

Modelling of the Dynamics of an immersed body in a microchannel with stenosis using the immersed boundary method

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ABSTRACT

In the present study, the combination of lattice Boltzmann and immersed boundary methods is used to simulate the motion and deformation of a flexible body. Deformation of the body is studied in microchannel with stenosis and the effect of the flexibility changes on its deformation is investigated. The obtained results in the present manuscript show that by increasing the elasticity modulus, the deformation of the body and its speed decrease. In this case, the flow pressure around the body increase. When the body is initially located outside the microchannel center, tank-treading motion occurs due to the difference in velocity of the shear layers. In addition, with a decrease in the size of microchannel stenosis, the body is less deformed and goes faster and reaches to the end of the microchannel in less time. The faster or slower movement of the biological membranes than the normal state causes the proper exchange of materials between the membrane wall and the surrounding flow and that disturbs its most important duty i.e. the exchange of materials with tissues. The analysis in this study shows that the results of the simulation are in good agreement with the available results and demonstrates the efficiency of the combination of lattice Boltzmann and immersed boundary methods to simulate the dynamic behavior of biological membranes, red blood cells and deformable particles inside the flow.

1. Introduction

Fluid-structure interaction (FSI) problems are of great important in fluid dynamics[1]. It is also used in biomechanics problems [2,3]. The immersed boundary method (IBM) is the most appropriate approach for solving such problems taking the advantage of a fixed uniform computational grid [4,5]. Therefore, the IBM can be easily used to simulate the medical and pharmaceutical contexts including red blood cells motion, and blood flow in vessels and heart valves. IBM is both a mathematical formulation and a numerical scheme. The mathematical formulation uses a combination of Eulerian and Lagrangian parameters. These parameters are linked together via interaction equations where the Dirac delta function plays an important role. In numerical implementation of IBM, the Eulerian variables are defined on a fixed Cartesian grid and the Lagrangian variables are defined on a curvilinear grid moving freely through the Eulerian grid. The basis of IBM is to add a forcing term as a source term to the Navier-Stokes or lattice Boltzmann equations [6]. In recent years, the lattice Boltzmann method (LBM) has developed into a promising numerical method for the simulation of complex fluid flows. Unlike conventional numerical schemes, which are based on discretization of macroscopic continuum equations, the LBM is based on microscopic models and mesoscopic kinetic equations. The LBM is a reliable alternative to the conventional computational fluid

dynamics methods for the simulation of complex problems including incompressible fluid flows, porous media flows, multi-phase flows and blood flow. When Mach number and Knudsen number are small enough, the LBM equation is a good approximation for Navier-Stokes (N-S) equations. In LBM, fluid is considered as a combination of virtual particles, which can move in a finite number of directions. This method comprises two steps: streaming and collision. In the streaming step, the particles move to the neighbor body lattice points. In the collision step, the particles arriving at the points, interact one another and change their velocity directions according to scattering rules. LBM has been found to recover the N-S equation using Chapman-Enskog expansion [7]. The most important features of the LBM are: explicit updating, algebraic operation and easy implementation on curved boundaries. There have been many researchers who have combined the IBM-LBM to solve the fluid flows involving rigid/elastic interfaces. Feng and Michaelides [8] were the first to combine the LBM with the IBM and simulated suspensions of rigid disks in 2D. Le and Zhang [9] used in their work a hybrid LBM-IBM and noticed that the computed velocity profiles can deviate greatly from theoretical ones even for very simple flow situations, both in the immersed boundary layer and the bulk region. Dupuis et al. [10] studied how the coupling method of the forcing term between the Eulerian and Lagrangian grids could affect the results for the flow over an impulsively started cylinder at moderate Reynolds (Re) number. Wu and Shu

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[11] proposed a new version of IBM-LBM, which could well consider the effect of external force on the momentum flux as well as the discrete lattice effect. JiSeok and SangHwan [12] presented a numerical scheme for fluid-structure interaction, especially for elastic structures. They employed a hybrid LBM-IBM using an improved direct forcing scheme for the fluid, and a finite element method with Euler beam elements for the elastic plate. Zhang et al. [13, 14] also used a combination of the IBM and the LBM to investigate the microscopic hemodynamic and hemorheological behaviors of discrete RBCs in shear flow. They noted that three-dimensional simulation of RBCs is required to attain accurate results. Cheng et al. [15] proposed a model to properly simulate the fast boundary movements and steep pressure gradient occurring in the fluid-body interaction. They simulated the mitral valve jet flow considering the interaction of leaflets and fluid. The combination of the Lattice-Boltzmann and the immersed boundary method has been used extensively in recent years in modeling biomechanics problems [16-19]. Recently, this method has been used to simulate the flow around rigid bodies [20-22], and to simulate the motion and deformation of the flexible membrane (fluid-structure interaction problem) [23-26]. Also recently, Boltzmann's method has been used for multiphase flows [27-31], non-Newtonian fluid [32] and solution of differential equations [33,34].

In the present work, the effect of elastic modulus changing and the initial location of the membrane and increasing the microchannel stenosis diameter on the dynamic behavior of the flexible boundary are investigated using combination of lattice Boltzmann and the immersed boundary methods.

