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Magnetic particle movement program to calculate particle paths in flow and magnetic fields

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ABSTRACT

We developed an analysis program for predicting the movement of magnetic particles in flow and magnetic fields. This magnetic particle movement simulation was applied to a capturing process in a flow cell and a magnetic separation process in a small vessel of an in-vitro diagnostic system. The distributions of captured magnetic particles on a wall were calculated and compared with experimentally obtained distributions. The calculations involved evaluating not only the drag, pressure gradient, gravity, and magnetic force in a flow field but also the friction force between the particle and the wall, and the calculated particle distributions were in good agreement with the experimental distributions. Friction force was simply modeled as static and kinetic friction forces. The coefficients of friction were determined by comparing the calculated and measured results. This simulation method for solving multiphysics problems is very effective at predicting the movements of magnetic particles and is an excellent tool for studying the design and application of devices.

1. Introduction

Magnetic separation is used in a variety of industrial fields. In drainage processors, contaminants are connected with magnetic matter, and removed from the water by using a strong magnetic field [1]. In in-vitro diagnostic detectors and separation processes in biotechnologies, magnetic micro or nanoparticles are used to carry target molecules such as proteins [2,3]. These particles are gathered in the magnetic field, and unbound molecules in a solution are removed. These instruments are complex multiphysics systems using flow and magnetic fields, and it is very important to accurately predict the distribution of magnetic particles in order to make them precise in their operation.

Many analytical and computational studies have dealt with the prediction of complex paths of magnetic particles in flow and magnetic fields. For example, Satoh developed the Lattice Boltzmann method based on the fluctuation hydrodynamics which is applicable to a flow problem of a suspension. Then he applied this method to a two-dimensional Poiseuille flow of a magnetic suspension between the two parallel walls in order to investigate the behavior of magnetic particles in a non-uniform applied magnetic field situation. He showed that the behavior of magnetic particles drastically changes due to which factor dominates the phenomenon much more significantly among the magnetic particle–particle interaction [4]. Haverkort et al. theoretically derived exact analytical solutions for a particle moving in a simple flow and constant magnetization force field [5]. This study treated a Poiseuille flow and a magnetic field generated by a current carrying wire. The fields became almost homogeneous. However, the above-mentioned studies only considered simple geometries, where in fact the flow and magnetic fields in bio- and mechanical engineering industrial products are rather complicated. On the other hand, Kim et al. recently developed a finite element and a level set method of predicting the paths of magnetic particles [6]. In this method, the coordinates of the particles are represented as functions of the level set in a fixed background mesh for the magnetic field. This method can be used to make predictions about real products with arbitrary geometries such as real products. However, the number of particles it can treat is limited by the computational resources; many meshes are needed to represent many particles. Moreover, Ravnik et al. combined the boundary element method and the Lagrange based particle tracking model. And they were applied to the motion of magnetic particles in fluid flow under the external non-uniform magnetic field. They showed that the collection efficiency decreased linearly with increasing flow rate [7,8]. On the other hand, Yang et al. calculated the motions of magnetic nanospheres under the magnetic field in rectangular microchannel and the calculated particle motions due to both the flow and magnetic field were in good agreement with

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experimental data [9]. The movements of magnetic particles on a wall have to be modeled in order to predict the particle distribution in practical situations. However, to the best of our knowledge, the previous research does not deal with particle movement on a wall.

We developed a method of simulating the movements of magnetic particles in flow, pressure gradient, gravity, and magnetic fields for the purpose of analyzing complicated commercial products. We applied it to magnetic particles in a capturing process of a flow cell and in a magnetic separation process in a small vessel in an immunoassay device. In this method, the path of a magnetic particle is calculated using the Newton equations in a background mesh for the flow and magnetic field. The flow and magnetic field calculations using a finite volume method and finite element method, respectively, are independent of the path calculation of the particle. The adsorption distribution of the magnetic particles on the wall has to be ascertained in order to predict the movement of the particles in a solution or on the wall. Therefore we added a friction force between the particle and the wall. The friction force was composed of static and kinetic forces with static and kinetic coefficients. We simulated the movements of magnetic particles in the capturing process of the flow cell and in a magnetic separation process in a vessel surrounded by magnets. We then compared the calculated distributions of the magnetic particles with experimental results on actual process systems.

2. Numerical simulation method

2.1. Analysis of particle moving in a flow

We developed a simulation tool that can predict the path of magnetic particles in a flow, pressure gradient, gravitational, and magnetic fields. The motion of magnetic particles is governed by the Newton equation with forces including drag, pressure gradient, gravity, and magnetism as shown in the following equation:

$$m_p \frac{d^2 \boldsymbol{r}_p}{dt^2} = \boldsymbol{F}(\boldsymbol{r}_p) \tag{1}$$

here, m_p, $\boldsymbol{r}_p$, and t are the mass of the particle, spatial coordinates of the particle, and time, respectively. $\boldsymbol{F}(\boldsymbol{r}_p)$ is the sum of the external forces on particle p. As shown in Eq. (2), the external force is composed of the drag force from the flow $\boldsymbol{F}_{drag}(\boldsymbol{r}_p)$, pressure gradient force $\boldsymbol{F}_{\nabla P}(\boldsymbol{r}_p)$, gravity and buoyancy force $\boldsymbol{F}_{gravity}$, and magnetic force $\boldsymbol{F}_{magnet}(\boldsymbol{r}_p)$.

