Particle based Droplet Simulation in Liquid-Liquid Two-phase Flow

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Abstract: The subarachnoid hemorrhage is a disease that damages brain function by rupture of cerebral aneurysm and, at the worst case, it leads to death. The subarachnoid hemorrhage is one of the dangerous diseases in Japan. And, clipping and coil embolization are selected as the preventive surgery; however, these surgeries do not have enough effect for distorted shape or enormous size of the cerebral aneurysm. On the other hand, liquid embolization that injects an embolic material having chemical curing property into the aneurysm is also used overseas. Liquid embolization can treat a distorted shape or enormous size of aneurysm that clipping and coil embolization cannot treat. However, liquid embolization has not been approved in Japan because there is a risk that the injected embolic material might flow out of the aneurysm and embolize peripheral blood vessels.

Then, we have developed an embolic material injection simulation using a particle method as a preliminary stage to validate the safety of the liquid embolization simulation, and have performed the quantitative evaluation by comparing the simulation result with the physical experiment in order to control the embolic material injection. In the study, we have performed the injection simulation of embolic material, which is injected from a circular tube imitating a catheter into a water tank imitating a cerebral aneurysm. In the previous research, however, the formed droplet did not contact with the tip of the circular tube.

Therefore, we consider that the previous simulation results are due to the interfacial tension model, and in this paper, we solve the problem by reconsidering the interfacial tension model. The interfacial model used in the previous research considered only the intermolecular potential force of in a single fluid. However, we have to consider the intermolecular potential force between different liquids because water in the water tank and the embolic material injected through a catheter are different. Therefore, we newly adopt an interface tension model that can consider the influence from the other liquid on the boundary of two different liquids. In this paper, we propose an interfacial tension model that considers liquid-liquid two-phase flow because the reference model of the potential force for two different fluids treats gas-liquid two-phase flow. As the result of the simulation, we have confirmed that the droplets formed by the simulation contacts with the tip of the catheter.

Figure 1 shows the result of the simulation. In the figure, the black line on the top of the droplet shows the tip of the catheter. In Figure 1 (a), the droplet does not contact with the tip of the catheter, while it contacts with the tip in Figure 1 (b).

Time = 1.03[s]

(a) Previous model (interfacial tension model for single liquid) (b) Proposed model (interfacial tension model for two different liquid)

Figure 1. Simulation results for the previous and the proposed models.

Keywords: *Physical simulation, particle method, liquid-liquid two-phase flow, interfacial tension*

1. INTRODUCTION

The subarachnoid hemorrhage, which gives serious damage to the brain by rupture of a cerebral aneurysm, is one of the top causes of the death in Japan. Clipping and coil embolization techniques are used in Japan as the preventive surgeries and they are the established surgical methods, which give a certain amount of therapeutic effect. However, these techniques cannot be applied to an enormous or distorted cerebral aneurysm. On the other hand, a liquid embolization technique, which injects an embolic material to the aneurysm through the catheter, is used over the sea (Molyneux, et al. 2004). The liquid embolization is an effective technique since it can embolize liquid in an enormous or distorted cerebral aneurysm. The liquid embolization technique, however, is not authorized yet in Japan because the flow control of an injected embolic material is difficult, and the material that flows out of the aneurysm might embolize normal blood vessels.

Then, we have developed an embolic material injection simulation as a preliminary stage to validate the safety of the liquid embolization, and have performed a quantitative evaluation by comparing droplets formed by the simulation and that in the physical experiment in order to research how to control the embolic material (Natsume et al. 2018; Natsume et al. 2019). In the study, MPS method, which is one of particle methods, was used as the analytical method that was suitable for incompressible fluid (Koshizuka and Oka 1996). The embolic material injection simulation was performed, which injects an embolic material through a circular tube that imitates the catheter into a water tank that imitates the cerebral aneurysm. In the previous simulation results, however, the droplet was not detached from the tip of the catheter or it did not contact with the tip of the circular tube even in the case that it was detached from the tip. Then, we assume that these simulation results are due to the interfacial tension models, and in this paper, we consider interfacial tension models to solve the issue. The interfacial model used in the previous research considered only the intermolecular potential force of a single fluid (Nomura et al. 2001; Kondo et al. 2007). However, for the simulation that considers the real surgery, two-phase liquid flow should be treated, where one liquid gives some influence to the other on the interfacial boundary.

