MANY-BODY HYDRODYNAMIC INTERACTIONS IN A MICROCHANNEL

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Summary We present the results of numerical calculations for colloidal particles confined to a cylindrical microchannel. In particular we calculate the mutual mobility coefficient of two spheres and short-time self-diffusion coefficients. Other results like single particle friction coefficient, velocities of polymeric chains of particles in parabolic flow will also be presented. Comparison with earlier results shows that the widely used method of reflections is insufficient for calculations of hydrodynamic interactions.

INTRODUCTION

Dynamics of colloidal particles in quasi-one-dimensional systems are of great interest in chemical engineering and biology [1, 2, 3]. The essential problem is the evaluation of many-body hydrodynamic interactions between the particles. Earlier theoretical works tended to focus on one hard sphere in a cylindrical microchannel. The problem was tackled either by the reflection method [4] valid for small particle radius or by the singular perturbation technique [5] valid for particle radius comparable to the radius of the cylinder. At the best the pair-wise contributions to hydrodynamic the interactions were considered [6].

Efficient methods that are based on the multipole expansion of the Stokes equations have been constructed and are readily available in a form of the HYDROMULTIPOLE code [7, 8]. These algorithms are meshless, fast, accurate and versatile in the sense that we can easily change the radius and the character of particles. Recently this method was extended and implemented for the case of suspension bounded by a microchannel [9, 10].

HYDRODYNAMIC INTERACTIONS IN CYLINDER - NOVEL ALGORITHM

We consider a cylindrical microchannel of radius b, filled with a suspension of N non-deformable spherical particles of radius a_i $(i = 1, ..., N)$ immersed in an incompressible viscous fluid. Each particle is described by the position of its center $\boldsymbol{R}_i$ $(\boldsymbol{\rho}_i, z_i$ in cylindrical coordinates), translational velocity $\boldsymbol{U}_i$ and rotational velocity $\boldsymbol{\Omega}_i$. The fluid is characterized by shear viscosity η. We assume low Reynolds number, creeping flow conditions and no-slip boundary condition on the cylinder surface and on the spherical particles. We also set $b = 1$ as our length scale.

For such a system, instead of solving Stokes partial differential equations for the fluid velocity and pressure, we can focus exclusively on the particle motion and solve the corresponding boundary integral equation for the density of the induced forces $\boldsymbol{F}_i$ on the particle surfaces S_i [8],

$$\boldsymbol{v}_i^{rb}(\boldsymbol{r}) - \boldsymbol{v}_\infty(\boldsymbol{r}) = \int \boldsymbol{Z}_i^{-1}(\boldsymbol{r}-\boldsymbol{R}_i, \boldsymbol{r}'-\boldsymbol{R}_i)\cdot \boldsymbol{F}_i(\boldsymbol{r}')\,d\boldsymbol{r}'$$

$$+\sum_{j=1}^{N}\int \left[1-\delta_{ij}\boldsymbol{T}_0(r-r') + \boldsymbol{T}_b(\boldsymbol{r},\boldsymbol{r}')\right]\cdot \boldsymbol{F}_j(\boldsymbol{r}')\,d\boldsymbol{r}', \boldsymbol{r}\in S_i, \tag{1}$$

where $\boldsymbol{v}_i^{rb}(r) = \boldsymbol{U}_i + \boldsymbol{\Omega}_i \times (\boldsymbol{r}-\boldsymbol{R}_i)$ is the rigid-body velocity field of the particle i and $\boldsymbol{v}_\infty(\boldsymbol{r})$ is the imposed ambient flow. $\boldsymbol{T}_0(\boldsymbol{r})$ denotes the Oseen tensor

$$\boldsymbol{T}_0(\boldsymbol{r}) = \frac{1}{8\pi\eta}\frac{\boldsymbol{1}+\widehat{\boldsymbol{r}}\widehat{\boldsymbol{r}}}{r}, \tag{2}$$

and $\boldsymbol{T}_b(\boldsymbol{r},\boldsymbol{r}')$ describes the flow reflected from the boundaries which confine the suspension. In the case of unbounded space $\boldsymbol{T}_b(\boldsymbol{r},\boldsymbol{r}') = 0$. The single-particle friction operator $\boldsymbol{Z}_i$ depends on the specific boundary conditions at the surface of particle i, and can be obtained by solving the Stokes equations for a particle subject to an external flow in an unbounded fluid. The main theoretical result of this presentation is the explicit expression for $\boldsymbol{T}_b(\boldsymbol{r},\boldsymbol{r}')$ in the cylindrical geometry. Projecting Equation (1) on a basic set of multipole functions and solving the resulting set of algebraic equations [8, 9, 10] we obtain the many-body hydrodynamic mobilities for a system of many particles confined in a cylinder.