2. Mathematical formulations

The discretized LBM equation is written in the form of Eq. (1).

$$f_i(\vec{x} + \hat{e}_i \Delta t, t + \Delta t) - f_i(\vec{x}, t) = \frac{f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)}{\tau} + \Delta t S_i \quad (1)$$

where $f_i(\vec{x}, t)$ is the density distribution function of a particle with speed \hat{e}_i located at position \vec{x} at time t . Δt is the time step, $f_i^{eq}(\vec{x}, t)$ is the equilibrium distribution function, τ indicates the relaxation time and S_i is the body force of the immersed body in the LBM equation. It should be noted that, the LBM equation can recover the N-S equations by the so-called Chapman-Enskog expansion. The velocities of the particles can be written in the form of Eq. (2):

$$\hat{e}_i = \begin{cases} (i, i) & ; i = 0 \\ (\cos \frac{\pi}{2}(i-1), \sin \frac{\pi}{2}(i-1))c & ; i = 1-4 \\ \sqrt{2}(\cos \frac{\pi}{2}(i-\frac{9}{2}), \sin \frac{\pi}{2}(i-\frac{9}{2}))c & ; i = 5-8 \end{cases} \quad (2)$$

In Eq. (2), $c = \Delta x / \Delta t$ and Δx is the distance between two adjacent nodes in the Eulerian grid. The equilibrium distribution function defined as follows,

$$f_i^{eq}(\vec{x}, t) = w_i \rho \left[1 + 3 \frac{(\hat{e}_i \cdot \vec{u})}{c^2} + \frac{9}{2} \frac{(\hat{e}_i \cdot \vec{u})^2}{c^4} - \frac{3}{2} \frac{|\vec{u}|^2}{c^2} \right] \quad (3)$$

where w_i is the weight coefficients given by,

$$w_i = \begin{cases} \frac{4}{9} & ; i = 0 \\ \frac{1}{9} & ; i = 1-4 \\ \frac{1}{36} & ; i = 5-8 \end{cases} \quad (4)$$

However, the elastic force in LBM is defined as Eq. (5),

$$S_i = (1 - \frac{1}{2\tau}) w_i \left[\frac{3(\hat{e}_i \cdot \vec{u})}{c^2} + \frac{9(\hat{e}_i \cdot \vec{u})}{c^4} \hat{e}_i \right] \cdot \vec{f} \quad (5)$$

Macroscopic fluid density is obtained by the following relation,

$$\rho = \sum_{i=0}^8 f_i \quad (6)$$

In addition, the macroscopic velocity field \vec{u} is defined as:

$$\vec{u} = \frac{1}{\rho} \left[\sum_{i=0}^8 f_i \hat{e}_i + \frac{1}{2} \vec{f} \Delta t \right] \quad (7)$$

The Lagrangian force density \vec{L} comprises two components of stretching/compression force \vec{L}_s and bending force \vec{L}_b defined as [23]:

$$\vec{L}(s, t) = \vec{L}_s(s, t) + \vec{L}_b(s, t) \quad (8)$$

The Lagrangian force density is related to the elastic energy density using the virtual work theorem:

$$\vec{L}(s, t) = - \frac{\partial \mathcal{E}}{\partial \vec{X}} = - \frac{\partial (\mathcal{E}_s + \mathcal{E}_b)}{\partial \vec{X}} \quad (9)$$

Therefore, the elastic energy density consists of stretching/compression \mathcal{E}_s and bending \mathcal{E}_b components, which are given in discretized form as:

$$\mathcal{E}_s = \frac{1}{2} E_s \sum_{j=1}^{N-1} \left(\frac{|\vec{X}_{j+1} - \vec{X}_j|}{\Delta s} - 1 \right)^2 \Delta s \quad (10)$$

$$\mathcal{E}_b = \frac{1}{2} E_b \sum_{j=2}^{N-1} \left(\frac{|\vec{X}_{j+1} - 2\vec{X}_j + \vec{X}_{j-1}|^2}{(\Delta s)^4} \right) \Delta s \quad (11)$$

The discretized form of the Lagrangian force density components is given by the following relations:

$$(\vec{L}_s)_k = \frac{E_s}{(\Delta s)^2} \sum_{j=1}^{N-1} \left\{ \begin{aligned} & (|\vec{X}_{j+1} - \vec{X}_j| - \Delta s) \times \\ & \vec{X}_{j+1} - \vec{X}_j \\ & \frac{|\vec{X}_{j+1} - \vec{X}_j|}{(\Delta s)^2} (\delta_{j,k} - \delta_{j+1,k}) \end{aligned} \right\} \quad (12)$$

$$(\vec{L}_b)_k = \frac{E_b}{(\Delta s)^4} \sum_{j=2}^{N-1} \left\{ \begin{array}{l} (\vec{X}_{j+1} - 2\vec{X}_j + \vec{X}_{j-1}) \\ (2\delta_{j,k} - \delta_{j+1,k} - \delta_{j-1,k}) \end{array} \right\} \quad (13)$$

In Eqs. (10) to (13), $k = 1, 2, \dots, N$ (N is the total number of Lagrangian nodes on the body), $(\vec{L}_s)_k$ and $(\vec{L}_b)_k$ are Lagrangian force density components associated with the node k on the body and $\delta_{j,k}$ is the Kronecker delta function. Interaction between the fluid and body can be achieved by obtaining a proper relationship between the Lagrangian parameters associated with the cell and Eulerian parameters associated with the fluid. In this section, it is shown how to transfer the Lagrangian force to the Eulerian frame and also how to interpolate velocities from Eulerian to Lagrangian coordinates. The Eulerian force density $\vec{f}(\vec{x}, t)$ is obtained by integrating the Lagrangian force density $\vec{L}(s, t)$:

$$\vec{f}(\vec{x}, t) = \int_{\Gamma} \vec{L}(s, t) \delta(\vec{x} - \vec{X}(s, t)) ds \quad (14)$$

where Γ represents the immersed elastic boundary and $\delta(\vec{x} - \vec{X}(s, t))$ is the Dirac delta function.

