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MD Simulation of Colloidal Particle Transportation in a Fiber Matrix

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Abstract: Surface glycocalyx, as a barrier to material exchange between circulating blood and body tissues, can be treated as a periodic square array of cylindrical fibers. Previous study treated the glycocalyx as porous media and simulated by continuum theory. However, it has recently been found that a relatively hexagonal fibre-matrix structure may be responsible for the ultrafiltration properties of microvascular walls. The fibre-matrix is an underlaying three-dimensional meshwork with a fibre diameter of 10∼12 nm and characteristic spacing of about 20 nm. The porous medium model does not consider the particle size, when the particle size is comparable to the fibre spacing, the porous medium assumption may not be appropriate to study the permeable characteristics of nanosize particle in such fibre-matrix structure.

Molecular dynamics (MD) simulation is a powerful method to simulate the fluid flow at the molecular level, it has been applied successfully in many fields including hydrodynamics and demonstrated surprising results at nanoscale which is different from their macroscopic counterparts. In this study we use MD to investigate the permeable characteristics of nano-particle in a quasi-periodic ultra-structure of the endothelial glycocalyx. As the first attempt, fibre-matrix is simplified as a two dimensional periodic system in which the colloidal particles, fluid solvent, fibers are all treated as atomic systems, and the study is focused on the effect of particle size on particle motion in fiber matrix.

1 Introduction

Microvessel permeability refers to material exchange between circulating blood and the body tissues. As a classical and important problem, people always try to figure out the ultrastructure of the inter-endothelial cleft and establish mathematical models for accurate description. Generally the structures include endothelial cell surface glycocalyx and junction strands in which glycocalyx plays an important role in the transport process, serving as molecular filtering (Fu, 2001). Recently a quasi-periodic fiber-matrix substructure in the glycocalyx was found using computed autocorrelation functions and Fourier transforms (Squire et al. 2001). The fibre-matrix is an underlying three-dimensional meshwork with a fiber diameter of 10∼12 nm and characteristic spacing of about 20 nm. However, in previous studies, the microvessel was considered as porous medium by Darcy law in which only one parameter is needed to describe the permeability, and the effect of detailed structure is typically ignored (Feng et al.,1998). Obviously, the porous medium model is not sufficient when the size of a particle is comparable to the fiber gap.

Molecular dynamics (MD) simulation is a powerful method to model the fluid flow at the molecular level (Rapaport, 1995). It has been successfully applied in many fields including hydrodynamics and demonstrated surprising results, such as slip boundary and density fluctuation, etc. (Travis and Gubbins 2000; Fan et al., 2002; Chen et al. 2005). Conventional fluid mechanics, which has many assumptions (such as no-slip boundary condition), may not be appropriate to describe the particle motion in nano-scaled enclosure. Numerical simulation has shown divergences aris-

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ing from the continuum analysis when the sphere moves in a fluid in the vicinity of a solid wall (Vergeles et al. 1995); and for confined brownian motion between two walls, deviations from the Stokes-Einstein law were also observed by experiment (Faucheux and Libchaber, 1994). The motion of colloidal particles (including sedimentation and diffusion) in fluid has been attracting people's attention for many years (Vergeles et al. 1995; Drazer et al. 2005). In this study, as the first attempt, the fiber-matrix is simplified as a two dimensional periodic system in which the colloidal particle, fluid solvent, fibers are all treated as atomic systems. The objective is to study the effect of particle size on transport properties and the effect of the fibers on particle motions, which is crucial to study the permeability of microvessel.

2 Numerical Method

A schematic view of the idealized brush structure of glycocalyx is shown in Fig. 1, the fibre-matrix is an underlaying three-dimensional meshwork with a fibre diameter of 10∼12 nm and characteristic spacing of about 20 nm, it is an approximately regular hexagon, therefore the spacing CD = 8nm and fibre diameter d = 12nm. Between the two rows of the fibres, there exists a channel which is indicated between lines m1 and m2. This channel would be the main path that the colloidal particle passes through. In order not to make the particle stagnated at the fibre, the particle is placed at a offset position from the central line of the middle row of fibres, as shown in Fig. 2.

The Lennard-Jones (LJ) potential is used:

$$\phi(r_{ij}) = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right], \qquad (1)$$

where $r_{ij} = \left|_{irj}\right|$, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, the parameter ε governs the strength of the interaction, σ defines a length scale, r_c is the cutoff distance, and corresponding force is $F = -\nabla\phi$. The variables, such as length, mass and energy, are dimensionless and normalized by σ, m, and ε, respectively. The non-dimensional parameters are the same as those proposed by Rapaport (1995). The potential is truncated at r_c = 2.2 in this study. The atoms representing the colloidal particles and the fibers are fixed at the lattice sites. The colloidal particles are composed of atoms of mass m_f = 20. The fibers are assumed to be rigid and at rest, while the motion of colloidal particles are treated as rigid body and the total force are calculated by summing the forces acting on the atoms representing the colloidal particles. The mainstream velocity is set as U_0= 0.3 while random velocities and periodic boundary conditions are applied. To improve the computational efficiency, cell subdivision and linked-list approach are adopted.

