

Analysis of Wettability Model Using Adhesional and Spreading Works

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Abstract: We have developed a new method of wettability, which is a feature for a liquid to keep the contact angle formed between a liquid and a solid body. Conventional models required the contact angle in advance for simulations, which angle can be measured by physical experiments. On the other hand, our new model does not need the contact angle and forms the shape of liquid on a solid body by considering adhesional and spreading works. We demonstrated that the proposed method was able to represent wettability by simulations without contact angles. This paper evaluates the proposed method by investigating the drop time of the liquid extruded from a thin tube.

1 INTRODUCTION

Liquid simulation is a very challenging issue since it deforms dynamically and the topology changes all the time with the separation and integration of many small molecules. The simulation where one kind of liquid drops in the air is relatively simple because the air is usually ignored and the simulation can be performed by considering just one type of liquid. On the other hand, the simulation where two kinds of liquid should be treated is very complex and difficult to perform.

One example is the simulation of an embolization material dropped in the cerebral aneurysm. In this case, two different kinds of liquid, which are embolization material and blood, should be considered in the simulation, and the interfacial tension works on the boundary between the two materials. The interfacial tension is different from free surface tension, which works between liquid and air that can be usually ignored.

For fluid simulations, two types of methods are usually used: grid-based Euler method and particle-based Lagrangian one. Grid-based Euler methods can perform simulations for large spaces, however, it is difficult to treat the interfacial tension that works on the boundary of two different kinds of fluid. On the other hand, particle-based Lagrangian ones can eas-

ily detect the boundary of two different kinds of fluid and can treat the topological change; however, the calculation accuracy is relatively low since it does not consider some particles that are outside of a constant range for the calculation.

For the safety verification of a new embolization method for a cerebral aneurysm, we have been trying to simulate the behavior of a droplet that is ejected from a thin tube, which is a real catheter, into a water tank, which imitates a cerebral aneurysm, using the MPS (Moving Particle Semi-implicit) method that is one of the particle methods and was developed for incompressive fluid. We have also evaluated our method by the comparison between the simulation results and the physical experiments. The method considered the effect of liquid-liquid two-phase flow; however, the droplet that came out of the catheter did not adhere to the edge of the catheter because we did not consider wettability.

To simulate wettability, which is a feature for a liquid to keep the contact angle between the liquid and the solid body, the contact angle is necessary and it can be measured by physical experiments. It means that we cannot perform the simulation unless the contact angle is known, which is decided depending on the physical features of two materials: liquid and solid.

Then, we developed a new wettability method that does not need the contact angle between a liquid and a

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solid and succeeded in representing wettability. However, we have not evaluated the method for the drop time of liquid by the comparison between the simulation results and the physical experiment. Therefore, this paper reports the evaluation of the new wettability method for the drop time of liquid. The maximal merit of our method is that it can represent wettability without contact angles, which must have been measured before simulations in the conventional methods. The proposed method can visualize wettability of a liquid on a solid body not by estimating the contact angle but by changing the liquid shape with adhesion and spreading works, which operate between liquid and solid body.

2 RELATED WORKS

For fluid simulations, mainly two types of methods are usually used: the grid-based Euler method and the particle-based Lagrangian one. The grid-based Euler method calculates physical features such as density and velocity of fluid at fixed positions. Then, it requires a lot of memories for simulations and it is difficult to determine the boundary where multiple fluids contact. On the other hand, the particle-based Lagrangian one simulates physical phenomena using many particles, and it can easily determine the boundary between different types of particles, but, the calculation accuracy is relatively low because it does not consider some particles outside of a constant range for the calculation. For the simulation of liquid embolization, particle-based methods are more suitable since they can treat the topological change and can calculate the interfacial tension on the boundary between two kinds of materials.

In general, two major particle methods are used depending on the purpose of the simulation: One is the SPH (Smoothed Particle Hydrodynamics) method that was developed by (Gingold and Monaghan, 1997) for compressive fluid, and the other is the MPS method that was developed by (Koshizuka and Oka, 1996) for incompressive one.