To enforce the no-slip condition on the fluid-body interface, the velocity of the body wall should be set equal to the adjacent fluid velocity, i.e.,

$$\vec{U}(s, t) = \vec{u}(\vec{X}(s, t), t) = \frac{\partial \vec{X}(s, t)}{\partial t} = \int_{\Gamma} \vec{u}(\vec{x}, t) \delta(\vec{x} - \vec{X}(s, t)) dx \quad (15)$$

It should be noted that in the present work, the fluid velocity $\vec{u}(\vec{x}, t)$ is obtained using the LBM.

Mathematically the Dirac delta function $\delta(\vec{x})$ is discontinuous and has to be smoothed for numerical implementation. There are different methods of smoothing this function. The following smoothed delta function is proposed by [6]:

$$\delta(\vec{x}) = \frac{1}{h^2} \phi\left(\frac{x}{h}\right) \phi\left(\frac{y}{h}\right)$$

$$\phi(r) = \begin{cases} \frac{1}{4} \left(1 + \cos \frac{\pi r}{2}\right) & ; |r| \leq 2 \\ 0 & ; |r| > 2 \end{cases} \quad (16)$$

where h is the distance between two Eulerian grid points and r denotes the distance between any two Eulerian and Lagrangian points.

3. Results

3.1. Validation

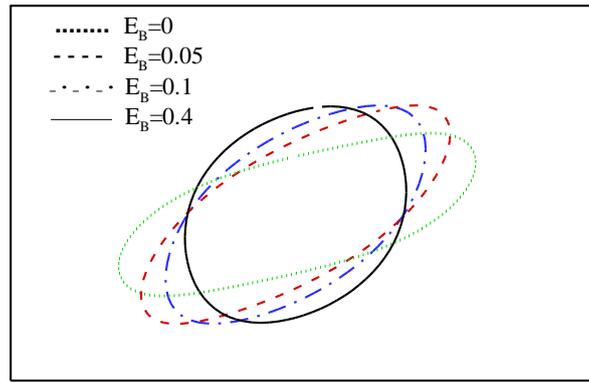
In this section, the motion of a circular elastic body in shear flow is studied. Length and width of the microchannel is considered to be 16 times of the original radius of the body. The body is positioned at the center of microchannel and 160 Lagrangian points have been used. In Fig.1a, capsule deformation and tank-treading movement are observed. where G

and E_B are 0.04 and 0.04 respectively. which are calculated by the equations $G = \frac{\mu k a}{E_s}$ and $E_B = \frac{E_b}{a^2 E_s}$. G is dimensionless shear rate, k is shear rate (1/s), a is initial capsule radius, E_s is elastic modulus (N/m), E_b is bending modulus (N.m) and E_B is dimensionless bending modulus. Taylor deformation parameter is defined as $D_{xy} = \frac{L-B}{L+B}$. In Fig. 1b, the introduced variables are shown. By increasing the bending modulus, the deformation of the body decreased. In Figs.1c and 1d present results have been compared with Sui and et.al [35] results. By increasing bending modulus, Taylor deformation parameter is decreased, which represents less deformation of capsule. In addition, it can be seen from Fig. 1 (d), by decreasing bending modulus, dimensionless angle $\frac{\theta}{\pi}$ is decreased. The result that is obtained from this section is that: by decreasing bending modulus, deformation of body increased and orientation of the body to the horizon decreased and its shape becomes oblique. In fact, the circle has become ellipse, and with the further decreasing of the bending modulus, the ellipse becomes more elongated. Present results are in good agreement with Sui et al. [35] results.

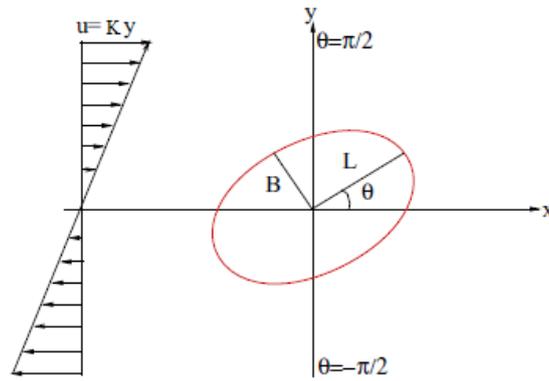
3.2. The behavior of a flexible body in passing through stenosis

A circular body with a diameter of $H=30 \mu\text{m}$ is considered in the poiseuille flow. Length and height of microchannel are $L=300 \mu\text{m}$ and $D=60 \mu\text{m}$ and in stenosis section (half oval in the middle of microchannel) is $d=20 \mu\text{m}$ ($d/D=1/3$). Reynolds number is $Re=0.5$ (Fig. 2). The bounce-back and periodic boundary conditions have been used on the walls and on the inlet and exit of the microchannel and the boundary condition BFL has applied on curvilinear boundaries [36]. First, the dynamics of the circular body which located at the center of the microchannel, in two case of high and low flexibility are examined with elastic and bending 14×10^{-19} N.m, 1×10^{-19} N.m and 5×10^{-5} N.m, 19×10^{-19} N.m respectively.