3 Results and Discussion

The computational code was validated elsewhere (Chen et al. 2005). The density is set as 0.8 (particle/area). Colloidal particles with three different radius, 2.5nm, 3.0nm and 3.8nm, are investigated and scaled by 0.34nm (the diameter of Argon atom), then the dimensionless radius is 7.35, 8.82 and 11.18, respectively. These three sizes of particle are composed of 137, 193 and 305 atoms respectively. One fiber is composed of 777 atoms, with dimensionless radius 17.65. The diameter of the colloidal particles is close to the fiber space. There are total 42500 atoms in the fluid domain, and the computation domain is $-176.47 \leq x \leq 176.47$, $-76.41 \leq y \leq 76.41$. It is found if the offset distance Δd is 0, the colloidal particle will attach to the most left fiber. In order to make the particle pass through the matrix, the offset distance Δd is set to be 5.0. Typical configuration is shown in Fig. 2. The colloidal particles are set at rest initially.

Fig. 3 shows the snapshots of the colloidal particles of three different radius with and without fibers at the same time t = 738 (dimensionless). From the figures, we can find that fibers have significant effect on the motion of colloidal particles with different radius. Without fibers, there is no big difference for the colloidal particle with different radius. With fibers, the colloidal particle of 2.5nm radius has successfully passed through the fibers, the colloidal particle of 3.0nm radius is stagnated between the fibers, and the colloidal particle of 3.8nm radius is just attached to the

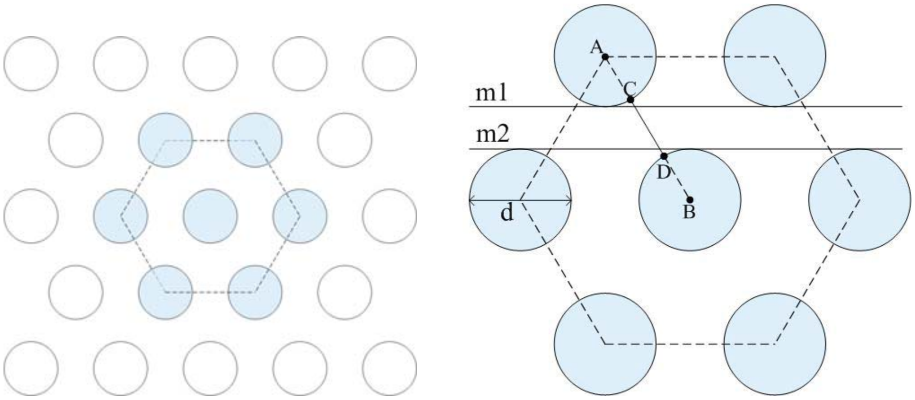


Figure 1: Schematic view of the fiber-matrix. CD = 8nm, d = 12nm.

