

**Computational Methods for
Interactions Between Swelling Solid and Fluid
using Eulerian-Lagrangian Approach**

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Abstract

The simulation of fluid and solid interactions is shown to be an important consideration in many engineering problems. In the situations where solid is experiencing large volume deformations such as swelling and distortion, the computations of these solid within fluid becomes challenging. The interaction that is affecting the movement of the solid also affecting the shape of the solid. Additionally, the deformations of the solid will also affecting the fluid movement. It is often that several aspects of this difficulties are ignored, leaving a simpler approach to reproduce some cases. However, due to the absence of the variables, sometimes it cannot give a bigger picture of the problem. For example, by omitting the existence of fluid in the problem, it may not account into the movement of the solid due to the fluid flow. In order to give the closest reproduction for these cases, we proposed several numerical methods that are considered simple and yet reliable to be used in different cases. As a representative for the swelling solid, superabsorbent polymer (SAP) particles and hydrogel particles are investigated. Several methods and model are proposed to be used depending on the case of the computation since it is considered to give more straightforward and yet accurate results compared to a one size fits all approach. First, experiments were conducted on the superabsorbent polymer particles and hydrogel particles. The experiments are then analyzed and the swelling behavior of the particles are observed. Following the experiment, computations are conducted in each case with the proposed methods. In the computations on the superabsorbent polymer particles, a 3D computations is conducted using multiphase incompressible-flow solver with collocated grid system (MICS) method by Ushijima. The computation is compared to the experiment in order to verify the applicability of the method. Additionally, since in some cases the focus of the fluid-solid interaction on swelling objects is the flow of the fluid through the solid layer, we adjusted the MICS method. By taking

advantage of the attribute used in MICS, we were able to calculate the case of seepage flow on a layer of swelling particles. The results and its applicability are then discussed. In the hydrogel particles case, a methods utilizing mass-spring model and direct-forcing immersed boundary method is introduced. Similar to the previous case, the computations are also compared with the obtained experiment results. In addition, various cases are also computed and the applicability of the methods are discussed.

Keywords: Fluid-solid interaction, Superabsorbent polymer particle, Hydrogel particle, Swelling, Mass-spring model, Immersed boundary method, VOF method

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1 Introduction

1.1 Motivation

In this study, the interaction between swelling solid and water is studied. Fluid-solid interactions remain a major challenge in various fields. The application of fluid-solid interaction is extensive. We can observe the interactions of fluid and solid almost everywhere everyday in science, engineering, and medicine. Fundamentally, in the fluid-solid interactions problems, the fluid and solid mutually influence each other. The motion of the fluid affects the motion of the solid, and as the solid moves, it also influence the fluid flow. The more this influence between the solid and fluid is dependent to each other, the more challenging the problem becomes. Furthermore, in some solid materials, there is the possibility that swelling or other deformations may occur. Since more variables such as the swelling characteristics of solid are introduced into the problem, more attention are needed in the coupling between the solid and fluid.

Generally, the computation of fluid-solid interactions is separated depending on the domain used in the fluid and solid calculation. A Computation where both the fluid and solid computations are taking place on the same Eulerian domain, such as inside a Cartesian grid is called as Eulerian-Eulerian method. In the past, a fluid-solid interactions computation in the Eulerian-Eulerian method is introduced by Sugiyama [1][2][3][4]). We have also investigated such computation in this method in the effects of free surface flows on soft body[5]. The proposed Eulerian-Eulerian method is able to robustly compute large deformation of solid objects without the need to reconstruct the computational mesh. However, it is also to be noted that in the proposed method, some limitations are found. Due to the usage of the solid/fluid volume of fraction (VOF) method, when a long duration computation was calculated, numerical dissipation on the fluid-solid interface may occur[1]. In order to reduce this numerical dissipation, special technique such as PLIC (piecewise linear interface calculation) [6][7][8] is needed. In

addition, implicit treatment on the stress computation is also necessary to stably calculate the deformation of solid objects with a broad range of physical properties [1].

Another approach where the calculations of fluid and solid phases are done separately in Eulerian and Lagrangian frameworks, called Eulerian-Lagrangian approach, is also widely used for fluid-solid interaction problems. In the Eulerian-Lagrangian approach, there are two frameworks in one model and we need to communicate the information obtained in one framework to another [9]. When dealing with multiple objects, and its distribution is not uniform, we need some techniques to balance the load in the parallelization with domain decomposition method [10][11][12]. Numerical diffusion in the interface between the fluid and solid does not occur. It is also easy to set up different physical properties for each object in the same computation. Consequently, in this dissertation, the Eulerian-Lagrangian method is used.

In the past studies of swelling objects, generally such objects are observed in particle-scale such as studied by Nagano et al (2020) [13], Sweijen et al. (2017) [14] and Guinea et al (2023) [15]. On some other cases, the particles are observed as a group of particles (macro-scale) such as studied by Diersch et al (2010) [16]. Within these studies, the use of different approaches can be observed. The use of a one-size fits all approach is appealing as it can give a better flexibility to various cases with one model. However, this may cause some simplification over the fairly complicated problem. Creating a model which is able to work on multiple problems is difficult. Consequently, it is often that some aspects of the problems are omitted. For instance, in the computation of superabsorbent polymer (SAP) particles by Sweijen et al. (2017) [14], the fluid computation is omitted, leaving a simpler computational using distinct element method (DEM). The omission of the fluid however, means that in some cases the influence of fluid into the solid is not accounted for. Since the conditions of the problems are fairly complicated, it is considered best to use different approaches for different problems.

In this study, alternative methods which are considered simple is proposed depending on the swelling solid characteristics. Using different approaches, it is expected that a close reproduction can be obtained. As a representative for the swelling solid, superabsorbent polymer (SAP) particles and hydrogel particles are investigated. SAP particles are hard crystallized particles consisted of entangled polymer chains. When these particles come into contact with water, the polymer chains expand, absorbing the water inside as the particle size increases [17]. In the

wet state, the particle become softer and transparent. Due to its water retaining and swelling capability, superabsorbent polymer used such as in hygienic products [18] , and water shutoff treatment [19] . SAP particles are able to absorb water and swell rapidly within seconds. The hydrogel particles are spherical and made of a type of superabsorbent polymer called sodium polyacrylate. These particles are commonly used as plant media and air freshener. Similar to the SAP particles, the hydrogel particles are able to swell multiple times its original size. The shape itself is round and easy to be observed. However, due to their large size, the swelling time is considerably longer.

For the SAP particles, the multiphase incompressible-flow solver with collocated grid system method by Ushijima [20] is proposed for the fluid-solid computation. The applicability of MICS had been discussed in past studies such as in the flow through granular bed [21], flow through multiple elastic bodies [22], and floating objects transported by tsunami flow through structures [23]. Multiple tetrahedron elements (T-type model) is used for the solid model. Using this method, a 3D particle-scale computation is conducted for the SAP particles and compared to the experiment. In some cases, the fluid flow penetrating into a SAP layer is the focus of the computation. For this problem, the MICS method is adjusted. Utilizing the volume fraction of solid variable used in MICS, the computation of seepage flow through a layer of swelling SAP particles are able to be conducted.

It is considered that in some cases the hydrogel particles shape may be distorted by the fluid flow or solid contact. Therefore, a model where the solid does not only swell, but also distorts is considered. In the preceding studies of the Eulerian-Lagrangian approach for soft solid, solid objects represented by unstructured mesh and finite element method (FEM) are often used for computations [24][25], however in more complex problem and large distortion on the solid, non-linear finite element method is needed and the computation may become complicated. A Method utilizing mass-spring model for the solid distortion is introduced. The fluid-solid interactions are calculated using direct-forcing immersed boundary method for the fluid-solid interaction. 2D Computations are considered to be suitable for this model. The applicability of the proposed method for a 3D computations is possible. However, since the mass-spring system used tend to become complex, more caution is required.

1.2 Overview

First, the swelling behaviors of SAP particles and hydrogel particles are observed. Different experiments were conducted for both materials.. From the experiment with SAP particles [26], the height change of SAP layer is measured. Additionally, the images of the experiment results are processed using OpenPIV. Particle Image Velocimetry (PIV) is a measurement technique to capture velocity fields through high spatial and temporal resolution that is used in various applications [27]. OpenPIV is an open-source software that performs PIV analysis from images and a variety of post-processing tools to track the change of the frames in time and extract the velocity fields [28]. From this velocity fields, the swelling rate and behavior of the particles are used as a condition for the computation. The size growths of hydrogel particles are measured. The size growths are then used as the swelling rate of the hydrogel particles computations

The computation utilizing proposed methods are then conducted for SAP particles and hydrogel particles. For the SAP particle computations, a 3D computations is conducted to be compared with the experiment results. The applicability of the proposed method is then discussed. By adjusting the variable used in MICS, the computation for seepage flow through a layer of swelling SAP particles is conducted and the results is discussed.

For the verification of the mass-spring model computation used in the 2D particle-scale computation, the obtained swelling rate on hydrogel particles are used in the computation, and compared to the experiment. Comparing the obtained results and past research of the computation of the sedimentation of a single swelling particle in fluid is also done. Additionally, in order to check the flexibility of the proposed method in various cases, the 2D computation of lid-driven cavity flow problems are conducted and its applicability are discussed.

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2 Numerical Methods

2.1 Fluid Computations in Collocated Grid

The governing equation for incompressible fluids are given by

$$\frac{\partial u_j}{\partial x_j} = 0, \quad (2.1)$$

$$\frac{\partial \rho_f}{\partial t} + \frac{\partial(\rho_f u_j)}{\partial x_j} = 0. \quad (2.2)$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_i u_j) = -\frac{1}{\rho_f} \frac{\partial p}{\partial x_i} + \frac{1}{\rho_f} \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + f_i \quad (2.3)$$

It is to be noted that the equations are written in Einstein notation. 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 Cartesian coordinate system, ρ_f is density, μ is dynamic viscosity, p is pressure, f_i is the external force in x_i direction. In addition, u_i is the mass-averaged liquid and gas phase velocity component. The phase between gas and liquid is governed by the volume fraction of fluid C . The value of C and its relation to the density ρ_f and velocity u_i is shown as

$$\rho_f = (1 - C)\rho_g + C\rho_l \quad (2.4)$$

$$u_i = \frac{(1 - C)\rho_g u_{g,i} + C\rho_l u_{l,i}}{\rho_f} \quad (2.5)$$

Here, g and l indicates the gas and liquid phase and C is $0.0 \leq C \leq 1.0$. Due to this relation, the convection equation becomes

$$\frac{\partial C}{\partial t} + \frac{\partial(Cu_j)}{\partial x_j} = 0. \quad (2.6)$$

2. Numerical Methods

In this study, the convection equation from Eq. 2.6 is used instead of the Eq. 2.2.

The fluid computations are conducted using the Finite Volume Method (FVM) in the collocated grid system consisting of prediction stage, pressure calculation stage, and correction stage. The flowchart of the fluid computation in the collocated grid system can be seen on Fig. 2.1.

Figure 2.1: Flowchart of the fluid computations in the collocated grid system

A simple illustration in the computation of 2D collocated grid system is shown in Fig. 2.2. In the collocated grid system, all variables are defined at the cell center as shown in Fig. 2.2 (a). While the convection and diffusion term of the Navier Stokes equation are calculated at the cell center, the velocity components are spatially interpolated on the cell boundaries in the pressure computations as shown in Fig. 2.2 (b).

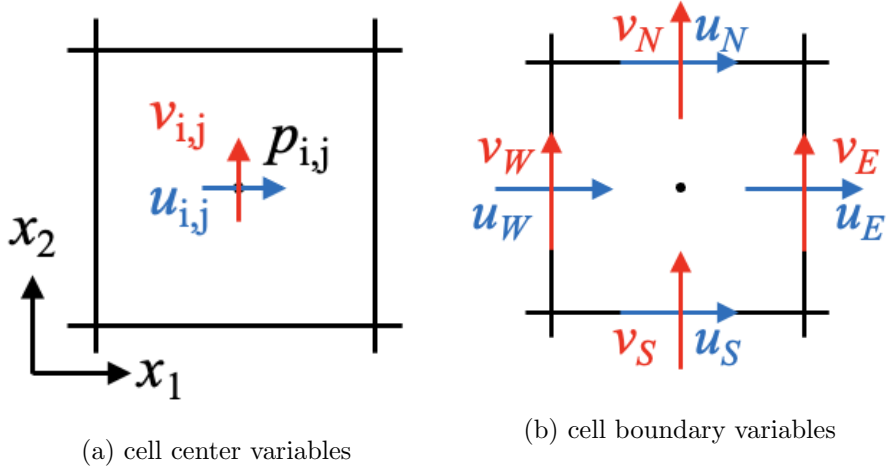


Figure 2.2: Variable placements on fluid cells

The notation i and j show the variable component in x_1 and x_2 direction. E, W, N, and S represent the variables at the cell boundary in each direction. In this study, uniform mesh is used in both 2D and 3D computations.

First, Eq. 2.3 is discretized and used to obtain the tentative velocity component. The convection term is solved explicitly using 5th order TVD scheme. The pressure Poisson equation (eq. 2.7) is solved using Bi-CGSTAB method.

$$\frac{\partial}{\partial x_i} \left(\frac{1}{\rho_f^n} \frac{\partial \psi}{\partial x_i} \right) = \frac{1}{\Delta t} \frac{\partial u_i^*}{\partial x_i} \quad (2.7)$$

Here, ψ is the time difference, $\psi = p^{n+1} - p^n$. In the correction stage, the obtained pressure from the pressure calculation stage is used to update the flow velocity as shown in eq. 2.8

$$u^{**} = u_i^* + \frac{\Delta t}{\rho} \frac{\partial}{\partial x_i} (p^{n+1} - p^n) \quad (2.8)$$

Next, the convection equation of C is calculated using THINC/WLIC method [1]. The next time step of C is calculated from a dimensional splitting algorithm as follows.

$$C^* = C^n - \Delta t \left\{ \frac{\partial C^n u_1^{n+1}}{\partial x_1} - C^n \frac{\partial u_1^{n+1}}{\partial x_1} \right\} \quad (2.9)$$

$$C^{n+1} = C^* - \Delta t \left\{ \frac{\partial C^n u_2^{n+1}}{\partial x_2} - C^n \frac{\partial u_2^{n+1}}{\partial x_2} \right\} \quad (2.10)$$

Afterwards, the value of ρ and μ are updated with the obtained value of C .

2.2 Fluid-Solid Interactions Computations

Two methods are proposed for the computations of SAP particles and hydrogel particles. In the SAP particle computations, multiphase incompressible-flow solver with collocated grid system (MICS) method is used. Meanwhile, Direct-Forcing/Immersed Boundary (DF/IB) method is used in the hydrogel particle computations.

2.2.1 Numerical Method Used in Superabsorbent Polymer Particles Computations

Different to the computation using DF/IB which utilizes the interpolation between Eulerian cells and Lagrangian points, computations using MICS only take place on the Eulerian cells. In order to differentiate between solid and fluid state, variable ϕ_s , the volume fraction of solid is used. The value of ϕ_s is set between 0 and 1.

The fluid forces acting on the objects are calculated with the pressure and viscous terms as

$$\mathbf{F}_{Cki} = \phi_s \rho_s \Delta V \left[-\frac{1}{\rho_f} \frac{\partial p}{\partial x_i} + \frac{1}{\rho_f} \frac{\partial}{\partial x_j} \left\{ \frac{\partial}{\partial x_j} (\mu \mathbf{u}_i) + \frac{\partial}{\partial x_i} (\mu \mathbf{u}_j) \right\} \right] \quad (2.11)$$

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

The mass-averaged velocity $\mathbf{u}_i$ is calculated as

$$\mathbf{u}_i = \frac{(1 - \phi_s) \rho_f \mathbf{u}_{f,i} + \phi_s \rho_s \mathbf{u}_{s,i}}{\rho} \quad (2.12)$$

2.2.2 Numerical Method Used in Hydrogel Particles Computations

Due to the consideration of the existence of solid within the fluid domain, the governing equation of the fluid of Eq. 2.3 should be modified with an additional term of fluid interaction forces λ_i in x_i direction. Therefore, in the DF/IB computation, equation 2.3 becomes

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} (u_i u_j) = -\frac{1}{\rho_f} \frac{\partial p}{\partial x_i} + \frac{1}{\rho_f} \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + f_i + \lambda_i. \quad (2.13)$$

The computation of DF/IB starts after the prediction stage of the fluid computation as shown by the orange bordered box in Fig. 2.3. After the DF/IB calculations, the computations continue to the rest of the fluid computation with SMAC method and entering the computation of deformations, solid-solid interactions, and swelling processes of the solids as shown in the green bordered box in Fig. 2.3. The solid model will be explained in detail in the next section.

The setup of Eulerian fluid cells and Lagrangian Points used in the DF/IB is shown in Fig. 2.4.

In detail, we can see the calculation of SMAC and DF/IB method in Fig. 2.5.

The white boxes show that the calculations take place in Eulerian framework, while grey boxes show that the calculations take place in the Lagrangian framework. The governing equations for incompressible fluids are first solved to obtain the tentative fluid velocities assuming that fictitious fluid exists inside the solid.

