Canadian Science Publishing | Canadian Journal of Physics

Active particle aggregate on complex bubble surfaces

Journal:	*Canadian Journal of Physics*
Manuscript ID	cjp-2017-0686.R2
Manuscript Type:	Article
Date Submitted by the Author:	21-Dec-2017
Complete List of Authors:	Akguc, Gursoy; Izmir Ekonomi Universitesi, Fizik
Keyword:	soft matter, Brownian motion, active particles, simulation, aggregate
Is the invited manuscript for consideration in a Special Issue? :	33rd International Physics Conference of Turkish Physical Society

Active particle aggregate on complex bubble surfaces

Gursoy B. Akguc[1, *]

[1]*Department of Physics,*

Izmir University of Economics, 05400, Izmir, Turkey

(Dated: May 28, 2018)

Abstract

Recently, colloids are shown to form complex structures on bubble surfaces on demand. With the help of a high power pulse laser shining on a thin water film, water bubbles can be formed and heat unbalance creates a convective flow which carries colloids on to the surface of this water bubbles to form aggregates.Here, active particles are studied in a similar set up and conditions are laid out to form aggregates on water bubble surfaces. The effect of motility and chirality of active particles on to form aggregate are discussed. The simulation results obtained here hopefully helps the experimental endeavors in future.

PACS numbers:

*Electronic address: gursoy.akguc@ieu.edu.tr

I. INTRODUCTION

Recently, rich complex behavior of colloidal particles has been shown by looking at crystal formation on the surface of bubbles with the help of a nonlinear laser sources.[1] A similar Brownian type of model is valid for active nano particles like the colloidal particles. In this paper, active nano particles under similar set up have been examined using numerical simulations in two dimensional model. There are recent works about active particles form aggregate so called life crystals,[2–4] but those set up requires an external potential to form aggregates. Here a flow forms and deforms aggregates, it is a self-organized system where particles form and deform on demand in the order of seconds.

Active nano particles different than colloids in addition to have motility and chirality in their motion.[5] A model of e-coli bacteria for instance can be considered having motility and chirality.[6] Active particles have inherent energy (such as pulling water in and pushing out by squeezing) hence system can not be considered an equilibrium statistical system. As a matter of fact the standard rules of thermodynamic and statistical mechanics are not applicable here.[7]

Recently, motion of microscopic life forms in water and laser manipulations of them attracts a lot of interest. For instance, it has recently been shown the wave guide behaviour emerging from bacteria-light non-linear interaction.[8] A powerful pulse laser in reference [1] is used for colloids but its aim is to form the convective flow to carry active particles on to the surfaces of water bubble.

A system of equations for heat and momentum balance in water is solved to get velocity profile at each point on liquid surface. A Finite Element Method (FEM) code is used for this part. No particle-fluid interaction is implemented in this study but there are ways to add this effect for instance multiparticle collision method may be one of them.[9–12] Than Langevin equation is solved with model motility and chirality parameters combined with the already obtained fluid flow. A hard-body interaction among particles is assumed.[13, 14] Aggregate formation is observed though not full scale due to both computational restrictions and the simplicity of inter particle forces. Yet it is quite interesting to see formation of crystal like aggregates formed without any help of external potential but just the convective flow.

In the next section, the numerical methods employed in calculations are discussed in details. The simulation parameters and three different type of motion and their aggregate

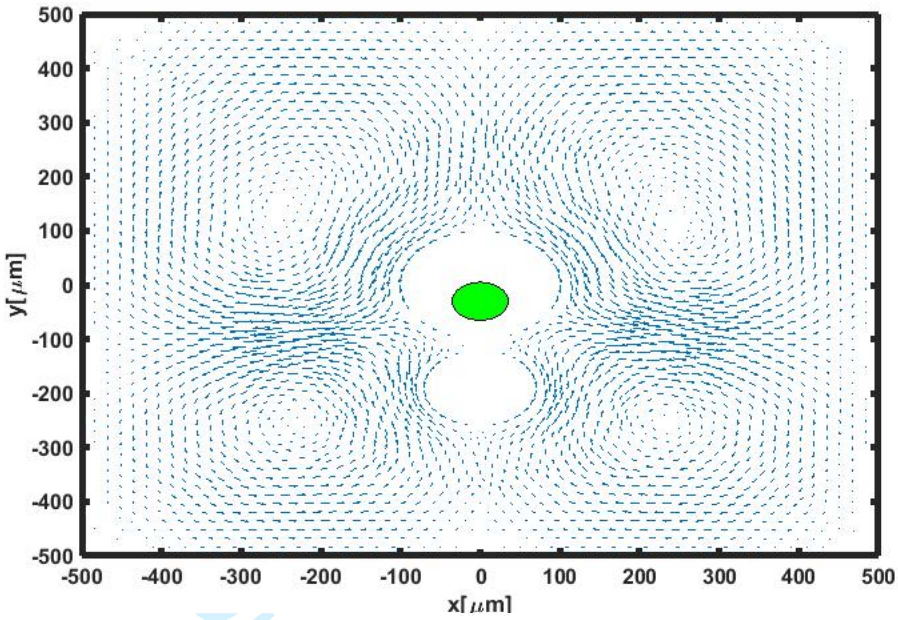

FIG. 1: Bubble set up and water flow around it.

formations described in section III and finally conclusion in section IV is given.