$$\boldsymbol{F}(\boldsymbol{r}_p) = \boldsymbol{F}_{drag}(\boldsymbol{r}_p) + \boldsymbol{F}_{\nabla P}(\boldsymbol{r}_p) + \boldsymbol{F}_{gravity} + \boldsymbol{F}_{magnet}(\boldsymbol{r}_p) \tag{2}$$

The drag on the particle, $\boldsymbol{F}_{drag}(\boldsymbol{r}_p)$, can be evaluated with Eq. (3). Here, $\boldsymbol{u}_p$ is the particle velocity, and $\boldsymbol{u}$ and ρ_f are the flow velocity and the density of the background fluid at the coordinate of particle p. A_p is the projected area of the particle, and C_d is the drag coefficient for a sphere in the Stokes region or Allen region, as shown in Eq. (4) [10]. Drag is calculated in terms of the relative velocity between the particle velocity and the flow velocity.

$$\boldsymbol{F}_{drag}(\boldsymbol{r}_p) = \frac{1}{2} C_d \rho_f A_p |\boldsymbol{u} - \boldsymbol{u}_p| (\boldsymbol{u} - \boldsymbol{u}_p) \tag{3}$$

$$C_d = \begin{cases} 24(1 + 0.15 Re_D{}^{0.687})/Re_D, & Re_D \le 10^3; \\ 0.44, & Re_D > 10^3 \end{cases} \tag{4}$$

Re_D is the Reynolds number, and it can be expressed using the density of the background fluid ρ_f, the diameter of the particles D_p, and the viscosity μ.

$$Re_D \equiv \frac{\rho_f |\boldsymbol{u} - \boldsymbol{u}_p| D_p}{\mu} \tag{5}$$

The force of the pressure gradient $\boldsymbol{F}_{\nabla P}(\boldsymbol{r}_p)$ is calculated by using Eq. (6). Here, V_p and P are a volume of the particle p and pressure of the background fluid, respectively.

$$\boldsymbol{F}_{\nabla P}(\boldsymbol{r}_p) = -V_p \nabla P \tag{6}$$

$\boldsymbol{F}_{gravity}$ includes the effect of gravity and buoyancy (Eq. (7)). Here, $\boldsymbol{g}$ is the gravitational acceleration

$$\boldsymbol{F}_{gravity} = (\rho_f - \rho_p) V_p \boldsymbol{g}. \tag{7}$$

The magnetic energy of a magnetic particle $U_{magnetic}(\boldsymbol{r}_p)$ with a magnetic moment $\boldsymbol{M}_p$ in a field with a magnetic flux density $\boldsymbol{B}$ is expressed as [11]

$$U_{magnetic}(\boldsymbol{r}_p) = -\boldsymbol{M}_p \boldsymbol{B}. \tag{8}$$

The magnitude of the magnetic moment $|\boldsymbol{M}_p|$ depends on the magnitude of the magnetic flux density $|\boldsymbol{B}|$ [12]. The magnetic particle is made by incorporated nanoparticles, which has a property as superparamagnetism, in porous monosized polymer beads. Then we use the hysteresis curve in this reference [12] for the magnetic moment of the magnetic particle. The magnetic force of the particle p is calculated as the gradient of the magnetic energy $U_{magnetic}(\boldsymbol{r}_p)$ as shown in the following equation:

$$\boldsymbol{F}_{magnetic}(\boldsymbol{r}_p) = \nabla U_{magnetic}(\boldsymbol{r}_p) = -\nabla(\boldsymbol{M}_p \boldsymbol{B}) \tag{9}$$

here, we suppose that the directions of $\boldsymbol{M}_p$ and $\boldsymbol{B}$ are parallel. As a result, $\boldsymbol{M}_p$ can be expressed as

$$\boldsymbol{M}_p = |\boldsymbol{M}_p| \frac{\boldsymbol{B}}{|\boldsymbol{B}|}. \tag{10}$$

Substituting Eq. (10) into Eq. (9), the magnetic force of the particle p becomes

$$\boldsymbol{F}_{magnetic}(\boldsymbol{r}) = -\nabla(|\boldsymbol{M}_p||\boldsymbol{B}|). \tag{11}$$

2.2. Analysis of particle moving on a wall

We estimate not only the force in a flow field but also the friction force between a magnetic particle and a wall. We use a friction force obeying the Amontons–Coulomb friction law [13,14], as shown in Fig. 1, the force is composed of static and kinetic components with static and kinetic coefficients, μ_s and μ_k. When the particle is on the wall, the force calculated by Eq. (2) is

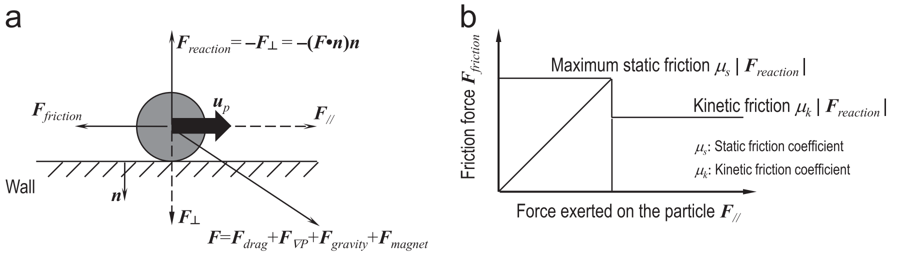

Fig. 1. Slip model for a particle on a wall. External force of the particle on the wall (a) and friction force of the particle using static and kinetic friction forces (b).