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#### **Short Communication**

### Friction coefficient of rod-like chains of spheres at very low Reynolds numbers. II. Numerical simulations

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Abstract. — Experiments on the sedimentation of chains of spherical particles in a viscous fluid are presented in the preceding paper [1]. In this paper, we compare the predictions of numerical simulations based on Stokesian dynamics to the experimental results reported in reference [1], and to analytical expressions available for this problem. For unbounded fluids, the experimental measured velocity and the numerical results are compared to slender body theory. This comparison shows a correct agreement for a ratio of the length of the chain to its diameter as small as 5. When the fluid is limited by a wall, we use the expression given by Brenner [3] for the friction coefficient of particles in a bounded fluid. We find that this relation holds even for distances that are smaller than the length of the chain. The good agreement between the numerical and the experimental results shows the reliability of the Stokesian dynamics for simulating the hydrodynamical interactions between all the particles and the wall.

The problem of the sedimentation of a chain of spheres lies in the determination of its friction coefficient which depends on the length of the chain. There is no general expression but for an unbounded medium and when the length of the chain is large compared to its diameter, one can use the slender body theory [2] to get the friction coefficient and then the sedimentation velocity.

Another difficulty arises from the hydrodynamic interactions of the chain with the walls of the vessel in which the experiment is performed. We need to know the true influence of the walls on the sedimentation velocity of the chains. This depends on the distance of the chain to the wall and on the length of the chain; there is an analytical result for the friction coefficient but only when the particles are far from the wall [3].

On the other hand, we have developed a numerical method, based on Stokesian dynamics [4, 5] which allows us to calculate the trajectories of groups of particles close to a plane in the limit of zero Reynolds number [6]. This method takes into account the many body hydrodynamic interactions between the particles and a planar wall, whatever the distance

between the particles and the wall.

In the first part we introduce the analytical theories available for the problem of the sedimentation of a slender body. We will then present a brief outline of the Stokesian dynamics. In the last part we compare the experimental results reported in [1] to those obtained by numerical simulations for different chains of various lengths, and at different distances from the wall. The limitation of the theoretical friction coefficient when the chain approaches the plane will be discussed in the conclusion.

#### 1. Analytical results.

We consider a chain of n spheres sedimenting under gravity in a viscous fluid. The particles are monodisperse spheres touching each other. The forces on the chain are its weight, the buoyancy forces and the Stokes drag. The velocity of the chain will depend on the friction coefficient which is a function of the number n of particles and of the distance h from the wall. At equilibrium, we have the relation:

$$\frac{4\pi}{3}a^3.\Delta
ho.g.n=6\pi\mu a.\xi_n.v_n$$

which relates the sedimentation velocity  $v_n$  of the chain to the number of particles, the dimensionless friction coefficient  $\xi_n$  ( $\xi_1 = 1$ ), the radius *a* of the particles and the difference of density between the particles and the fluid  $\Delta \rho$ . This gives the final velocity:

$$v_n = \frac{2}{9} \frac{a^2 \cdot \Delta \rho \cdot g}{\mu} \frac{n}{\xi_n} = v_1 \frac{n}{\xi_n} \tag{1}$$

where  $v_1$  is the velocity of an isolated sphere. All the results are then expressed as the ratio  $v_n/v_1$  which depends only on n and h. However, the experimental value of  $\Delta \rho$  may vary [1], and so does  $v_1$ . We then decide to choose  $v_1$  so that the numerical and the experimental results for  $v_n$  are equal for large values of n and h.

1.1 UNBOUNDED FLUID. — In the case of a chain of spheres sedimenting in an unbounded fluid, one is interested in the behaviour of the velocity of the chain as a function of its length l = 2na.

When n is large or, equivalently, when the chain is long, one can use the slender body theory [2] which gives useful analytical expressions for the friction coefficients of thin elongated bodies of various shapes. Here we consider a cylinder of length l and radius a ( $l \gg a$ ). The case of an ellipsoid is presented in reference [1], and the two models give similar results. Replacing l with 2na, we obtain the coefficient  $\xi^{\parallel}$  for a motion parallel to the main axis, and  $\xi^{\perp}$  for a motion perpendicular to it

$$\xi^{\parallel} = \frac{2}{3} \frac{n}{\ln(2n)} \left[ \frac{1 + 0.307\varepsilon}{1 - 0.5\varepsilon} + O\left(\varepsilon^2\right) \right] \qquad \xi^{\perp} = \frac{4}{3} \frac{n}{\ln(2n)} \left[ \frac{1 + 0.307\varepsilon}{1 + 0.5\varepsilon} + O\left(\varepsilon^2\right) \right] \tag{2}$$

where  $\varepsilon = (\ln 2n)^{-1}$ 

From those coefficients one can calculate the sedimentation velocity as a function of n, using the relation (1).