II. MODEL AND METHOD

In the simulation, thin water film between two glass substrate is modeled with a two dimensional non-isothermal fluid. As shown in Fig. 1 two bubbles located with radii $r_1 = 100\mu m$ and $r_2 = 70\mu m$ with laser source near the lower part of central bubble shown as solid circle in the figure. The channel width is given as $d_{12} = 20\mu m$. Water flows due to temperature difference between edges of the square box and the lower half of central bubble surface in the center. The flow pattern is obtained by solving Navier-Stokes equation with coupled to the heat equation. The coupling depends on temperature difference between bubble surface temperature which is assumed $300K$ and edges at $293K$. When flow velocity is found it is interpolated to each particles positions in second part of calculations.

As shown in Fig. 2a, an amount of 225 particles has been prepared initially to start the motion near the bubbles. Water molecules kick active particles with each has radius $r = 1\mu m$. This can be modelled as a Langevin equation. It is a standard approximation to take inertial term zero near friction term due to high viscosity effect at nano scale.

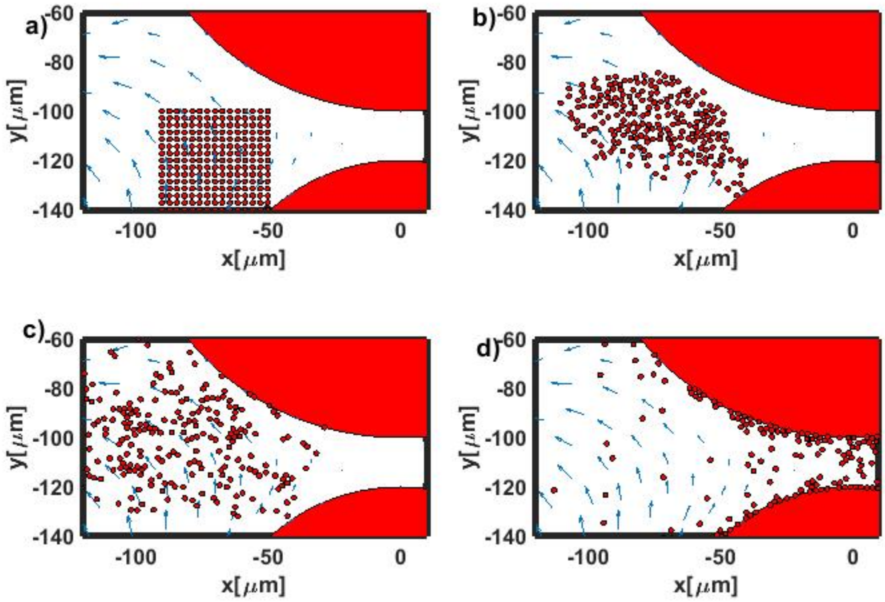

FIG. 2: a) initial configuration b) colloids with no motility and chirality c) active particles with chirality d)active particles with motility only.

Active nano particles in water can be described with the following set of equations in two dimensions,

$$\frac{d}{dt}\varphi(t) = \Omega + \sqrt{2D_R}W_T$$
$$\frac{d}{dt}x(t) = v\cos(\varphi(t)) + \sqrt{2D_T}W_x$$
$$\frac{d}{dt}y(t) = v\sin(\varphi(t)) + \sqrt{2D_T}W_y \quad (1)$$

where D_R and D_T rotational and translational diffusion constants. For water analytic results of sphere in 3D flow at low Reynolds number is used in calculations, i.e. specifically $D_R = 6DT/(8R^2)$ and $D_T = DT = kBT/\gamma$ where $\gamma = 6\pi R\eta$. The effect of water molecules on nano particles are represented by Wiener processes in above equation given by W_x, W_y, and W_T corresponds to a random number drawn from uniform Gaussian distribution. Here the velocity v is called motility to represent directed motion of active particle and Ω represent chirality. The boundary conditions on bubble surfaces and square box surfaces are implemented such that no motion allowed out of water. Hard body interaction is also important so that aggregate formation can be observed. Each particles has $1\mu m$ radius and

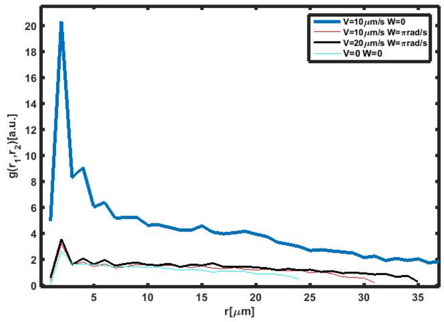

FIG. 3: Pair correlation function of passive particles and active particles with motility and active particles with chirality.

they can not penetrate or pass through each other.