Therefore, in this paper, we develop a model that gives the influence from one fluid to the other on the interface boundary by the interfacial tension, and investigate if the droplet formed in the simulation contacts with the tip of the catheter and also if the droplet is detached from the catheter.

2. ANALYTICAL METHOD

2.1. Governing equations

The embolic material and the water treated in this study are assumed to be incompressible fluids, and the governing equations are the equation of continuity and the Navier-Stokes equation.

$$\frac{D\rho}{Dt} = 0 \tag{1}$$

$$\frac{D\boldsymbol{u}}{Dt} = -\frac{1}{\rho}\nabla \boldsymbol{P} + \nu\nabla^2\boldsymbol{u} + \boldsymbol{g} + \frac{1}{\rho}\boldsymbol{F}^{inter} \tag{2}$$

where, $\rho, t, \boldsymbol{u}, \boldsymbol{P}, \nu, \boldsymbol{g}$, and $\boldsymbol{F}^{inter}$ are density, time, velocity vector, pressure, kinematic viscosity coefficient, gravitational acceleration vector, and interfacial tension force, respectively, and items in the right side of Eq. (2) are pressure, viscosity, gravitational acceleration, and interfacial force terms, respectively. MPS method we use as the analytical method in the paper differentiates physical quantities using interparticle interaction models. However, the MPS method developed by Koshizuka et al. (Koshizuka and Oka 1996), has a numerical instability due to the pressure oscillation that should be suppressed in the simulation. Then, in this research, the methods developed by Tanaka et al. (Tanaka and Masunaga 2010) and Iribe et al. (Iribe and Nakaza 2011), are employed in order to suppress the pressure oscillation.

2.2. Interfacial tension model

The previous research used the interfacial tension model that considered only the volume force or intermolecular potential force of a single fluid, and then the droplet formed in the simulation was not detached from the catheter or the droplet did not contact with the tip of the catheter even in the case that it was detached. Then, we employ the interfacial tension model proposed by Ishii et al. (Ishii and Sugii 2012), which considers the influence by the pressure gradient on the interface boundary between two different materials, and this paper proposes a new interfacial model that can be applied to liquid-liquid two-phase flow. The model developed by Ishii et al. (Ishii and Sugii 2012) is based on the method (Kondo et al. 2007), and employs the potential model shown in the following equation.

$$\boldsymbol{F}_i = C \sum_{j \neq i} \boldsymbol{f}_{ij}(r_{ij}) \frac{(\boldsymbol{r_j} - \boldsymbol{r_i})}{r_{ij}} \tag{3}$$

where, $\boldsymbol{F}_i, C, \boldsymbol{f}_{ij}, r_{ij}$, and $\boldsymbol{r_i}$ are interparticle force of i, potential coefficient, potential force between particle i and j, distance between particle i and j, and particle coordinate vector of i, respectively. The potential force is calculated by the potential function as follows.

$$\boldsymbol{f}_{ij}(r_{ij}) = \begin{cases} (r_{ij} - l_0)(r_{ij} - r_e^{it}) & (r_{ij} \leq r_e^{it}) \\ 0 & (r_{ij} > r_e^{it}) \end{cases} \tag{4}$$

where, l_0 and r_e^{it} are the initial distance between particles and the radius of influence for interfacial tension, which is 3.1 times of the initial particle distance (Ishii and Sugii 2012). The normal pressure at particle i is calculated with the following equation.

$$P_i^n = \frac{\boldsymbol{F}_i \cdot \boldsymbol{n_i}}{A_i} \tag{5}$$

where, $P_i^n, \boldsymbol{n_i}$, and A_i are normal pressure, normal unit vector, and small area element of particle i, respectively. Here, $\boldsymbol{n_i}$ is calculated with the interparticle force of i ($\boldsymbol{F}_i$) as follows.

$$\boldsymbol{n}_i = \begin{cases} \boldsymbol{F}_i / |\boldsymbol{F}_i| & (|\boldsymbol{F}_i| / |\boldsymbol{F}_i|_{flat} \geq \gamma) \\ 0 & (|\boldsymbol{F}_i| / |\boldsymbol{F}_i|_{flat} < \gamma) \end{cases} \tag{6}$$

where, $|\boldsymbol{F}_i|_{flat}$ and γ are interparticle force magnitude at zero interfacial curvature and coefficient of interfacial decision that is 0.2, respectively. On the other hand, the small area element A_i for particle i is calculated as the following.