For the simulation of a droplet that is ejected from a thin tube, force balance should be considered. The droplet drops when the gravitational force becomes more than the attractive force caused by the interfacial tension. Two kinds of models are usually used for interfacial tension calculation. One is the CSF (Continuum Surface Force) model developed by (Brackbill et al., 1992), and the other is a potential energy model. (Morris, 2000) applied the CSF to the interfacial model of the SPH method, while (Nomura et al., 2001) used the CSF to the MPS method. On

the other hand, (Tartakovsky and Meakin, 2005) utilized the potential energy model for the SPH method, while (Shirakawa et al., 2001) proposed an interfacial tension model based on potential energy for the MPS method.

Wettability is caused by the attractive force that works to support the droplet against the gravitational force. (Wang et al., 2005) proposed a wettability model with a level set method, while (Zhang et al., 2012) established the model by using a mesh method. They both represented a droplet with wettability, where the liquid adheres to a solid body.

In addition, (Akinci et al., 2013) proposed a method considering adhesion wetting, while (Yang et al., 2016) investigated another model with potential energy by considering the interaction between liquid and air. (Hattori and Kohizuka, 2019) also represented a droplet that slides down on a slope by using potential energy and the MPS method.

(Natsume et al., 2019b) investigated the droplet behavior by using the MPS method and the comparison between the simulation result and a physical experiment, and (Natsume et al., 2019a) performed a droplet simulation with a particle method for liquid-liquid two-phase flow. On the other hand, (Ruan et al., 2021) proposed a method to model the contact interaction using a hybrid Euler-Lagrangian framework, and (Xing et al., 2022) simulated surface tension flow with a position-based dynamics (PBD) framework. In addition, (Natsume et al., 2021a) also simulated the viscous fluid injection by considering the effect of the force working between two kinds of liquid. These methods, however, did not consider wettability. For the simulation considering wettability, the contact angle, which is the angle formed between a liquid and a solid body, is necessary. Unless the contact angle is known, the wettability simulation cannot be performed.

(Kondo and Matsumoto, 2021) proposed a surface tension model and expressed wettability by introducing the interaction ratio between fluid and wall; however, it required contact angle calculation. On the other hand, (Natsume et al., 2021b) proposed a wettability method based on surface free energy between a liquid and a solid body, not by specifying the contact angle but by calculating the interfacial tension based on surface free energy. In addition, (Natsume et al., 2022) proposed another method to represent wettability by considering adhesion and spreading works and (Mukai et al., 2022) performed a liquid injection simulation with the new wettability method. The paper demonstrated that the liquid ejected from the catheter adhered to the solid body; however, it did not investigate the drop time of each

droplet. Then, this paper evaluates the proposed wettability method by the comparison of the drop time between the simulation results and the physical experiment in the same environment. The biggest merit of the proposed method is to be able to simulate wettability without contact angles that were necessary for the simulations using conventional methods.

3 METHODS

3.1 Governing Equations

The purpose of the paper is to simulate the behavior of the droplet ejected from a thin tube to a water tank and to investigate the drop time by the comparison between the simulation results and a real physical experiment. We employ the MPS method for the simulation because particle methods can easily treat the topological change caused by the detachment of the droplet extruded from a tube, and the embolization material and water are considered as incompressible fluid.

The governing equations for the liquid behavior analysis are the equation of continuity and the Navier-Stokes equations described as follows.

$$\frac{D\rho}{Dt} = \frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\mathbf{u}) = 0, \quad (1)$$

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g} + \mathbf{f}^{Tension}, \quad (2)$$

where, ρ is the density, t is the time, \mathbf{u} is the velocity, p is the pressure, μ is the viscosity coefficient, \mathbf{g} is the gravitational acceleration, and $\mathbf{f}^{Tension}$ is the interfacial tension.

For incompressible fluid, $\nabla \cdot \mathbf{u} = 0$ is true. Then, Eq. (1) can be written in the following.

$$\frac{\partial\rho}{\partial t} = 0 \quad (3)$$

3.2 Wettability Model

Wettability is a feature that liquid on a solid body keeps the contact angle between them, and there is the following relationship between the contact angle and the surface tensions as shown in Fig. 1 and Eq. (4), which is called Young' formula.

$$\gamma^s = \gamma^l \cos\theta + \gamma^{sl}, \quad (4)$$

where, θ is the contact angle, γ^s , γ^l , and γ^{sl} are the surface tensions of solid, liquid, and solid-liquid, respectively.