In the DF/IB calculation, in order to calculate the fluid force acting on a solid body, tentative velocities on the center points of fluid cells in the prediction stage are first interpolated into setup Lagrangian points as shown in Fig. 2.6.

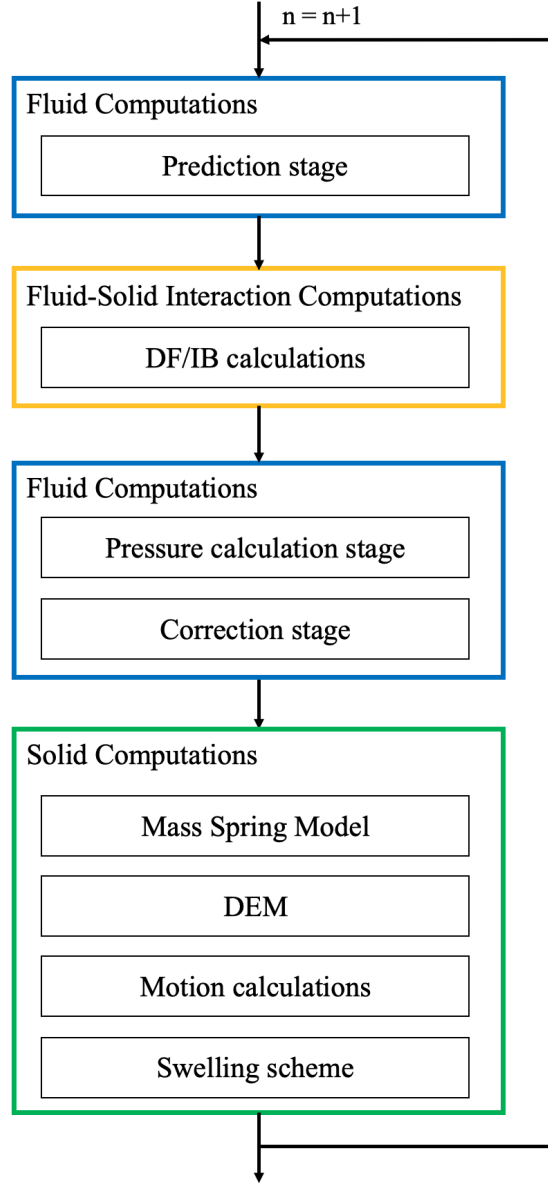


Figure 2.3: Flowchart of the computations

For the interpolation and spreading between Eulerian cells and Lagrangian points, a sharp discrete delta functions [2] is used, as shown in

$$\Phi(r) = \begin{cases} 1 - |r|, & |r| < 1 \\ 0, & \text{otherwise.} \end{cases} \quad (2.14)$$

Then we calculate the δ_h using

$$\delta_h(\mathbf{x} - \mathbf{X}) = \frac{1}{h^2} \Phi\left(\frac{\mathbf{x} - \mathbf{X}}{h}\right) \Phi\left(\frac{\mathbf{y} - \mathbf{Y}}{h}\right). \quad (2.15)$$

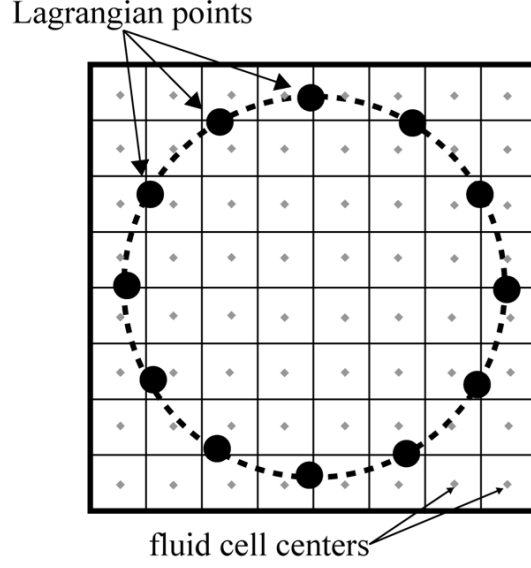


Figure 2.4: Setup of fluid cells and Lagrangian points for DF/IB

The interpolation of velocity are calculated using the following formula

$$U^*(\mathbf{X}_l) = \sum_{p=1}^{n_x} \sum_{q=1}^{n_y} \mathbf{u}^* \delta_h(\mathbf{x}_{p,q} - \mathbf{X}_l) h^2. \quad (2.16)$$

With the interpolation, the velocity values on the Lagrangian points are obtained and fluid interaction force $\mathbf{F}_f(\mathbf{X}_l)$ is calculated using

$$\mathbf{F}_f^{n+1}(\mathbf{X}_l) = \frac{\mathbf{U}_s^n(\mathbf{X}_l) - \mathbf{U}^*(\mathbf{X}_l)}{\Delta t}. \quad (2.17)$$

The obtained fluid interaction force $\mathbf{F}_f(\mathbf{X}_l)$ is then returned into the surrounding Eulerian fluid cells using the spreading functions

$$\lambda^{n+1}(\mathbf{x}_{p,q}) = \sum_{l=1}^{N_l} \mathbf{F}_f^{n+1}(\mathbf{X}_l) \delta_h(\mathbf{x}_{p,q} - \mathbf{X}_l) \Delta V_l. \quad (2.18)$$

The spreading of the fluid interaction force can be seen on Fig. 2.7.

Here we are using the same discrete delta function used in the interpolation step. Finally, we update the value of tentative velocity obtained in the prediction stage of SMAC method with the fluid interaction force as follows

$$u_i^{*'} = u_i^* + \Delta t \lambda_i^n. \quad (2.19)$$

Exiting the computation of DF/IB, The updated tentative velocity are obtained and used in the pressure calculation and correction stage of SMAC method.

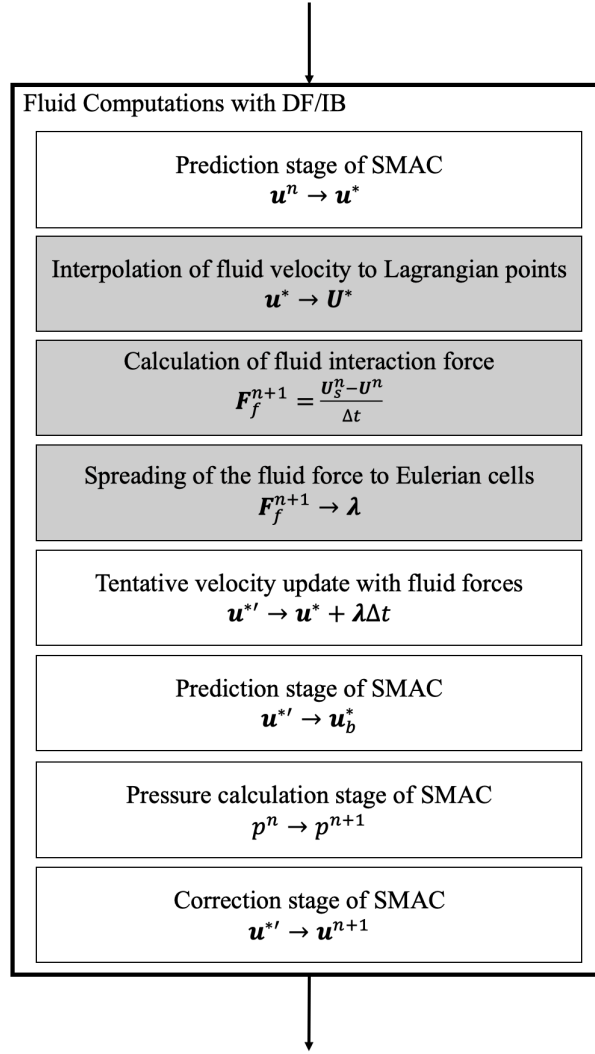


Figure 2.5: Flowchart of the computation of DF/IB

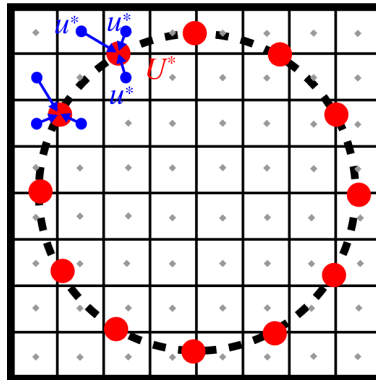


Figure 2.6: Interpolation of fluid velocity into Lagrangian points

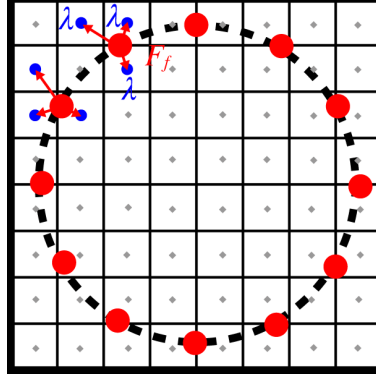


Figure 2.7: Spreading process of force value into fluid cells

2.3 Swelling Solid Computations

Different solid model is used for different solid characteristics in this study complementing the fluid-solid computation used. In the SAP particle computations, the distortion of the solid due to fluid flow and external forces is not considered. The solid in SAP particle computation is represented by multiple tetrahedron elements (T-type model) and by the volume fraction of solids. While using the multiple setup of spring and dashpot, the distortion of elastic bodies by fluid flow in hydrogel particle computations can be reproduced.

2.3.1 Swelling Solid Model Used in Superabsorbent Polymer Particles Computations

Solid objects in the SAP particle computation is represented by multiple tetrahedron elements (T-type model). Using this T-type model, the approximations of volume, mass and inertia tensors are more accurate. It is to be noted, that due to the computational cases introduced in this study, the solid objects computed using MICS are treated as rigid body.

The movement of the solid is then calculated by solving the translation and rotational motions due to the fluid force. The translation and rotational motion equations can be seen on Eq. 2.20 and Eq. 2.21.

$$M_b \dot{\mathbf{u}}_s = \mathbf{F} \quad (2.20)$$

$$\dot{\boldsymbol{\omega}} = \mathbf{I}^{-1} \left[\mathbf{R}^{-1} \mathbf{N} - \boldsymbol{\omega} \times \mathbf{I} \boldsymbol{\omega} \right] \quad (2.21)$$

Here, $\mathbf{F}$ is the summation of $\mathbf{F}_{CK}$ in all fluid cells, torque $\mathbf{N}$ is the summation of moments $r_{GC} \times \mathbf{F}_{CK}$, where r_{GC} is the vector from the object center $\mathbf{x}_{c,k}$ to the center of a fluid cell as shown in Fig. 2.8

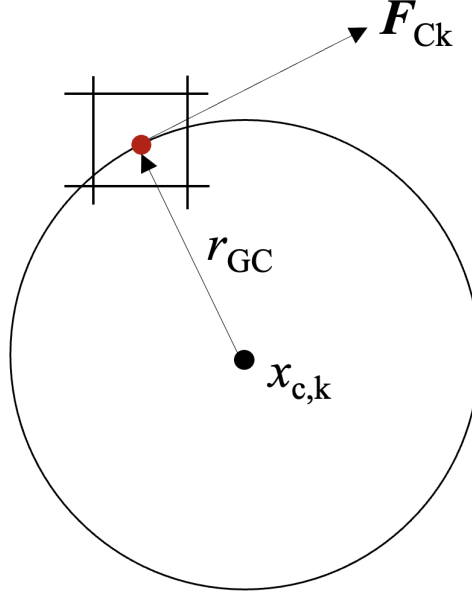


Figure 2.8: Fluid forces acting on the solid object

On the seepage flow case, 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 as $0.0 \leq \phi_s \leq 1.0$. The value of $\mathbf{u}_{s,i}$ in macro-scale computation is set as 0 as the solid is treated as a single unit of stationary solid. The value of ϕ_s is set as a function of time from the initial value. It is assumed that as the SAP particles come into contact with water, they absorb water resulting in the increase of porosity, slowing down the flow. This is represented in the increase of ϕ_s . As the value of ϕ_s increases, the mass-averaged velocity calculated by Eq. 2.12 is largely influenced by $\mathbf{u}_{s,i}$ which is 0, resulting in the decrease of fluid flow.

In the seepage flow computations, the increase of SAP layer is calculated as shown in Fig. 2.9. The absorption line, represented by the dotted line is set on the initial setting of the solid boundary line. As the water flow under the absorption line, the solid layer increases by the same

number as the submerged solid cell.

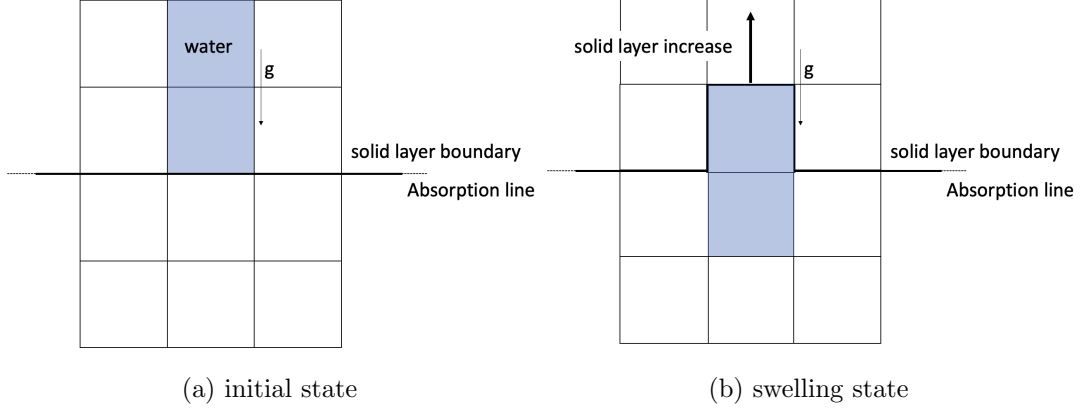


Figure 2.9: Swelling computation on the macro-scale model

For the MICS 3D computations, the swelling is applied by increasing the length of the tetrahedron elements.

2.3.2 Swelling Solid Model Used in Hydrogel Particles Computations

For the solid model in the hydrogel particle computations, the mass-spring model is used, and the placements of mass points, springs, and dashpots used can be seen in Fig. 2.10 (a). In addition, the DEM is used to predict the solid-solid interactions and the placements of the CDS can be seen in Fig. 2.10(b). The positions of each Lagrangian points on the solid boundary is updated, and the swelling of the solid is calculated by changing the length of the spring's natural length. Figure 2.3 using the combination of modified DF/IB and mass spring model (MSM-DF/IB) is proposed. The setup for DF/IB, mass spring model, and contact detection spheres used in the computation can be seen in Fig. 2.10

The detailed outline of our computation method for the deformable solid can be seen in Fig. 2.11.

In the solid computation, we need to update the movement of each points as given by

$$M\dot{\mathbf{U}}_s = \mathbf{F}_s + \mathbf{F}_f + \mathbf{F}_c + \mathbf{F}_e, \quad (2.22)$$

where $\mathbf{U}_s$ is the vector of the mass point/Lagrangian point velocity, and the dot sign represents the time derivative. M is the mass of each point given by $M = \rho_s V_s / N_l$, where ρ_s is the solid density, V_s is the total volume of the solid object, and N_l is the number of mass points

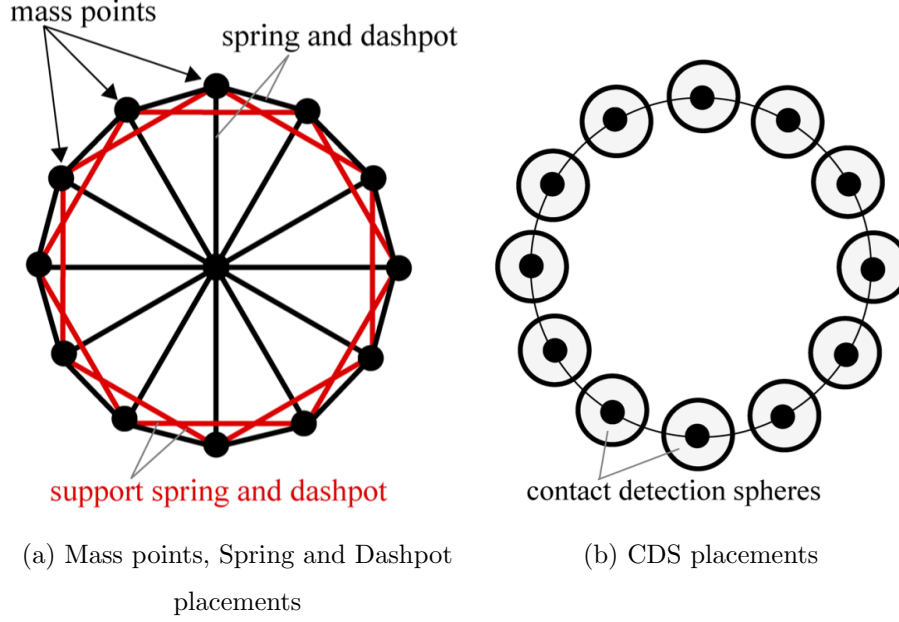


Figure 2.10: Solid model of swelling deformable solid

(Lagrangian points). $\mathbf{F}_s$ is the vector of the force calculated by the spring-dashpot model, $\mathbf{F}_f$ is the vector of the fluid forces calculated with DF/IB, explained on the Chapter 2. $\mathbf{F}_c$ is the vector of the contact force calculated with contact detection spheres and DEM, and $\mathbf{F}_e$ is the vector of the external forces.