$$A_i = A_0 \frac{1}{N} \sum_{j \neq i} sin\,\varphi_{ij} \tag{7}$$

where, A_0, N, and φ_{ij} are interfacial area occupied by one particle, particle number in the radius of influence, and the angle between the normal vectors of particle i and j, respectively. The interfacial force $\boldsymbol{F}_i^{inter}$ is calculated as the pressure gradient at the particle i with Eq. (8), where two different materials (liquid and gas) exist.

$$\boldsymbol{F}_i^{inter} = \nabla P_i = \frac{d(P_{liquid} - P_{gas})}{h} \boldsymbol{n}_i \tag{8}$$

where, d and h are spatial dimension number and interfacial thickness that equals to the initial particle distance, respectively. The model developed by Ishii et al. (Ishii and Sugii 2012), considered gas-liquid two-phase flow as shown in Eq. (8). However, the embolic material simulation has to treat two different liquids (embolic material and water) so that $\boldsymbol{F}_i^{inter}$ becomes the following.

$$\boldsymbol{F}_i^{inter} = \frac{d(P_{embolic} - P_{water})}{h} \boldsymbol{n}_i \tag{9}$$

where, $P_{embolic}$ and P_{water} are pressure of embolic material and average pressure of water in the radius of influence, respectively. P_{water} is calculated as follows.

$$P_{water} = \frac{1}{N} \sum_{j \neq i} P_{water}\, \omega(r_{ij}) \tag{10}$$

$$\omega(r_{ij}) = \begin{cases} 1 & (r_{ij} \leq r_e^{ave}) \\ 0 & (r_{ij} > r_e^{ave}) \end{cases} \tag{11}$$

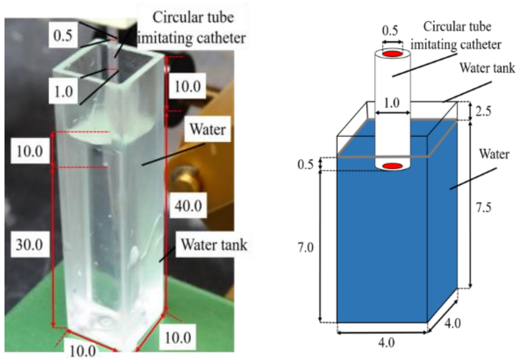
where, r_e^{ave} is the radius of influence used for the calculation of average pressure, and equals to the initial particle distance l_0 since the interfacial tension $\boldsymbol{F}_i^{inter}$ is solved with the interfacial thickness h that also equals to l_0 (see Eq. (9)).

2.3. Simulation condition

Table 1 shows the condition for both of the physical experiment and the simulation. In addition, Figure 2 shows the environments of the physical experiment for the quantitative assessment and the simulation model. In Figure 2, the size of the catheter in the simulation is the same as that in the physical experiment, however, the size of the water tank in the simulation is smaller than that in the physical experiment due to the computational resource. Table 2 shows the environment of the simulation.

Table 1. Condition of the physical experiment and the simulation.

Parameter	Value	Unit
Density of embolic material	1.18×10^3	kg/m^3
Density of water	1.00×10^3	kg/m^3
Kinematic viscosity of embolic material	628×10^{-6}	m^2/s
Kinematic viscosity of water	1.00×10^{-6}	m^2/s
Gravitational acceleration	9.8	m/s^2
Interfacial tension coefficient	10.8×10^{-3}	N/m
Injection flow velocity	8.5×10^{-3}	m/s
Initial particle distance (simulation only)	1.0×10^{-4}	m
Time step (simulation only)	1.0×10^{-4}	s



(a) Physical experiment (b) Simulation

Figure 2. Dimensions of the physical experiment and the simulation model.

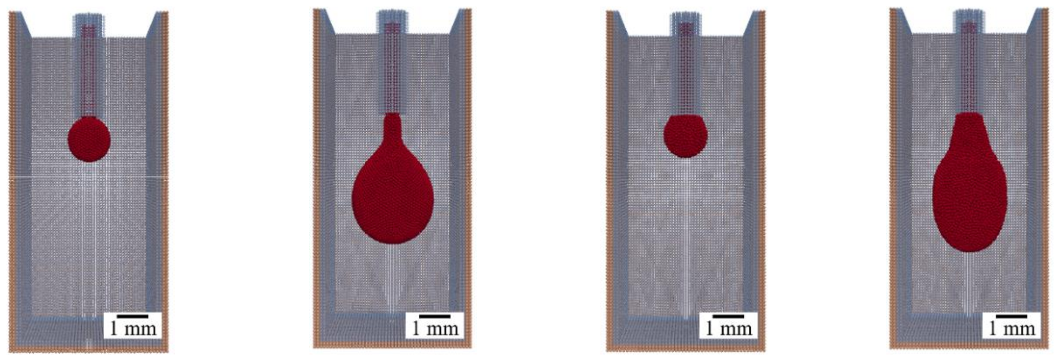
Table 2. Environment of the simulation.