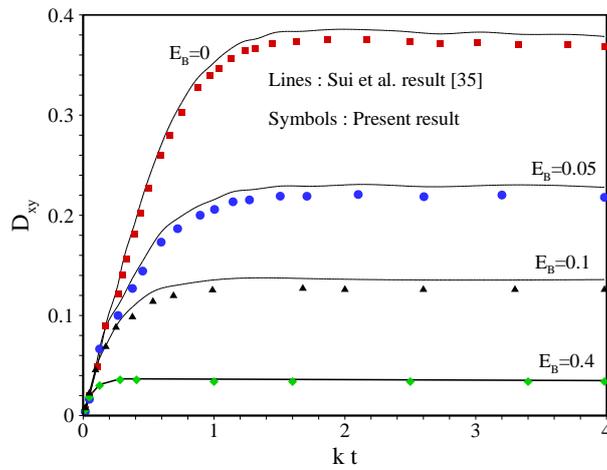
In Figs. 3 and 4, motion of the body, with high and low flexibilities at different times, is observed while passing the stenosis. Pressure is considered in grid unit. One can see in Fig. 3 that body with high flexibility is stretched more and reaches the end of microchannels in less time. The low-flexible body (Fig.4), reduces somewhat the effective cross-sectional area of the fluid behind the body due to its high hardness. In fact, it is similar to blocking a greater amount of flow path (relative to the body with high flexibility), which reduces the flow velocity behind the body and increases the flow pressure behind the immersed body according to Figs. 3b and 4b. In both cases, since the boundary is located in the center of the microchannel and the axial flow is symmetrical, a balance is occurred between the upper and lower lift forces acting on the body. Thus, the body is not displaced vertically. The difference in pressure created behind and in front of the body causes it to move in the longitudinal direction of the microchannel. The greater pressure on the back side relative to front, makes the rear side form concave shape, while the front is stretched more and in after. Therefore, it's shape become convex before stenosis.



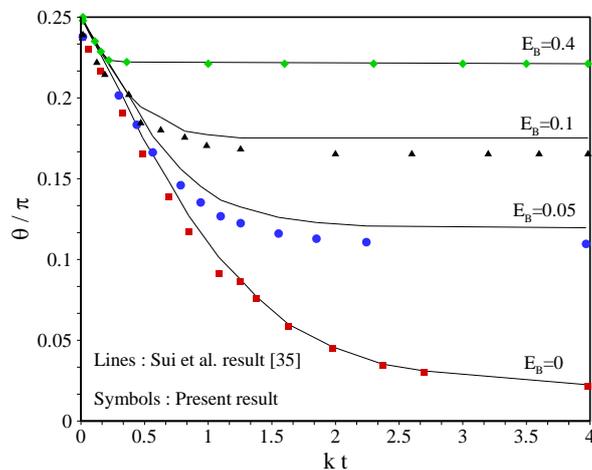
(a)



(b)



(c)



(d)

Figure 1. a) The effect of bending modulus on deformation of circular body (present result) ; b) represent L, B, θ ; c) Taylor deformation parameter changes for

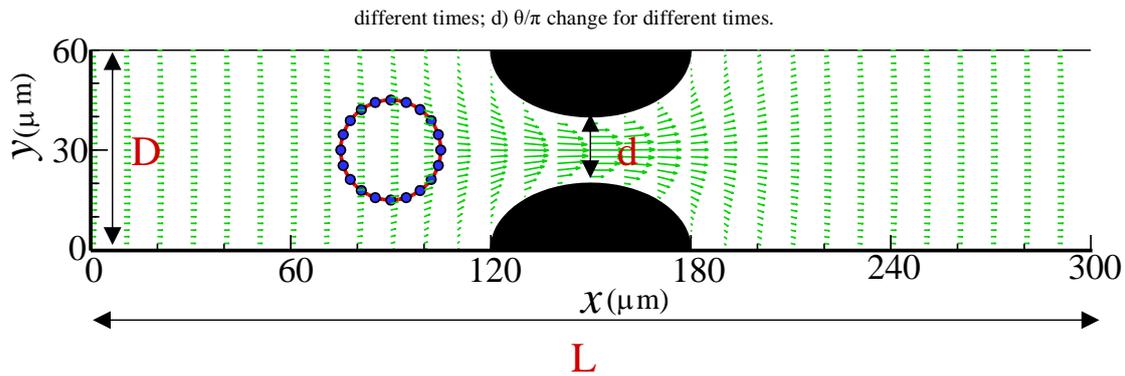


Figure 2: The initial position of the immersed body located at the center of the microchannel

Figure 5 shows that a body with a high elasticity modulus has a lower rate of velocity than the body with a low elastic modulus. This matter is also observed in the results of others researches [37, 38]. It should be noted that the acceleration or deceleration movement of biological membranes than the normal state, results in the lack of proper exchange of materials between the membrane wall and the surrounding flow and interferes with its most important task, ie, the exchange of materials with tissues. The body with high flexibility, reaches the end of the microchannel at a shorter time due to its faster velocity. In both cases, the body appears to be faster when it comes to stenosis due to increased flow velocity in this area.

Figure 6 shows that the A/B ratio is higher for more deformable body due to its low elasticity modulus. When the immersed body reaches to stenosis, it is most deformed due to the increase in speed in this area. In this case, the body in the moment of passing through stenosis is more stretched and passes through the stenosis more easily with less energy from the fluid. After exiting from stenosis, the body reaches convex at front and reaches concave at behind it (Fig. 3d) due to its high flexibility. While the body with low deformability, maintains its circular shape after exiting from stenosis.

In Fig. 7, the initial location of the body is placed under the center of the microchannel. The body's rotation (tank-treading) is caused by the shear force of the fluid around it. Due to the rotational phenomenon, a lifting force is applied to the deformed membrane and directs it towards the center of the microchannel. In the rotational movement, after a change in the initial shape, the shape and the movement direction of the body remain constant during the movement (after the stenosis); because the flow inside the microchannel is viscous, so it has shear layers. The shear is caused by horizontal component of the fluid velocity. It means that, the velocity in the vertical axis varies within the shear layers. Therefore, when fluid collides to the boundary, the upper part of the boundary is affected by higher velocity than the lower part. This difference in momentum on the body causes it to rotate. As a result of this rotation, an upward lift force from the fluid to the body is applied and directs it to the center of the microchannel.

