Simulation of single particle flowing in a microfluidic device using molecular dynamics method

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Abstract. Blood cells are modeled as spherical particles that flow through a microfluidic device with one inlet and two outlet channels, which is designed as a separator of blood particles. Molecular dynamics (MD) method was used intuitively in the simulation with the help of Semi-Circle Segmented Path Generator (SCSPG) as an approximation in creating fluid profile along the device channel. The trajectories generated from SCSPG was advanced using a fully developed Poiseuille flow with maximum fluid speed on the trajectories and the tails of speed distribution which was extended to the size of the channel with speed of zero at the channel walls. It has been observed that for a single particle trajectory the outlet channel was chosen by the particle depends on the axial position of the particles. Mass of particle determines how hard the particle deflects due to fluid profile. A better design is proposed in this work for separating two groups of particles with different size.

1. Introduction

A blood cells separation (BCS) system which imitates a microfluidic device is simulated in this work. Microfluidic devices have successfully separated blood cells by taking advantages of some physical properties e.g. viscoelasticity [1], flow fractionation [2], or dielectrophoresis [3]. There is also experiment result in the form of video showing that cells with different inertia are flowing through different channel in a separation system. In this work, red blood cell (RBC) and white blood cell (WBC) were simplified into spherical cells that interact through collision, which was modeled using soft-sphere scheme with linear spring-dashpot model [4]. The numerical method was using simple Euler algorithm or forward finite difference method, where the whole simulation system was also known as molecular dynamics method. There is also drag force from fluids
that makes the cells move along the channel. A Y-junction or fork one was designed to collect different type of blood cell, RBC or WBC, based on its inertia and elasticity. Flow field of the fluid was obtained from another work, which has been confirmed in experiment. Blood cells can move through the channel using the field. It is observed that cells with larger mass were having difficulties to turn at the junction, while cells with larger cross section area will follow the flow better than the cells with smaller cross section area. Width and length of the channel before and after the junction are also varied to show how these parameters influence the separation process.

2. Simulation

A BCS system, which is design to separate red blood cells (RBCs) and white blood cells (WBCs), is shown in figure 1.

![Figure 1. Type of forces considered in this work: gravitational force ($\vec{G}_i$), buoyant force ($\vec{B}_i$), drag force ($\vec{D}_i$), normal force ($\vec{N}_{ij}$), and attractive force ($\vec{A}_{ij}$).](image)

As reference $(x_0, y_0)$ or point 0 is chosen and all other points will be described using the reference. Points 1-5 will be defined using

\[
\begin{align*}
    &x_1 = x_0 + l, \quad y_1 = y_0, \\
    &x_2 = x_0, \quad y_2 = y_0 + w_s, \\
    &x_3 = x_2 + l_{23}, \quad y_3 = y_2, \\
    &x_4 = x_5 - l_{45}, \quad y_4 = y_5, \\
    &x_5 = x_1, \quad y_5 = y_1 + w_{D0}.
\end{align*}
\]

Two points, points 20 and 21, were defined as center of circular arcs that connect points
4-6 and points 3-7. Then it can be obtained that

\[ x_6 = x_4 - R_{20} \sin \theta, \quad y_6 = y_4 - R_{20}(1 - \cos \theta), \quad (6) \]
\[ x_7 = x_3 + R_{21} \sin \phi, \quad y_7 = y_3 - R_{21}(1 - \cos \phi), \quad (7) \]

with a relation

\[ \phi = \pi - \theta. \quad (8) \]

between \( \phi \) and \( \theta \). The last two points are

\[ x_8 = x_6 + l_{68} \cos \theta, \quad y_8 = y_6 - l_{68} \sin \theta, \quad (9) \]
\[ x_9 = x_7 + l_{79} \cos \theta, \quad y_9 = y_7 - l_{79} \sin \theta, \quad (10) \]

and the relation of

\[ x_9 = x_8 + w_{D1} \cos \theta, \quad y_9 = y_7 - w_{D1} \sin \theta, \quad (11) \]

should be held.

