the geometric shape of the walls of the micromixer. After further modification by introducing the obstacles into microchannels, we conclude that these changes have led to a significant improvement of the efficiency of mixing and reduced the length required for mixing. This makes possible to integrate the micromixer into a complex of more complicated microdevices [H. A. Stone et al., 2004] and thus provide a more efficient mixing of fluid in a shorter mixing channel.

5. Conclusions

This paper presents the 2D simulation of modified microfluidic T-shape micromixer with the lattice Boltzmann method, using palabos library for simulation, that runs on multi-core CPUs and GPUs. T-micromixer is modified with obstacles in the form of circles, walls of micromixer are modified to triangular shape. This modifications allows to achieve better mixing efficiency of fluids in microchannels at small channel length. As well small channel length allow to integrate micromixer in complex microfluidic device. Results of simulation for lattice Boltzmann method shows better results and higher performance in comparison with other methods. The modeling was performed by using the palabos library for D2Q9 LBM lattice.

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