In this case, the maximum deformation of the body is observed when it passes through the stenosis. The body with high elasticity (Fig. 7a) is more stretched when passing through the stenosis compared to the body with low elasticity (Fig. 7b), while the body with low elasticity blocks a greater pass of flow that reduces the velocity and increases the pressure around the body. The red solid points are related to the rotation of the body (tank-

treading movement). This type of motion has been observed in the experimental and numerical results [39-41]. In Figs. 7c and 7d, the velocity vector of Lagrangian points of immersed body with high and low elasticity are observed at the exit of stenosis. The body with high elasticity adapts itself to the flow path and passes stenosis with less energy. A body with low elasticity blocks the outlet span of stenosis for a moment. The velocity vector of the Lagrangian points in comparison to the previous one cannot easily fit itself with the streamline. In this case, a higher pressure is applied to the back of the body so that the flow can pass the body from the stenosis. This behavior of body in the passing the stenosis leads to slowing down its motion.

Figure 8 shows the effects of decreasing the height of the stenosis for the body with low flexibility (Fig. 4). Figure 8a shows deformation of body with low flexible for case $d/D = 2/3$. Reducing the stenosis causes reduction in the deformability of the body. The body has the least deformation in the case without stenosis (Figure 8b). It is seen from the Figure 8c that the velocity of the body increases with decreasing stenosis height. By creating stenosis, the loss due to obstruction increases and as a result, the body velocity decreases. Stenosis causes the body to slow down before and after the stenosis and increases its velocity value when crossing the stenosis.

4. Conclusion

In the present study, the combination of the lattice Boltzmann method and the immersed boundary method was used to simulate the motion and deformation of a flexible body in a viscous flow. By increasing the elasticity modulus, the deformation and velocity of the body decreased. In this case, the pressure of the flow around the body increased. In addition, by decreasing the size of stenosis of the microchannel, the body was less deformed and had higher velocity, resulting in less time to reach at the end of microchannel. Also, the results of the simulation were in good agreement with the available results. By performing this numerical study and study of a number of different parameters, one can study the physics of flow and the effect of solid and fluid interaction on each other. Each individual behavior of these parameters gives the reader a view that does not feel the vacuum of experimental works in this field. Investigating various parameters affecting fluid flow and immersed membrane helps to understand biological systems. It is also possible to observe the lattice Boltzmann-immersed boundary method's ability to model the dynamic behavior of biological membranes, red blood cells, and other deformable particles in the flow and compare the simplicity of programming and convergence rate of this method with other CFD methods.

