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DEVELOPMENT OF SURFACE TENSION MODEL WITH MANY-BODY POTENTIAL FORCE

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Abstract. A new approach to calculate surface tension in a particle method is proposed. In particle methods, one way to calculate surface tension is introducing pairwise potential force, which is long-range attractive and short-range repulsive. However, the potential force acts not only on the surface but also inside the fluid bulk, which causes unrealistic pressure increase in the droplet or shrinkage of the droplet. In this study, a many-body potential is introduced for surface tension calculation instead of the pairwise potential. The new approach is tested in the droplet oscillation calculation, capillary pressure calculation and capillary rise calculation. The surface tension could be estimated consistently in these calculations.

1 INTRODUCTION

One of the advantage of particle methods is to capture the complex motion of the dynamic free-surface flows. It is important to take surface tension into consideration to calculate the free surface flows, especially in analysing fluid motion in microstructures or droplet break up behaviours. There are mainly two ways to calculate surface tensions in particle methods [1,2]. One is to introducing surface tension force by discretising the continuum surface force (CSF) model [3]. However, the first approach does not conserve linear momentum of the particle system, and it might cause strange motion of droplet. Another way is to introduce pairwise potential force, which is long-range attractive and short range repulsive [4-6]. This approach can conserve linear momentum and the formulation is much simpler than the CSF approach. Since the mechanical energy conservation is good with the potential force, its numerical stability is also good. However the pairwise potential force acts not only on the surface of the fluid but also acts inside the fluid bulk. Because of this force inside, unrealistic pressure increase in the droplet or the droplet shrinkage occurred [5]. The pairwise force tends to be large, and the time step width has to be small enough, which is not favourable for numerical efficiency.

In this study, a new model for surface tension calculation is developed. A many-body potential force is introduced instead of the pairwise potential force in the context of Moving Particle Full-implicit (MPF) [7] method, and the new model is tested in the calculations of droplet oscillation, capillary pressure and capillary rise, and the surface tensions are estimated through these calculations.

2 NUMERICAL METHOD

2.1 Incompressible calculation [7]

To simulate incompressible free surface flows, Moving Particle Full-implicit method [7] was used in this study. In the method, the following governing equation was adopted.

$$\rho \frac{du_i}{dt} = \frac{\partial}{\partial x_j} \mu \dot{\varepsilon}_{ij} + \frac{\partial}{\partial x_i} (\lambda \dot{\varepsilon}_{kk} + \kappa \varepsilon_{kk}) + \rho g_i \tag{1}$$

Since this equation approaches to the usual incompressible Navie-Stokes (NS) equation when we set the parameters λ and κ large enough, it can be used instead of the incompressible NS equation. The first term on the right hand side is the viscosity term and the second term is equivalent to the pressure term in the general NS equation for incompressible flow. Here, the pressure is expressed as

$$P = -(\lambda \dot{\varepsilon}_{kk} + \kappa \varepsilon_{kk}) . \tag{2}$$

In particle methods, the governing equations are replaced by particle interaction forces. The interaction is limited in a finite range using an effective radius r_e and a weight function w^{ij} as

$$\begin{aligned} w^{ij} &= \frac{W^{ij}}{N_0} \\ W^{ij} &= \begin{cases} (r_e - d^{ij})^2 & (d^{ij} < r_e) \\ 0 & (d^{ij} > r_e) \end{cases} \\ N_0 &= \sum_{init} W^{ij} \end{aligned} \tag{3}$$

In this study, the particle interaction models for gradient, divergence and Laplacian operators are formulated as

$$\begin{aligned} \nabla \phi &\approx \sum_j (\phi^j + \phi^i) \mathbf{r}^{ij} \frac{w'^{ij}}{d^{ij}} \\ \nabla \cdot \mathbf{A} &\approx \sum_j (\mathbf{A}^j - \mathbf{A}^i) \mathbf{r}^{ij} \frac{w'^{ij}}{d^{ij}} \\ \nabla^2 \phi &\approx \sum_j (\phi^j - \phi^i) \frac{w'^{ij}}{d^{ij}} \end{aligned} \tag{4}$$

where w^{ij}' is the differential of the weight function shown in Eq. (3). The particle interaction models are formulated in a similar manner compared to the Smoothed Particle Hydrodynamics (SPH) [1] formulation, however, the weight function (Eq. (3)) instead of the SPH kernel function is used in this study. The differential of this weight function is non-zero at d^{ij}=0 so as to keep the particle arrangement uniform.