When we consider a computation of multiple objects, the contact force between solids $\mathbf{F}_c$ need to be included into the computations. In the computation, contact detection spheres are arranged on the solid object surface as shown in Fig. 2.4 (right) and the distinct element method (DEM) is used for the calculation of solid-solid and solid-wall contact forces [3]. Shown in Fig. 2.12 is the contact scheme between two objects A and B. For the calculation, we need the relative velocity $\mathbf{v}_r$ between the two points.

The computation of contact forces $\mathbf{F}_c$ is done by

$$\mathbf{F}_c = \mathbf{F}_{cn} + \mathbf{F}_{ct}. \quad (2.23)$$

Here, $\mathbf{F}_{cn}$ and $\mathbf{F}_{ct}$ are normal and tangential contact forces respectively, calculated by

$$\mathbf{F}_{cn} = -k_n d_n \mathbf{n} + c_n \mathbf{v}_{rn} \quad (2.24)$$

$$\mathbf{F}_{ct} = -k_t d_t + c_t \mathbf{v}_{rt}. \quad (2.25)$$

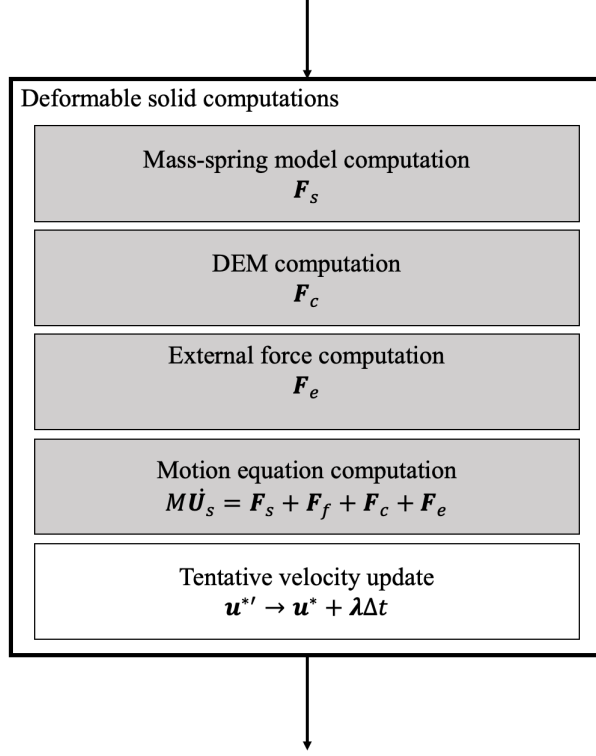


Figure 2.11: Flowchart of the deformable solid computations

In the normal contact force calculation, k_n and c_n are the spring constant and damping coefficient in normal direction. $\mathbf{n}$ is the unit normal vector. The relative velocity on normal direction $\mathbf{v}_{rn}$ is calculated as $\mathbf{v}_{rn} = (\mathbf{v}_r \cdot \mathbf{n})\mathbf{n}$. In the tangential contact force calculation, k_t and c_t are the spring constant and damping coefficient in tangential direction. The relative velocity on tangential direction $\mathbf{v}_{rt}$ is calculated as $\mathbf{v}_{rt} = \mathbf{v}_r - \mathbf{v}_{rn}$. Additionally, d_t is calculated as $d_t = \mathbf{v}_{rt}\Delta t$. The damping coefficient used in our method is calculated using

$$c = 2\sqrt{\left(\frac{mk(\ln e_b)^2}{\pi^2 + (\ln e_b)^2}\right)}, \quad (2.26)$$

where e_b is the coefficient of restitution, the ratio of relative velocity after and before collision.

The solid objects with circular shapes in the initial condition are calculated in the 2D field. Multiple mass points are arranged on the surface and a central point of the object as shown in Fig. 2.4 (center), where the points on the surface correspond to the Lagrangian points used in DF/IB (Fig. 2.4 (left)). Spring and dashpot represented by the lines in Fig. 2.4 (center) are assumed to exist between mass points.

We calculate the stretch and compression of springs between two points A and B as shown in

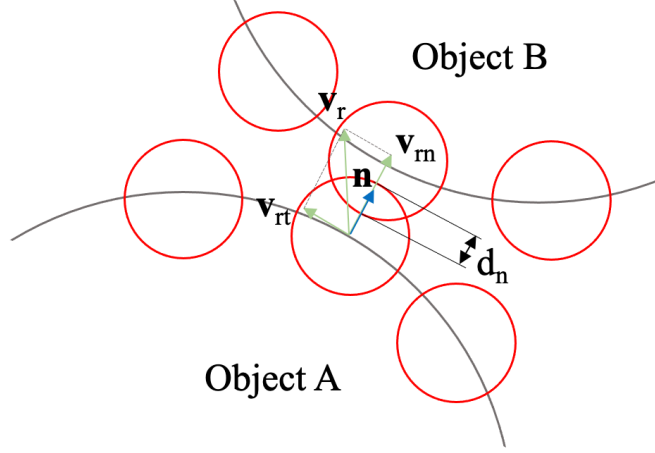


Figure 2.12: Contact scheme between two objects

$$\mathbf{F}_{s,AB} = -k \left(\|x_{AB}^n\| - \|x_{AB}^0\| \right) \mathbf{n}_{AB} + c (\mathbf{U}_A - \mathbf{U}_B). \quad (2.27)$$

Here, $\mathbf{F}_{s,AB}$ is the spring force between the two points, k is the spring stiffness constant, c is the damping coefficient. Additionally, $\mathbf{n}_{AB}$ is the unit normal vector described as

$$\mathbf{n}_{AB} = \frac{x_A - x_B}{\|x_A - x_B\|}. \quad (2.28)$$

Then, the total spring forces in each points is calculated to obtain the $\mathbf{F}_s$. It is to be noted that we set additional springs and dashpot, shown as blue lines in Fig. 2.4 (center), to act as supports in order to reduce the oscillation that occurs on the objects' surfaces when subjected to very large deformations.

When fluid get absorbed through the solid object surface, we assume that the fluids simply change its phase into solid. Therefore, the fluids absorption property is implemented by increasing the object size uniformly. In our method, we propose the size increase by utilizing the natural spring length $\|x_{AB}^0\|$ used in our proposed mass spring model in Eq. 2.27. The natural length of the spring between two points at step $n+1$, $\|x_{AB,0}^{n+1}\|$, is a function of time, and the function will be different depending on the property and material of the object as shown in Fig. 5.2. Simply, it can be written as

$$\|x_{AB,0}\| = f(t). \quad (2.29)$$

As the value of L_{AB} increases, the restoring force of the spring works and pull the position of the mass point to a new location as shown in Fig. 2.14. In this study, the objects are assumed to absorb surrounding water at the same rate as the swelling process. The density of the object is assumed to be constant resulting to the increase of the mass of the object when swelling occurs. As the objects swell, the distances between CDS increase and create empty spaces which allow objects to infiltrate each other during contact. In order to avoid this, the CDS radiuses are set to increase in the same rate as the increase of the natural spring length.

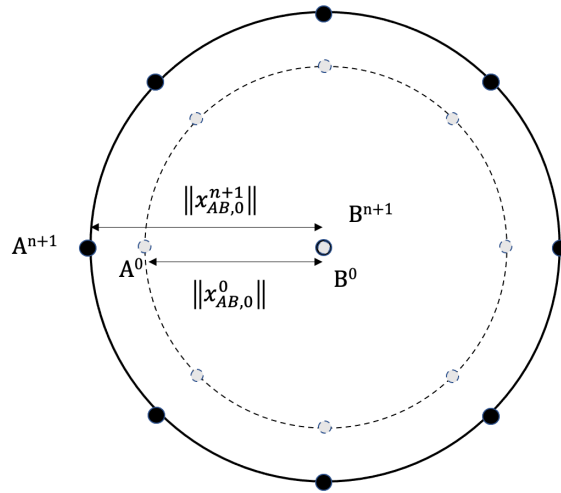


Figure 2.13: Swelling computation of the solid object

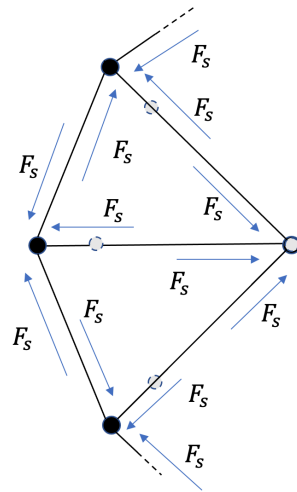


Figure 2.14: Free-body diagram of the spring forces due to swelling

References

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3 Experiments on Swelling Deformable Solids

3.1 Experiment on Superabsorbent Polymer Particles

In order to observe the swelling behavior of a group of SAP particles, an experiment with setup shown in Fig. 3.1 (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. 3.2 (b). The height of SAP particles on $t = 0$ [s] is set as h_0 . The particles are allowed to swell until $t = 5$ [s] as shown in Fig. 3.2 (c) and the height growth of the layer is recorded.

The obtained experimental results are processed using OpenPIV. Particle Image Velocimetry (PIV) is a measurement technique to capture velocity fields through high spatial and temporal resolution that is used in various applications [1]. OpenPIV is an open-source software that performs PIV analysis from images and a variety of post-processing tools to track the change of the frames in time and extract the velocity fields [2]. Pictures obtained from the experiment are altered into black and white and filtered to show sharp boundaries of the particles. After processed with OpenPIV, the velocity fields are shown in Fig. 3.3. In order to observe the swelling behavior of SAP particles on different layers, the obtained u_2 velocity at $t \approx 5$ [s] on $l_1/2$ is plotted as shown as blue points in Fig. 3.4. The regression line of the extracted velocities are represented by the dotted line. In addition, the red line shows the expected velocity when all particles on different layers swell on the same rate. From the graph, it can be observed that a deviation between the dotted and red line exists. The deviation shows that the particles on different layers do not swell on the same rate. The extracted velocity has gentler slope meaning

that particles on the top layer swell faster than the particles on the bottom.

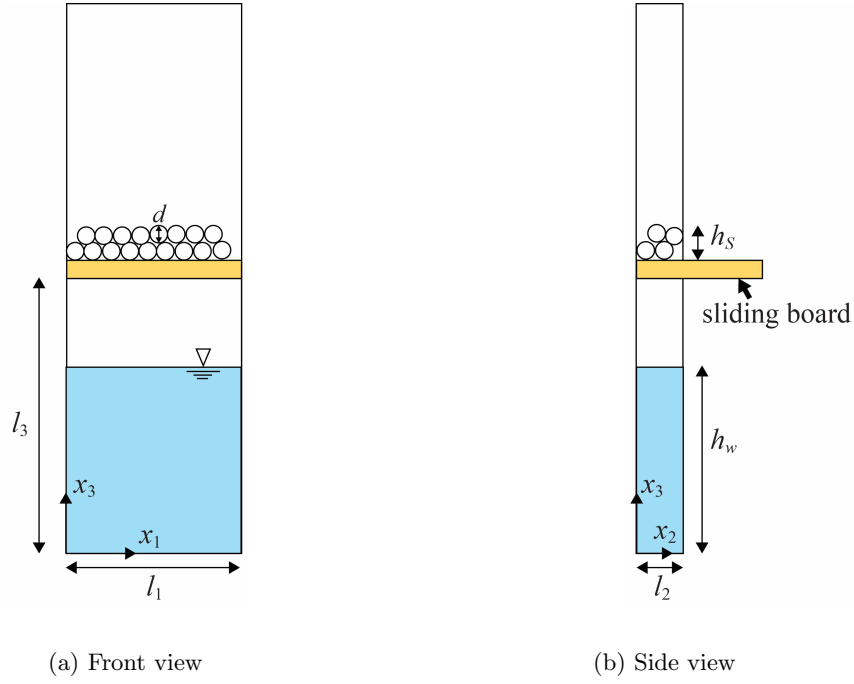


Figure 3.1: Experiment setup of SAP particles dropped in water

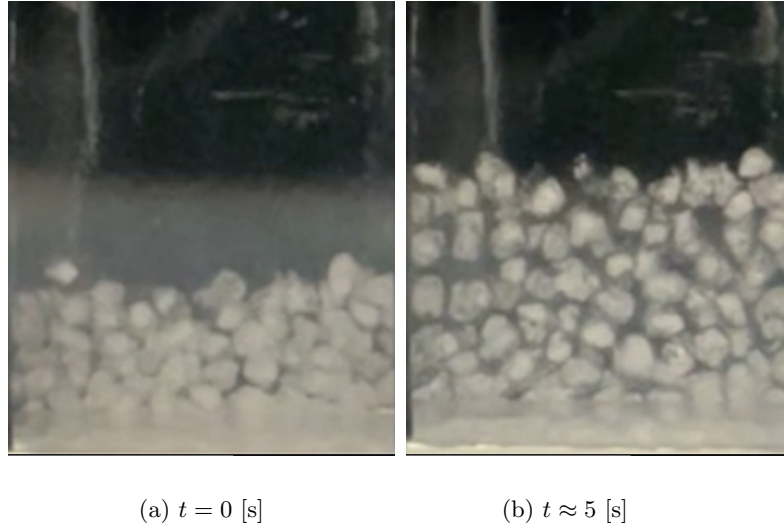


Figure 3.2: Experiment results of SAP particles dropped in water on different times

3.2 Experiment on Hydrogel Particles

The diameter growth of hydrogel particles are observed and applied into the computational method. The total of twenty hydrogel particles with three colors are put inside the water as shown in Fig. 3.5.

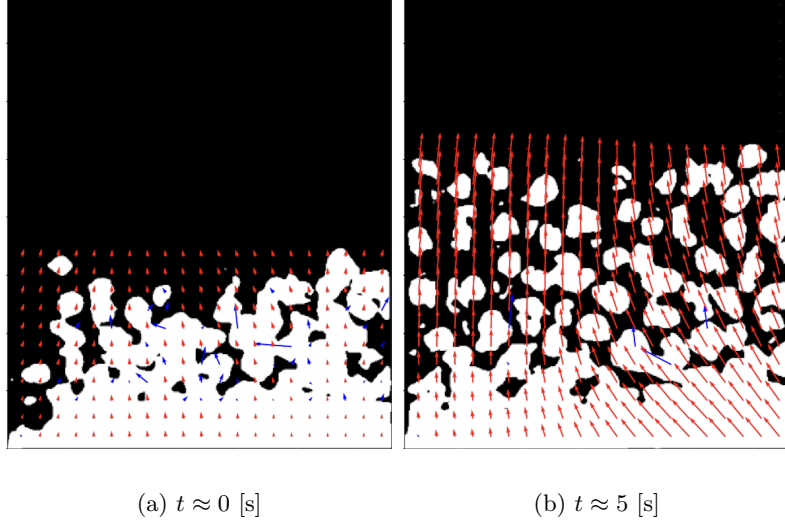


Figure 3.3: Velocity fields on experiment images processed using OpenPIV

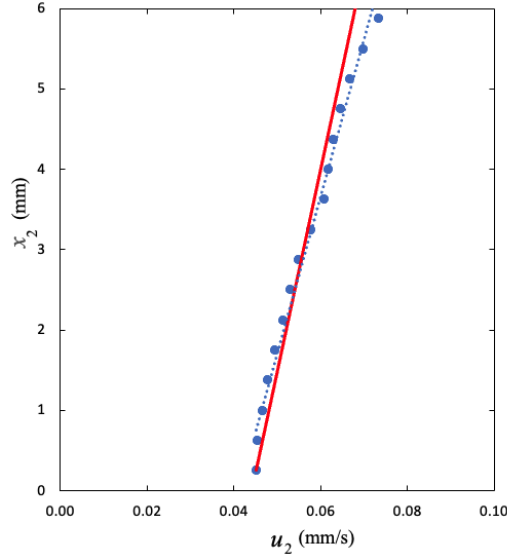


Figure 3.4: Velocity u_2 on $l_1/2$ at $t \approx 5$ [s]

We let the particles to swell for around 10 [hrs] until the particles are saturated and reach their maximum sizes. The black colored hydrogel particles are easier to be seen, we also notice that the distribution on the maximum sizes are more uniform than the other color, therefore, the swelling behavior of the black hydrogel particles are chosen to be used in our computation. The diameter of black particles are then measured, and the growths are recorded as shown in Fig. 3.6.