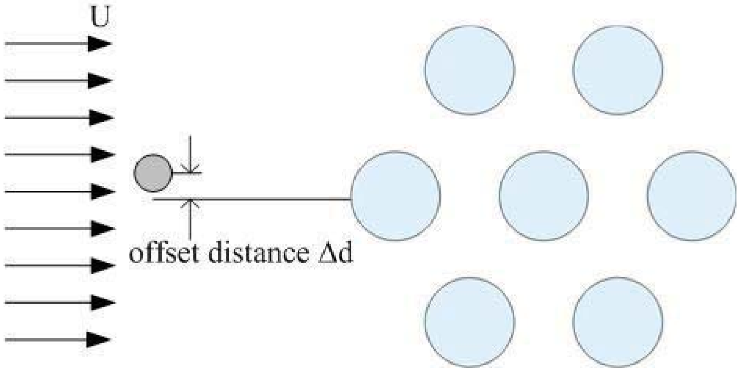
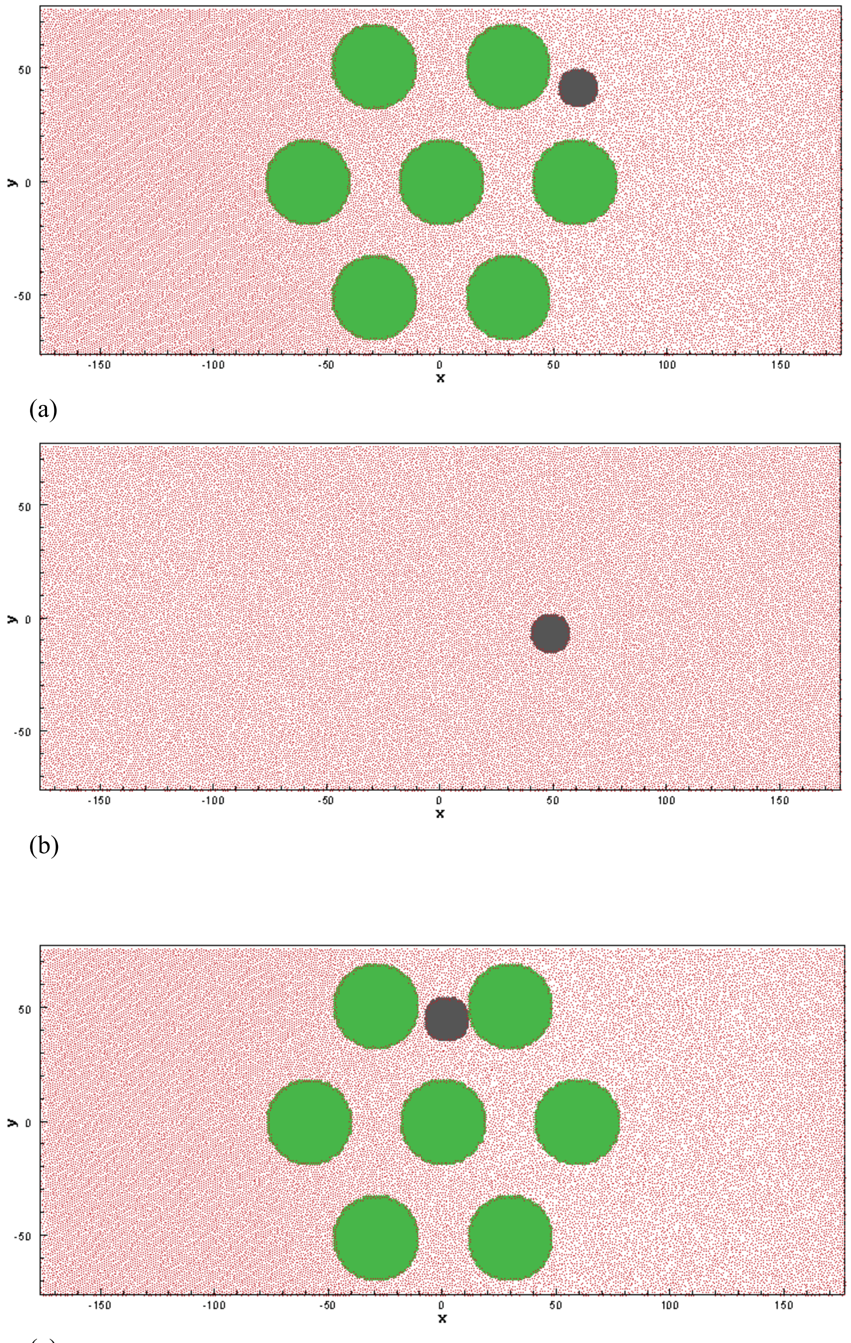


Figure 2: Schematic view of the problem for a colloidal particle with the fiber matrix.

most left fiber. It is obviously that the matrix would block bigger particles. After a long trip, the particles with 3.0 nm and 3.8nm radius eventually pass through the matrix at t = 1818, as shown in Fig. 4. The traveling time of bigger particle is much longer than that of smaller one.

To thoroughly investigate the effect of particle size on the permeability of fiber matrix, Figs. 5-10 show the trace of the colloidal particle passing through the domain with/without fiber matrix. It is interesting to note, even without fiber matrix, the particle trace deviates in y-direction, most likely it is due to the thermal fluctuation. The bigger particle seems more stable and the deviation is smaller. For particle of 2.5nm radius, as shown in Figs. 5-6, the matrix seems not hinder the particle motion in x-direction, and even makes the particle move faster than that without matrix. It is not surprised, since the volume flow rate is the same, with narrow cross-section area the flow rate would be higher. Before the particle reaches the middle fiber (x = 0), it moves slowly compare to that without matrix; when it approaches the middle fiber (x = 0), it may stagnate on the fiber for a while, then move out of the matrix with higher speed. In y-direction, the particle oscillates due to the variation of the flow channel. With increasing the particle radius to 3.0 nm, the matrix blocks the particle seriously. In x-direction, the particle moves much slower than that of without matrix, and the stagnation of particle is quite long that results in a plateau in the x-t diagram of Fig. 8.