When we discretize the governing equation (Eq.(1)) with the particle interaction models, the force acting on the particles are formulated as

$$\rho_0 \frac{d\mathbf{u}^i}{dt} = \mu \sum_j (\mathbf{u}^j - \mathbf{u}^i) \frac{w'^{ij}}{d^{ij}} - \sum_j (P^j + P^i) \mathbf{r}^{ij} \frac{w'^{ij}}{d^{ij}} + \rho_0 \mathbf{g} \ , \tag{5}$$

where

$$P^i = -\lambda \sum_j (\mathbf{u}^j - \mathbf{u}^i) \cdot \mathbf{r}^{ij} \frac{w'^{ij}}{d^{ij}} + \kappa (1 - \sum_j w^{ij}) \tag{6}$$

Since the potential energy and dissipative function for the discretized equation can be written, thermodynamic consistency of the particle system after discretization is assured. It implies that the mechanical energy of the system monotonically decrease, and this property is important for stable calculation.

The equations (5) and (6) will be a linear matrix equation whose unknowns are the velocity **u** and the pressure *P*. Since the coefficient matrix is symmetric, it can be solved by conjugated residual (CR) method.

2.2 Surface tension model using many body potential

The surface tension is calculated in the similar manner to the SPH pressure calculation, where another normalized weight function

$$\begin{aligned} w_s^{ij} &= \frac{W_s^{ij}}{N_{s0}} \\ W_s^{ij} &= \begin{cases} \left(1 - \left(\frac{d^{ij}}{r_{es}}\right)^2\right)^2 & (d^{ij} < r_{es}) \\ 0 & (d^{ij} > r_{es}) \end{cases} \\ N_{s0} &= \sum_{init} W_s^{ij} \end{aligned} \tag{7}$$

is used. The parameters like density and pressure are calculated as

$$\begin{aligned} \rho_s^i &= \sum_j m w_s^{ij} \\ P_s^i &= -a(\rho_0 - \rho_s^i) \end{aligned} \tag{8}$$

where ρ_0 is the bulk density at the initial state, and a is a coefficient to control the magnitude of surface tension. The interaction force with respect to surface tension is formulated as

$$\mathbf{F}_s^{ij} = \frac{m}{\rho_0} \sum_j (P_s^j + P_s^i) \mathbf{r}^{ij} \frac{w_s^{ij'}}{d^{ij}} \tag{9}$$

Because of the low particle number density close to the surface, the pressure P_s will be negative, and it yields the long-range attractive force, which can simulate surface tension.

Since the force can be derived from the potential formulated as

$$E_s = \frac{a}{2\rho_0} \sum_i (\rho_0 - \rho_s^i)^2 \tag{10}$$

$$F_s^i = -\frac{\partial E_s}{\partial \mathbf{x}_i}, \tag{11}$$

it conserves mechanical energy and also the linear momentum of the system.

3 CALCULATIONS

Using the same set of the parameters shown in Table 1, droplet oscillation, capillary pressure and capillary rise will be calculated, and surface tension σ were estimated through each calculation. For the uniform arrangement of the particles during the calculation, the effective radius for the surface tension term r_{es} should be larger than the effective radius for the pressure term r_e. It is because the range of the attractive force due to the surface tension term is to be larger than the range of the repulsive force due to the pressure term.