1.2 WALL EFFECT. — We now look at the sedimentation of a chain of spheres in a fluid bounded by some rigid boundaries. The effect of these boundaries on the friction coefficient can be estimated using the expression [3]

$$\frac{\xi}{\xi_{\infty}} = \left[1 - k \frac{\xi_{\infty}}{h/a}\right]^{-1}$$

In this relation,  $\xi$  is the dimensionless Stokes friction coefficient at distance h from the wall,  $\xi_{\infty}$  is the friction coefficient in an infinite medium and h/a is the ratio of the distance from the wall on the radius of the spheres. The value of the constant k has been determined for various situations. For a motion parallel to a single planar rigid wall, k is equal to 9/16, and for a chain of spheres sedimenting midway between two infinite rigid walls we have k = 1.004.

From (1), we get for the sedimentation velocity

$$v(h) = v_{\infty} \left[ 1 - k \frac{\xi_{\infty}}{h/a} \right]$$
(3)

This result can be rederived using the solution given by Blake [7] for the velocity field induced by a point force acting on the fluid near a wall.

The force exerted by the sedimenting body is  $F \approx 6\pi\mu a\xi_{\infty}(v+v')$ , where v is the sedimentation velocity of the chain relatively to the wall and v' is the backflow generated by the wall. But v' depends on F, and we find from [7]:  $v' = 3F/32\pi\mu h$ . This gives  $F \approx 6\pi\mu a\xi_{\infty}v/(1-9\xi_{\infty}a/16h)$  and  $\xi \approx \xi_{\infty}/(1-9\xi_{\infty}a/16h)$ . We thus recover the solution (3) with the correct value of k.

#### 2. Numerical method.

The numerical method is based on the solutions of the Stokes equations for the interactions of spherical particles in a viscous fluid and has been extended to include the effect of a rigid plane wall limiting the suspension. This method takes into account both lubrication forces and many-body interactions, using the resistance and the mobility formulation.

For *n* particles, we defined the  $6 \times n$  force vector  $\mathbf{F} = (f_1, \dots, f_n, t_1, \dots, t_n)$  and the  $6 \times n$  velocity vector  $\mathbf{V} = (v_1, \dots, v_n, \omega_1, \dots, \omega_n)$  where  $f_1, \dots, f_n, t_1, \dots, t_n$  are the forces and torques acting on the particles and  $v_1, \dots, v_n, \omega_1, \dots, \omega_n$  are the velocities of the particles (for translation and rotation). They are related through the  $6n \times 6n$  resistance matrix  $R_{2b}$  and mobility matrix M.

The resistance matrix  $R_{2b}$  contains the solutions of the lubrication theory for two spheres almost in contact and the solution for each individual sphere close to a rigid wall.

The mobility matrix M includes the first two moments of the force distribution on each sphere resulting from the motion of the other particles and from the reflexion of the velocity field on the plane. The elements of M are calculated from the solutions given in [7]. More details of this calculus and references can be found in [6]. Inverting M gives the many-body contribution to the total force. This procedure allows us to take into account the hydrodynamic interactions between two spheres induced by the presence of the wall, which permitted us to study, for example, the trajectories of particles near a rigid boundary [6].

To get the total resistance matrix R, we add the two matrices  $R_{2b}$  and  $M^{-1}$  The forces and the velocities are then given by the relation

$$F = R.V$$
 where  $R = R_{2b} + M^{-1}$ 

For a chain of spheres which all move at the same velocity without rotation, the total force on a particle  $\alpha$  is the sum of the contributions of all the particles, including itself. If  $R^{\alpha\beta}$  is the 6×6 submatrix relating the force on the particle  $\alpha$  to the velocity of the particle  $\beta$  we have

$$F_{i}^{\alpha} = \sum_{\beta=1}^{n} R_{ij}^{\alpha\beta} \cdot v_{j}^{\beta} = \left[\sum_{\beta=1}^{n} R_{ij}^{\alpha\beta}\right] \cdot v_{j}$$

