DYNAMIC SIMULATIONS OF THE INSTABILITY OF SEDIMENTING FIBERS

David Saintillan*, Eric Darve*, Eric S. G. Shaqfeh**
*Department of Mechanical Engineering, Stanford University, Stanford CA 94305, USA
**Departments of Chemical and Mechanical Engineering, Stanford University, Stanford CA 94305, USA

Summary The concentration instability of sedimenting fiber suspensions at zero Reynolds number is investigated by means of large-scale numerical simulations. Large systems are simulated, allowing the capture of several inhomogeneities. The structure of the suspension is studied in both the vertical and horizontal directions, providing new insight into the formation and dynamics of the inhomogeneities, as well as the mechanisms behind the wavenumber selection process of the instability.

INTRODUCTION

It has been known for over a decade that sedimenting suspensions of non-spherical particles such as fibers undergo a concentration instability, by which an initially homogeneous suspension evolves towards a very inhomogeneous state where high-concentration streamers are surrounded by clarified fluid. The instability was first predicted theoretically by Koch and Shaqfeh [1] as a consequence of a coupling between the fluctuations of the mean flow and the anisotropic mobility of the particles. It was subsequently observed both in experiments [2] and in numerical simulations [3]. While the origin of the instability is now fairly well understood, several important questions remain unanswered: what are the mechanisms behind the wavenumber selection of the instability? And what therefore determines the size of and spacing between the inhomogeneities in the suspension, which have a strong influence on the sedimentation rate?

In their previous simulations, Butler and Shaqfeh [3] captured most of the qualitative features of the instability; however only fairly small systems were typically simulated and the wavenumber selection could not be observed. In this paper we use a fast summation algorithm to perform simulations of larger systems in order to study the suspension microstructure in more detail.

METHOD OF SIMULATION

The simulation method used here follows the previous work by Butler and Shaqfeh [3]. The motion of the fibers is described using Batchelor's slender-body theory, which represents the disturbance of the fibers on the flow as line distributions of point forces or Stokeslets [4]. The force distributions are expanded in a Legendre polynomial along the fiber length in which only the first two moments are retained, namely the total force and dipole term, which can be expressed in terms of the total torque and particle stresslet [5]. The lubrication approximation is used to capture close particle pair interactions [6].

Periodic boundary conditions are used to simulate infinite suspensions, and the velocity disturbance created by the fibers is calculated using the periodic Green's function for Stokes flow [7]. The evaluation of this velocity disturbance constitutes the most time-consuming part of the simulations, and is accelerated using a Smooth Particle-Mesh Ewald (SPME) method previously used in molecular dynamics simulations [8]. The SPME algorithm is similar in many ways to the Accelerated Stokesian Dynamics method of Sierou and Brady [9], and is based on a decomposition of the slowly decaying Green's function into two fast-converging sums: the first one involves the distribution of point forces and is evaluated rapidly over close particle pairs, while the second one is expressed in terms of the Fourier transform of the force distribution and is computed efficiently on a Cartesian grid using Cardinal B-spline interpolation and the Fast Fourier Transform algorithm. The total cost of the algorithm scales as $O(N \log N)$, and therefore results in a significant speedup.

SIMULATION RESULTS

Suspension microstructure and cluster formation

Figure 1 shows the evolution of a suspension of 512 fibers of aspect ratio $A = 11$ and average volume fraction $nl^3 = 0.05$ for a simulation box of high aspect ratio. Starting from a well-mixed suspension, small clusters form and converge towards a high-density streamer. The streamer is composed of several inhomogeneities, with new fibers constantly entering and leaving the clusters. A procedure was implemented to systematically determine the number and size of the clusters inside the streamer (where we define clusters as regions where the local concentration peaks beyond 1.3 times the average concentration). Statistics could therefore be performed, and the graph in Figure 1 shows the evolution of the numbers of small and large clusters (i.e. containing more or fewer than 30 fibers) inside the streamer. The two curves initially present slow oscillations, which are easily interpreted: during the transient phase of the instability, a periodic mechanism is observed by which small clusters merge into larger clusters, which again break up into small clusters. After a while the oscillations subside and a steady state is reached where a combination of clusters of different sizes coexist on average. The average spacing between clusters in the vertical direction at steady state can be estimated at 10 fiber lengths.

Increasing one of the lateral dimensions of the box also allowed to observe several high-concentration streamers as shown in Figure 2. The structure of the suspension is quite interesting as it exhibits large regions of shear between the streamers and the clarified fluid where the fibers are aligned with gravity and slowly converge towards the streamers as