As it can be seen, the black hydrogel particles grow more than triple in size from the initial diameter of around 3 [mm] within 2 [hrs] and the growth rate slowly decreases and the particles

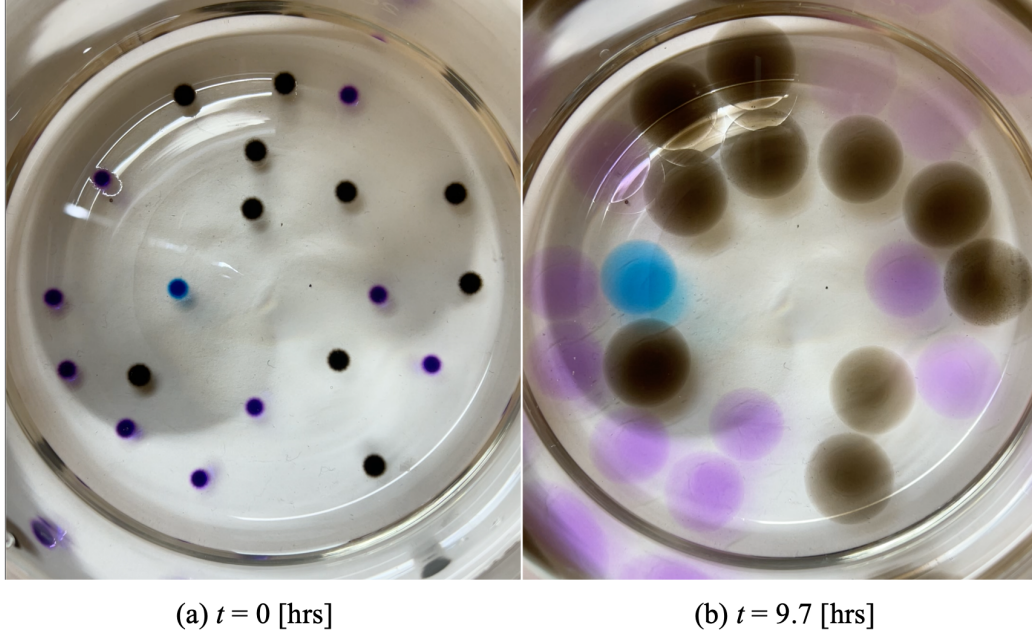


Figure 3.5: Experiment on hydrogel particles at (a) $t = 0$ [hrs] and (b) $t = 9.7$ [hrs]

reach a stable size at around 13.5 [mm] after around 9 [hrs]. In addition, we do a regression analysis using computer software (KaleidaGraph 4.5) and find out the relation between time (t) and diameter of the particles (D). The equation for the relation of t and D for $0 < t < 9.7$ [hrs] is shown in the Eq. 3.1.

$$D = -4.38 \times 10^{-26}t^6 + 5.88 \times 10^{-21}t^5 - 3.36 \times 10^{-16}t^4 + 1.04 \times 10^{-11}t^3 - 1.85 \times 10^{-7}t^2 + 0.002t + 2.98 \quad (3.1)$$

The obtained Eq. 3.1 is used to calculate the change of the natural length of the spring $\|x_{AB}^0\|$ as explained in Chapter 5.

3.3 Summary

In this chapter, two kind of experiments on hydrogel particles and superabsorbent polymer particles are introduced. In the experiments on hydrogel particles, we observed the swelling rate of the particles by measuring the diameter growth over time for around 10 hours. Using KaleidaGraph software, we are able to obtain the equation of the diameter growth to time and this equation will be used in the next chapter for validation of the proposed method for 2D

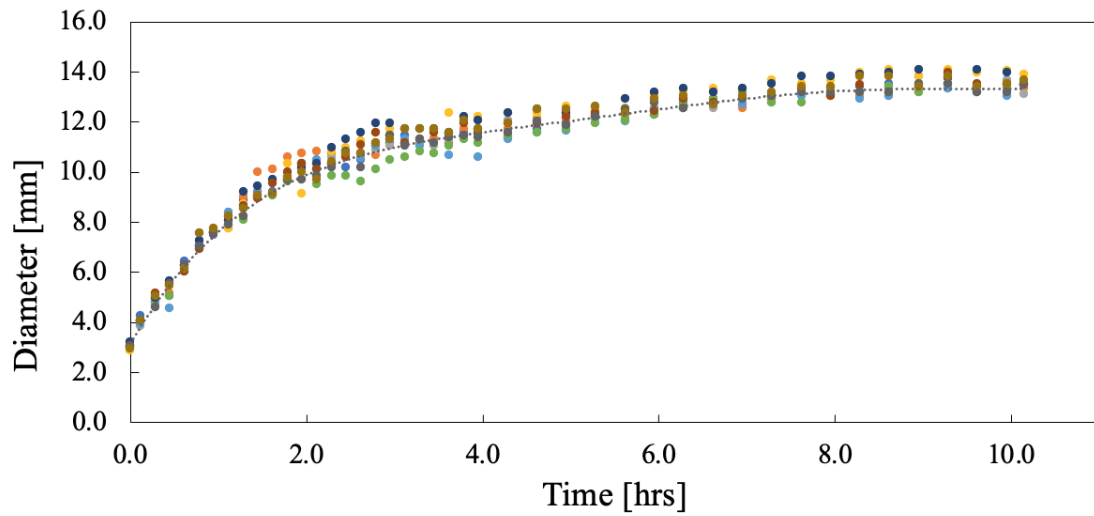


Figure 3.6: Observed size growth of hydrogel particles

particle-scale computations. In the experiments on Superabsorbent Polymer Particles, a group of particles are dropped into a chamber filled with water. the height growth of this group of particles are measured for around 5 second. Using OpenPIV algorithm, we are able to obtain the swelling rate of the SAP particles and the rate will be used for the validation of 3D particle-scale computations in the next chapter.

References

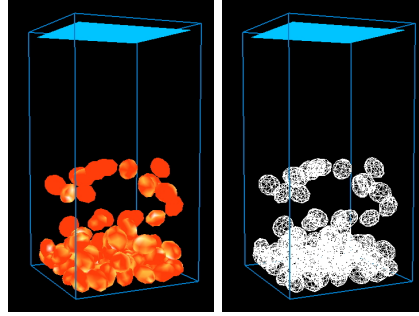
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4 Computations on Superabsorbent Polymer Particles

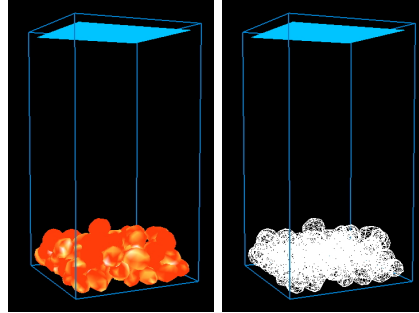
4.1 Computations on Multiple Particles in Fluid

A 3D numerical prediction with the same dimensions as the experiment is then computed as shown in Fig. 4.1 (a) and (b). The same swelling rate is used in the computation. In the beginning, the particles are set to fall freely from the setup position at $t = -0.40$ [s]. Similar to the recorded experimental results, after the particles piled up at the bottom, the swelling starts. The swelling computation is also setup so that the particles on different layers swell on different rate. In order to compare the computed results to experimental results, the height of the particle layers are recorded. Ratio between present and original layer height h/h_0 between the computational and experimental results are compared as shown in Fig. 4.1 (c).

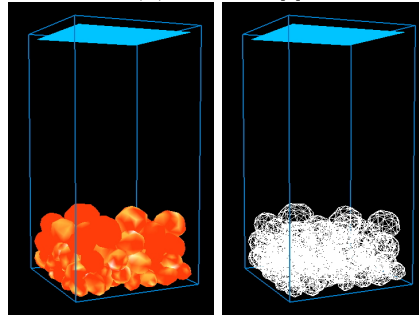
The computation shows a good agreement with the experimental results. As the computational conditions follow the obtained experimental data, it might be expected. However, the condition of the computation is fairly complicated, especially due to the accumulation behavior of the particles.



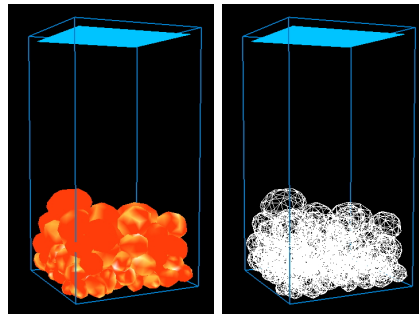
(a) $t = -0.40$ [s]



(b) $t = 0.50$ [s]



(c) $t = 3.50$ [s]



(d) $t = 5.00$ [s]

Figure 4.1: Calculated SAP particles in water surface (left) and wire frame (right)

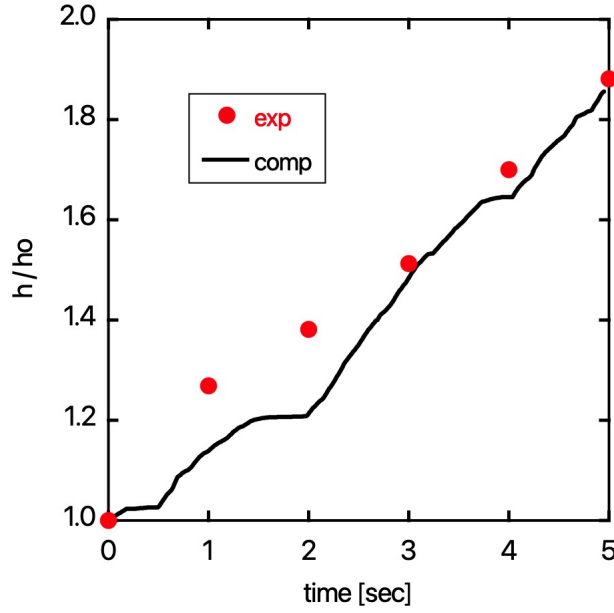


Figure 4.2: SAP height change with time

4.2 Computations on Fluid Flow Through Swelling Porous Layer

In addition to the 3D scale computation of SAP particles, a 2D macro-scale computation using MICS is conducted. This computation focuses on the seepage flow of a fluid through a swelling porous solid layer. A column of water is set on a bed of solid as shown in Fig. 4.3 (a). Due to the gravity, water flow through the porous 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 and density between air and solid layer causes fluid to flow slower and spread through the layer. As the fluid flow into the solid, the solid swell upward using a swelling computation that is included in the model. The results of the computations can be seen in Fig. 4.3 (b) and (c).

In this first case, the volume fraction of solid ϕ_s is set as a constant value. Due to the constant value, after entering the solid layer, water flow on the same rate, preserving the shape and showing an unnatural condition.

In order to avoid this problem, as mentioned before, the constant value of ϕ_s is changed into a function of time, following the equation

$$\phi_{s,t} = \phi_{s,0} + 0.2t. \quad (4.1)$$

Here, $\phi_{s,t}$ shows the volume fraction of solid value at time $= t$. Respectively, $\phi_{s,0}$ is the initial volume fraction of solid value at $t = 0$. Using this new mechanism, it is assumed that the porosity of the solid which come in contact with water increases. Hypotetically, it is the same as when water flow through a layer of SAP particles, the particles on that area swell, increasing the porosity of the layer. The computation is then calculated using the same condition as the first case. The results is shown in Fig. 4.4, and the change in ϕ_s can be seen in Fig. 4.5. The same behavior as the initial computation can be observed as water spread and slowed down when entering the solid layer. Afterwards, it can be observed that the due to the increase of the ϕ_s value, after entering the solid layer water is trapped around the surface. The water flow can be observed to be spread wider than the previous model. From Fig. 4.5, it can be observed that the ϕ_s is getting into a darker color, showing the increase in value around the solid surface which come in contact with water. This result shows a more natural condition where water absorption only occur near the surface of SAP layer as reported by Jockusch et al (2009) [1].

4.3 Summary

In this section, the computations of the SAP particles are the main focus. Following the experiment in the previous section, a 3D computation with the similar setup is conducted. The observed swelling behavior of SAP particles such as swelling rate and the different rate of swelling between different layers are included in the computation. The height change of the computation is then measured and is compared to the experiment. It can be seen that a good agreement is obtained between the results. On the different case, the computation of seepage flow of fluid through swelling SAP layer is conducted. By taking advantage of the volume fraction of solid attribute which is used in the MICS method, the porosity of solid can be reproduced. The swelling characteristics of the solid layer is also implemented using the change of this volume fraction of solid attribute. Additionally, the discussion of water trapping mechanism is introduced to reproduce the realistic physical condition.

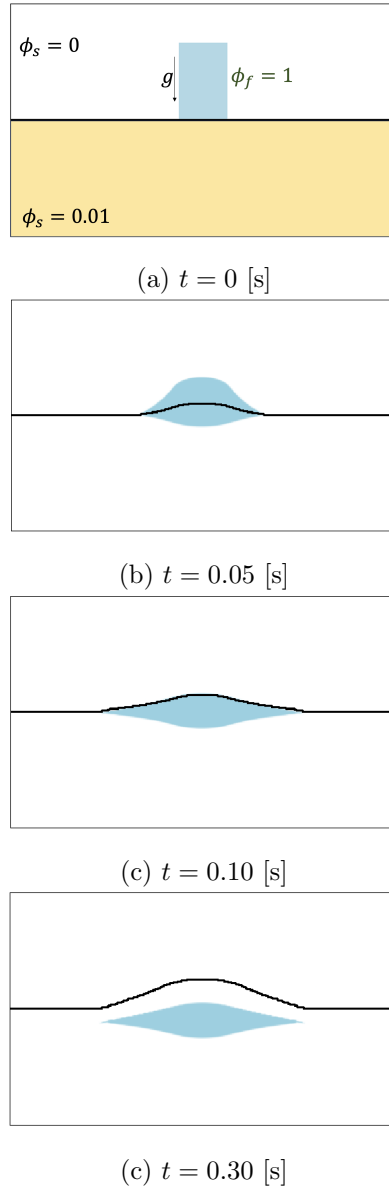
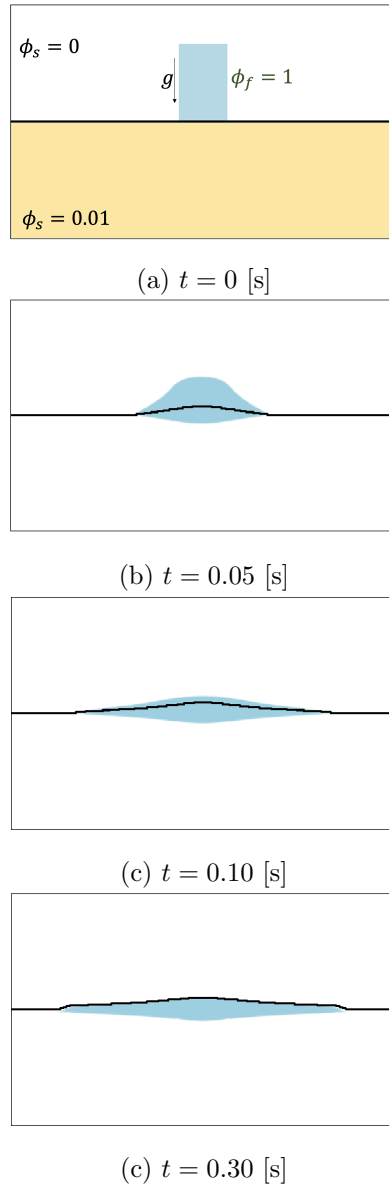
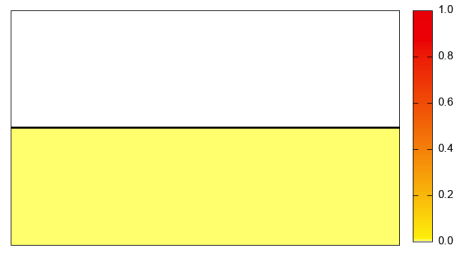
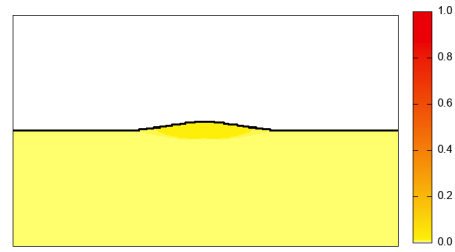


Figure 4.3: Computational results using constant value of ϕ_s

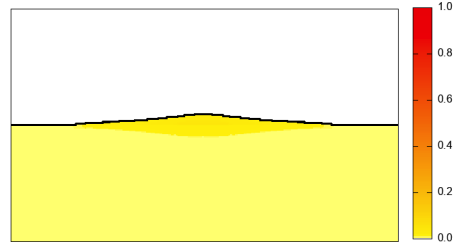
Figure 4.4: Computational results using increasing value of ϕ_s



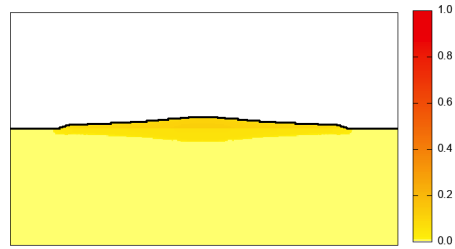
(a) $t = 0$ [s]



(b) $t = 0.05$ [s]



(c) $t = 0.10$ [s]



(c) $t = 0.30$ [s]

Figure 4.5: The change of volume fraction of solid ϕ_s with time

References

- [1] Jockusch, S., Turro, N. J., Mitsukami, Y., Matsumoto, M., Iwamura, T., Lindner, T., Flohr, A., and di Massimo, G., 2009. “Photoinduced surface crosslinking of superabsorbent polymer particles”. *Journal of Applied Polymer Science*, **111**(5), pp. 2163–2170.

