Electrophoresis simulation of charged particles with thin double layer

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イオン電解質内に薄い電気2重層を持った粒子が分散した系について考える。位置 $\boldsymbol{r}$ における粒子表面のゼータ電位が $\zeta(\boldsymbol{r})$ となるときに、すべり速度 $\boldsymbol{v}^s = -\epsilon\zeta(\boldsymbol{r})/\eta\boldsymbol{E}(\boldsymbol{r})$ を考えた結果を述べる。ここで、$\epsilon, \eta, \boldsymbol{E}(\boldsymbol{r})$ は溶媒の誘電率、粘度、電場である。

1 Theory

Electrophoresis simulation for the arbitrary shaped and charged particle with thin electric double layer is presented. The particle is dispersed in Newtonian fluid with viscosity η and permittivity ϵ. The surface of the particle has non-uniform zeta potential distribution as $\zeta(\boldsymbol{r})$ where $\boldsymbol{r}$ is the position on the particle surface. The velocity $\boldsymbol{v}(\boldsymbol{r})$ on the particle with linear velocity $\boldsymbol{V}$ and angular velocity $\boldsymbol{\Omega}$ under external electric field $\boldsymbol{E}$ is expressed as

$$\boldsymbol{v}(\boldsymbol{r}) = \boldsymbol{V} + \boldsymbol{\Omega} \times (\boldsymbol{r} - \boldsymbol{r}_c) - \frac{\epsilon\zeta(\boldsymbol{r})}{\eta}\boldsymbol{E}(\boldsymbol{r}) \tag{1}$$

where $\boldsymbol{r}_c$ is the center of the particle and $\boldsymbol{E}(\boldsymbol{r})$ is the local electric field on the position $\boldsymbol{r}$. Since the physics of the electric effect is imposed in the above equation, the following Stokes and Poisson equations are solved only,

$$\eta\nabla^2\boldsymbol{v} - \nabla p = 0, \qquad \nabla^2\phi = 0 \tag{2}$$

where $\boldsymbol{v}$, p and ϕ are the velocity, pressure and electric potential respectively. The boundary condition of the electric field on the particle is $\nabla\phi \cdot \boldsymbol{n} = 0$ where $\boldsymbol{n}$ is the normal of the particle since we consider the non-conducting particle. This condition says the electric field $\boldsymbol{E}(\boldsymbol{r})$ in equation (1) is tangential component of the particle surface.

The results of computational simulation using boundary element method are shown in next section.

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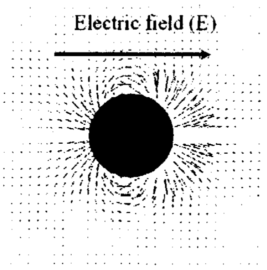
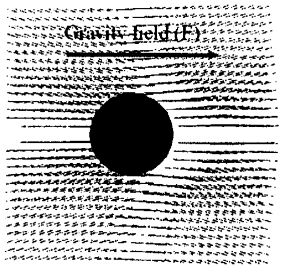
2 Results

The flows of electrophoresis and sedimentation are compared.



The uniform charged particle under external electric field produces the dipole velocity field as Fig.1. The flow is expressed as $O((a/r)^3)$.

Fig. 1: Dipolar flow



The particle under gravity field produces the flow denoted by Oseen tensor as Fig.2. The order is as $O(a/r)$.

Fig. 2: Oseen flow

Next the zeta potential of the spherical particle is expanded as spherical harmonics function using monopole M, dipole $\boldsymbol{D}$ and quadrupole $\boldsymbol{Q}$ as

$$\zeta(\boldsymbol{r}) = M + 3\boldsymbol{D}\cdot\boldsymbol{n}(\boldsymbol{r}) + \frac{5}{2}\boldsymbol{n}(\boldsymbol{r})\cdot\boldsymbol{Q}\cdot\boldsymbol{n}(\boldsymbol{r}). \tag{3}$$

When $M = 0$, $\boldsymbol{D} = \boldsymbol{e}_z$ and $\boldsymbol{Q} = \boldsymbol{e}_x\boldsymbol{e}_x + \boldsymbol{e}_y\boldsymbol{e}_y - 2\boldsymbol{e}_z\boldsymbol{e}_z$, the electric mobility is depend on the strength of the electric field as shown in Fig.3.

The uniform charged spheres in the vincinity of the wall come near each other as shown in Fig.4. The electric field is applied to the normal direction of the wall normal. On the other hand, in the sedimentation, the particles move away as shown in Fig.5.

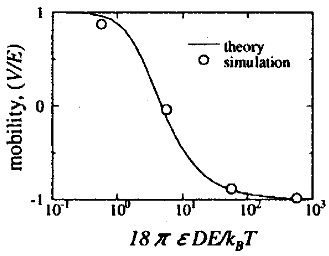


Fig. 3: Mobility of non-uniform charged particle as a function of electric field

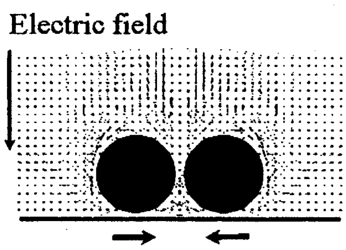


Fig. 4: Two particles near a wall under electric field

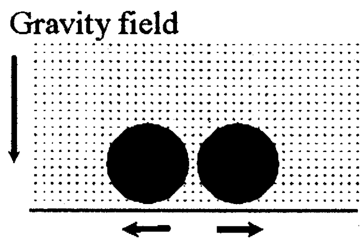


Fig. 5: Two particles near a wall under gravity field

Acknowledgment

This work is supported by the Japan Science and Technology Agency (JST/CREST).