Direct numerical simulation of the self-assembly of colloidal particles in a micro-channel

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Summary

In recent experiments, clustering of droplets of size 5μm and 50μm have been observed in unique microfluidic devices. Depending on the flow condition, number of droplets, etc., particles self-assemble into different 2D or 3D structures, yet the mechanism for such dynamics is unclear. Here, direct numerical simulations using the Immersed Boundary Method has been performed, assuming neutrally buoyant, rigid particles transported in a channel flow. A Lennard-Jones-like interaction potential is introduced to model the overall attraction and repulsion among particles. Results show that, for four particles, a planar diamond is formed under weak potential while a 3D tetrahedron is formed under strong potential, which agree qualitatively well with experiements.

Keywords: Microfluidics, colloidal particles, self-assembly, colloidal interaction potential, direct numerical simulation

1. Introduction

In the field of colloidal science, much progress has been done on the synthesis of complex building blocks mimicking molecular structures to elaborate innovative materials. The constraint, however, is that the rates at which these building blocks are obtained are far too low to approach industrial applications. The recent discovery by the group at ESPCI, France [1], of a new hydrodynamic mechanism that reorganizes droplet clusters into well-defined configurations during their transport in microfluidic devices may potentially unlock this bottleneck. It is observed that, once a number of droplets are produced in the micro-channel, they can form 2D or 3D clusters, including chains, triangles, diamonds, tetrahedrons, heterotrimers, etc. With chemical or magnetic anisotropies, directional bonding can also be enabled [1]. Then the questions remain as what attribute to such self-assembly mechanism, and how to deepen and harness it under high throughput conditions.

2. Numerical set-up and results

The goal of the present work is to simulate the clustering of neutrally-buoyant, monodisperse particles in a channel flow and examine the effect of an interaction potential on the final configuration. In the experiments in [1], the droplet Capillary number is exceedingly small (of order 10^{-5}); hence, very little deformation is expected and the droplets are simulated as rigid spheres using a second-order accurate Immersed Boundary Method, see e.g. [2]. The particle Reynolds number is order 10^{-2} to 10^{-3}; to speed up the computation without changing the result a value of 0.03 is used. The channel height is three times the particle diameter. The flow is governed by the incompressible Navier-Stokes equations, discretized using a second-order finite volume method and advanced in time by a third-order Runge-Kutta scheme. 16 grid points per particle diameter are used, and grid independence has been verified with higher resolution.

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In addition to the viscous force due to the surrounding flow and collisions if hitting the wall, the particles experience an interaction potential mimicking attractive/repulsive forces, written as

$$E^n_{i,j} = \epsilon[(r_m/r_{i,j})^{12} - 12/n(r_m/r_{i,j})^n] \tag{1}$$

where $E^n_{i,j}$ is the potential between particle i and j based on an integer parameter n, ϵ is the potential well depth, $r_{i,j}$ is the distance between particle centers, r_m is the equilibrium distance where the potential is minimum. By varying these non-dimensional parameters, we alter the strength and range of the potential and study the particle motion in different conditions.

Figure 1 shows snapshots from numerical simulation of four particles under weak or strong potential, in comparison with experimental observations. In the case of plot (a), the parameters in Equation (1) are chosen to yield a short-range potential where particles separated by one particle diameter away cannot feel each other. In this case, a planar diamond is formed and transported steadily thereafter. This agrees qualitatively well with experimental result shown in plot (c), where 50μm droplets self-assemble into 2D diamonds. Plot (b) corresponds to to a potential much stronger and longer in range. As a result, a compact tetrahedron is formed, which is consistent with plot (d) where smaller droplets are in a highly adhesive environment. In our final contribution, we shall examine the relative particle velocities and the interactions leading to the different clusters. The effect of the slip at the droplet interface will also be considered as possible control parameter.

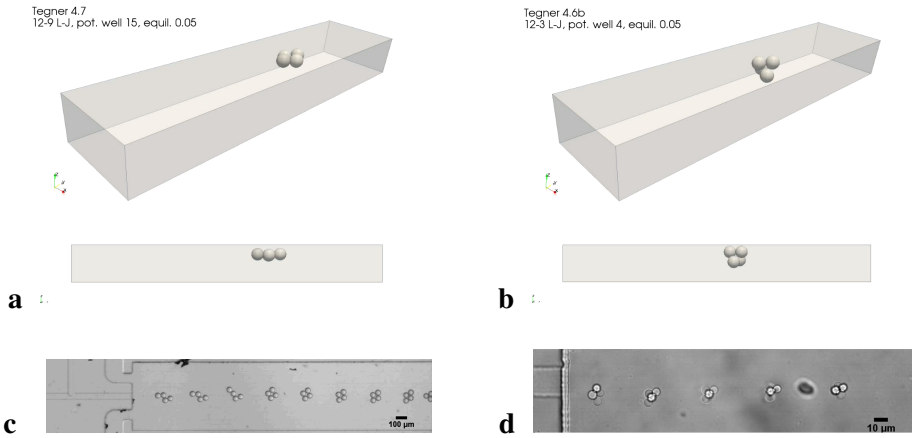

Figure 1. Clustering of four particles. (a) "Weak" potential characterized by r_m=1.05, ϵ=15, n=9. (b) "Strong" potential characterized by r_m=1.05, ϵ=4, n=3. Initial shape of the particles is a "chain" similar to that in (c). The lower view is from the side. (c)(d) Experimental observation of clustering of 50μm and 5μm droplets, viewing from top of the channel.

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