CPU	Intel(R) Xeon(R) CPU E5-1650 v3 (3.5GHz)
GPU	Tesla K40 (12GB)
OS	Arch Linux
Memory	32GB

3. RESULT AND DISCUSSION

3.1. Comparison of methods

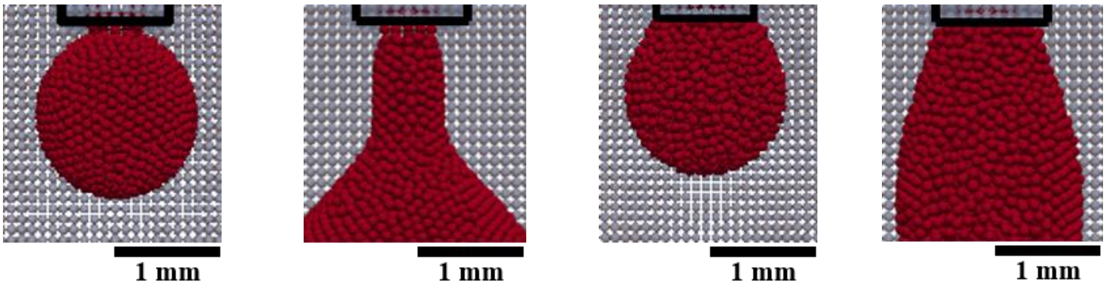
Figure 3 shows the comparison of the previous and the proposed models in the simulation. Figure 4 shows the zoomed view in the vicinity of the catheter tip in Figure 3.



Time = 1.03[s] Time = 8.00[s] Time = 1.03[s] Time = 8.00[s]

(a) Previous model (interfacial tension model for single liquid) (b) Proposed model (interfacial tension model for two different liquid)

Figure 3. Comparison of the previous and the proposed models.



Time = 1.03[s] Time = 8.00[s] Time = 1.03[s] Time = 8.00[s]

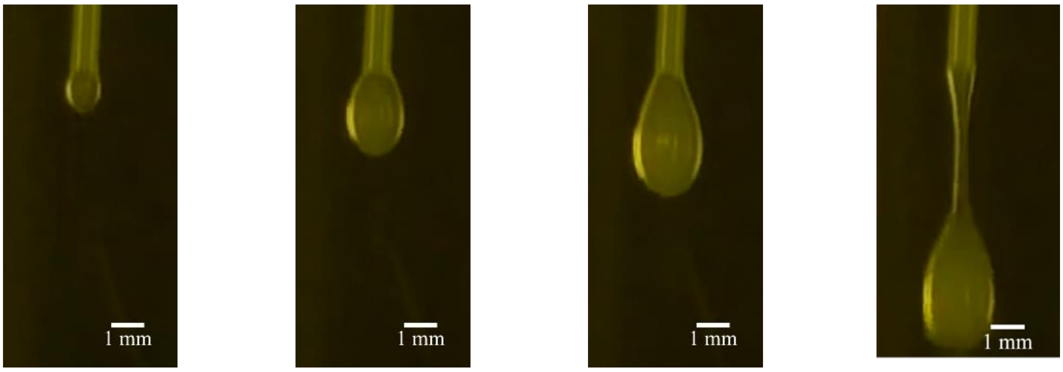
(a) Previous model (b) Proposed model

Figure 4. Comparison of the previous and the proposed models (zoomed).