When increasing the radius to 3.8nm, the particle attaches to the first fiber for a while, it experiences stick-slip motion, and then is squeezed out of the matrix. This behavior was also found by Drazer et al. (2005) when they investigated the motion of a colloidal particle in nanoflows. Based on the x-t curves, we can roughly estimate that the time ratio for the colloidal particles with different radius to



(a)

(b)

(c)

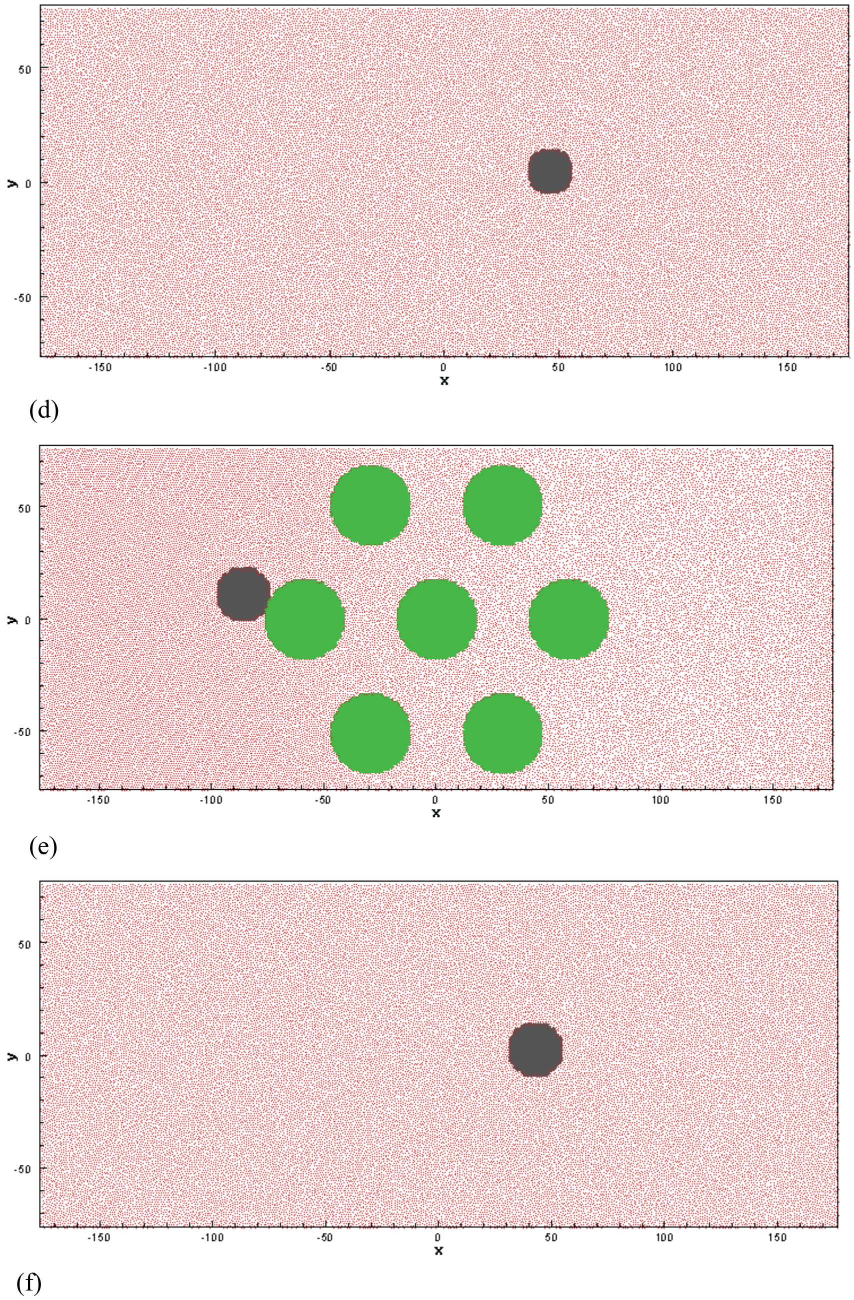
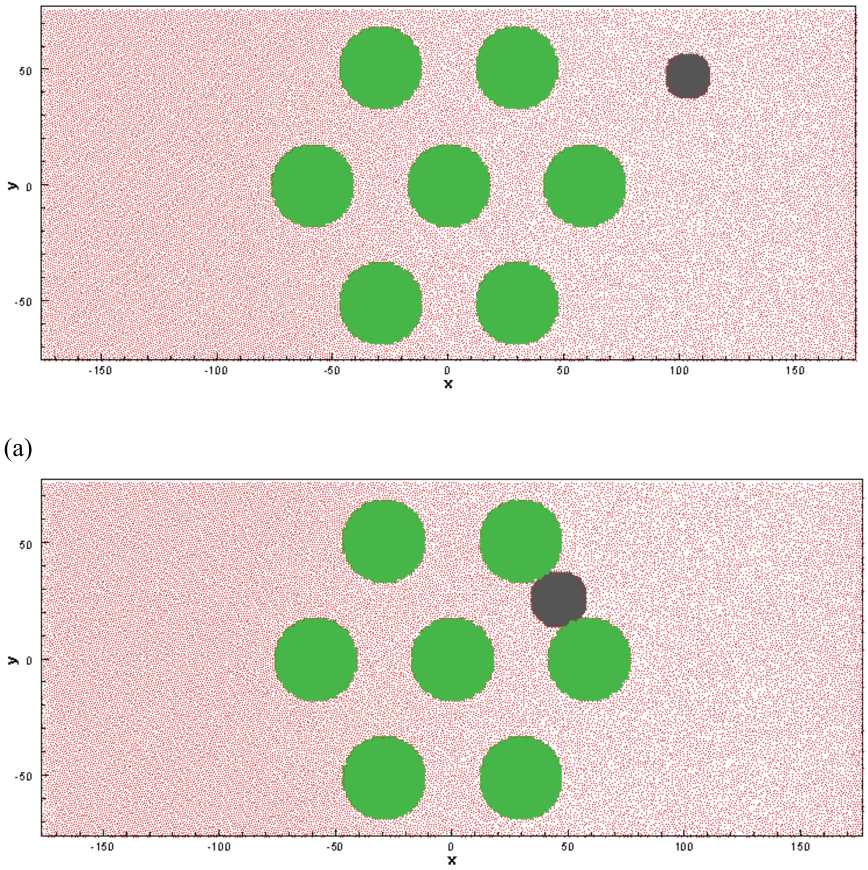


