The swapping-trajectory effect: lattice evolution and buckling transition in wall-bounded hydrodynamic crystals

Jerzy Blawdziewicz\textsuperscript{1} and Eligiusz Wajnryb\textsuperscript{2}

\textsuperscript{1}Department of Mechanical Engineering, Texas Tech University, Lubbock, TX 79409, U.S.A.

\textsuperscript{2}Institute of Fundamental Technological Research, Warsaw, Polish Academy of Sciences

E-mail: jerzy.blawdziewicz@ttu.edu

Abstract.

We analyze novel structural transformations in perturbed periodic square monolayers of microspheres in parabolic flow between two parallel walls. We find that a perturbed monolayer is initially stabilized by the swapping-trajectory mechanism that causes the particles to fluctuate between faster and slower streamlines in such a way that particle collisions do not occur. The fluctuations slowly decay in time, and the array achieves nearly perfect rectangular order. Surprisingly, after the fluctuations have dissipated, the particle lattice undergoes a sudden buckling instability that produces coherent vertical displacements of particle rows oriented in the flow direction. The instability results in formation of a disordered phase in which particles are arranged into meandering strings, similar to the structures observed in recent experiments [2012 PNAS 109 63]. We show that the behavior of the system is controlled by the swapping-trajectory interactions at all stages of the evolution.

1. Introduction

Collective hydrodynamic phenomena in microconfined suspensions figure prominently in many scientific fields ranging from dynamics of living cells and active matter [1–3] to microfluidics [4–6]. A number of recent studies [5–15] have demonstrated an unexpectedly complex phenomenology of strongly confined dispersion flows, in systems where the channel thickness is comparable to the particle size. Such geometry is frequently encountered in microfluidic devices, so strongly confined dispersions are not only of fundamental but also of practical interest (e.g., for separation of particles of different properties [16]).

Even though suspensions and emulsions in pores and narrow channels are common in natural and engineered systems, distinct phenomenology of strongly confined dispersion flows has been recognized only recently. It has been shown that particle interactions with confining walls can produce macroscopic effects such as intrinsic convection [17–19], enhanced hydrodynamic diffusion [20, 21], complex instabilities of particle jets [22], and enhanced breakup of suspension drops [23]. Particle-wall interactions can also cause microstructural changes, e.g., suspension layering [24] and development of complex micro-scale patterns in confined emulsion [4, 11, 25, 26] and suspension [12, 27] flows.
Our paper focuses on the behavior of non-Brownian rigid particles under creeping-flow conditions in parallel-wall channels with wall separation comparable to the particle diameter. Wall-induced collective evolution that is observed in such systems includes propagation of dissipative displacement waves in particle or drop trains [6, 10, 12], topological transitions in quasi-two-dimensional (2D) monolayers of microspheres [12], and unusual stability of square particle lattice [12, 28].

Our recent simulations [28] of an initially ordered particle monolayer in confined Poiseuille flow have revealed other striking and unexpected hydrodynamic phenomena, such as stabilization of an ordered particle monolayer by random fluctuations, spontaneous decay of such fluctuations with time, and a sudden instability of the particle lattice that happens right after the fluctuations have disappeared. This instability results in a new suspension microstructure with particles arranged into meandering strings. In the present study we elucidate the nature of these phenomena and discuss them in detail.

2. Evolution of a particle monolayer

We consider evolution of an infinite array of spheres of diameter \(d\) in Poiseuille flow in a parallel-wall channel of width \(H\). The walls are in the planes \(z = 0\) and \(z = H\) (where \(z\) is the transverse coordinate), and the flow is in the \(x\)-direction. As depicted in Fig. 1, the particles are initially arranged on a square lattice, with the lattice vectors along the flow direction \(x\) and vorticity direction \(y\), in an off-center plane parallel to the walls. The lattice is organized into uniform parallel strips separated by particle-free gaps. Periodic boundary conditions are applied in the \(x\) and \(y\) directions.

The simulations presented in this paper were performed for the following system parameters: the normalized channel width is \(H/d = 1.9\), the initial normalized interparticle distance is \(W/d = 2\), and the initial position of the particle monolayer is \(z/H = 0.37\). We note, however, that a similar behavior to the one described below has been observed also for other parameter values. In what follows, the dimensionless time \(t\) is normalized by the time in which an isolated particle in the reference plane \(z/H = 0.37\) travels the distance equal to its diameter.
Figure 2. Evolution of a particle monolayer (top view). The panels show the projection of the particle outlines onto the $x$--$y$ plane at time as labeled. Simulation cell is $14 \times 14$ particles; two periodic cells are shown in the $x$ direction and 1.5 periodic cell in the $y$ direction. (Also see supplemental video movie_1.mov.)
The simulations in this paper were performed using our Cartesian representation method [29], which combines the HYDROMULTIPOLe technique [30] with expansion of the flow field in the wall presence into lateral Fourier modes [29]. The periodic boundary conditions were implemented using the far-field Hele–Shaw form of the flow in the channel [31, 32].