The total force and the friction coefficient of the chain are then

$$F_i = \sum_{\alpha=1}^n F_i^{\alpha}$$
 and  $\xi_{ij} = \sum_{\alpha=1}^n \sum_{\beta=1}^n R_{ij}^{\alpha\beta}$ 

Because of the geometry of a chain, the coefficients  $\xi_{ij}$  are zero for  $i \neq j$ . With i = j = 1 we get the coefficient  $\xi^{\parallel}$  corresponding to a motion parallel to the main axis of the chain. With i = j = 2 or 3, the coefficient is  $\xi^{\perp}$ , corresponding to a motion perpendicular to the main axis ( $\xi_{22}$  and  $\xi_{33}$  are equal far from the wall). The ratio  $v_n/v_1$  is then calculated as in (1).

#### 3. Results and discussion.

The results for a motion respectively parallel and perpendicular to the chain axis and far from the walls are given in figures 1 and 2. Our numerical method, however, does not apply when the particles are influenced by two walls as is the case for the experimental results given in [1]. Therefore the numerical values presented here and calculated for an unbounded medium are corrected using (3) with k = 1.004. We do the same with the results obtained from the slender body theory. We find a good agreement between experimental and numerical results for all values of n. For the smallest values (n < 5), the slender-body theory predicts a sedimentation velocity which can be more than two times lower than the experimental one. This was expected because the body is no longer slender ( $\varepsilon = 0.43$  for n = 5), but nevertheless we notice that this theory holds in a wide range of values of n and is already correct for n > 6 ( $\varepsilon = 0.33$  for n = 10).

Curves 3 and 4 show the velocity of a chain sedimenting parallel to the wall, as a function of the distance from the wall. The distance h is ranging from 3a to 300a, and the number of spheres is n = 17 and n = 98. We can here neglect the influence of the other wall on the experimental values. Again we find a good agreement between the experiments and our simulations, except for the smallest values of h. This discrepancy seems to be due to the experimental uncertainty in the determination of h in a domain where the slope of the curve is important.

The analytical solution (3), with k = 9/16, becomes very different from the experimental results for rather small values of h/l, depending on the length of the chain. The agreement is correct (1% error) for h greater than a limiting value  $h_{\text{lim}}$  which depends on n. For n = 17, we have  $h_{\text{lim}} \approx 26a$  and  $h_{\text{lim}}/l \approx 0.76$ . With  $\xi_{\infty} \approx 4.15$  this corresponds to a ratio  $\xi_{\infty}/h_{\text{lim}} \approx 0.16/a$ . For n = 98, we have  $h_{\text{lim}} \approx 97a$ ,  $\xi_{\infty} \approx 15$  and  $\xi_{\infty}/h_{\text{lim}} \approx 0.15/a$ . The ratios  $\xi_{\infty}/h_{\text{lim}}$  are very close, so we see that  $\xi_{\infty}/h$  is the quantity which gives the influence of the wall, because the effect of the wall depends on the force exerted by the chain on the fluid, i.e. the friction coefficient, which varies more slowly than the length of the chain.



Fig. 1. — Normalized sedimentation velocity  $v_n/v_1$  for a chain of spheres versus the number n of particles in the chain. The motion is parallel to the chain axis, far from the boundaries. Experimental data ( $\Box$ ), numerical results (—) and theoretical results for cylinder (- - -). Fig. 2. — The same as figure 1 for a motion perpendicular to the chain axis.



Fig. 3. — Normalized sedimentation velocity  $v_n/v_1$  for a chain of 17 spheres versus the normalized distance h/a from the wall. The motion is parallel to the chain axis and the wall. Experimental data ( $\Box$ ), numerical results (—) and theoretical results from (3) (- - - -). Fig. 4. — The same as figure 3 for a chain of 98 spheres.

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#### 4. Conclusion.

We have found that the analytical expressions given by the slender body theory (see also Ref. [1]) predict correct results for rather small values of the number of particles in the chains, and that the influence of a limiting wall on the friction coefficient can be well estimated using (3), even for distances from the limiting wall which are smaller than the length of the body.

The numerical method agrees quite well with the experiment for any distance and any number of particles. This verification allows us to use it with confidence to study other problems related to particles and wall hydrodynamic interactions in a viscous fluid, such as the layering of particles sedimenting on a plane.

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