Figure 3: Snapshots of the transportation of colloidal particle in the flow domain with/ without fibers at the same time t = 738. (a) Radius of 2.5nm with fiber-matrix; (b) radius of 2.5 nm without matrix; (c) radius of 3.0nm with matrix; (d) radius of 3.0nm without matrix; (e) radius of 3.8nm with matrix; and (f) radius of 3.8nm without matrix.



(a)

(b)

Figure 4: Snapshots of the transportation of colloidal particle in the flow domain with/ without fibers at the same time t = 1818. (a) Radius of 3.0nm with matrix; (b) radius of 3.8nm with matrix.

transport through the fiber matrix is about 1: 2: 2.5.

Generally, in the presence of fibers, the colloidal particle moves forward in a wavelike or oscillatory way, with main channel between lines m1 and m2 as shown in Fig. 1. To quantify the effect of particle size on permeability, we define the permeability as

$$\text{Permeability} = \frac{\text{particle displacement in x direction with fibres}}{\text{particle displacement in x direction without fibres}} \tag{2}$$

Then the permeability is 1.12 at particle size of 2.5 nm; 0.45 at particle size of 3.0 nm; and 0.44 at particle size of 3.8 nm. The reason that the permeability is higher than unity at particle size of 2.5 nm is due to the higher flow rate caused by the narrowing flow channel.

4 Conclusion

The motion of a colloidal particle passing through a fiber matrix was investigated by molecular dynamics. It has been found that the particle size has significant effect on the permeability. For the colloidal particle with radius 2.5nm, fibers have little effect in x direction. Bigger colloidal particles experience a much slower motion, due to the block of the fibers. Stick-slip motion occurs for bigger particles. The particle can stay at a point for a quite long time then move forward. This can help us to understand the mechanism of permeability.

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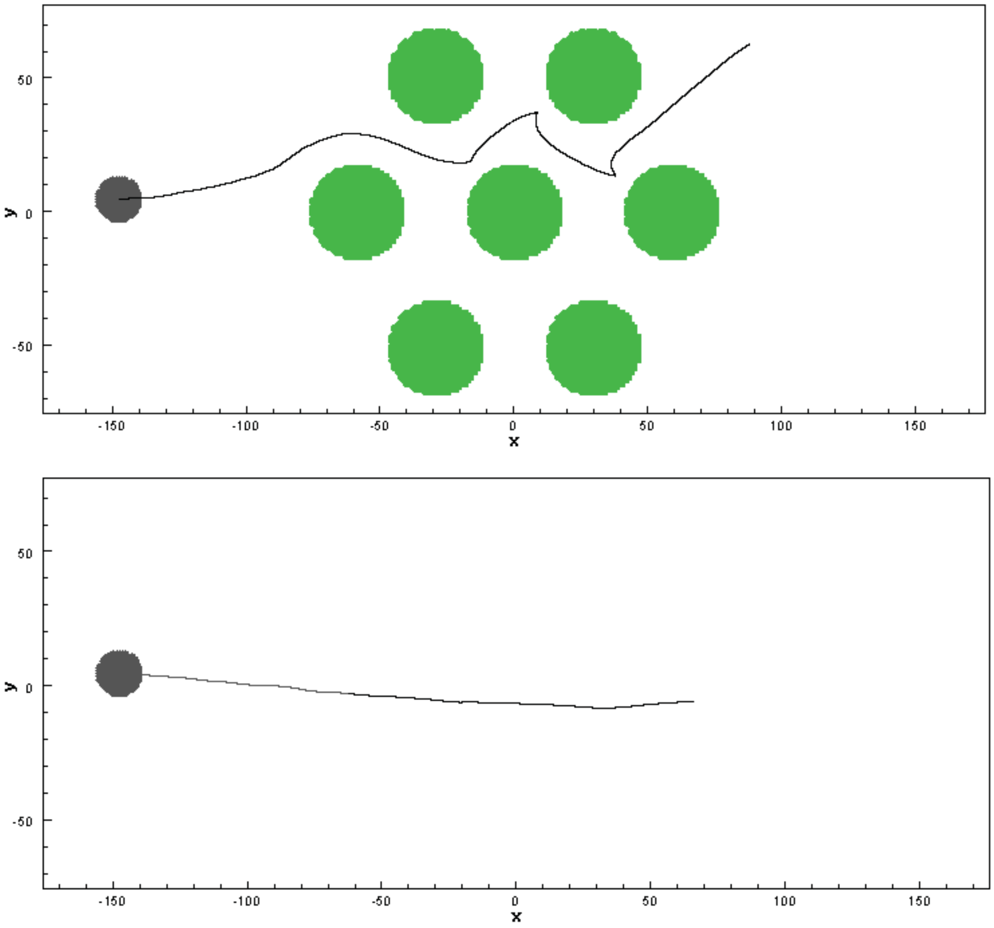