2.1. Microstructural evolution

The dynamics of the microstructure of the particle monolayer are depicted in Figs. 2 and 3, which show top view of the suspension in the channel (i.e., a view in the $x$–$y$ plane). The system exhibits several distinct stages of evolution, and it undergoes a sudden microstructural transition. The key dynamical events, illustrated in Fig. 2 and 3, can be characterized as follows:

(i) At the first stage of evolution (cf. frames $t = 9$ and $t = 48$), individual strips of the particle lattice expand, until they completely fill the particle-free gaps, and the system forms an approximately uniform rectangular lattice.

(ii) At the second stage (cf. frames $t = 112$ and $t = 653$), the distance between $y$-rows in the particle lattice fluctuates significantly, but the particles remain well aligned in the $y$-direction, and the lattice preserves its integrity. The magnitude of the fluctuations slowly decreases in time, and at $t \approx 650$ the fluctuations nearly completely disappear.

(iii) At the third stage of evolution, when the fluctuations have decayed and a nearly perfect uniform lattice has been formed, the lattice undergoes a sudden instability (described in Sec. 2.3) and the particle monolayer exhibits coexisting local regions with square and hexagonal symmetry (cf. frame $t = 720$). As depicted in Fig. 3, the instability develops over a short time period $\Delta t \approx 10$, and afterwards the system evolves further into a new stable disordered microstructure.

(iv) At the fourth stage (cf. frame $t = 840$), the monolayer forms a complex stationary microstructure with particles arranged into meandering strings whose orientations vary between the flow and the vorticity directions. Our numerical simulations show that the system can remain in this phase for a very long time.

(v) At very long times (cf. frame at $t = 12700$) the suspension randomly undergoes another instability, resulting in formation of particle clusters that move slower than individual particles in the monolayer. The clusters gradually grow, creating particle-depleted void regions around them.
Figure 4. (a) Near-field and far-field flow produced by a particle moving in a channel: far from the particle (compared to the wall separation) the flow field assumes the parabolic Hele–Shaw form (side view). (b) The backflow pattern associated with 2D Hele–Shaw pressure dipole produced by a particle in an external flow (top view). (c) The swapping-trajectory effect: wall reflection of scattered flow produced by particle $P_1$ makes particle $P_2$ migrate cross-streamline, from slow moving to fast moving fluid region. As a result of this effect, particles that initially approach each other separate without collision, after switching (swapping) their cross-streamline positions (side view).

2.2. Hele–Shaw dipoles and swapping-trajectory mechanism

We argue that the complex evolution of a suspension monolayer described in Sec. 2.1 stems from two wall-induced hydrodynamic phenomena, schematically illustrated in Fig. 4. The first effect is due to the far-field Hele–Shaw dipolar flow produced by the particles [7, 33] at distances exceeding the wall separation [cf. Fig. 4(b)], and the second is the swapping-trajectory (ST) effect [21, 24, 34] associated with near-field wall-mediated scattered flow [cf. Fig. 4(c)]. While for pressure-driven particle arrays the dipolar flow affects both center-plane and off-center particle positions, the ST mechanism influences only particles that are in an off-center configuration in a local shear flow.

The role of interparticle hydrodynamic interactions associated with dipolar scattered flow has been described in our previous studies of particle monolayers moving in the midplane of a channel [12, 28]. We have shown that dipolar interactions stabilize square arrangements of hydrodynamically coupled particles, and such arrangements can withstand significant deformations (while maintaining the particle alignment). The dipolar scattered flow plays a similar stabilizing role in the particle configuration considered here. Therefore, since this phenomenon has already been well documented, in what follows we focus on the ST mechanism, which in Poiseuille flow occurs for asymmetric off-center configurations.

