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Particle-Scale and Macro-Scale Computations on the Swelling Process of Superabsorbent Polymer Particles

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Abstract. In this study, an experiment where SAP particles are dropped into water was conducted. As the particles accumulated on the bottom area, swelling starts. The height change of the particle layer is measured. The swelling behavior of SAP particles are also tracked using OpenPIV. In addition, the swelling process was numerically predicted with a three-dimensional computation method which deals with fluid-solid and solid-solid interactions (MICS) to confirm its applicability. On the macro-scale, MICS is used to simulate a seepage flow through SAP layer. As water flow through the layer, it is absorbed by the SAP layer and the particles swell upward. The applicability and improvability of the computations are then discussed.

Keywords: Superabsorbent polymer particles, Fluid-solid interaction, Particle-scale swelling process, SAP particle experiment, 3D Multiphase computational model, Macro-scale model

1. Introduction

In this paper, the swelling behavior of Superabsorbent Polymer Particles (SAP) is studied. SAP particles in the dry state are hard crystallized particles with entangled polymer chains. When the particles come in contact with water, the polymer chains expand, absorbing the water inside as the particle size increases.[1] In the wet state, the particle become softer and transparent. These particles are able to retain the water inside.

In the past studies of SAP particles, the particles are commonly treated either as a single particle or as a group of particles (macro-scale).[2] In order to understand the swelling behavior of SAP particles better, the swelling behavior on particle-scale of multiple SAP particles is included in this study. Firstly, an experiment using SAP particles was conducted.[3] An open source algorithm used for Particle Image Velocimetry (PIV) image analysis and post-processing named OpenPIV is used on the experimental results to track the movement of the

particles. In addition, the swelling rate of the particles obtained through the experiment are used for the 3D computation. Multiphase Incompressible-flow solver with Collocated grid System (MICS) by Ushijima[4] is used to calculate the fluid-solid interaction computation. A good agreement of the particle height between the 3D computational results and experiment is obtained. On the second case, a macro-scale computation of seepage flow through a bed of SAP particles which swell is conducted using MICS. The computation shows a reasonable results as the fluid flow through the permeable solid layer.

2. Numerical Computation

The computation for the incompressible fluid is governed by

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

where u_j is the velocity component in x_j direction in two-dimensional Cartesian coordinates, t is time, x_i is the component of the Cartesian coordinate system, ρ_f is fluid density, ν is kinematic viscosity, and p is pressure. In addition, u_i is the velocity component and f_i is the acceleration component of the external force. The governing equations are discretized on finite volume method and solved with SMAC method on collocated grid system. The fluid forces acting on the objects are calculated with the pressure and viscous terms as

$$F_{Cki} = \phi_s \rho_s \Delta V \left[-\frac{1}{\rho_f}\frac{\partial p}{\partial x_i} + \frac{1}{\rho_f}\frac{\partial}{\partial x_j}\left\{\frac{\partial}{\partial x_j}(\mu u_i) + \frac{\partial}{\partial x_i}(\mu u_j)\right\}\right]$$

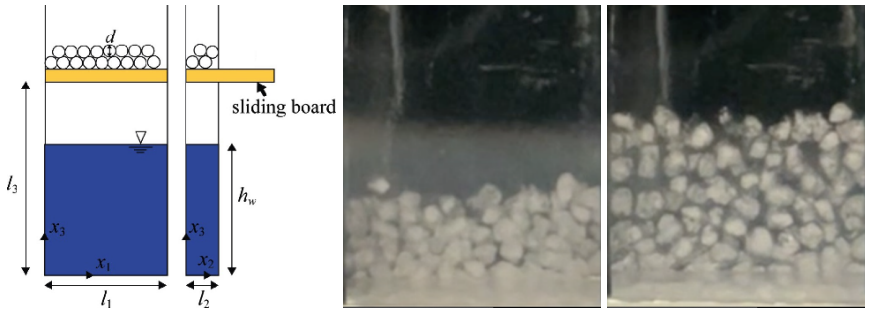
where F_{Ck} is the fluid force vector in fluid cell C acting on object-k and its x_i component is given by F_{Cki}. In addition, ΔV is the volume of a fluid cell, ρ_s is the density of the solid and ϕ_s is the volume fraction of solid.

On the particle-scale 3D computation, the solid is represented by multiple tetrahedron elements and introduced to the computational method for a multiphase field. On the macro-scale computation, the same method is used for the computation. However, as the solid is treated as a single unit of solid, the setup of multiple tetrahedron elements is not needed. In addition, in order to allow the liquid to flow through the solid, the volume fraction of the solid ϕ_s is set between 0 and 1.