III. ACTIVE PARTICLE AGGREGATION

The possibility of active particle aggregation between two water bubbles in a thin water film is investigated. The water flow drags active particles towards the channel between two bubbles. In Fig.2b active particles with no motility and chirality (equivalent to the case of colloids) have been shown after $t = 10sec$ of simulation time. In this case particles follow flow streamline due to drag effect. There is no appreciable aggregate formation partly due to no other force added and flow is unchanged with addition of particles. In Fig. 2c, the particles with chirality are shown and they rotate with an angular velocity given by $w = \pi rad/sec$ as well as stochastic motion due to the kicks of water molecules. A partial crystal formation is observed due to particles rotates. And finally in the case Fig. 2d the active particles with motility of $10\mu m/sec$ to the right are shown after $t = 10sec$ of propagation and they show the strongest effect of forming life crystal due to crowding at the channel.

To quantify the crystall formation the pair correlation function $g(r)$ for corresponding three cases has been calculated. Pair correlation function shows the probability of finding the center of a particle for a given distance from the center of another particle. It is a measure of crystalline order in the system. In Fig. 3 the case with only motility show strong indication of crystal formation.[15] The other cases show less correlations. It is possible to get aggregation with active particles even further by simulating large numbers of particles and include effect of change of flow.

IV. CONCLUSION

It has been shown that active particles with motility tends to form aggregates at the bubble surfaces on two dimensional thin water film. The other cases where there is chirality and motility the effect is comparatively less which can be seen from pair correlation function. The reason is due to crowding at the channel and constriction of the movement by the boundaries. As soon as the laser turned off water flow towards the bubble will stop and particles at the channel will leave that region as well. All this happens under few seconds. It is self organized for the given boundary configuration. These findings may have applications in drug delivery and fight against diseases as well as understanding biological systems better. It is also important to understand statistical behavior of active particles as unequilibrium statistical systems. The effect of particle-fluid interactions, different type of species in flow (binary systems) more variety to the flow and more complex inter particle interactions are the future directions one can go for this system.

[1] S. Ilday, G. Makey, G. B. Akguc, Ö. Yavuz, O. Tokel, I. Pavlov, O. Glseren and F. Ö. İlday, NATURE COMMUNICATIONS, 8, 14942 (2017).

[2] S. Jahanshahi, H. Löwen, B. Hagen, PHYSICAL REVIEW E 95, 022606 (2017).

[3] W. Yang W. Vyacheslav, R. Misko, J. Tempere, M. Kong, and F. M. Peeters, PHYSICAL REVIEW E 95, 062602 (2017).

[4] A. Zöttl and H. Stark PRL 112, 118101 (2014).

[5] H. Behringer and R. Eichorn, THE JOURNAL OF CHEMICAL PHYSICS, 137, 164108 (2012).

[6] A. P. Petroff, Xiao-Lun Wu and A. Libchaber, PRL 114, 158102 (2015).

[7] F. Smallenburg and H. Löwen PHYSICAL REVIEW E 92, 032304 (2014).

[8] A. Bezryadina, T. Hansson, R. Gautam, B. Wetzel, G. Siggins, A. Kalmbach, J. Lamstein, D. Gallardo, E. J. Carpenter, A. Ichimura, R. Morandotti, ve Z. Chen, PRL 119, 058101 (2017).

[9] I. O. Götze ve G. Gompper, PHYSICAL REVIEW E 82, 041921 (2010).

[10] P. Mueller and J. Thiffeault PHYSICAL REVIEW FLUIDS 2, 013103 (2017).

[11] D. Perumal And A. Dass ALEXANDRA ENGNEERNG JOURNAL, 54, 955-971 (2015).

[12] A. Zöttl and H. Stark 2014, PRL 112, 118101 (2014).

[13] C. Bechinger, R. Leonardo, H. Löwen, C. Reichhardt, S. G. Volpe, and G. Volpe REVIEWS OF MODERN PHYSICS, VOLUME 88, 1., (2016).

[14] Volpe G, and S. G. Volpe 2014, AMERICAN JOURNAL OF PHYSICS 82, 659 (2014).

[15] J. Stenhammar, C. Nardini, R. W. Nash, D. Marenduzzo, A. Morozov PRL 119, 028005 (2017).