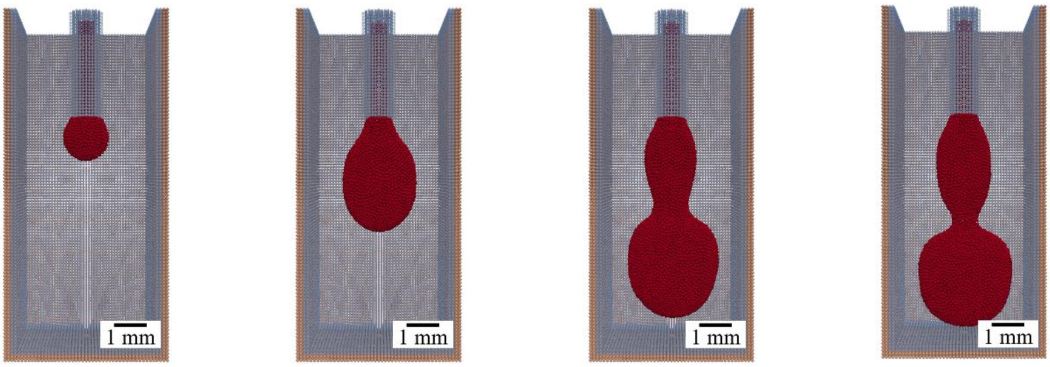
In Figure 3 and 4 (a), the droplet does not contact with the tip of the catheter at the both times of 1.03[s] and 8.00[s], while it contacts with the tip of the catheter at those times in Figure 3 and 4 (b). Figure 3 and Figure 4 show that the proposed method is more suitable for this study.

3.2. Comparison of physical experiment and simulation

Figure 5 shows the comparison of the physical experiment and the simulation with the proposed model, where the water particles in the water tank are not drawn to improve the visibility of the embolic material.



(a) Physical experiment



(b) Simulation

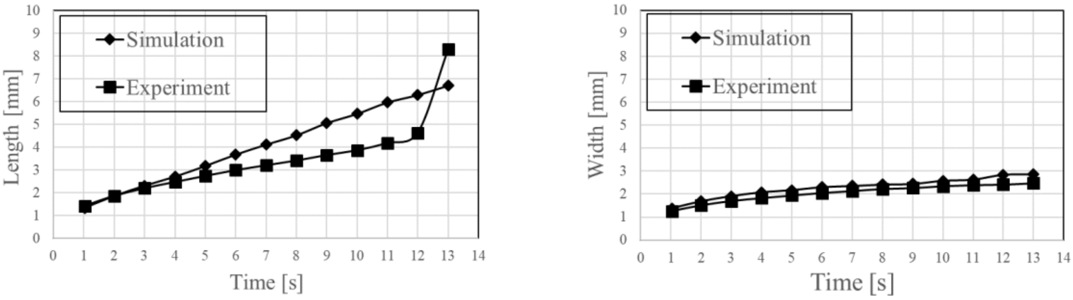
Time = 1.03[s] Time = 6.00[s] Time = 12.00[s] Time = 13.00[s]

Figure 5. Comparison of the droplets between the physical experiment and the simulation

In Figure 5, the shapes of the droplets formed by the physical experiment and the simulation with the proposed model are similar at the times of 1.03[s] and 6.00[s]. The droplet formed by the simulation at the times of

12.00[s] and 13.00[s] are different from those in the physical experiment. On the other hand, the detached times were 13.38[s] and 13.60[s] for the physical experiment and the simulation, respectively, which are very close.

In addition, Figure 6 (a) shows the length change of the droplets by the physical experiment and the simulation, and they are very close until 5.0[s], however, the lengths of droplets are gradually departed after 5.0[s]. On the other hand, Figure 6 (b) shows the width change of the droplets by the physical experiment and the simulation, and they are very close all the time.



(a) Length (b) Width

Figure 6. The length and width change of the droplets

4. CONCLUSION

As a preliminary simulation to verify the safety of liquid embolization surgery, we have performed an embolic material injection simulation with an interfacial tension model that considers liquid-liquid two-phase flow. In the previous results, the droplet was not detached from the catheter or it did not contact with the tip of the catheter even in the case it was detached from the catheter. On the contrary, the simulation result with the proposed model shows that the droplet contacts with the tip of the catheter and is detached from the catheter. In addition, although the shapes of the droplets by the physical experiment and the simulation are different, the detached time in the simulation is very close to that in the physical experiment. However, it is not sure if the fact that the droplet contacts with the tip of the catheter is related to the wettability, and it is not also clear if the proposed model has a relation with the wettability, because we did not consider the contact angle for the wettability in the simulation and the contact angle should not be fixed in advance but change dynamically in the process of the droplet forming. Therefore, in the future, we have to investigate the relation between the proposed model and the wettability.

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