However, we cannot simulate liquid behavior with wettability unless the contact angle is known. On the

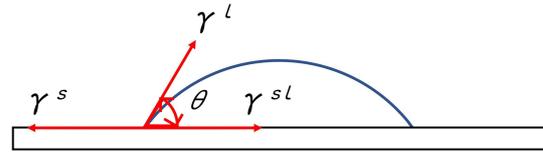


Figure 1: Relationship between the contact angle and the surface tensions.

other hand, there is a work that separates the solid and the liquid from the condition where they are attached, which is called ‘‘adhesional work’’. In addition, there is another work that restrains the liquid to spread out on the solid body, which is called ‘‘spreading work’’. There are also the following relationships between these works and the surface free energies according to Dupr e’s formula.

$$W^a + E^{sl} = E^s + E^l, \quad (5)$$

$$W^d + E^{sl} = E^s - E^l, \quad (6)$$

where, W^a and W^d are the adhesional and the spreading works, respectively. E^s , E^l , and E^{sl} are the surface free energies of the solid, the liquid, and the solid-liquid, respectively. Here, the unit of surface free energy is J/m^2 and $J = N \cdot m$. Then, the unit of surface free energy becomes N/m , which is the same unit as surface tension, and Eqs. (5) and (6) can be written as Eqs. (7) and (8), respectively.

$$W^a + \gamma^{sl} = \gamma^s + \gamma^l, \quad (7)$$

$$W^d + \gamma^{sl} = \gamma^s - \gamma^l. \quad (8)$$

Finally, the potential force that works at a particle i is defined in the following by replacing works and surface free energies with forces.

$$\mathbf{f}_i^a = \mathbf{f}_i^s + \mathbf{f}_i^l - \mathbf{f}_i^{sl}, \quad (9)$$

$$\mathbf{f}_i^d = \mathbf{f}_i^s - \mathbf{f}_i^l - \mathbf{f}_i^{sl}, \quad (10)$$

$$\mathbf{f}_i^k = C_i^k \sum_{j \neq i} f^p(r_{ij}) \frac{\mathbf{r}_j - \mathbf{r}_i}{r_{ij}}, \quad (11)$$

$$C_i^k = \frac{\gamma^k}{l_0(T_i^n - T_i^t)}, \quad (12)$$

$$T_i^n = \frac{1}{A_0} \sum_j^{N_n} f^p(r_{ij}) \frac{\mathbf{r}_j - \mathbf{r}_i}{r_{ij}} \cdot \mathbf{n}_i^p, \quad (13)$$

$$T_i^t = \frac{1}{A_0} \sum_j^{N_t} f^p(r_{ij}) \frac{\mathbf{r}_j - \mathbf{r}_i}{r_{ij}} \cdot \mathbf{t}_i^p, \quad (14)$$

$$f^p(r_{ij}) = \begin{cases} (r_{ij} - l_0)(r_{ij} - r_e^p) & (r_{ij} \leq r_e^p) \\ 0 & (\text{Otherwise}), \end{cases} \quad (15)$$

$$r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|, \quad (16)$$

where, \mathbf{f}_i^a and \mathbf{f}_i^d are the potential forces of a particle i for the adhesional and the spreading works, respectively. k means s , l or sl , C_i^k (C_i^s , C_i^l , and C_i^{sl}) are

the potential coefficients of \mathbf{f}_i^k (\mathbf{f}_i^s , \mathbf{f}_i^l , and \mathbf{f}_i^{sl}) of a particle i , respectively, f^p is the strength of the force working between particles, and \mathbf{r}_i and \mathbf{r}_j are the position vectors of particles i and j , respectively. l_0 is the initial distance between particles, A_0 is the small area element at the curvature 0, N_n and N_t are the numbers of particles in the normal and the tangential directions, respectively. \mathbf{n}_i^p and \mathbf{t}_i^p are the normal and the tangential vectors for the calculation of the potential coefficients C_i^k (C_i^s , C_i^l , and C_i^{sl}) of a particle i , respectively. r_e^p is the radius of influence for the calculation of potential forces. r_e^p is 3.1 times of the initial distance between particles (l_0), and other parameters are defined in the above equations.