The system is considered as two-dimensional system where thickness of the system \( H \) is in \( z \) direction. Inlet fluid flow can be approximated through

\[ Q_s \approx v_s W_s H, \quad (12) \]

and there are two outlet flow

\[ Q_{D0} \approx v_{D0} W_{D0} H, \quad (13) \]
\[ Q_{D1} \approx v_{D1} W_{D1} H. \quad (14) \]

Flow conservation requires that the relation

\[ Q_s = Q_{D0} + Q_{D1} \quad (15) \]

holds. Due to fluid viscosity this two-dimensional system a channel width \( W \) will give a velocity profile of

\[ v_y(x) = 12c \left( \frac{1}{4} W^2 - x^2 \right) \quad (16) \]

where \( x \) direction is along the channel length \( L \) and \( y \) is perpendicular to \( x \), which can be obtained from the general solution for this problem [5]. The constant \( c \) depends on fluid viscosity \( \eta \) and pressured difference \( \Delta p \) over a distance \( \Delta x \). For second outlet with width \( W_{D1} \), the \( x \) and \( y \) direction is rotated about \( \phi \) in clockwise direction from its original direction as shown in figure 1. Using Equation (16), fluid flow can be calculated through

\[ Q = 12cH \int \left( \frac{1}{4} W^2 - x^2 \right) dx \quad (17) \]

which gives better approximation than Equations (12)-(14). By integrating from \(-W/2\) to \(W/2\) Equation (17) will produce

\[ Q = ch \left[ 3W^2x - 4x^3 \right]_{-W/2}^{W/2} = cH \left( 3W^3 - W^3 \right) = 2cHW^3. \quad (18) \]
Substituting Equation (18) into Equation (15) will give the relation of

\[ c_s W_s^3 = c_{D0} W_{D0}^3 + c_{D1} W_{D1}^3 \]

which relates the \( \Delta p \) and \( \Delta x \) of the three channels \( S, D_0 \) and \( D_1 \) since \( \eta \) is the same for all channels. The constant \( c \) is also related to the maximum velocity \( v_{max} \) in each channel. If pressure difference is not considered in this work, then we can relate \( v_s, v_{D0}, \) and \( v_{D1} \) through

\[ v_s W_s^3 = v_{D0} W_{D0}^3 + v_{D1} W_{D1}^3 \]

for simplicity, which will define the velocity profile along the system.

In this work, the steady state velocity profile was assumed to be already developed, where it actually requires some distance from the inlet in rectangular ducts [6], the influence of fluid component, e.g. soap films [7] and pressure difference that can flatten the parabolic velocity profile [8] were not considered. This simplification is chosen due to complexity of pressure and velocity distribution of junctions [9], where such approach is often used even when the observational results deviated from the simple theory [10], such as its implementation in biological system [11] and using various polymer-based microfluidic devices [12].

System in figure 1 can be further simplified using similar method as defining arbitrary trajectory consisted of straight and semi-circular lines [13], which is the base of single fluid element method (SFVE) [14].

### 3. Results and Discussion

Simulation is conducted using parameters value listed in Table 1, where all values are in SI unit. Parameter variation is tested in the simulation, where there are more than single value for a parameter put in a parentheses.

| Parameter | Value   | Unit     |
|-----------|---------|----------|
| \( w_s, w_{D0}, w_{D1} \) | 50, 50, 50 | \( \mu m \) |
| \( v_s, v_{D0}, v_{D1} \) | 10, 5, 5 | \( \mu m/s \) |
| \( \theta \) | 0.8726 | rad |
| \( l, l_{21}, l_{45}, l_{68}, l_{79} \) | 400, 50, 100, 200, 310 | \( \mu m \) |
| \( R_{20}, R_{21} \) | 25, 50 | \( \mu m \) |
| \( D \) | 4, 8, 12, 16, 20 | \( \mu m \) |
| \( \rho, \eta \) | 1000, 10, 0.01 | kg/m\(^3\), Pa\(\cdot\)s |
| \( t_{beg}, t_{end}, \Delta t, T_{data} \) | 0, 600, 1, 1 | S |

Using straight and semi-circular lines [13], the design proposed in figure 1 can be implemented as shown in figure 2, where the three lines consisted of number in the software interface are information for drawing the channel wall in the form of

\[ x y \theta_{i1} \theta_{i1} N_1 \cdots \theta_{M-1,i} \theta_{M-1,i} N_{M-1} \theta_{M,i} \theta_{M,i} N_M, \]

(21)
if there are \( M \) different segments in a trajectory. Index \( i \) and \( f \) stand for initial and final direction of a segment.