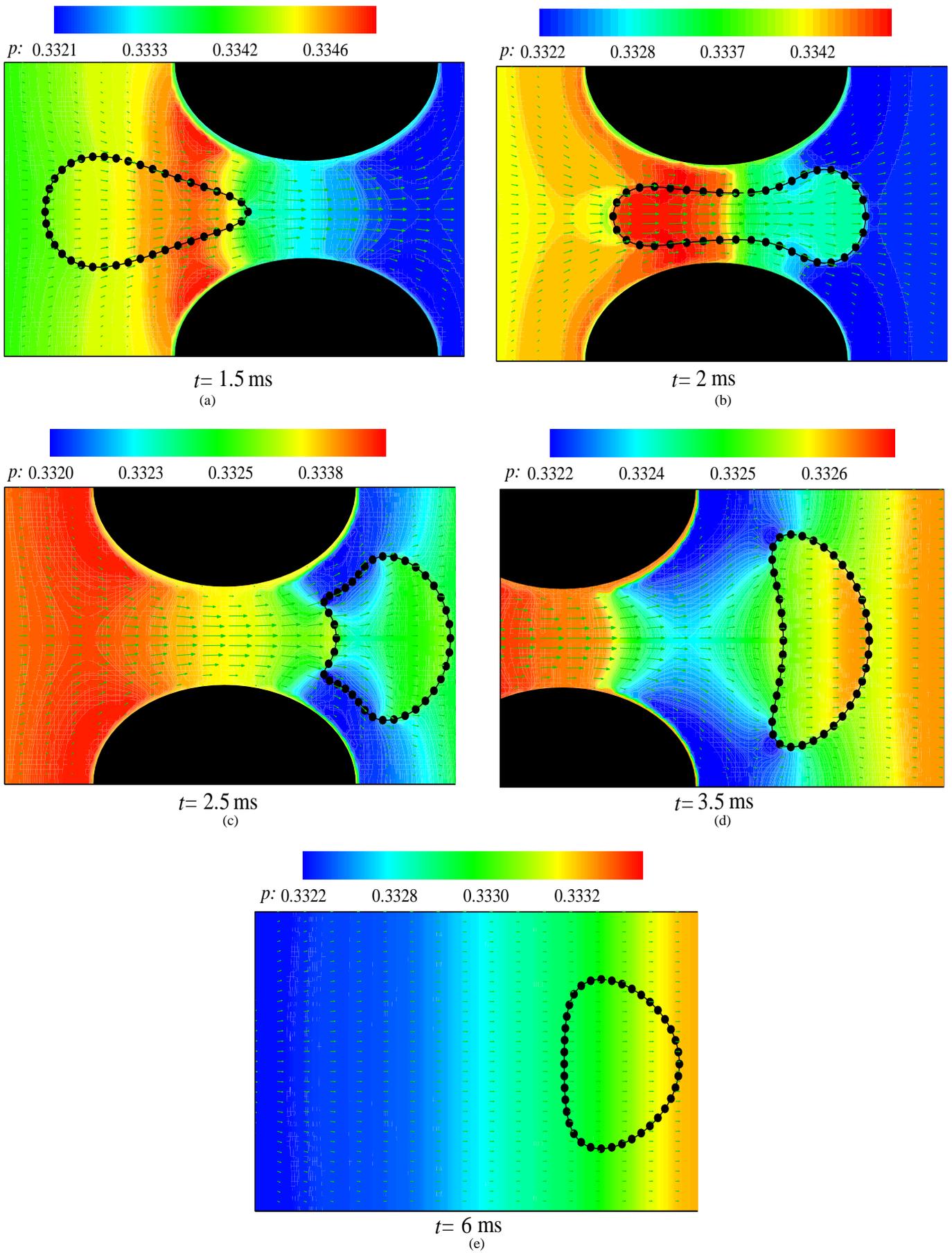


Figure 3. Motion of the body with a high flexibility passing stenosis at the times a) $t = 1.5$ ms, b) $t = 2$ ms, c) $t = 2.5$ ms, d) $t = 3.5$ ms and e) $t = 6$ ms

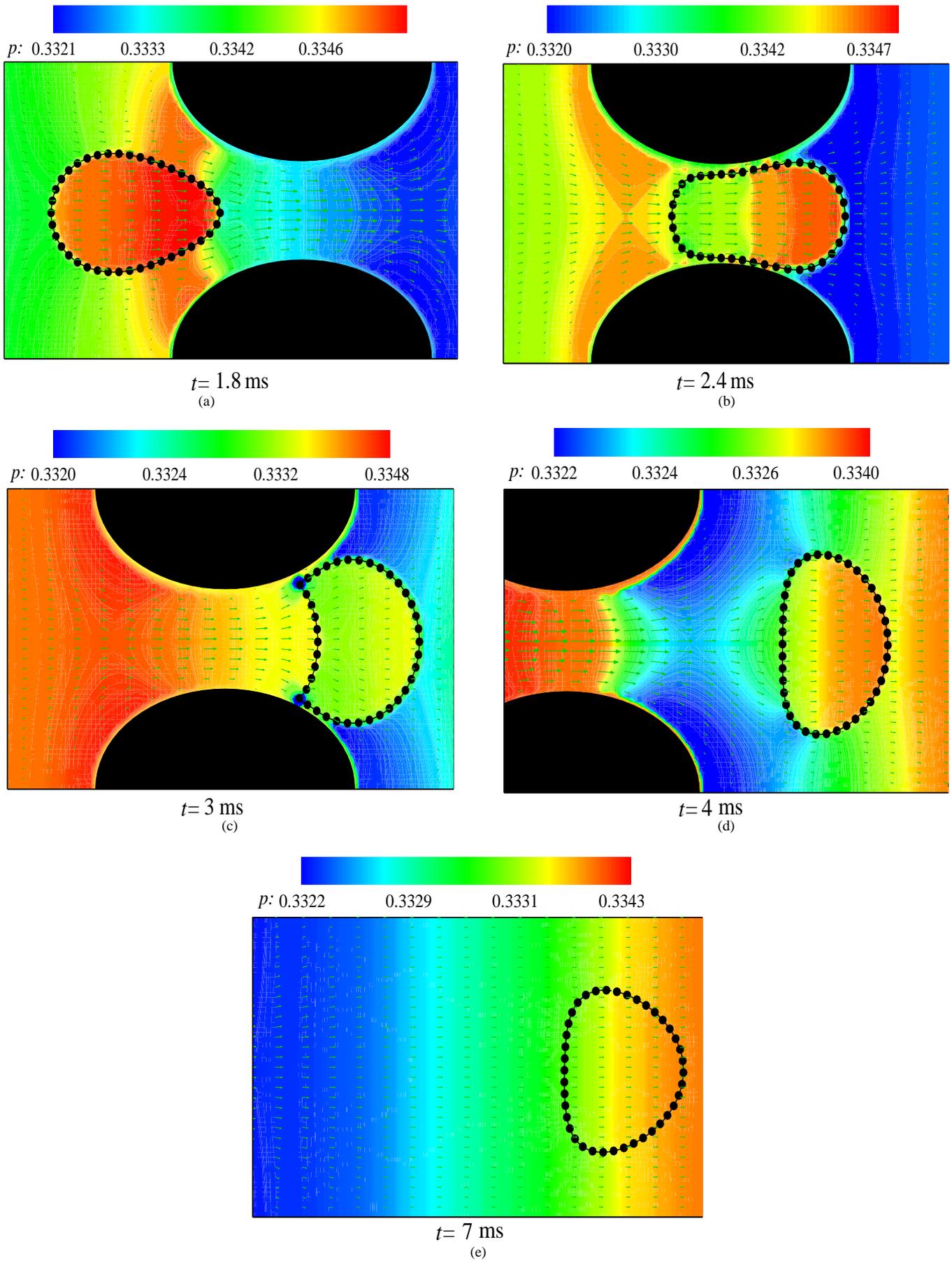


Figure 4. Motion of the body with a low flexibility passing stenosis at the times a) $t = 1.8$ ms, b) $t = 2.4$ ms, c) $t = 3$ ms, d) $t = 4$ ms and e) $t = 7$ ms.