5 Computations on Hydrogel Particles

5.1 Computation on The Swelling Process of a Single Particle

In our computation, we set up a stationary particle with the initial diameter of 3 [mm] within a computation area of 30 [mm] $\times$ 30 [mm]. Since the focus is to verify the swelling solid model, the fluid and contact forces computation is omitted. We use the mass points number N_l as 20, with the spring constant $k = 10^6$ [N/m] and coefficient of restitution $e_b = 0.8$. Additionally, we use the solid density as 1500 [kg/m³]. We calculate the model with $\Delta t = 5 \times 10^{-3}$ [s]. Figure 5.1 shows the computation of single hydrogel particle with our proposed method. We connect the 20 mass points used in our computation to represent the surface of the solid, with the additional line to the center point to distinguish the rotation movements of the solids in our computation. The figures show the initial ($t = 0$ [hrs]) and final ($t = 9.7$ [hrs]) diameter of the hydrogel particle as 3 [mm] and 13.5 [mm] respectively. Additionally, we observe no rotation on the particle.

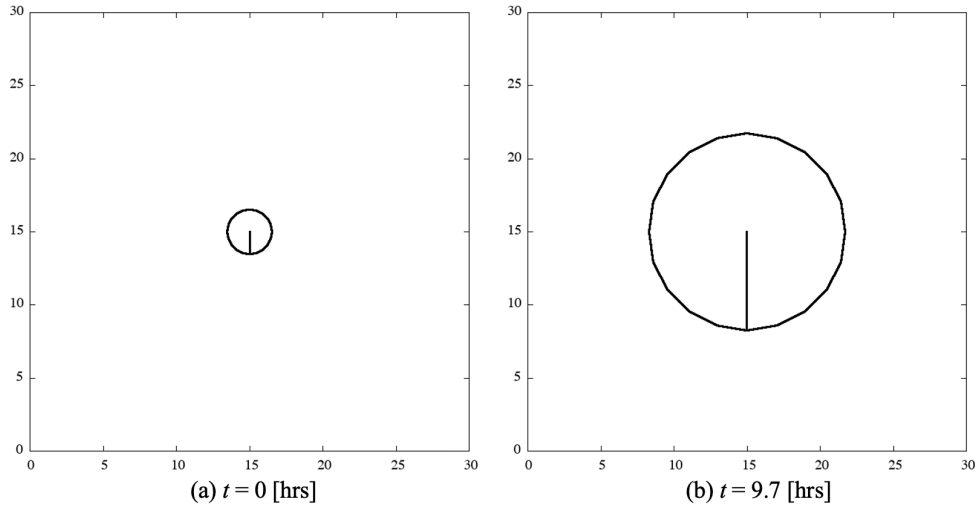


Figure 5.1: Computation of single hydrogel particle at (a) $t = 0$ [hrs] and (b) $t = 9.7$ [hrs] (particle outline)

Figure 5.2 shows the comparison between experimental data (exp), expected growth from regression analysis (reg), and our calculated results (cal). The calculated results show that the

solid grows quickly with a smooth curve from the initial diameter until around 2 [hrs], then slowing down until it reaches the stable size of around 13 [mm], showing a good agreement with the experimental data and the expected growth from Eq. 3.1.

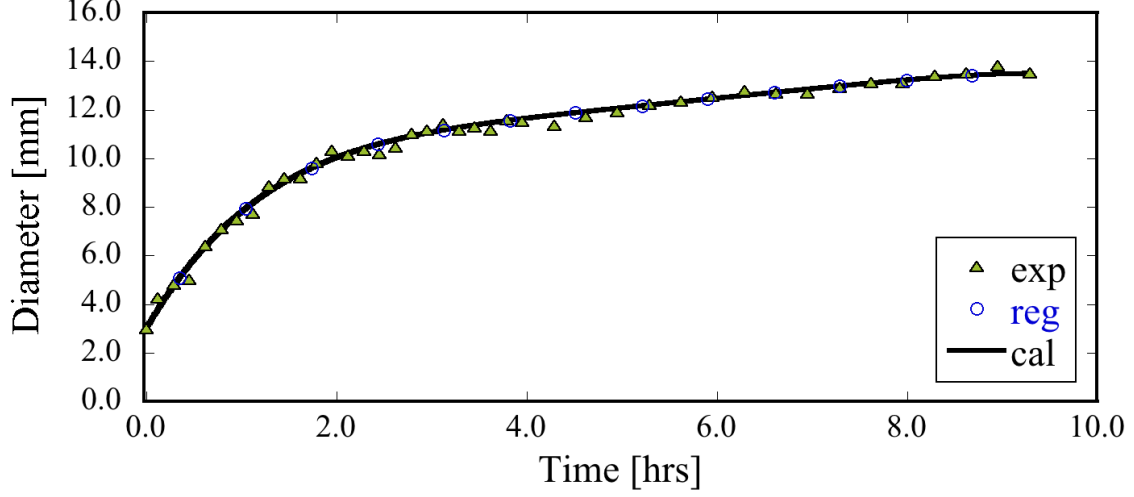


Figure 5.2: Computed diameter of hydrogel particle (cal) compared to experiments (exp) and predicted results (reg)

In addition, two values of N_l are computed to check the convergences of the Lagrangian points. Between the two values of $N_l = 10$ and $N_l = 20$, it can be seen that there are almost no differences as shown in Fig. 5.3.

5.2 Computations on The Sedimentation of a Single Particle in Fluid

It is to be emphasized that the proposed method is using a different DF/IB computation. Compared to the original DF/IB for rigid bodies, in which the total force of the Lagrangian points is calculated, and used to update the movement of the center point, the proposed method uses the interaction forces on each point to update the motion separately. This method allows the deformations of the solids to be predicted. As the first step, it is important to confirm that the proposed method will give the same results as the original DF/IB for rigid bodies. the proposed method is applied to a case of sedimentation of a single particle in fluid [1][2].

A single particle with diameter $D = 0.25$ and density $\rho_s = 1.25$ is set inside a 2×6 area from

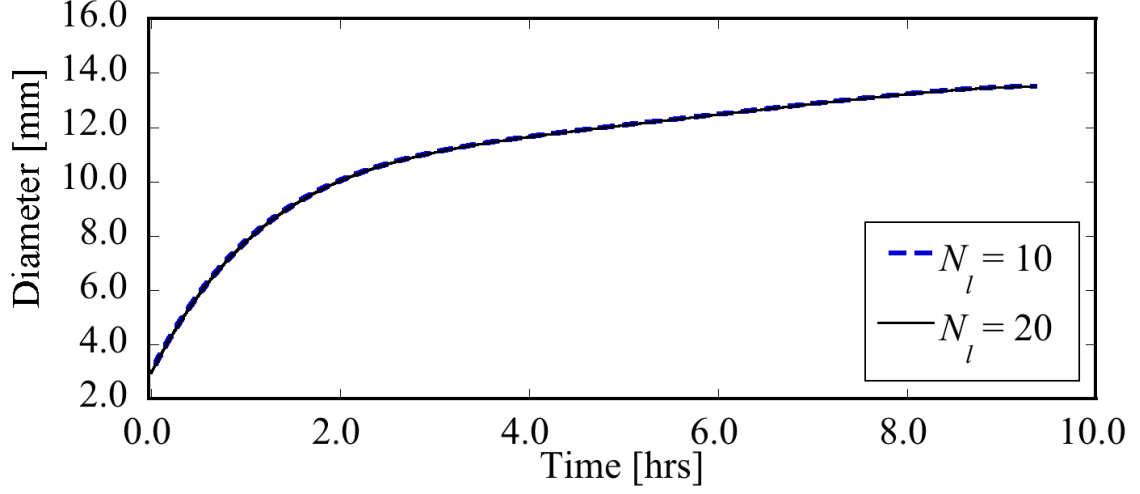


Figure 5.3: Effects of Lagrangian Points number N_l on the time histories of diameter of hydrogel particle

the initial position of (1, 4) and falls freely with the gravity acceleration of -980 as shown in Fig. 5.4. The number of fluid cells used in the computation is 200×600 and the number of Lagrangian points N_l is 70. The surrounding sides are treated as non-slip boundaries. The fluid density ρ_f and kinematic viscosity ν are 1.0 and 0.1 respectively,

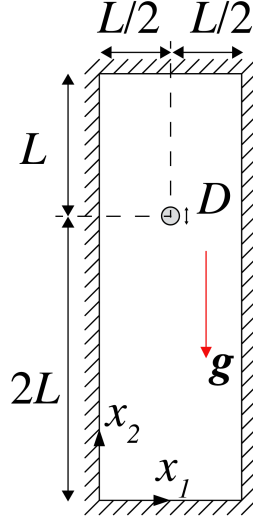


Figure 5.4: Computational area for sedimentation of a single particle

The spring constant and coefficient of restitution of mass spring model k_s and e_s used are 4×10^6 and 0.5. A large enough k_s is used so that the solid doesn't deform and acts similar to a rigid body. The spring constants for the DEM calculation $k_{D,n} = k_{D,t} = 1 \times 10^5$ and

coefficient of restitution for the DEM calculation $e_D = 0.5$ are used. The radius of the contact detection spheres is $0.2D$. The model is calculated with $\Delta t = 5 \times 10^{-3}$. It is to be noted that non-dimensional parameters are used in this computation. The calculated value of particle velocity in y-direction v_s is observed and compared to the computation with original DF/IB for rigid body and past references [1][2]. Figure 5.5 shows the computation of the sedimentation of a single particle. The solid is shown in the initial position (1,4) and falls straight to the bottom side of the computational area. Some velocities inside the solids can be observed. DF/IB method only overwrite the velocity of the boundary, leaving the velocity of the imaginary fluid inside the solid. It is to be noted that the velocity inside of the fluid has no effects on the solid movements.

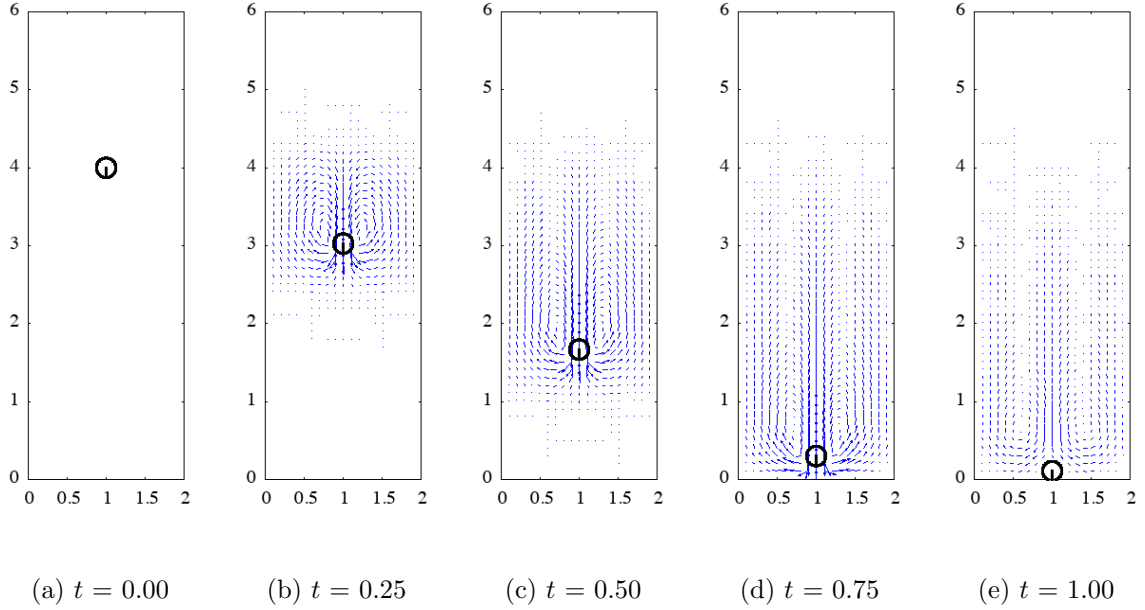
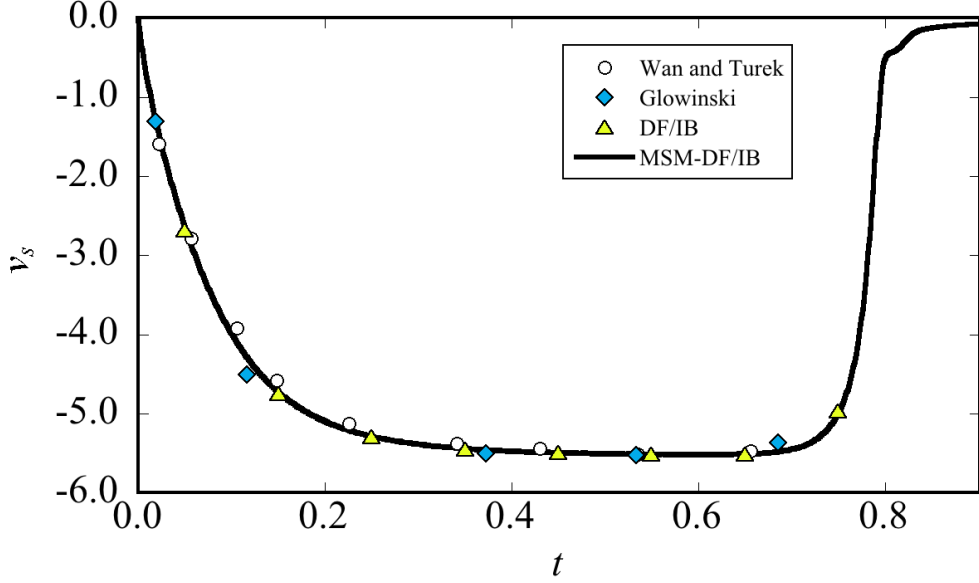


Figure 5.5: Sedimentation of a single particle with MSM-DF/IB (velocity vectors and particle outline)

Figure 5.6 shows the time histories of v_s . As the particle falls from the initial position, the velocity increases until it reaches the terminal velocity with $|v_s|$ around 5.5 at $t = 0.3$ until the solid moves closer to the bottom side of the computational area and the $|v_s|$ decreases until to zero and settles there. The time histories of velocity from the proposed method give a good agreement with the original DF/IB method and references.

In order to check for the mesh convergence, the computation is checked for different N_f . In

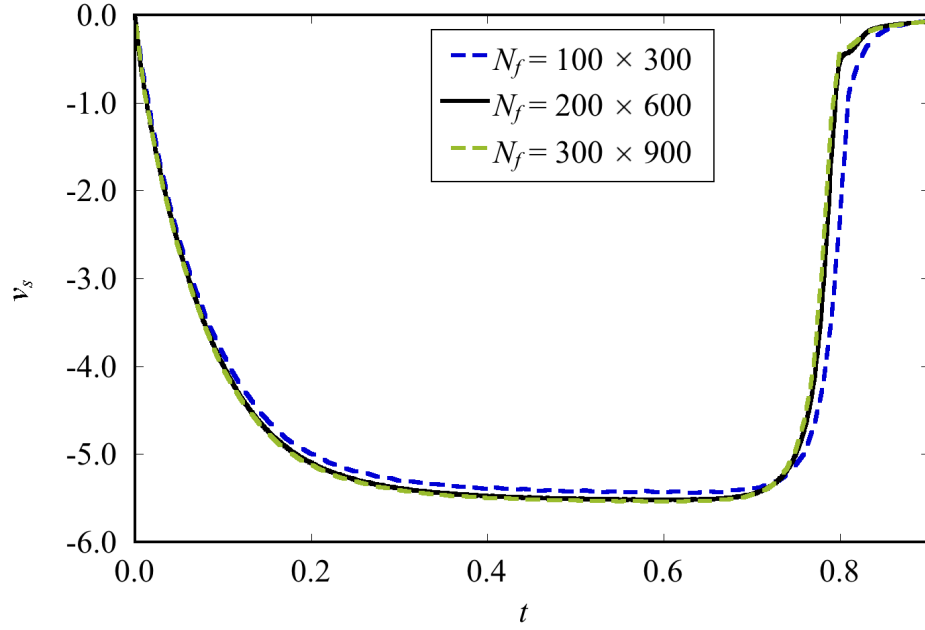

 Figure 5.6: Time histories of v_s with $D = 0.25$ and references

addition to the previous computation, a rougher resolution with $N_f = 100 \times 300$ and finer resolution with $N_f = 300 \times 900$ is computed. The results of the three computations can be seen on Fig. 5.7. It is shown that the computation is able to reach good results even at rougher mesh resolution, with more accurate results at mesh number 200×600 and the number of cells inside solid at around 25.

In order to check the effect of swelling on the terminal velocities, the computation is recalculated with initial position of the solid at (1,6). The solid is treated as a swelling solid with the diameter of the solid increases linearly from $D = 0.25$ to the maximum size $D = 0.30$ linearly with slope = 0.25 or can be written

$$D = \begin{cases} 0.25t + 0.25, & 0.3 \leq t < 0.5 \\ 0.30, & t \geq 0.5. \end{cases} \quad (5.1)$$

In order to give comparison to the terminal velocities of the swelling particle, the results of the minimum and maximum size of non swelling particle, is also calculated. For convenience, the case with $D = 0.25$ will be called case A, the case with $D = 0.30$ as case B, and the case with a swelling particle in which the diameter changes from the $D = 0.25$ to 0.30 as case C. The relation between the time and diameter of the three cases can be seen in Fig. 5.8. Other


 Figure 5.7: Effects of mesh sizes on the time histories of v_s

computational parameters used in the additional two cases are the same as case A. The changes of the particle diameter and the time history of the particle velocities can be seen on Fig. 5.8.