![Implementation of design using an in-house software based on JavaScript.](image)

**Figure 2.** Implementation of design using an in-house software based on JavaScript.

![Motion of particle from inlet channel \( S \) to outlet channel \( D_0 \) (top row) and outlet channel \( D_1 \) (bottom row).](image)

**Figure 3.** Motion of particle from inlet channel \( S \) to outlet channel \( D_0 \) (top row) and outlet channel \( D_1 \) (bottom row).

Results from figure 3 are obvious since the particle experienced only nearly laminar fluid profile in the two cases. In the case of outlet \( D_0 \), the top left figure of figure 4 shows the developing velocity along \( x \) axis for different diameter \( D = 4, 8, 12, 16, 20 \, \mu m \), where zero velocity is the initial condition. Particle with 4 \( \mu m \) diameter developed its velocity instantly and achieved near-maximum velocity at the outlet \( D_0 \), which was 5 \( \mu m/s \), while the largest particle with 20 \( \mu m \) could achieve only 1 \( \mu m/s \). Velocity \( v_y \) is not shown since it still have zero value when particles is through the outlet \( D_0 \).

It can be seen from the top right and bottom figure of figure 4 that smaller particle \((D = 4 \, \mu m)\) is easier to deflect than the larger one \((D = 20 \, \mu m)\), where the time they
Figure 4. Particle velocity from inlet $S$ to outlet $D_0$ (top left) and for $S$ to outlet $D_1$ (top right and bottom) for different value of diameter $D$.

start to turn are 50, 85, 150, 165, and 210 for $D = 4$, 8, 12, 16, 20 $\mu$m, respectively.

Figure 5. Particle velocity components from inlet $S$ to outlet $D_1$ for different value of diameter $D$.

Figure 5 shows the relation between particle $v_y$ and $v_x$ that confirms again for zero velocity as initial condition, only smaller particles were capable to develop their velocities approaching outlet velocity. Other interesting aspect to discuss is the condition when the particle hit the upper wall of outlet channel $D_1$, where for $D = 4$, 8, 12, 16, 20 $\mu$m and time $t = 136$, 237, 337, 437, 537, where the positions are shown in figure 6.

From the bottom-right figure in figure 6, particles with different diameter were observed to hit different places along the upper wall of the outlet channel $D_1$. For diameters of 12–20 $\mu$m, the position can be hardly distinguished but for diameter of 4 $\mu$m the position difference was well observed and already larger than the particle diameter.
Figure 6. Position where the particle hit upper wall of the outlet channel $D_1$.

According to the results from figure 6, a better, hopefully working in practice, microfluidic device can be proposed as shown in figure 7, which would be effective only to separate two different sizes of particles.

Figure 7. Proposed model of microfluidic device for separating particles in two groups of particles with size of 4 $\mu$m (green thin line) and 8 – 20 $\mu$m (red thick line).

Design in figure 7 will be the future plan of this work, where with the additional two outlets the velocity profile will also be changed and may not produce the desired results. Collision between particles is also interesting to discuss since it will also plays a role in determining whether the particle will go through the outlet $D_0$ or $D_1$. The proposed design only takes into account the case where the particle go through outlet $D_1$. A better approximation in creating fluid velocity profile will also be considered since it also plays an important role in determining particles motion in the microfluidic
device.

4. Conclusion

Flowing single particle in a microfluidic device has been performed intuitively using molecular dynamics method. The results showed that the particle initial position in vertical direction determined the final channel in which the particle will flow through. Larger particle was more difficult to turn than the smaller one. Better design of particles separation device has been proposed using this feature.

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