Here, the adhesional force works vertically to separate the liquid and the solid. Then, the vertical force of W^a is used as the adhesional force, and the vertical component is described as \mathbf{f}^{an} . Finally, \mathbf{f}^{an} and \mathbf{f}^d are connected with the Heaviside function (H), and $\mathbf{f}_i^{Tension}$ is calculated as the interfacial tension of a particle i , and applied to $\mathbf{f}^{Tension}$ in Eq. (2). \mathbf{f}_i in Eq. (17) is designed so that the larger surface tension of a particle i ($\mathbf{f}_i^{Tension}$) is used for the smaller spreading work of a particle i (\mathbf{f}_i^d).

$$\mathbf{f}_i = \mathbf{f}_i^{an} - H\mathbf{f}_i^d, \quad (17)$$

$$\mathbf{f}_i^{an} = (\mathbf{f}_i^a \cdot \mathbf{n}^{Surf})\mathbf{n}^{Surf}, \quad (18)$$

$$\mathbf{f}_i^{Tension} = S_i \frac{d}{V_0} \left[\left(\frac{1}{N_i} \sum_j \sin\phi_{ij} \right)^{-1} - 1 \right] \mathbf{f}_i, \quad (19)$$

where, \mathbf{n}^{Surf} is the normal vector on the boundary surface. S_i is 1 or -1 for the convex or the concave boundary surfaces of a particle i , respectively. d is the dimensional factor, V_0 is the volume of one particle, N_i is the number of particles within the radius of influence for a particle i , and ϕ_{ij} is the angle between the normal vectors of particles i and j .

Fig. 2 and Eq. (20) show the approximate Heaviside function.

$$H = \begin{cases} 1 & (x < -\frac{\Delta x}{2}) \\ 1 - \frac{1}{2} \left(\frac{2x + \Delta x}{\Delta x} + \frac{1}{\pi} \sin \frac{2\pi x}{\Delta x} \right) & (|x| \leq \frac{\Delta x}{2}) \\ 0 & (x > \frac{\Delta x}{2}) \end{cases} \quad (20)$$

The domain and the range of the Heaviside function are $[0, 180]$ for the contact angle and $[0, 1]$ for the value, respectively. The outputs of 1 and 0 correspond to the inputs of 0 and 180, respectively. The contact angle, however, cannot be measured during the simulation. Then, the domain should be decided without the contact angle, and it is defined by the potential force instead of the contact angle in our method. The maximum value of the potential force was 75% of the

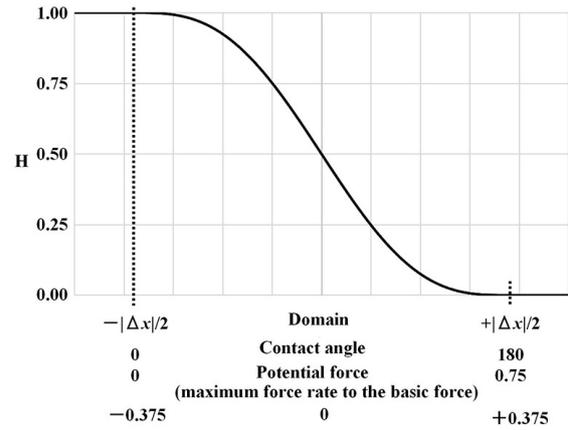


Figure 2: Approximate Heaviside function.

basis one, which is measured at the curvature 0. Finally, the domain becomes $[-0.375, +0.375]$ because the center of the domain should be 0.

4 SIMULATIONS AND RESULTS

Fig. 3 shows the environment of the physical experiment and the model of the simulation, which are the same ones for easier comparison. In the physical experiment, SCR780 was used as the liquid that was injected into a water tank from a thin tube that is a real catheter, which inner and outer diameters are 0.5 [mm] and 1.0 [mm], respectively.

Tables 1 and 2 show the parameters used in the simulation and the surface free energies of solid, liquid, and solid-liquid, respectively. In fact, the theoretical contact angle between the embolization material (SCR780) and the catheter (Teflon tube) is 26.2° . The number of particles dynamically changes during the simulation because the particles of the embolization material (SCR780) are injected into the water tank through the catheter. The detail is shown in Table 3. Table 4 shows the specification of the PC used in the simulation.

Fig. 4 shows the comparison between the simulation results and the physical experiment in 4 [s] after the injection starts. Fig. 4 (a) is the simulation image by the method without wettability, it does not show the feature of wettability, while Fig. 4 (b) shows the feature and the liquid adheres to the surface of the tube, which is similar to the image of the physical experiment shown in Fig. 4 (c). The contact angle (θ) in Fig. 4 (b) is about 25.0° , which is similar to that in Fig. 4 (c) that is about 28.0° , although the theoretical angle is 26.2° . These results show that the proposed method is effective for the wettability representation.