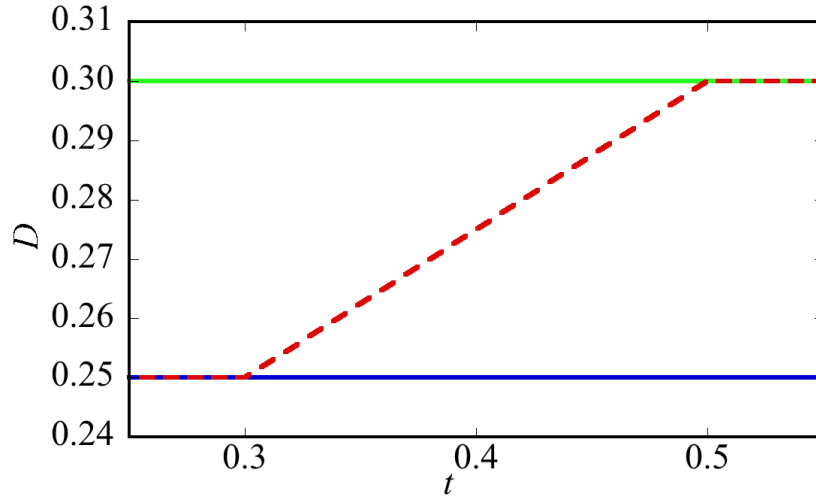


Figure 5.8: Changes of particles diameter

The velocity vector and particle outline of the three cases can be seen in Figs. 5.9, 5.10 and 5.11. When $t = 0.00$, the three particles are setup in the same position and dropped. At $t = 0.30$, the particle in case B with largest initial diameter size and mass is the closest to the bottom

5. Computations on Hydrogel Particles

than the particles in cases A and C. In addition, in this time step, the position of the solid in cases A and C is similar as only small swelling occur to the particle in case C. At $t = 0.60$, the particle in case B almost hits the bottom. The diameter of the particle in case C is already at the $D = 0.30$, and the position is closer to the bottom than in the case A. In the next time step at $t = 0.90$, the particle at case B is the closest to the bottom, followed by particle at case C, and particle at case A is the furthest from the bottom. At $t = 1.20$, all three particles settle on the bottom.

The particle velocities shows reasonable results between the three computations. On the non-swelling particles, the terminal velocity of the particle with smaller diameter (blue line) is smaller, causing the particle to reach the bottom side later than the particle with larger diameter (green line). The red line represents the velocity of the swelling particle. Prior to $t = 0.30$, the velocity of the swelling particle is equal to the blue line where the particle is identical in size. Afterward, the particle starts to swell and the velocity gradually reaches the green line. In addition, due to the increase of the particle velocity on the swelling particle, it reaches the bottom side before the particle with $D = 0.25$ and after the particle with $D = 0.30$.

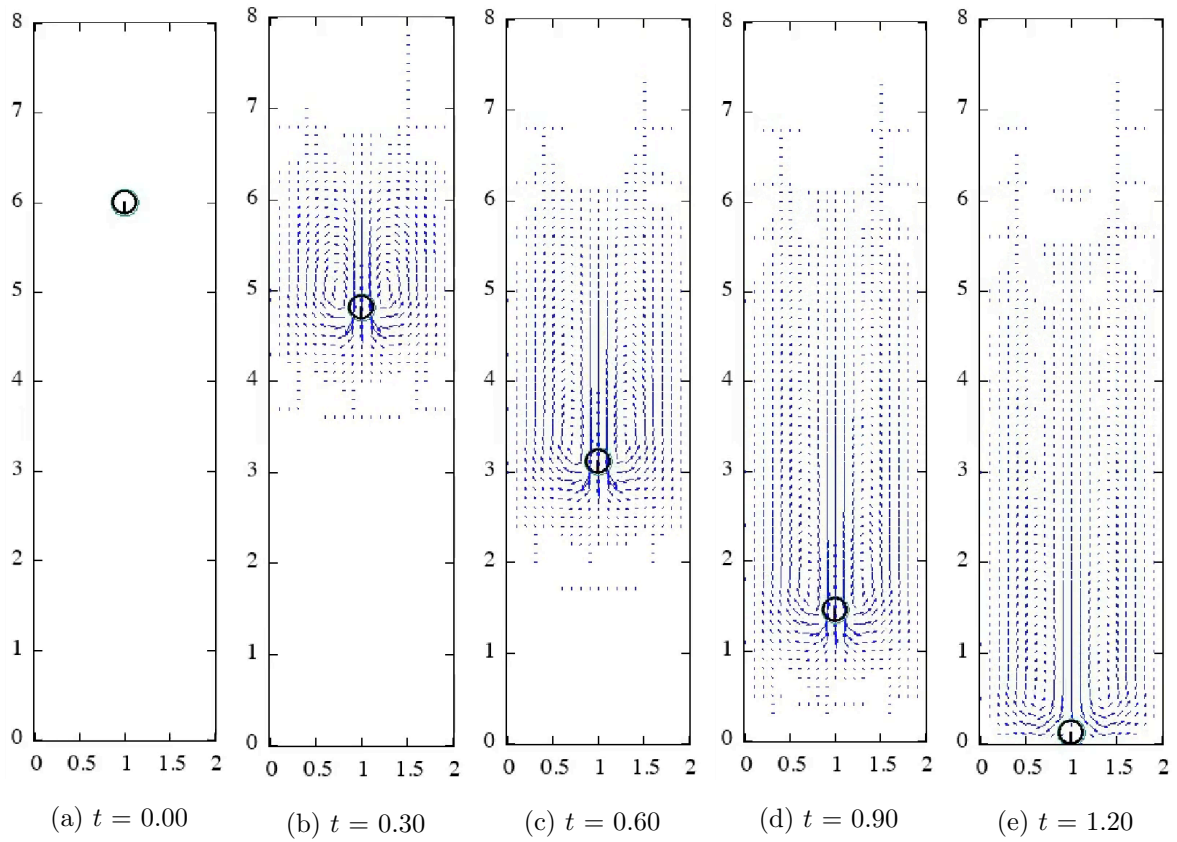


Figure 5.9: Sedimentation of a single particle in fluid for case A (velocity vectors and particle outline)

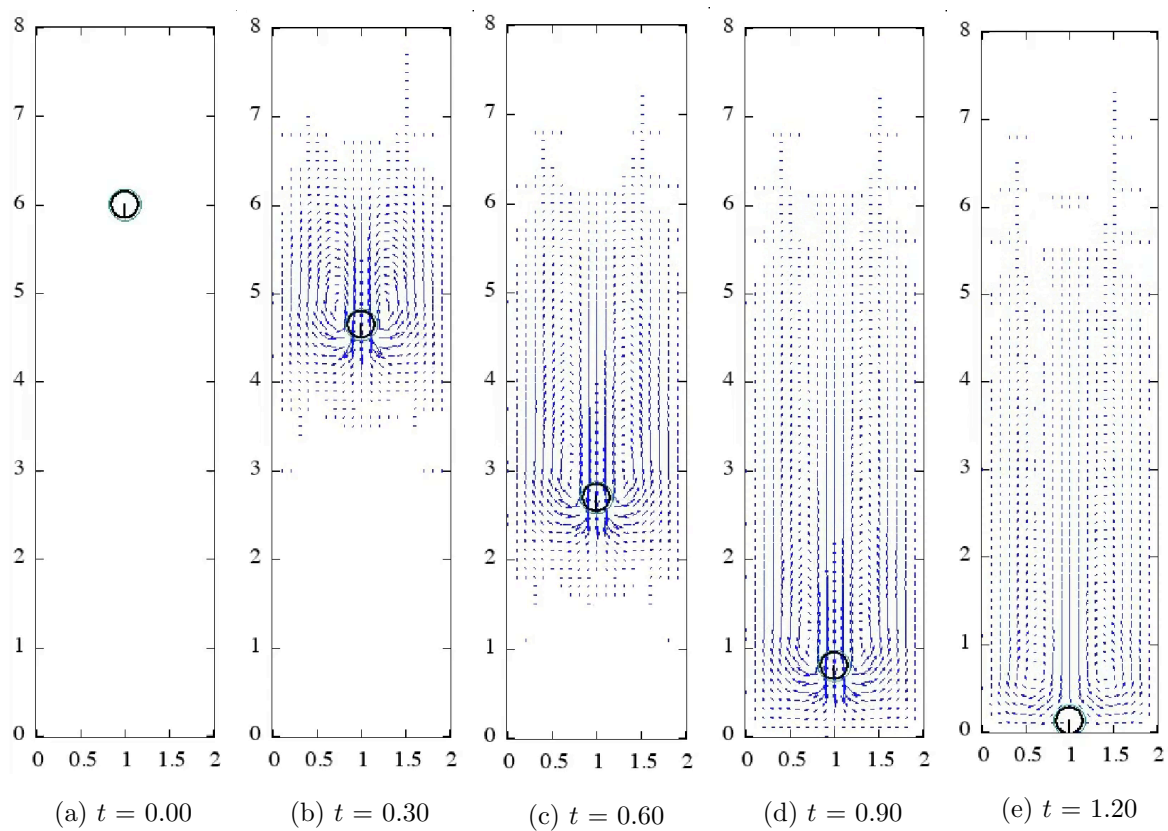


Figure 5.10: Sedimentation of a single particle in fluid for case B (velocity vectors and particle outline)

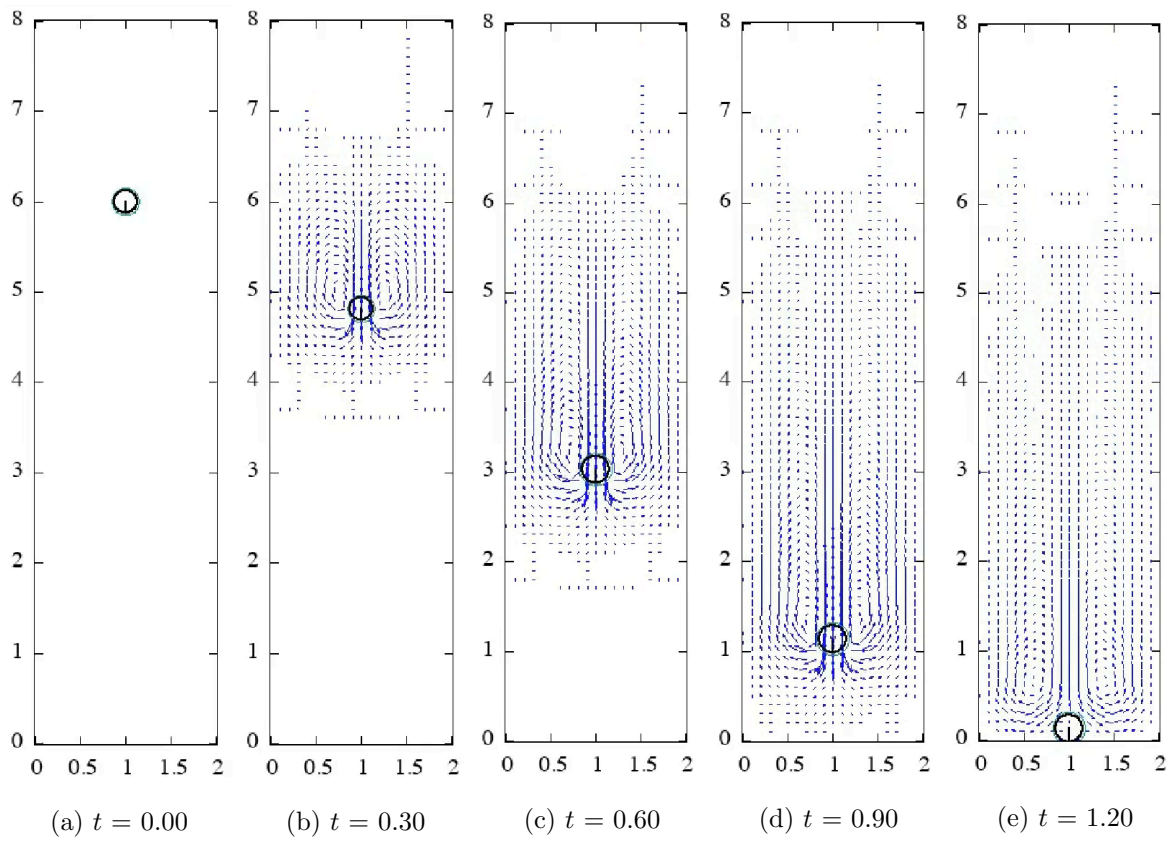
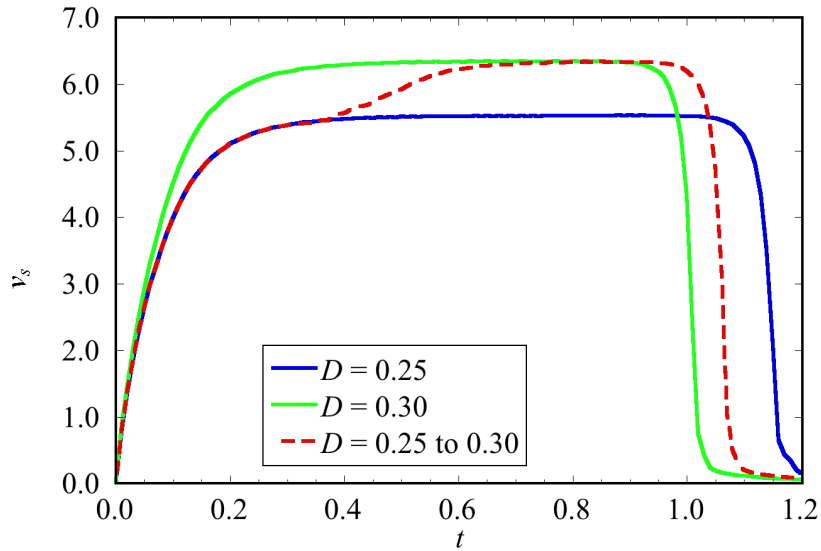


Figure 5.11: Sedimentation of a single particle in fluid for case C (velocity vectors and particle outline)

The v_s obtained in the three cases are compared in Fig. 5.12. The time history of v_s shown by the blue solid line for the case A is the same as the one computed previously in Fig. 5.6 as the size of the particle is the same. In case B, as the size and mass of particle are larger than the case A, the terminal velocity is larger, obtained at $|v_s|$ around 6.3 at $t = 0.3$ (green line). The red line represents the velocity of the swelling particle in the case C. The particle falls from the initial position with initial diameter $D = 0.25$. As the particle's diameter and mass increase, the $|v_s|$ also increases continuously until reaching the terminal velocity of around 6.3 similar to the terminal velocity of particle in the case B. From Fig. 5.6.

The terminal velocity of the particle with smaller diameter (blue line) is smaller and lighter, causing the particle to reach the bottom side later than the particle with larger diameter. Prior to $t = 0.3$, the velocity of the swelling particle is equal to the blue line where the particle is identical in size. Afterward, the particle starts to swell and the velocity gradually reaches the green line. In addition, due to the increase of the particle velocity on the swelling particle, it reaches the bottom side before the particle with $D = 0.25$ and after the particle with $D = 0.3$.



(b) Time histories of particle velocity

Figure 5.12: Comparison of diameter and particle velocities between the three cases

5.3 Computations on Lid-Driven Cavity Flow with Multiple Particles

5.3.1 Soft Particles

Multiple deformable solid solids are arranged inside the 2D computational area filled with the fluid as shown in Fig. 5.13.

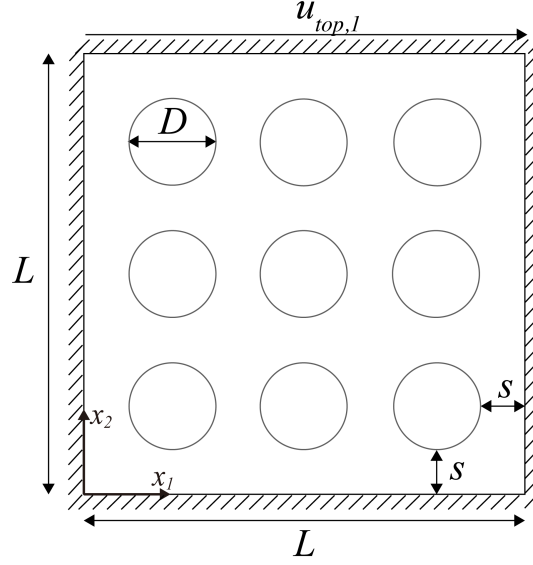


Figure 5.13: Computational area with deformable solids

The computational area is a square with the length $L = 1.0$. Initially, the total of 9 solids with the constant diameter $D_0 = 0.2$ and solid density $\rho_s = 1500$ are set up inside the computational area with the space between solids and wall $s = 0.1$. The surrounding side walls are treated as non-slip boundaries. For the fluid, the number of fluid cells used is 100×100 . Velocities $u_{top,1} = 0.1$ and $u_{top,2} = 0$ are applied on the top wall. We use kinematic viscosity $\nu = 0.01$, fluid density $\rho_f = 1000$, and the Reynolds number $Re = u_{top,1}L/\nu = 10$.