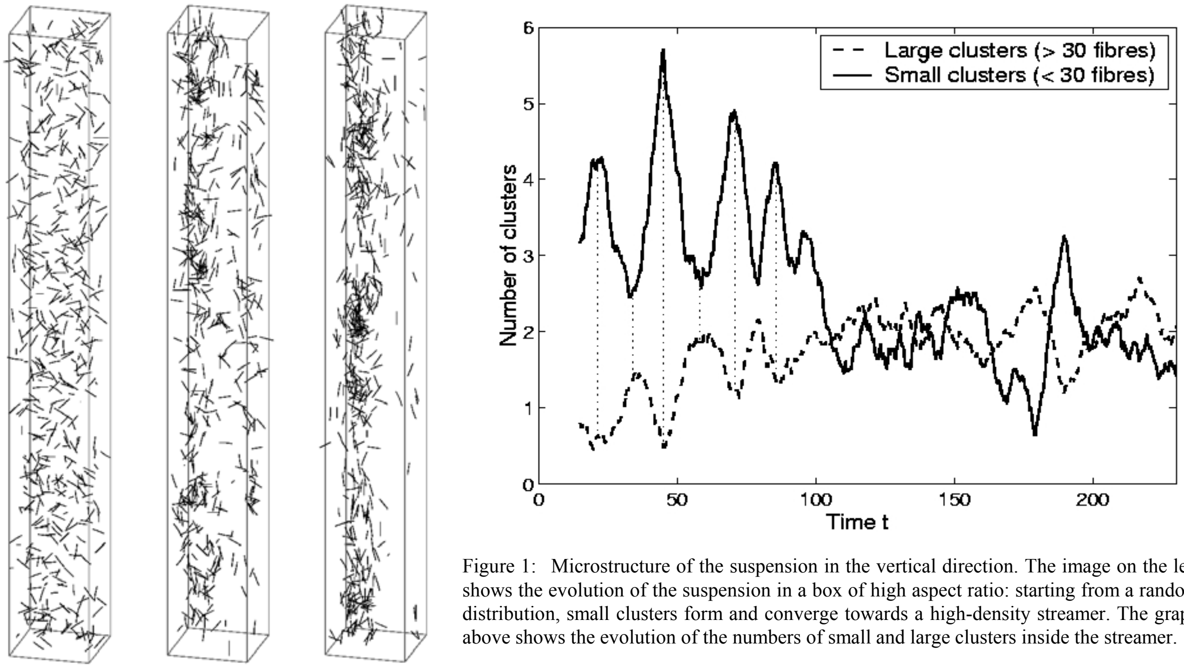


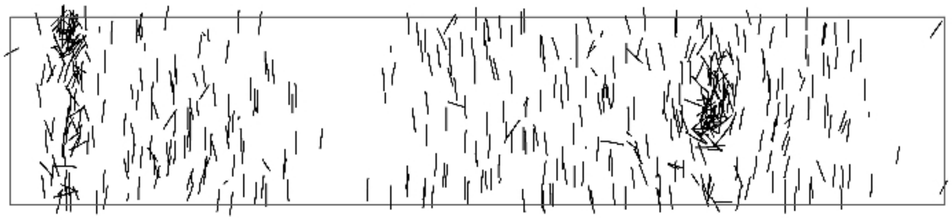
Figure 1: Microstructure of the suspension in the vertical direction. The image on the left shows the evolution of the suspension in a box of high aspect ratio: starting from a random distribution, small clusters form and converge towards a high-density streamer. The graph above shows the evolution of the numbers of small and large clusters inside the streamer.

a result of hydrodynamic dispersion. The average spacing between the streamers is typically quite large, on the order of 20 fiber lengths or higher, and seems to be determined to a large extent by the concentration fluctuations in the initial distribution. More precisely, low-wavenumber concentration fluctuations create backflows in the disturbance velocity field, which seem to act like barriers for the fibers. Because of the quasi one-dimensionality of these simulations in wide boxes, one should be prudent however in extending these conclusions to full-scale suspensions.

Orientation and velocity statistics

Statistics were also obtained for the orientations and velocities of the fibers, and were compared to the experimental results of Herzhaft and Guazzelli [2]. Using very wide boxes in the horizontal direction (such as in Figure 2) allows to obtain very good orientation statistics, where a very large portion of the fibers is essentially aligned in the vertical direction. The fiber velocities and the average sedimentation rate however still greatly depend on the dimensions of the simulation box, and are typically better in very high boxes (such as in Figure 1). We hope that simulations in large boxes in the both the horizontal and vertical directions using parallel computing will allow to reconcile the statistics for orientations and velocities.

Figure 2: Distribution of fibers at t = 140 for a very elongated box in the lateral direction. Two distinct streamers separated by clarified regions can be observed. Between the streamers and the clarified fluid, fibers are aligned with gravity and slowly migrate towards the streamers as a consequence of velocity fluctuations.



References

[1] Koch D. L., Shaqfeh, E. S. G.: The instability of a dispersion of sedimenting spheroids. *J. Fluid Mech.* **209**:512-542, 1989.
[2] Herzhaft B., Guazzelli E.: Experimental study of the sedimentation of dilute and semi-dilute suspensions of fibres. *J. Fluid Mech.* **384**:133-158, 1999.
[3] Butler J.E., Shaqfeh E. S. G.: Dynamic simulations of the inhomogeneous sedimentation of rigid fibres. *J. Fluid Mech.* **468**:205-237, 2002.
[4] Batchelor G. K.: Slender-body theory for particles of arbitrary cross-section in Stokes flow. *J. Fluid Mech.* **44**:419-440, 1970.
[5] Harlen O. G., Sundararajakumar R. R., Koch D. L.: Numerical simulations of a sphere settling through a suspension of neutrally buoyant fibres. *J. Fluid Mech.* **388**:355-388, 1999.
[6] Claeys I. L., Brady J. F.: Lubrication singularities of the grand resistance tensor for two arbitrary particles. *PhysicoChem. Hydrodyn.* **11**:261-293, 1989.
[7] Hasimoto H.: On the periodic fundamental solution of the Stokes equations and their application to viscous flow past a cubic array of spheres. *J. Fluid Mech.* **5**:317-328, 1959.
[8] Essmann U., Perera L., Berkowitz M. L., Darden T., Lee H., Pedersen L.G.: A smooth particle mesh Ewald method. *J. Chem. Phys.* **103**:8577-8583, 1995.
[9] Sierou A., Brady J. F.: Accelerated Stokesian Dynamics simulations. *J. Fluid Mech.* **448**:115-146, 2001.