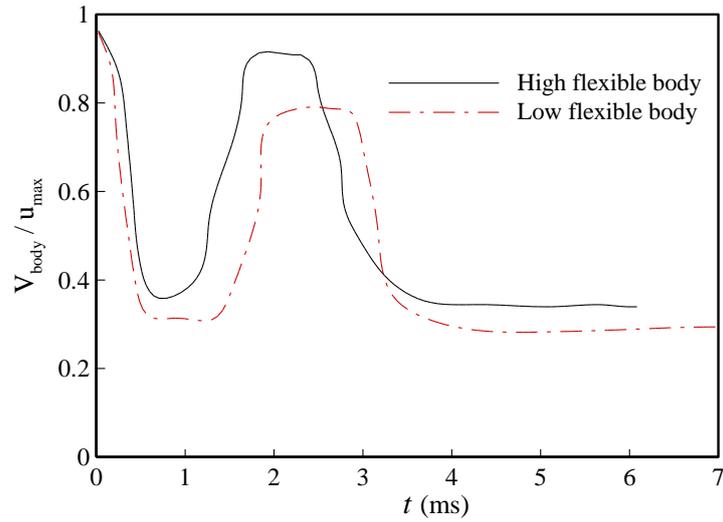


Figure 5. Comparison of velocity between high flexibility and low flexibility bodies.

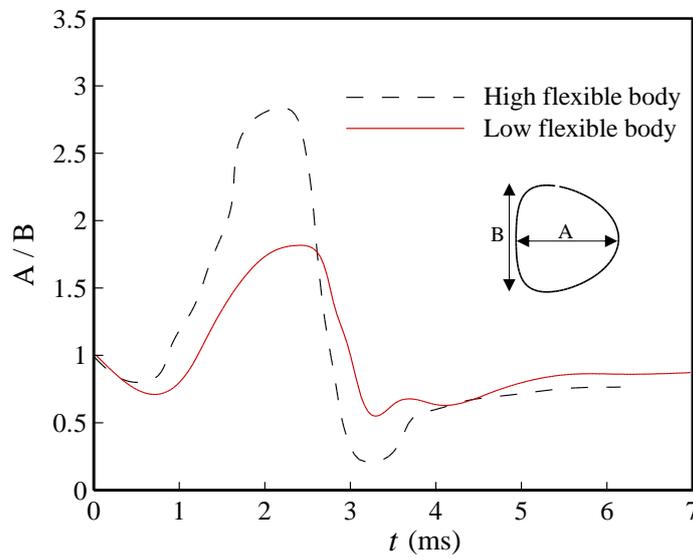
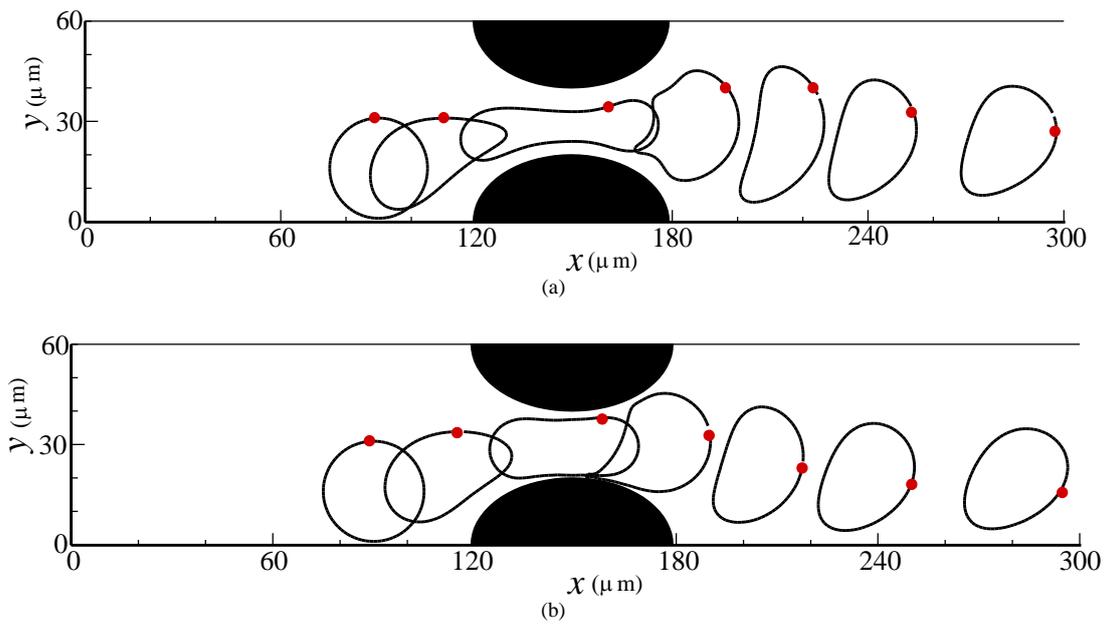


Figure 6. Comparison of A / B ratio of high elasticity body and low elasticity body



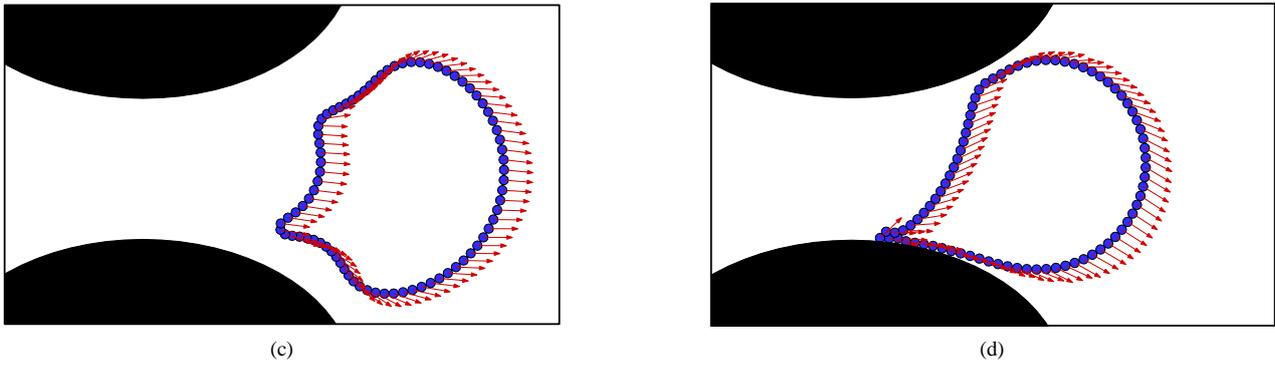


Figure 7. a) Tank -treading motion of immersed body with high flexibility; b) Tank -treading motion of immersed body with low flexibility; c) Lagrangian points velocity vector of immersed body with high flexibility at the threshold of stenosis; and d) Lagrangian point velocity vector of immersed body with low flexibility at the threshold of stenosis