Fig. 5 shows the comparison between the simula-

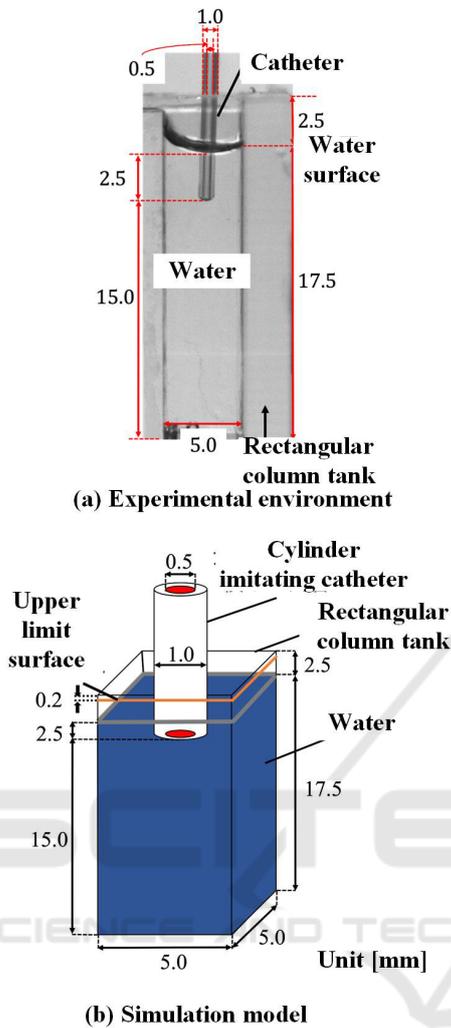


Figure 3: Experimental environment and simulation model.

tion result with the wettability method and the physical experiment. In Fig. 5, the comparison starts at 1.03[s] from the beginning because there is no liquid in the tube at 0.0[s] in the physical experiment, while there should be some particles in the simulation at the initial state. After one droplet is dropped, there is some liquid remaining in the tube, which amount corresponds to the volume in 1.03[s] after the injection starts. Then, both initial states can start at 1.03[s] by setting some particles that correspond to the volume of the real liquid at 1.03[s] after the injection starts.

In the figure, both liquid states are almost the same; however, the liquid in the simulation elongates vertically more than that in the physical experiment, and the liquid almost forms a droplet at 10.0[s] in the simulation, while a droplet has not been formed yet in the physical experiment. Table 5 shows the drop time for one droplet.

Table 1: Parameters used in the simulation.

Parameter	*	Value	Unit	
Density	Water	ρ	1.00×10^3	kg/m^3
	Liquid		1.18×10^3	
Viscosity coefficient	Water	μ	1.00×10^{-3}	$Pa \cdot s$
	Liquid		7.42×10^{-1}	
Injection speed	u	8.50×10^{-3}	m/s	
Gravity	g	9.80	m/s^2	
Particle radius (=Initial distance)	l_0	1.00×10^{-4}	m	
Time step	Δt	5.00×10^{-5}	s	

* Symbol

Table 2: Surface free energies used in the simulation. [J/m^2]

Material	γ^s	γ^l	γ^{sl}
Thin tube	10.5	—	0.8
Embolization material	—	10.8	—

Table 3: Number of particles used in the simulation.

Particle type	Numbers
Water	453,150
Wall	190,804
Catheter	3,384
SCR 780 (Minimum)	1,070
SCR 780 (Maximum)	44,072
Total (Minimum)	648,408
Total (Maximum)	691,410

Table 4: Specification of the PC used in the simulation.

CPU	Xeon E5-1650 v3 3.5GHz
Main memory	32GB
GPU	Tesla K40 with 12GB memory
OS	Arch Linux

In Table 5, the drop time in the simulation is shorter than that in the physical experiment except for the first drop. On the first drop, there is the same volume of the liquid in the tube, and they drop at almost the same time. However, there are more amounts of liquid remaining in and on the tube in the sim-

Table 5: Drop time for one droplet.

