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Computation of Micro-particle Dynamics in a Filtration Process with the Coulomb Interaction

Nobuyuki Hirooka[1,*] and Satoru Ushijima[2]

[1]Department of Civil and Earth Resources Engineering,Doctoral Program,Kyoto University
[2]Academic Center for Computing and Media Studies (ACCMS), Kyoto University

*hirooka.nobuyuki.85e@st.kyoto-u.ac.jp

Abstract. Particle dynamics in a filtration process with electric effects are numerically simulated using the MICS (Multiphase lncompressible flow solver with Collocated grid System) for multiphase flows and the DEM (Discrete Element Method). This study deals with micro-particles and fluid flows through a single pore, which is larger than the particle size, modeled with two solid obstacles at the micro-scale. For an understanding of the effect of the electrostatic force between the electric-charged particles and the porous structure, it is implemented based on Coulomb's law. The computational results indicate that the number density in the rear or the center of the porous structure tends to be high by giving the electrostatic attractive force between the negatively charged particles and the positively charged porous structure.

Keywords: Particle dynamics, Coulomb's force, Porous media, Filtration

1. Introduction

Filtration is an indispensable technology and is used in our lives and industry. It allows liquid or gas to pass through filter media and remove solid pieces or other unnecessary substances from the fluids. Recently, the demand for masks has risen for virus protection. The semiconductor manufacturing process is requiring high-performance filters with the spread of 5G, IoT (Internet of Things), and AI (Artificial Intelligence). As the detailed understanding of the mechanism at the micro-scale is difficult to realize experimentally, the filtration of a particle suspension under a dead-end and constant pressure has been simulated numerically by the LBM (Lattice Boltzmann Method) and the DEM [1]. Our previous computational study shows that there is some possibility of improving the retention performance by giving the electrostatic attractive force between the negatively charged particles with a diameter of 2.5 mm and the positively charged porous structure at the macro-scale. Based on the computational methods, the filtration performance and mechanism under a dead-end and constant inlet velocity have been investigated numerically using particles with a diameter of 8.0 μm at the micro-scale. The effect of the electrostatic attractive force between the micro-particles and the porous structure according to Coulomb's law is discussed in this study.

2. Governing equations

The incompressible condition and the momentum equations [2] for incompressible Newtonian-fluid flows can be written respectively as

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_i u_j) = f_i - \frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{1}{\rho}\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] \tag{2}$$

where x_i is components of the Cartesian coordinate system. Here u_i and f_i are components of the mass-averaged velocity of fluid, external force acceleration in x_i direction respectively. The volume-averaged variables ρ, p and μ are density, pressure, and the coefficient of viscosity respectively. The basic equations are solved numerically by the finite volume method with a collocated grid arrangement. The components of the fluid force F_{Cki} in a mesh cell C acting on a solid body k in x_i direction can be calculated from [2] :

$$F_{Cki} = \alpha_k \sigma_k \Delta V_C \left[-\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{1}{\rho}\frac{\partial}{\partial x_j}\left\{\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right\}\right] \tag{3}$$

where α_k, ΔV, and σ_k are the volume fraction of a solid phase in a mesh cell, the volume of a mesh cell, and the density of a solid body respectively. The mesh cell size is smaller than a particle. The sum of F_{Cki} for the mesh cells of a particle k is the fluid force on the particle.

The equations for the translational and rotational motions of a particle with the fluid force $\boldsymbol{F}_f$, the contact force $\boldsymbol{F}_s$, the adhesive force $\boldsymbol{F}_v$ and the electrostatic force $\boldsymbol{F}_e$ are given respectively by

$$m\frac{\partial \boldsymbol{v}}{\partial t} = \boldsymbol{F}_f + \boldsymbol{F}_s + \boldsymbol{F}_v + \boldsymbol{F}_e \tag{4}$$

$$I\frac{\partial \boldsymbol{w}}{\partial t} = \boldsymbol{m}_c \tag{5}$$

where $\boldsymbol{v}$ is the velocity vector of a particle. Here m, I, $\boldsymbol{w}$, $\boldsymbol{m}_c$ are the particle mass, the moment of inertia, the angular velocity vector, and the external torque vector respectively. The contact force between particles or a particle and a wall is calculated based on the DEM [3]. The adhesive force due to the van der Waals force [4] between particles of the diameter D_{pi} and D_{pj} is given by

$$\boldsymbol{F}_v = \sum_{pi \neq pj} \frac{A}{12z^2}\left(\frac{D_{pi}D_{pj}}{D_{pi} + D_{pj}}\right)\boldsymbol{n} \tag{6}$$

where z, A and $\boldsymbol{n}$ are the separate distance, the Hamaker constant, and the unit vector from the center of a particle pi to the center of a particle pj respectively. The electrostatic force between the particle pi and pj due to Coulomb's law is given by

$$\boldsymbol{F}_e = \sum_{pi \neq pj} -\frac{Q_{pi}Q_{pj}}{4\pi\varepsilon_0 r^2}\boldsymbol{n} \tag{7}$$

where Q_{pi} and Q_{pj} are the electric charge of the particle pi and pj. Here ε_0 and r are the permittivities of free space and the distance between the particle pi and pj respectively.