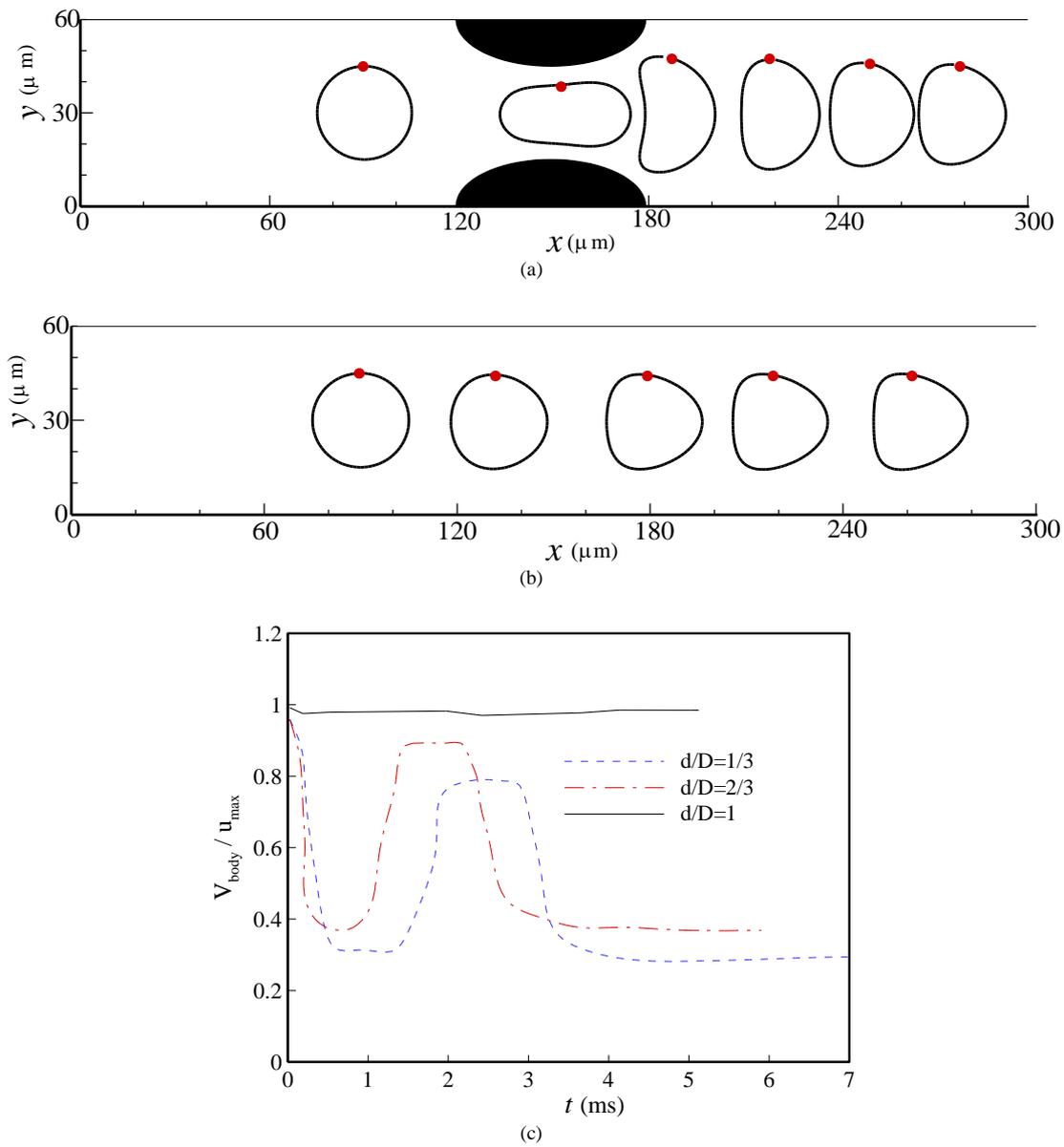


Figure 8. a) Deformation of body with low flexible for case $d/D = 2/3$, b) Deformation of body with low flexible for case without stenosis and $d/D = 1$, and c) comparison velocity for various sizes of stenosis.

5. Acknowledgment

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6. Appendix

The used Nomenclature in the manuscript is as follow as

c	particle streaming speed
\hat{e}_i	discrete particle speeds
E_s	elastic modulus
E_b	bending modulus
f_i	density distribution function
f^{eq}	equilibrium distribution function
f	force density of the fluid
L	Lagrangian force density
S_i	external force
\mathcal{E}	elastic energy density
N	total number of Lagrangian nodes
s	Lagrangian coordinate
u	fluid velocity
U	body velocity
X	position on the membrane
x	Eulerian coordinate
ρ	fluid density
w_i	weight coefficients in direction i
τ	relaxation time
δ	delta function
Δt	lattice time step
Δx	lattice spacing

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