We use two different values of spring constant k for the application, k as 1000 for case 1 and 100 for case 2. Additionally, the coefficient of restitution e_D for the two cases are 0.8. For the DEM calculation, the spring constants k_n, k_t in both cases are 5×10^4 , and the radius of the contact detection spheres is $0.2D$. and the number of mass points (Lagrangian points) N_l is 21. The gravity acceleration is assumed to be zero in both cases. It is to be noted that

5. Computations on Hydrogel Particles

non-dimensional parameters are used in this computation.

Comparing the results of the two cases shown in Figs. 5.14 and 5.15, we can see that from the initial position, the horizontal velocity to the right side on the top wall affects the fluids in the computational area, causing a clockwise movement in the fluid flow. The solids are transported by the fluid, causing rotational and linear motion around the computational area. As the solids move, they also make contact with the surrounding solids and the wall. Due to the smaller spring constant on case 2, as the solids get transported by the flow, the deformation can be clearly seen especially closer to the moving top wall, where velocity is higher, and also as the solid-solid and solid-wall contact occur.

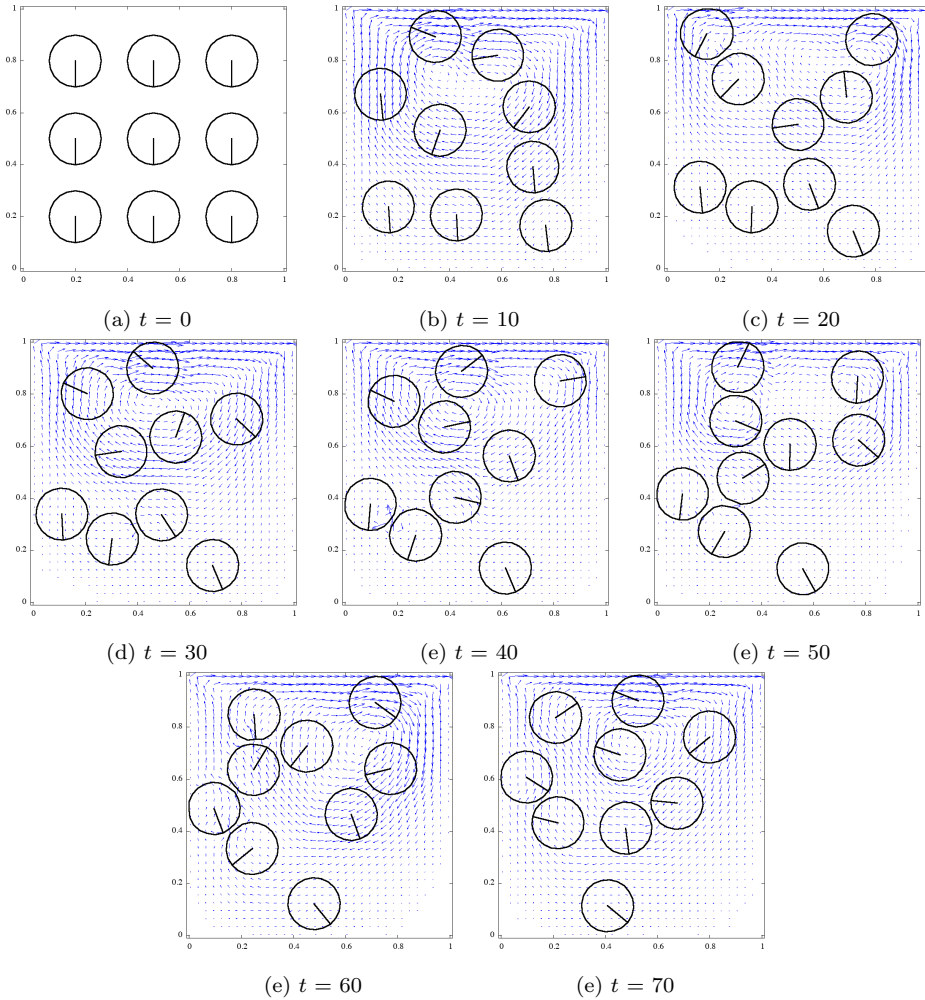


Figure 5.14: Cavity flow with deformable solids (velocity vectors and solid outlines) with $k = 1000$ at time (a) $t = 0$, (b) $t = 10$, (c) $t = 20$, (d) $t = 30$, (e) $t = 40$, (f) $t = 50$, (g) $t = 60$, (h) $t = 70$

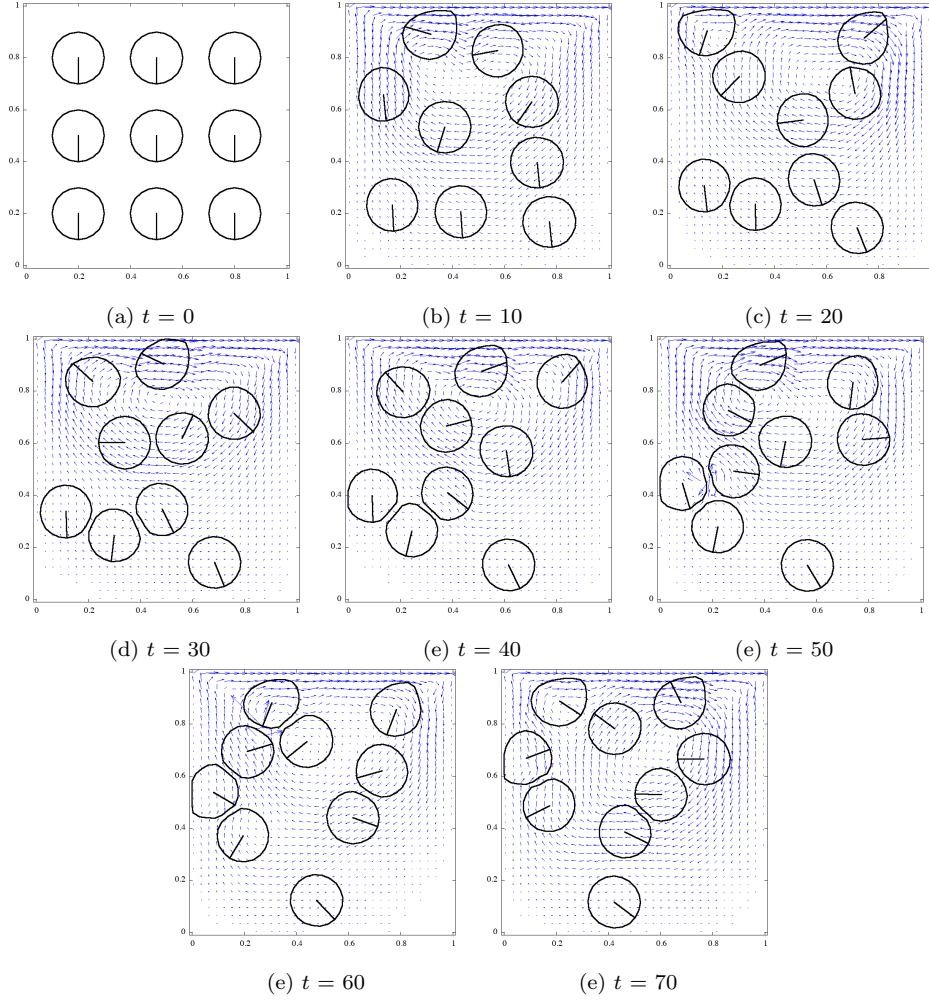


Figure 5.15: Cavity flow with deformable solids (velocity vectors and solid outlines) with $k = 100$ at time (a) $t = 0$, (b) $t = 10$, (c) $t = 20$, (d) $t = 30$, (e) $t = 40$, (f) $t = 50$, (g) $t = 60$, (h) $t = 70$

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In the earlier version of our computational method, we observe the need to implement the additional spring as explained in Chapter 2. Without the support spring, when we compute the cavity flow with multiple deformable solids at $k = 100$, some overlapping of the surface spring on the solid as shown in the red circle in Fig. 5.16 may occur.

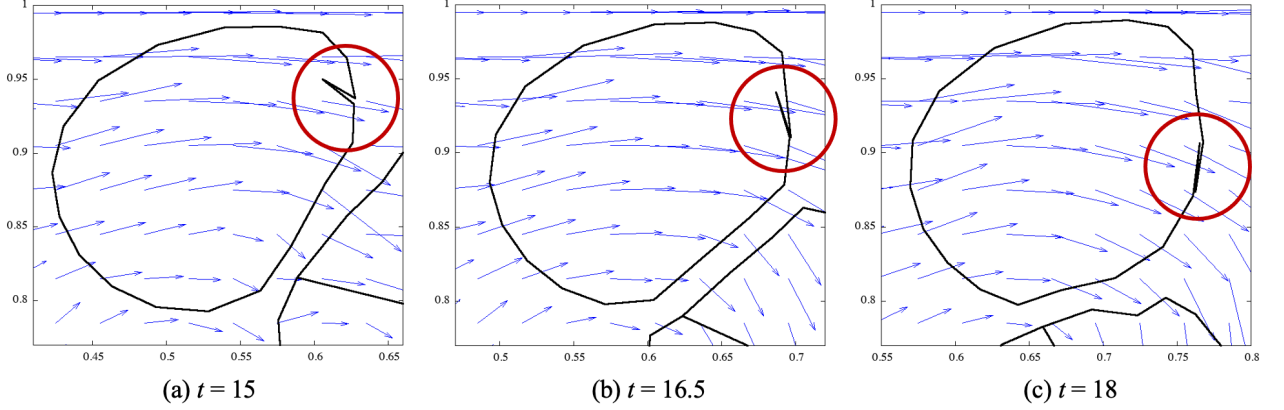


Figure 5.16: Computation results without support springs at (a) $t = 15$, (b) $t = 16.5$, and (c) $t = 18$

5.3.2 Swelling Soft Particles

Similar to the previous computation, multiple deformable solid solids are arranged inside the 2D computational area filled with the fluid as shown in Fig. 5.17. The computational area is a square with the length $L = 1.0$, and the total of 16 solids with the diameter $D_0 = 0.12$ are setup with space between solids and wall s as 0.104. Other parameters of fluid and solid used in this computation are the same with the previous computation on previous section. Additionally, the solids swell linearly with slope 6×10^{-4} , until the maximum size D_{max} of $1.5D_0$ as can be seen in Eq. 5.2

$$D = \begin{cases} 6 \times 10^{-4}t + 0.12, & 0 < t < 100 \\ 1.8, & t \geq 100. \end{cases} \quad (5.2)$$

The computations of swelling deformable solids with two spring constants $k = 1000$ and $k = 100$ can be seen in Figs. 5.18 and 5.19. Non-dimensional parameters are used in this

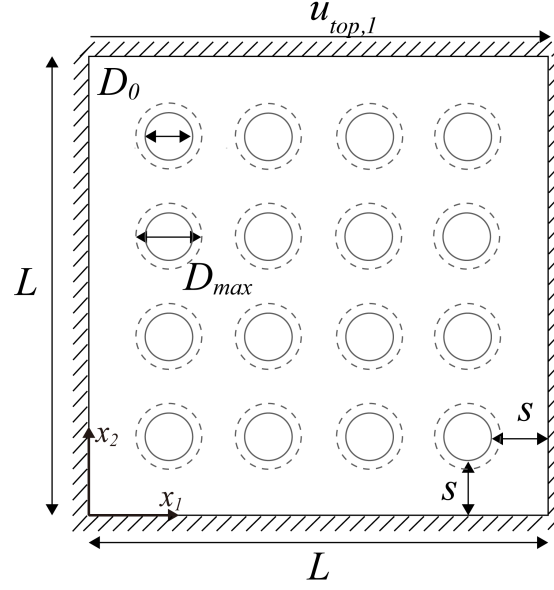


Figure 5.17: Computational area with the swelling deformable solids

computation. Similar to the computation on previous section, At first, the horizontal velocity to the right side on the top wall affects the fluids in the computational area, causing a clockwise movement in the fluid flow. The solids are transported by the fluid, causing rotational and linear motion around the computational area. Additionally, the diameter of the solids increase with the introduced swelling condition. As the solids swell, the computational area is filled with the solids and slower movements can be observed as seen in the flow velocity vector distribution on Figs. 5.18 and 5.19 when $t = 110$. In addition, between the two cases of spring constant k , we can see that on the second case where spring constant is smaller than the first case, larger deformation can be observed similar to the previous computations.

5.4 Computations on Multiple Particles Transported in Two-Sided Lid-Driven Cavity Flow

Multiple deformable solid particles with various sizes are arranged inside the 2D computational area filled with fluid as it can be seen on Figs. 5.20 (a) and 5.21 (a). The computational area is filled with fluid with kinematic viscosity $\nu = 0.01$ and fluid density $\rho_f = 1.0$. It is to be noted that non-dimensional parameters are used in this computation. The surrounding walls

5. Computations on Hydrogel Particles

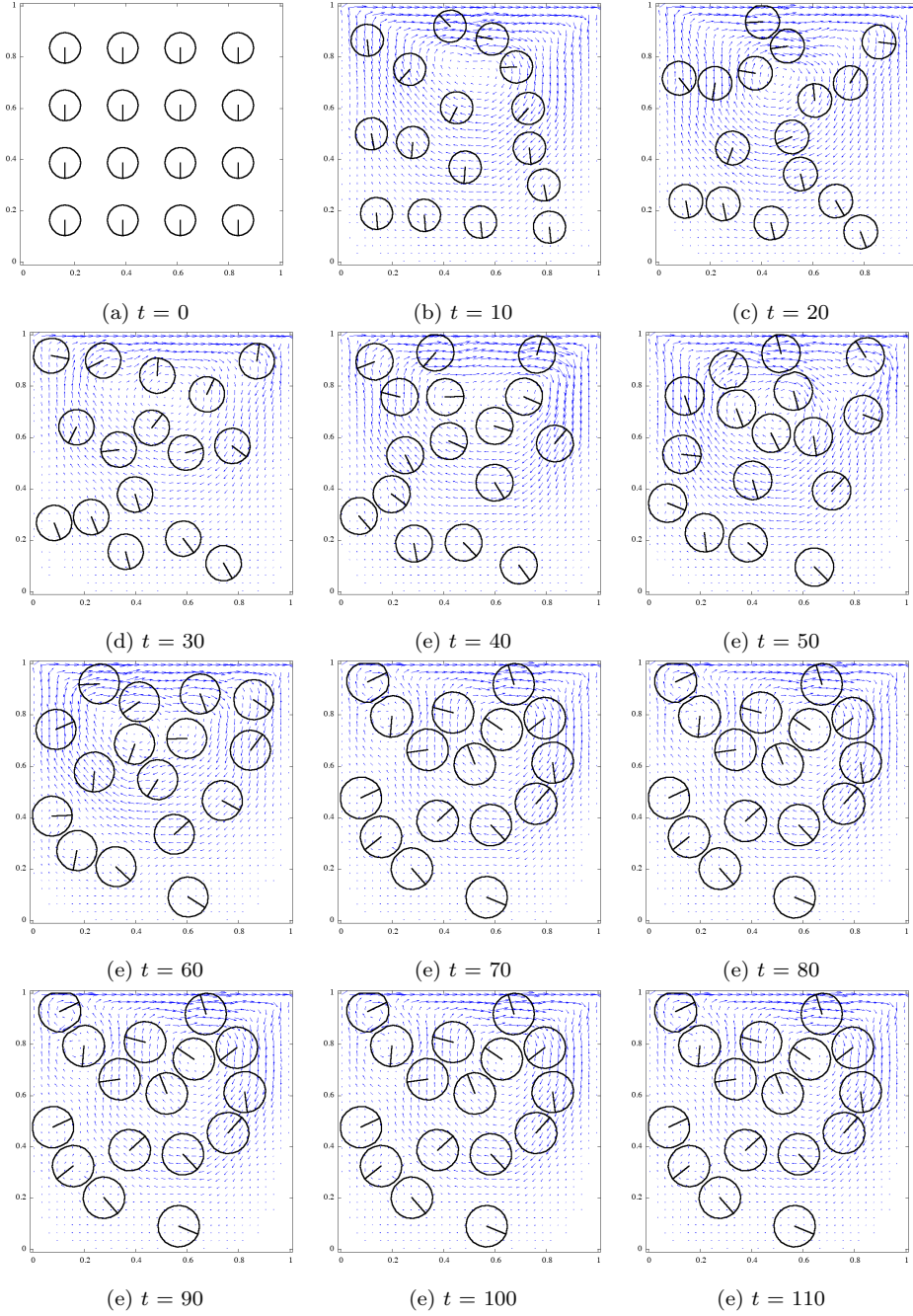


Figure 5.18: Cavity flow with deformable swelling solids (velocity vectors and solid outlines) with $k = 1000$ at time (a) $t = 0$, (b) $t = 10$, (c) $t = 20$, (d) $t = 30$, (e) $t = 40$, (f) $t = 50$, (g) $t = 60$, (h) $t = 70$, (i) $t = 80$, (j) $t = 90$, (k) $t = 100$, (l) $t = 110$

are treated as non-slip boundaries. The top and bottom walls move in horizontal direction with velocities $u_{top,1} = 1.0$, $u_{top,2} = 0.0$, $u_{bottom,1} = -1.0$, and $u_{bottom,2} = 0.0$. The Reynolds number Re is 100. 16 particles with the initial diameter D_0 varied between 0.1 and 0.15 with density