As illustrated in Fig. 4(c), the ST mechanism originates from the scattering of local incoming shear flow by one of the particles [21]. The scattered flow is then reflected from a wall and acts on the other particle, displacing it across streamlines to a fluid region moving with a different velocity. The ST phenomenon is present both in two-particle and multiparticle systems. In the case of a particle chain aligned in the flow direction (cf. Fig. 5), the ST effect causes the trailing particle to move towards the closer wall while the leading particle moves away from this wall. Since the flow is slower near the wall, the trailing particle stays behind, and the leading particle accelerates. As a result of this behavior the particle chain expands. We demonstrate below that entire strips of particle lattice depicted in Fig. 2 are affected by a similar ST mechanism.

The influence of the ST effect on the motion of the particle monolayer described in Sec. 2.1

---

1 We note that chain expansion can also be produced by dipolar interactions (for particles in the midplane) [35], but in our off-center system the dominant effect comes from the ST mechanism.
Figure 5. Swapping-trajectory effect in a three-particle system (side view).

Figure 6. Evolution of a particle monolayer (side view). The panels show the projection of the particle centers onto the $x$-$z$ plane at times as labeled. Note that the vertical scale is magnified. (Also see supplemental video movie 3.mov.)
can be easily observed in the side view (i.e., the flow–gradient $x$–$z$ plane) of the evolving system. In Fig. 6 we show positions of particle centers in the $x$–$z$ plane at the times corresponding to the frames depicted in Fig. 2. We note that for configurations where particle rows are perfectly aligned in the $y$ direction (which is the case for $t = 9, 48, 112, 653$) only the centers of the front particles are visible in the figure.

The results shown in Fig. 6 for $t = 9$ are consistent with the predictions of our analysis of the ST mechanism (illustrated in Fig. 5). The front end of the strips moves upwards and speeds up, and the trailing end moves down and slows down. After the front row of particles in a given strip catches up with the trailing row of the next strip (cf. frame $t = 48$), significant ST interactions are established between these rows, and therefore, the entire rows change the direction of their vertical motion.

Subsequently, mutual ST interactions between neighboring particle rows give rise to their random motion in the vertical direction $z$ and lead to corresponding fluctuations of the row distances in the flow direction $x$ (cf. frames $t = 112$ in Figs. 2 and 6). The incoherent vertical motion of particle rows causes gradual cancellation of the fluctuations, and this cancellation results in a well-aligned rectangular lattice with regular interparticle spacing (cf. frames $t = 653$ in Figs. 2 and 6).

However, the lattice instability that takes place at $t = t_b \approx 700$ (cf. Fig. 3) entirely changes the system behavior: not only does a transition from a regular crystalline-like suspension microstructure to a disordered state occur, but also the particle alignment in the $y$ direction suddenly breaks down (cf. frames $t = 720$ and $t = 840$ in Figs. 2 and 6). We examine the nature of this buckling instability in Sec. 2.3.

### 2.3. Buckling instability

Figure 7 shows the front view of the system just before the lattice instability event ($t = 695$) and just after the onset of the lattice breakup process ($t = 718$). Before the instability occurs the particles are well aligned along lines parallel to the flow direction $x$. The lack of vertical displacements indicates that the fluctuations observed at the earlier stages of the evolution have dissipated nearly completely. However, after the instability event significant vertical displacements take place (although the particles still preserve some alignment in the direction $x$).

In the new transient microstructure of the particle monolayer every other $x$-row of particles...
Figure 8. Buckling instability mechanism: a particle row that is ahead due to a random displacement (dark particles) receives a lift produced by the flow scattered from the particles in the neighboring rows that stay behind (light). The dark row is thus pushed up into a faster moving streamline and gets ahead even more. (a) Top view of the system, i.e., in the plane $x-y$; (B) side view.

is displaced up and every other $x$-row is displaced down, as seen in the right panel of Fig. 7. A comparison of the frames at $t = 695$, 710, and 720 in Fig. 3 indicates that $x$-rows of particles that have been displaced up move faster than the others. The consecutive $x$-rows of particles are displaced in opposite directions, and this buckling instability causes the decomposition of the previously well-aligned particle monolayer.

Qualitatively, the hydrodynamic mechanism of the buckling instability can be explained as follows. If a given $x$-row of particles is displaced up (i.e., away from the closer wall), it starts to move faster, and gets slightly ahead of the other $x$-rows, as illustrated in Fig. 8(a). Particles in the neighboring rows that are slightly behind produce scattered flow that gives lift to the upper displaced row of particles (similar to the lift that causes the ST effect depicted in Fig. 5). As a result, the displaced $x$-row moves even further from the wall, and speeds up more, leading to a rapid growth of the initial perturbation.