3. Particle-Scale Computation of SAP particles

In order to observe the particle-scale swelling behavior of a group of SAP particles, an experiment with setup shown in Fig. 1 (a) is conducted. The experimental area is separated into two chambers separated by a sliding board. 50 particles with size d around 0.5 mm to 0.71 mm are set on the upper chamber. On the lower chamber, an area with dimension of $l_1 = 8$ mm, $l_2 = 3$ mm is filled with water with elevation $h_w = 10$ mm. As the sliding board is pulled out, the particles on the upper chamber fall into the water. Almost immediately, the particles piled up on the bottom area and that time is assigned as $t = 0$ [s] of the swelling

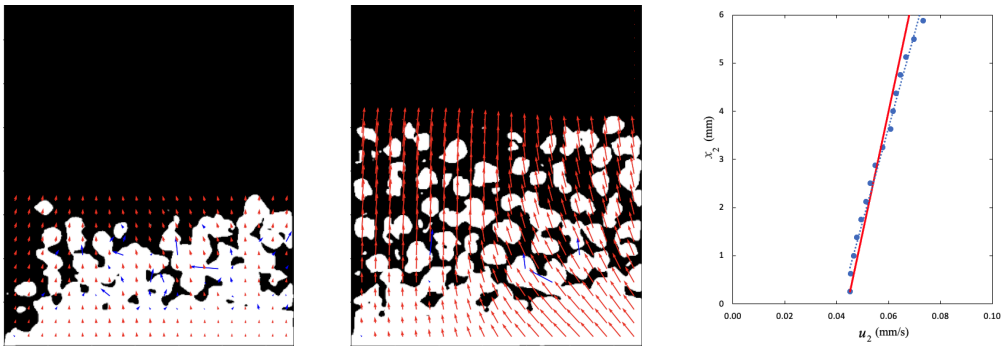
process as shown in Fig. 1 (b). The height of SAP particles on $t = 0$ [s] is set as h_0. The particles are let to swell until $t = 5$ [s] as shown in Fig. 1 (c) and the height growth of the layer is recorded.



(a) Experimental setup (b) $t \approx 0$ [s] (c) $t \approx 5$ [s]

Figure 1: Experimental setup and results of SAP particles on different time

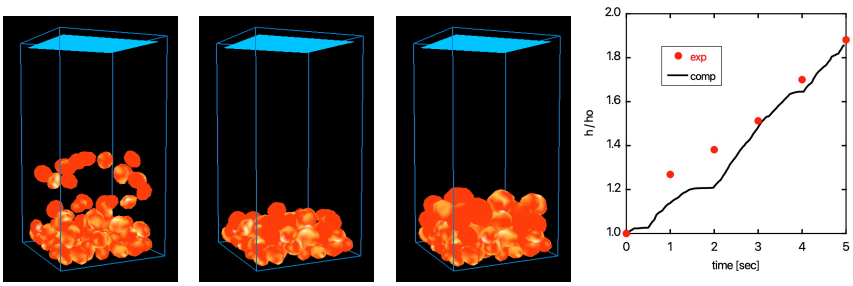
The obtained experimental results are then processed using OpenPIV. Using OpenPIV, the change of the frames in time can be tracked. In this study, the change is the position change and velocity of SAP particles as shown in Fig. 2 (a) and Fig.2 (b). The obtained u_2 velocity in x_2 direction on $l_1/2$ is shown in Fig. 2 (c). The red line shows the expected velocity of particles when all particles swell on the same rate and the dotted line shows the regression line of the extracted velocity. It can be observed that a deviation between the dotted and red line exists. The deviation shows that the particles do not swell on the same rate in different layers. The extracted velocity has gentler slope meaning that particles on the top layer swell faster than the particles on the bottom.



(a) $t \approx 0$ [s] (b) $t \approx 5$ [s] (c) u_2 on $l_1/2$ at $t \approx 5$ [s]

Figure 2: Extracted velocity using OpenPIV

A 3D numerical prediction with the same dimensions as the experiment is then computed as shown in Fig. 3 (a) and (b). The h/h_0 of SAP particle layers between the computational and experimental results are then compared as shown in Fig. 3 (c). The computation shows a good agreement with the experimental results.

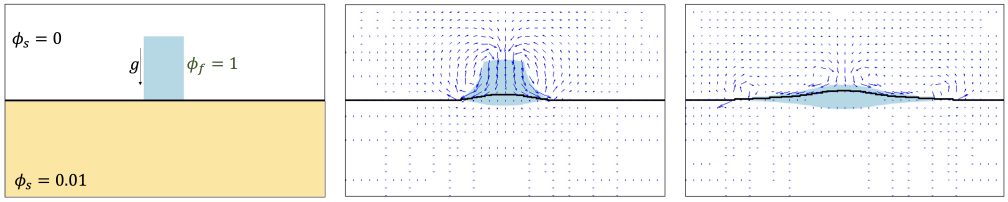


(a) t = −0.40 [s] (b) t = 0.50 [s] (c) t = 3.50 [s] (d) SAP height change with time

Figure 3: Calculated SAP particles in water and comparison with experimental data

4. Macro-Scale Computation of SAP Particles

In addition to the particle-scale computation, a macro-scale computation using MICS is conducted. A column of water is set on a bed of SAP layer as shown in Fig. 4 (a). Due to the gravity, water flow through the permeable SAP layer. The porosity of the SAP layer is represented as the volume fraction of solid used in MICS computation ϕ_s and the value is set as 0.05. Different porosity between air and SAP layer causes water to flow slower and spread through the layer. The SAP layer swell upward using a swelling computation that is included in the model. The results of the computations can be seen in Fig. 4 (b) and (c).



(a) t = 0 [s] (b) t = 0.04 [s] (c) t = 0.09 [s]

Figure 4: Computational setup at t = 0 [s] and results

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