3. Computational methods and results

As shown in Fig. 1, two semicircular objects with a diameter D_t = 64 [μm] are placed. The overall scale is L = 225 [μm] in length and W = 100, 120 [μm] in width. The spatial resolution was fixed at $\Delta x = \Delta y = 1.0$ [μm]. The inlet fluid velocity U_{in} is 0.05 m/s. Micro-particles with a diameter D_m = 8 [μm] are injected upstream at the rate of 10 particles/ms when W = 100 [μm] and 12 particles/ms when W = 120 [μm]. The particles that flow outside the domain are deleted. Slip boundary conditions for the fluid are applied at the upper and bottom walls. The computations were conducted for the three different charge densities: (a) 0.0, (b) 0.015 and (c) 0.025 [C/m^3]. The porous structure is charged positively and the particles are charged negatively. Figure 2 shows the simulation results when W = 100 [μm]. The contour indicates the fluid velocity in x_1 direction normalized by the inlet velocity U_{in}.

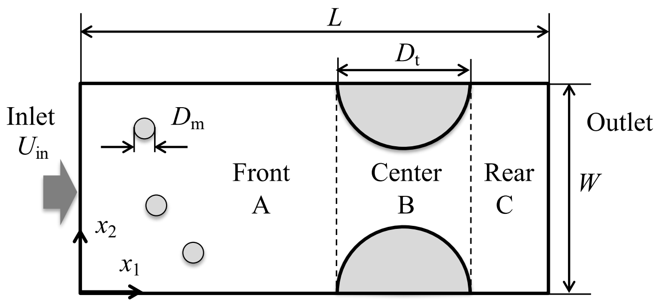

Figure 1: Schematic diagram of the computational domain.

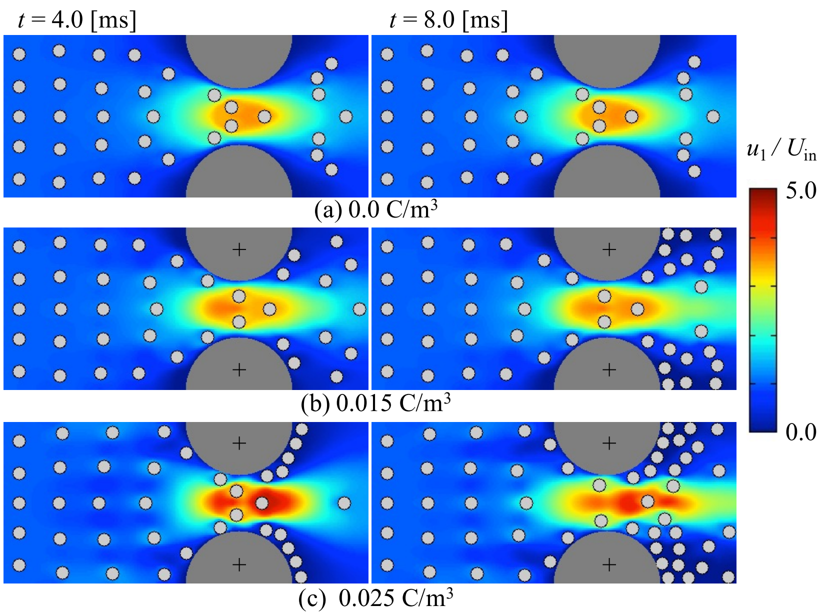

Figure 2: Micro-particle flows through the single pore when W = 100 [μm].

The number density of the charged micro-particles increases at Rear C when W = 100 [μm] and tends to increase at Center B when W = 120 [μm], varied depending on the charge density and the width W as shown in Fig. 3. It seems reasonable to think that the particles and the porous structure are attracting each other according to the electrostatic attractive force and that the charged particles are retained more as the force increases.

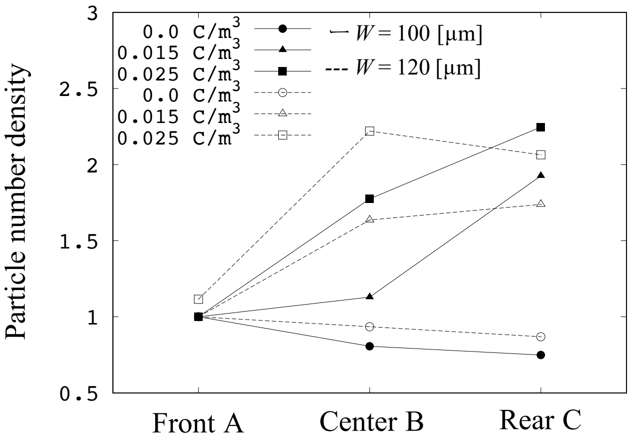

Figure 3: Normalized particle number density by one at Front A with 0.0 C/m^3.

4. Conclusions

The computational methods including the MICS and the DEM were applied to the filtration process on a micrometer scale. The electrostatic attractive force between micro-particles and a porous structure is implemented based on Coulomb's law. The micro-particles and fluid flows through a single pore under a constant inlet velocity is simulated numerically. As a result, it is confirmed that the number density of the particles increases in the rear or the center of the porous structure according to the electrostatic attractive force and the width W.

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