We note that a displacement of an individual particle does not produce a similar effect. The displaced faster moving particle approaches the particle in front of it and slows down, due to the ST interaction. Therefore, a one-particle perturbation does not grow. The unstable modes through which the particle lattice decomposes thus involve coherent displacements of entire segments of $x$-rows of particles, consistent with the transient structure of the system seen in Fig. 2 at $t = 720$.

An important issue that remains unsolved is the mechanism through which the particle lattice is stabilized against buckling at the earlier stages of the evolution. Since the only difference between the unstable state with well-aligned particles at $t = t_b$ and the fluctuating stable states for $t < t_b$ is the existence of lateral and transverse displacements of $y$-rows of particles, such displacements must be responsible for the array stabilization. The behavior of the particle monolayer qualitatively resembles stabilization of an elastic sheet by a transverse deformation wave. Such a wave, oriented along one direction, prevents buckling of the sheet in the orthogonal direction. While this analogy provides some useful intuition, a specific hydrodynamic mechanism stabilizing the particle array still needs to be investigated.
3. Conclusions

Our numerical simulations of an initially ordered particle monolayer driven by Poiseuille flow in a parallel-wall channel have revealed very interesting and rich dynamics. As depicted in Figs. 2 and 6 the system can heal large gaps in the particle lattice, and lattice fluctuations can spontaneously decay, leading to a well-aligned rectangular configuration. We have also described a new buckling instability of the particle monolayer, and prior lattice stabilization through displacements of particle rows orthogonal to the buckling direction. All of these phenomena, which occur in the Stokes-flow regime, are purely hydrodynamic in their nature and arise from the ST effect.

Our simulations have demonstrated the existence of a new hydrodynamically stabilized disordered suspension phase. In this phase, particles are arranged into meandering strings, with orientations changing between the flow direction \(x\) and the vorticity direction \(y\). This phase (briefly discussed in our earlier study [28]) closely resembles the microstructure of particle layers that spontaneously form in oscillatory shear flow, as observed in recent experiments [27]. These experiments also show spontaneous formation of a square particle lattice (as opposed to a hexagonal configuration resulting from excluded-volume effects). The structures in our simulations and in experiments [27] are strikingly similar, although the respective results were obtained for different flows and system geometries. Therefore, the observed patterns (i.e., hydrodynamically stabilized square lattice and string-like particle correlations) underscore the generality of our findings.

Our analysis of the dynamics of a particle monolayer has revealed an important role of the ST effect. The ST mechanism, which influences the system at all stages of its evolution, is associated with wall-mediated hydrodynamic interactions between particles in a local shear flow. The ST phenomenon causes cross-streamline displacements of approaching particles: the particles move in opposite directions normal to the wall, and as a result of this position swapping across the streamlines, the particles reverse their relative motion and separate without collision.

The multiparticle ST interactions in confined suspension flows have far-reaching and diverse consequences. On the one hand, the ST mechanism stabilizes fluctuating quasi-2D monolayers by preventing particle collisions. On the other hand, it has a destabilizing effect in perfectly ordered 2D monolayers by causing buckling of the particle lattice. The resulting string-like microstructure is, again, stabilized by the ST effect. Other phenomena produced by the ST effect were discussed in our earlier studies: the ST mechanism can produce spontaneous suspension layering [24], and it can lead to enhanced hydrodynamic diffusion [21].

While our study is focused on the dynamics of infinite quasi-2D particle monolayers, we expect that similar phenomena also occur in microfluidic flows that involve particle arrays of finite extent. In particular, we predict stabilization and realignment of linear particle trains via cancellation of random fluctuations, i.e., due to a mechanism similar to the one seen in Fig. 6 for \(t \leq 653\). (In fact, this mechanism is likely to play a significant role in the recently observed spontaneous particle ordering at non-zero Reynolds numbers [14, 15].) We propose that experiments to observe the buckling effect (illustrated in Fig. 7) can be carried out using a multi-orifice flow-focusing devices [36] to generate synchronized parallel particle trains in a channel with a rectangular crosssection of high aspect ratio. Such experiments would help to explore the diverse consequences of the ST effect in confined particulate flows.

Acknowledgments

3.1. Acknowledgments

We acknowledge financial support by NSF grant CBET 1059745 (JB) and Polish Ministry of Science and Higher Education grant N N501 156538 (EW). JB wishes to thank François
Feuillebois for exposing him to the science of wall-bounded suspensions and to the art of French living during the author’s stay in Laboratoire d’Aérothermique du CNRS and ESPCI in 1993 and 1994.