Figure 5: The trace of the colloidal particle with radius 2.5nm, with and without fibers.

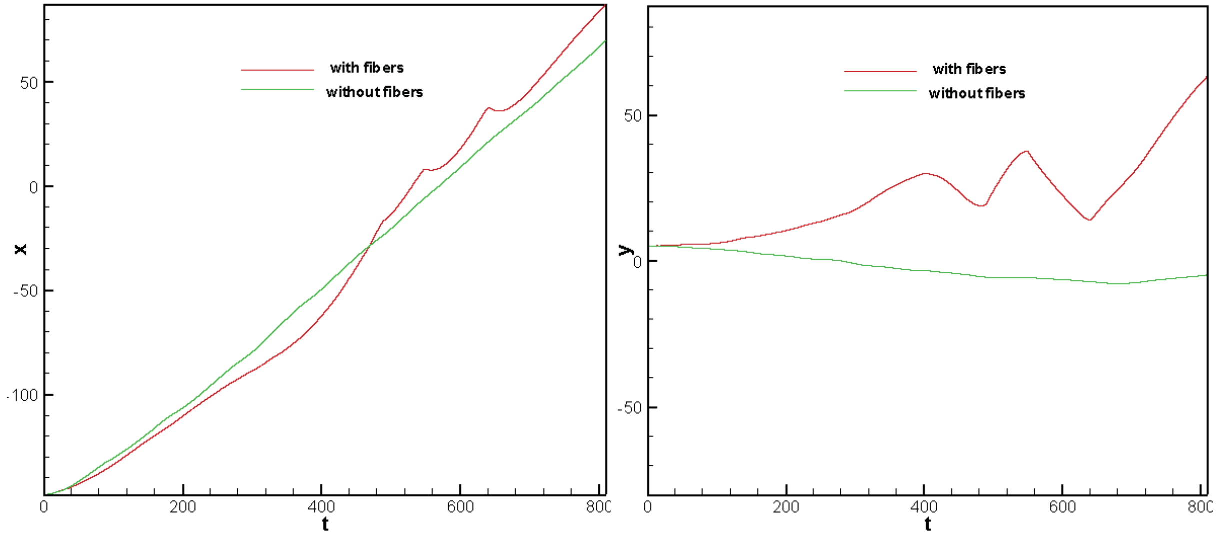

Figure 6: x-t and y-t curves for the colloidal particle of 2.5nm with and without matrix.