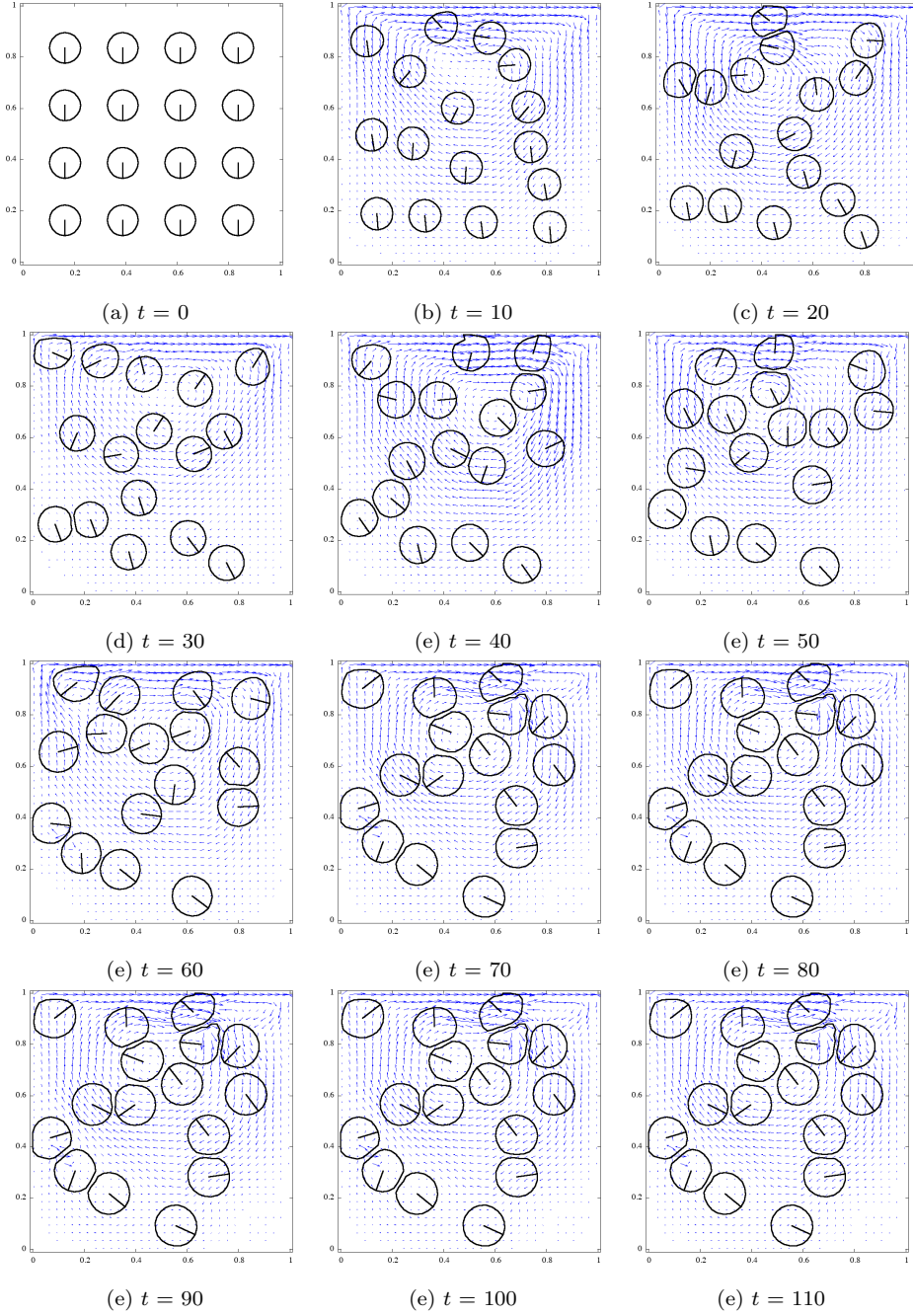


Figure 5.19: Cavity flow with deformable swelling solids (velocity vectors and solid outlines) with $k = 100$ at time (a) $t = 0$, (b) $t = 10$, (c) $t = 20$, (d) $t = 30$, (e) $t = 40$, (f) $t = 50$, (g) $t = 60$, (h) $t = 70$, (i) $t = 80$, (j) $t = 90$, (k) $t = 100$, (l) $t = 110$

$\rho_s = 1.5$ are set up on the computational area. The spring stiffness k_s of the particles are set between 0.56 and 0.88, with the coefficient of restitution $e_s = 1.0$. For the DEM computation, the values of spring constant $k_{D,n}$ in normal direction is 1.0×10^7 . Tangential contact forces is

5. Computations on Hydrogel Particles

assumed to be 0 in this computation. The coefficient of restitution e_D of DEM computation is 1.0, and the radius of the contact detection spheres is $0.167D$. The number of fluid cells used is 100×100 , while the number of mass (Lagrangian) points N_l is 21. In addition, the time increment Δt is 1.0×10^{-4} . Two cases are computed in this study. In both cases, velocities on top and bottom walls are stopped after $t = 10$. Non-swelling particles are introduced in the first case, while swelling particles are on the second case. The particles on the second case are set to swell linearly with the slope of 3×10^{-3} until the maximum size D_{max} of $1.5D_0$, following the equation

$$D = 3 \times 10^{-3}t + D_0, \quad D \leq 1.5D_0. \quad (5.3)$$

Figures 5.20 and 5.21 show the computation results on the non swelling and swelling particles. The black lines represent the line connecting the mass (Lagrangian) points, and red lines represent the line connecting the outer side of the contact detection spheres. Additional lines are drawn connecting the surface and the center of the solid to help observe rotation on the particles. Due to the movement of the top and bottom wall, deformations can be observed especially closer to the moving top and bottom wall where velocity is higher and when the solid-solid and solid-wall contacts occur. After the velocities are stopped on $t = 10$, we can see the particles move only with their remaining speed and finally stopped. The trajectories of the center points of the particles for $10 \leq t \leq 20$ can be seen on Fig. 5.22. It can be observed that the non-swelling particles are moving further than the swelling particles after the velocities are stopped. In addition, after the velocity is stopped, the particles on the second case are still swelling. As a result, the particles push each other, causing slight movement as it can be observed on the discontinuous lines on Fig. 5.22 (b).

5.5 Summary

In this section, the computations of the hydrogel particles are the main focus. Different to the previous section, the particles are considered to be able to distort and warped by external and fluid forces. This capability is simulated by the mass-spring model computation. First, in order to check the proposed method, several computations are introduced. In the first part, the main

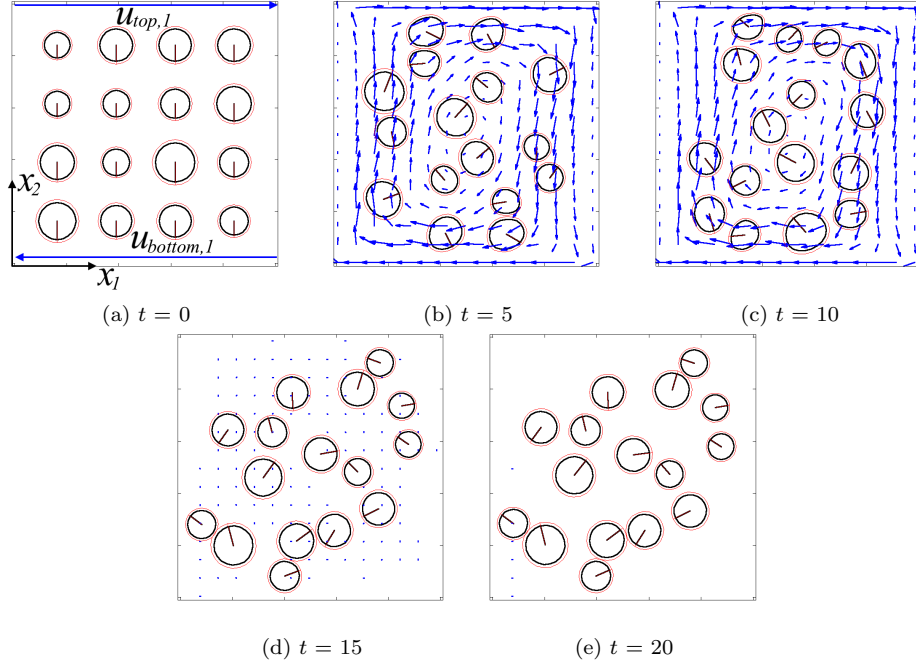


Figure 5.20: Computation of non-swelling particles

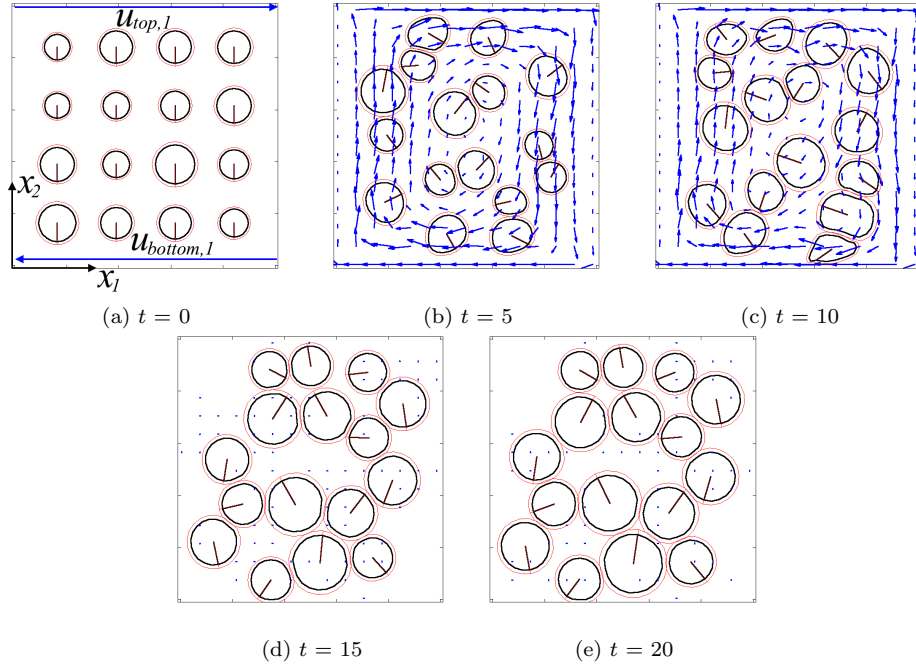


Figure 5.21: Computation of swelling particles

target is to observe the swelling mechanism of the proposed method. Therefore, the existence of fluid is ignored. A Computation for the swelling process of a single particle is conducted and compared to the experiment of hydrogel particles. A good agreement between experiment and computation results can be seen. Then, the integration of the fluid-solid interaction computations is considered in the computation. In this part, the distortion capability of the particles

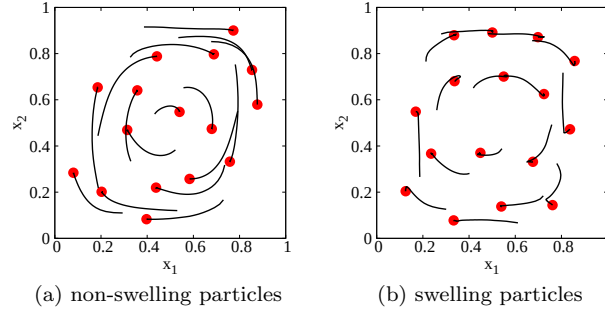


Figure 5.22: Trajectories of non-swelling and swelling particles for $10 \leq t \leq 20$ (red points mark the position of the particles at $t = 20$)

is ignored. In the sedimentation of a single particle computation, the computation results are compared to past studies. As a good agreement is observed, the same computation is repeated for a swelling particle. The terminal velocity of the computation is observed and discussed within different cases of non-swelling particles of minimum and maximum size. It can be seen that the terminal velocity of the swelling particles grows between the minimum and maximum sized particle, showing a reasonable outcome. Finally, several computations of particles inside cavity flow computation is conducted in order to confirm the robustness of the proposed method. On the lid-driven cavity flow problem, different values of spring stiffness coefficient is calculated. Both cases shows a reasonable result on the condition, showing the capability of the proposed method in various stiffness value. Within the computation of multiple objects in various size inside the two-sided lid-driven cavity flow, the difference of the particle trajectories between swelling and non-swelling computations are discussed. It is shown that after the velocity is stopped, the non-swelling particles move further than the swelling particles. This is considered reasonable as since the swelling particles have larger size, the drag on the particles is larger than the non-swelling particles.

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6 Conclusions

In this research, several fairly simple methods had been proposed to simulate the interactions between fluid and swelling solid. The proposed method was applied to several different computations and some was compared to the experiment results. For the SAP particle computation, first an experiment using multiple SAP particles was conducted. Multiple SAP particles are dropped into a chamber filled with water. The computation results were processed and the velocity field obtained through OpenPIV was observed. The time histories of height increase of the layer were also recorded. Through this experiment, the swelling rate of the particles was obtained. Additionally, the fact that SAP particles on different layer swell on different rate can be recognized. Next, A 3D computation with similar setup was conducted. The swelling behavior observed through the experiment was implemented into the 3D computation. The height increase of the particle layer was compared between experiment and computation. From the comparison, a good agreement between experiment and computation can be observed.

The same MICS method was used for the seepage flow through swelling SAP layer problem. The SAP particles layer was treated as a single layer of solid. The porosity of the layer is represented by utilizing the value of ϕ_s between 0.0 and 1.0. In the macro-scale computation, a column of water was dropped above a bed of porous layer. At first, the model is proposed with constant value of ϕ_s . As water flow through the solid layer, it slowed down and spread. the solid boundary then increased, imitating the swelling behavior of SAP layer. Afterwards, water flow on the constant rate under the solid layer, showing an unnatural condition. A modified model was introduced where the ϕ_s is changed into a function of time. The value of ϕ_s on cells that came in contact with water is set to increase as time elapses. Due to the increase of ϕ_s , the flow gets slowed down and spread more within the solid layer. Using this modified model, a more natural, reasonable flow through the porous layer can be observed.

In the hydrogel particle computations, first, we conducted an experiment on several hydrogel

particles and the time histories of the diameter growth was recorded. A regression analysis was then conducted to the data and the equation for the relation between time and diameter was obtained and used in our proposed method to calculate single hydrogel particle in 2D. Since the target is the swelling mechanism, the existence of fluid is omitted. The calculated results were then compared back to the experimental data and the regression equation. We confirmed that our proposed method is able to give a good agreement to the observed swelling of hydrogel particles.

In the second 2D application, as the fluid-solid interaction computations is considered, we compared our proposed method to past studies by calculating the sedimentation of single particle in fluid. In this computation, distortion of the solid is ignored by setting a large value on the spring constant. We confirmed that the proposed method gives a good agreement with the original DF/IB for rigid body and references. In addition, we calculated a case of sedimentation of single swelling particle. A particle is dropped from the initial position with the minimum diameter inside fluid and as it falls to the bottom side of the computational area, the diameter D increases from 0.25 to the max value of 0.30. We compared the absolute value of particle velocity in y direction $|v_s|$ for the swelling particle with the $|v_s|$ of the non swelling particles with $D = 0.25$ and 0.30. A reasonable results can be observed in the computation of swelling object as the time history of v_s fit between the other two cases. We also observed that the computation with swelling particle reached its terminal velocity with the same value as the non swelling object at $D = 0.30$ before hitting the bottom side of the computational area. Next, we apply our method to the computation of lid-driven cavity flow with multiple objects. We separate our computation to the non swelling soft objects and swelling soft objects. In both cases, two values of spring stiffness values are investigated. In the non swelling case, we observed that as the soft solids are transported through the fluid flows, the objects are moving in linear and rotational motions and larger distortions can be seen on the second case with smaller spring stiffness value. It can be confirmed from these computations that the proposed method is able to reproduce either hard or soft solid by changing the spring stiffness value. In the swelling case, the solids are similarly transported through the fluid flows and moving in linear and translational motions as the diameter is slowly increasing. It can be observed from the fluid velocity vector distribution that the movement of the objects become slower as the size increases and filled the

6. Conclusions

computational area. Similarly, two cases of spring stiffness values are also investigated, we can see larger deformation of the second case with smaller spring stiffness value, especially on the top side of the moving wall and when the solid-solid contact occurred.

Finally, a computation with multiple objects in various size inside the two-sided lid-driven cavity flow was conducted. In this computation, velocity was applied on the top and bottom side of the computational area. At $t = 10$, the velocity is stopped and the movement of the objects are tracked. Two cases were introduced with swelling and non-swelling objects, and the trajectory of the particles between the two cases are studied. It can be seen that in the case where the particles do not swell, the particles move further than the swelling particles. This shows a reasonable results that since the particles are larger on the swelling case, the drag is also larger than the non-swelling particles.

In both cases of computations, the proposed method is able to give good and reasonable results, responding well to the given computational conditions. Depending on the necessity, the proposed model can be adapted for various other material with different characteristics. A further detailed study is also considered for future works. On the 3D SAP particles computation, the particles are treated as a rigid particles. For condition such as cases with soft solid, there is a need to introduce a distortion computation on the particles. Such computation is considered possible by modifying the wireframe method with similar spring model computation as the one proposed for the hydrogel particle computations.

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