References

[1] Riedel I H, Kruse K and Howard J 2005 Science 309 300–303
[2] Lenz P and Ryskin A 2006 Phys. Biol. 3 285–294
[3] Underhill P T, Hernandez-Ortiz J P and Graham M D 2008 Phys. Rev. Lett. 100
[4] Garstecki P and Whitesides G M 2006 Phys. Rev. Lett. 97 024503
[5] Hashimoto M, Mayers B, Garstecki P and Whitesides G M 2006 Small 2 1292–1298
[6] Beatus T, Trusty T and Bar-Ziv R 2006 Nature Phys. 2 743–748
[7] Cui B, Diamant H, Lin B and Rice S A 2004 Phys. Rev. Lett. 92 258301–1–4
[8] Koppl M, Henseler P, Erbe A, Nielaba P and Leiderer P 2006 Phys. Rev. Lett. 97 208302
[9] Garstecki P 2006 Nature Phys. 2 733–734
[10] Beatus T, Trusty T and Bar-Ziv R 2007 Phys. Rev. Lett. 99 124502
[11] Hashimoto M, Garstecki P, Stone H A and Whitesides G M 2008 Soft Matter 4 1403–1413
[12] Baron M, Bławzdziewicz J and Wajnryb E 2008 Phys. Rev. Lett. 100 174502
[13] Bonthuis D J, Meyer C, Stein D and Dekker C 2008 Phys. Rev. Lett. 101 108303
[14] Humphry K J, Kulkarni P M, Weitz D A and Stone H A 2010 Phys. Fluids 22
[15] Lee W, Amini H, Stone H A and Di Carlo D 2010 PNAS 107 22413–22418
[16] Pasol L, Martin M, Ekiel-Jezewska M L, Wajnryb E, Bławzdziewicz J and Feuillebois F 2011 Chem. Eng. Sci. 66 4078–4089
[17] Bruneau D, Feuillebois F, Anthore R and Hinch E J 1996 Phys. Fluids 8 2236–2238
[18] Bławzdziewicz J and Feuillebois F 1995 Fluid Mech. Research 22 66
[19] Bruneau D, Feuillebois F, Bławzdziewicz J and Anthore R 1998 Phys. Fluids 10 55–59
[20] Zaragà I E and Leighton D T 2002 Phys. Fluids 14 2194–2201
[21] Zurita-Gotor M, Bławzdziewicz J and Wajnryb E 2007 J. Fluid Mech. 592 447–469
[22] Alvarez A, Clement E and Soto R 2006 Phys. Fluids 18 083301
[23] Mylky A, Mele W, Brenn G and Ekiel-Jezewska M L 2011 Phys. Fluids 23
[24] Zurita-Gotor M, Bławzdziewicz J and Wajnryb E 2012 Phys. Rev. Lett. 108 068301
[25] Vananroye A, Van Puyvelde P and Moldenaers P 2006 Langmuir 22 2273–2280
[26] Tufano C, Peters G W A and Meijer H E H 2008 Langmuir 24 4494–4505
[27] Cheng X, Xu X, Rice S A, Dinner A R and Itai C 2012 PNAS 109 63–69
[28] Bławzdziewicz J, Goodman R H, Khurana N, Wajnryb E and Young Y N 2010 Physica D 239 1214
[29] Bhattacharya S, Bławzdziewicz J and Wajnryb E 2005 Physica A 356 294–340
[30] Cichocki B, Felderhof B U, Hinsen K, Wajnryb E and Bławzdziewicz J 1994 J. Chem. Phys. 100 3780–3790
[31] Bhattacharya S, Bławzdziewicz J and Wajnryb E 2006 J. Comput. Phys. 212 718–738
[32] Bławzdziewicz J and Wajnryb E 2008 Phys. Fluids. 20 093303
[33] Bhattacharya S, Bławzdziewicz J and Wajnryb E 2005 J. Fluid Mech. 541 263–292
[34] Bossis G, Meunier A and Sherwood J D 1991 Phys. Fluids A 3 1853–58
[35] Janssen P J A, Baron M D, Anderson P D, Bławzdziewicz J, Loewenberg M and Wajnryb E 2012 Collective Dynamics of Confined Rigid Spheres and Deformable Drops arXiv:xxx
[36] Hashimoto M, Shevkoplyas S S, Zasonska B, Szymborski T, Garstecki P and Whitesides G M 2008 Small 4 1795–1805