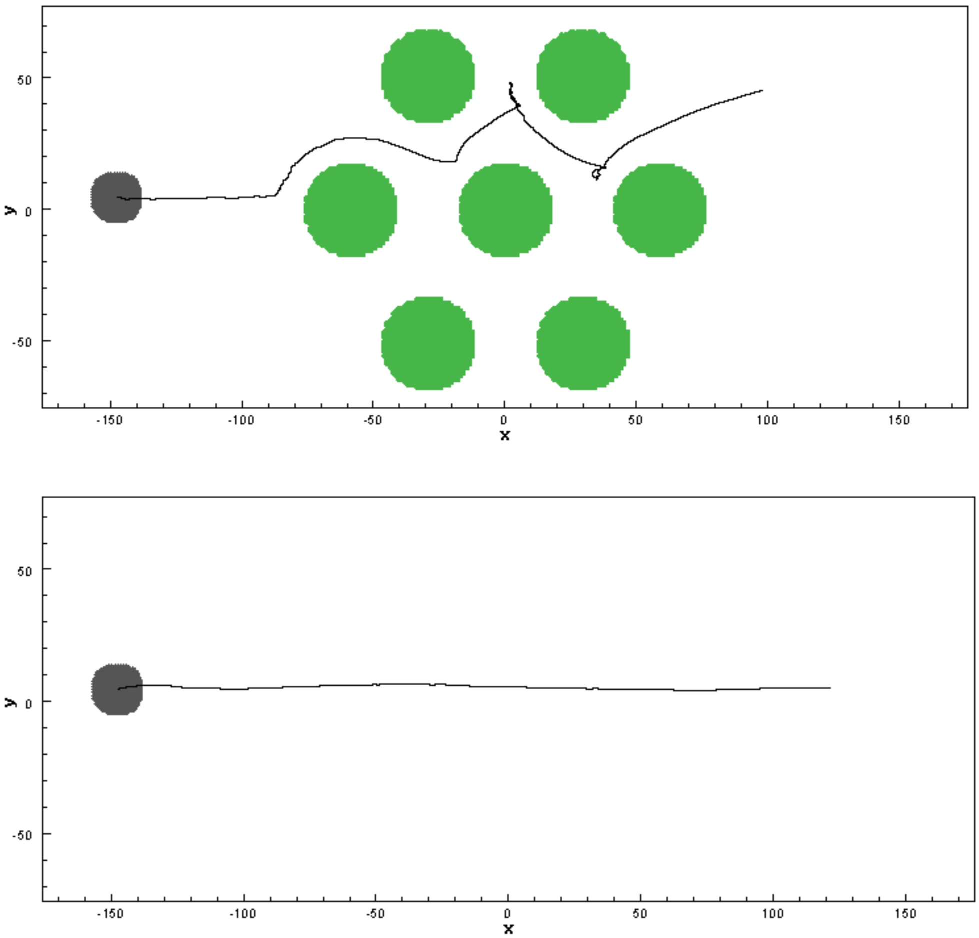

Figure 7: The trace of the colloidal particle with radius 3.0nm, with and without fibers.

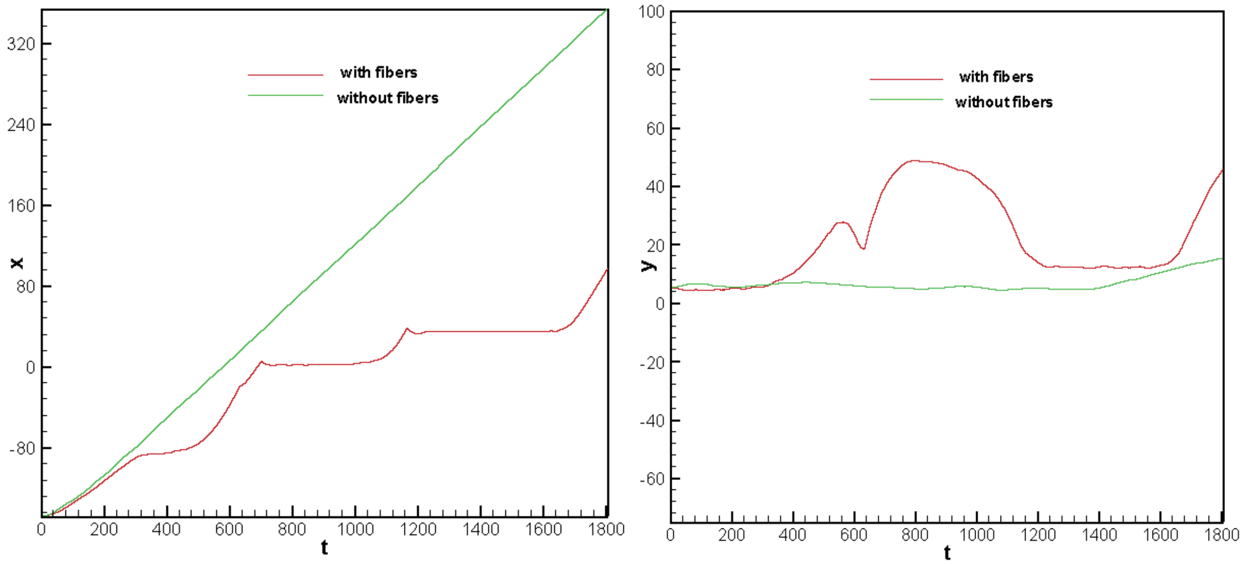

Figure 8: x-t and y-t curves for the colloidal particle of 2.5nm with and without matrix.