HYDRODYNAMIC INTERACTIONS IN CYLINDER - EXAMPLES

Example 1: We consider two particles on the axis of the cylinder. In [11] a peculiar effect for point particles at large distances (inter-particle distance z_{12} larger than 2) is reported. These particles inhibit each other's motion rather than aid it. In our case this should be seen as a negative mutual axial mobility coefficient μ_{12}^{tt}. With our method we can compute μ_{12}^{tt} for finite particles. Figure 1 presents the results for $a_1 = a_2$ and $a_1 \neq a_2$. We see that the effect is observable also

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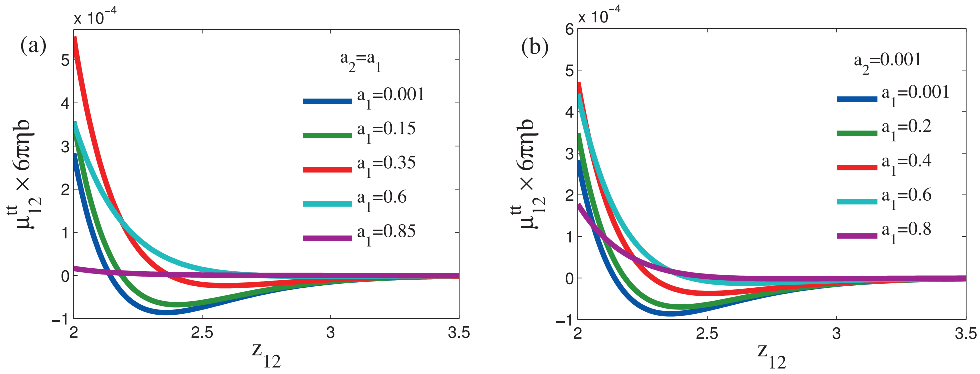

Figure 1. Normalized mutual mobility coefficient as a function of inter-particle distance.

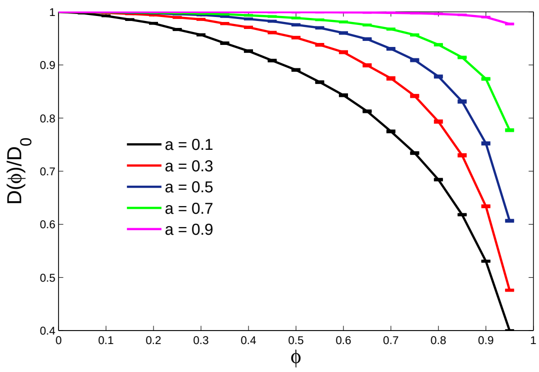

Figure 2. Normalized self-diffusion coefficient $D\left(\phi\right)/D_0$ as a function of the packing fraction ϕ.

for finite particles and it diminishes with increasing particle radius. Moreover, comparing results for $a_1 = a_2 = 0.6$ and $a_1 = 0.001, a_2 = 0.6$, we see that the negative coupling is stronger when one particle is small.

Example 2: The short-time self-diffusion coefficient, for the infinite ($1d$ periodic) array of particles confined in microchannel, is given by the initial slope of the mean-square displacement [12]

$$D = \lim_{t\to 0} \frac{1}{2}\frac{d}{dt}\left\langle \left[z_1\left(t\right) - z_1\left(0\right)\right]\right\rangle = \frac{k_B T}{N}\left\langle \sum_{i=1}^{N} \mu_{ii}\left(1,...,N\right)\right\rangle_{eq}. \quad (3)$$

In Equation (3) we used the many-body Smoluchowski equation which allows to express D as an equilibrium ensemble average of the N-particle self-mobility matrix [13]. Here k_B is the Boltzmann constant and T is the temperature. Figure 2 presents the normalized self-diffusion coefficient $D\left(\phi\right)/D_0$ as a function of the packing fraction ϕ for a wide range of packing fractions. We do not show the error bars because the statistical error is smaller than the line width. We see that the larger particle radius the decay of $D\left(\phi\right)$ is slower, which is consistent with the computed virial expansion [10]. This behavior can be accounted for by the strong screening of hydrodynamic interactions in a cylindrical microchannel, i.e. the larger particles interact effectively with fewer partners so their self-diffusion coefficient is less dependent on the packing fraction.

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