Number	Experiment	Simulation
1	10.69	10.01
2	10.33	5.38
3	10.41	5.88
Average	10.32	7.09

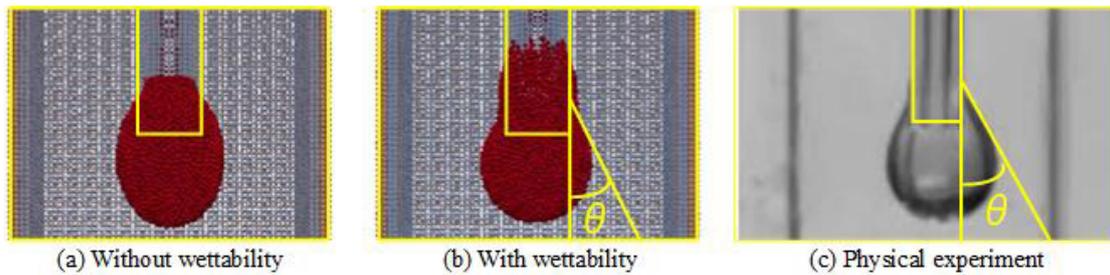
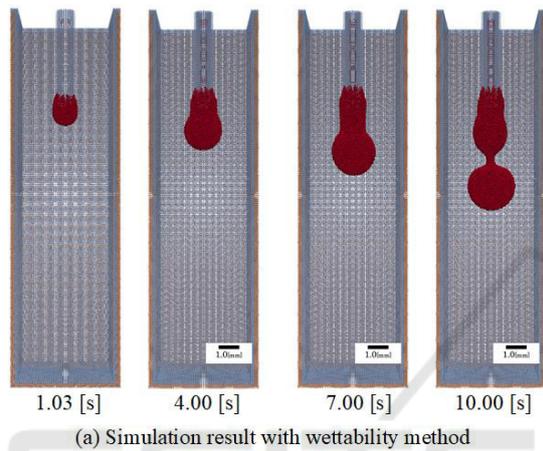
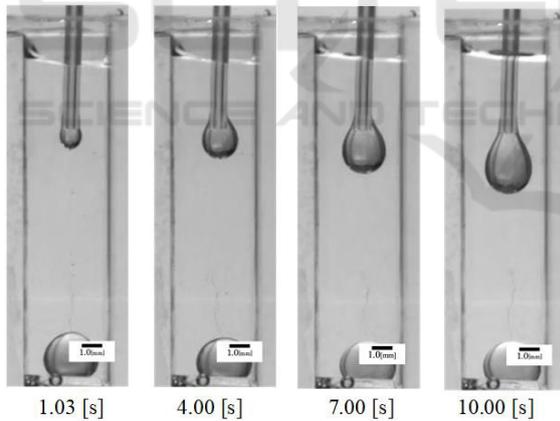


Figure 4: Comparison between the simulation results and the physical experiment for wettability.



(a) Simulation result with wettability method



(b) Physical experiment

Figure 5: Comparison between the simulation result and the physical experiment for the drop time.

ulation by introducing the wettability method. The volume of the droplet in the physical experiment was about $1.80 \times 10^{-8} [m^3]$, while that in the simulation was about $8.84 \times 10^{-9} [m^3]$ in average, which is about the half of the real droplet volume. This means that the interfacial tension of the particle in the simulation is weaker than that in the real liquid. Then, the drop time in the simulation becomes faster than that in the physical experiment.

5 CONCLUSIONS AND FUTURE WORKS

The conventional methods needed contact angles to represent wettability since simulations were not able to be performed without them. This means that we could not represent wettability for the materials, which contact angles are unknown. Then, we have developed a new wettability method that does not need to specify the contact angle but change the liquid shape using adhesional and spreading works, and we became able to represent wettability of materials even if the contact angles were not known. In addition, we have confirmed that the proposed method can represent wettability that is similar to the physical phenomenon by the comparison between the simulation results and the physical experiment,

However, the liquid elongated vertically more than that in the experiment, and the drop time was shorter. It seems that there are three main reasons for the difference. One is that more liquid remains in and on the tube by introducing the wettability method. The second is that the interfacial tension based on potential energy in the simulation is weaker than the real force. The last one is that we did not consider the visco-elastic feature of the liquid. The material is a visco-elastic fluid so it has both characteristics of viscosity and elasticity. This simulation, however, considered only viscosity and did not consider elasticity.

Then, we plan to perform the droplet simulation by reconsidering the wettability method and the interfacial tension model and also by introducing the visco-elastic feature of the liquid in the future.

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