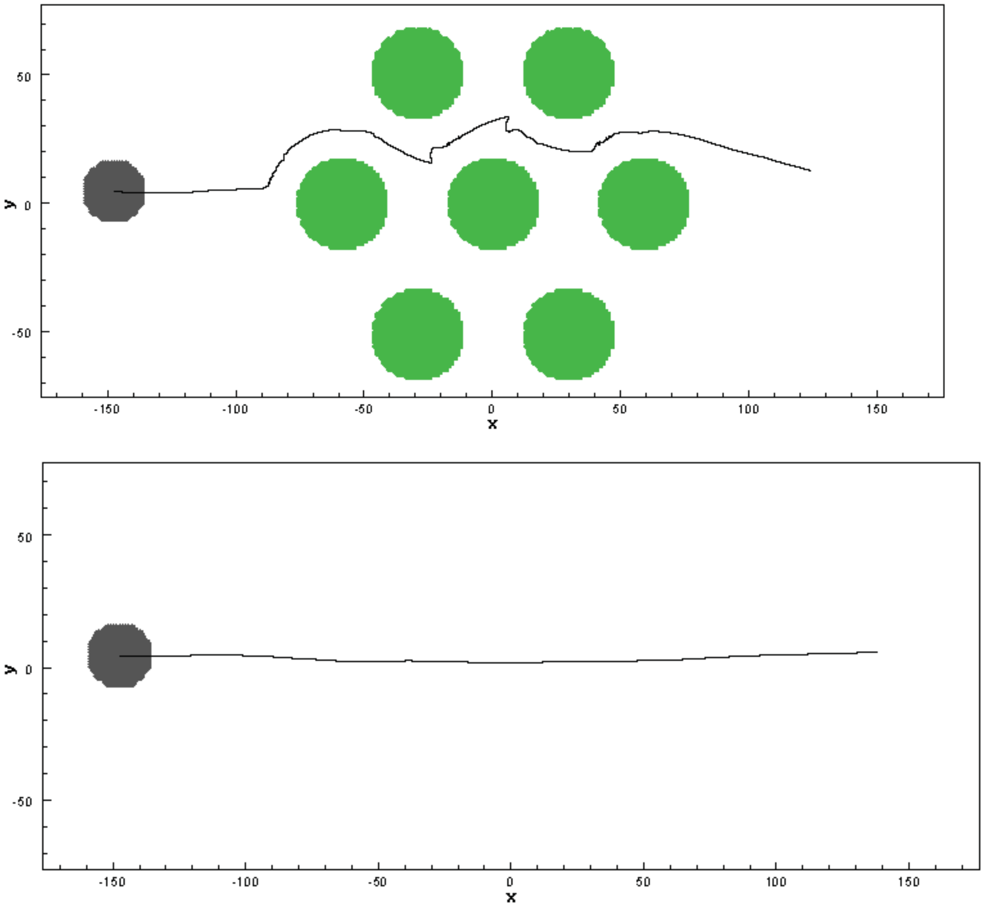

Figure 9: The trace of the colloidal particle with radius 3.0nm, with and without fibers.

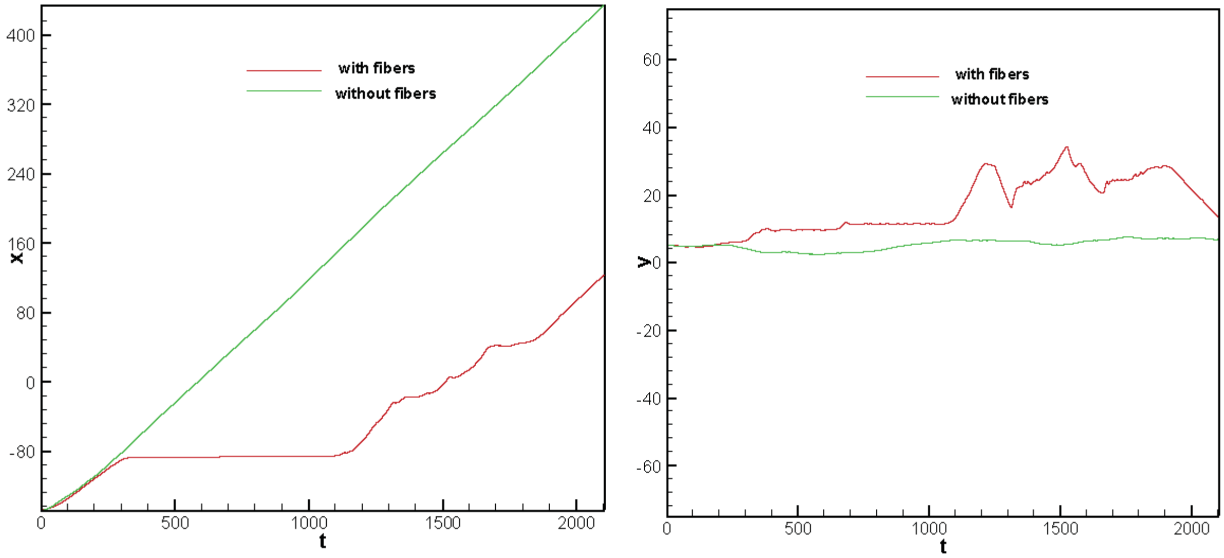

Figure 10: x-t and y-t curves for the colloidal particle of 3.8 nm with and without matrix.

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