Table 1: Parameters used in the calculations

Parameters	Values
Time step Δt	0.001
Particle spacing l_0	0.01
Mass m	0.0001
Viscosity μ	1.0×10^{-10}
Effective radius for pressure and viscosity terms r_e	0.015
Bulk viscosity κ	100
Bulk modulus λ	10000
Effective radius r_{es}	0.032
Coefficient in the surface tension calculation a	0.01

3.1 Droplet oscillation calculation

Figure 1 shows the initial state of the droplet oscillation calculation. The radius of the droplet is R=0.3 and the shear rate of 1.0 is given at the initial state. The snapshots of the calculation is shown in Figure 2, where the oscillating droplet can be seen. The time history of the x radius of the oscillating droplet is shown in Figure 3. Even when the viscosity is set very small value, the oscillation decay occurred. It is because the particle method has its intrinsic viscosity. The surface tension σ can be estimated using the theoretical period of oscillation [4]

$$\tau = 2\pi\sqrt{\frac{R^3\rho}{6\sigma}} \tag{12}$$

Since the theory is applicable for the oscillation in a small fluctuation, the oscillation period after decay was used to calculate the surface tension coefficient σ. With this calculation, it was estimated that σ=0.044.

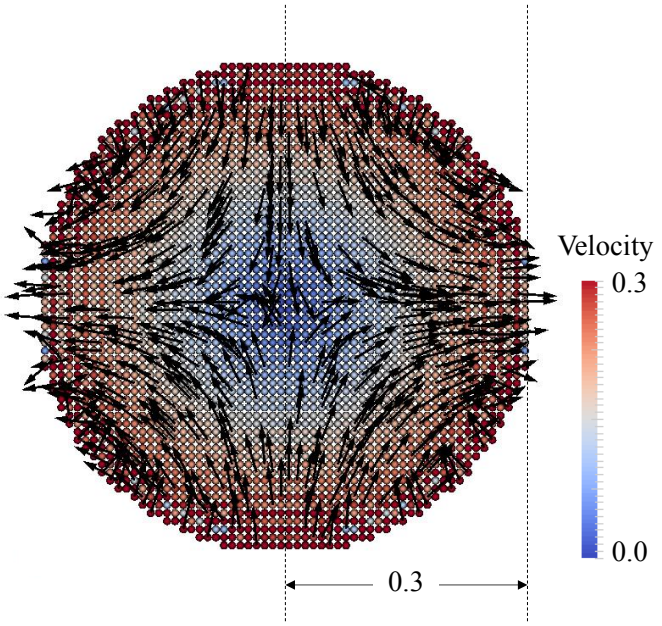

Figure 1: Initial velocity in the droplet oscillation calculation

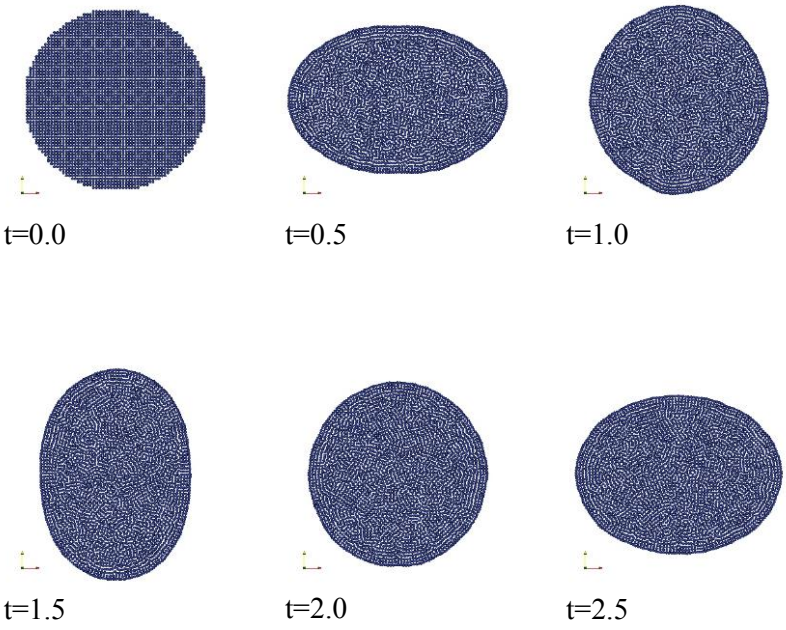

Figure 2: Droplet oscillation calculation

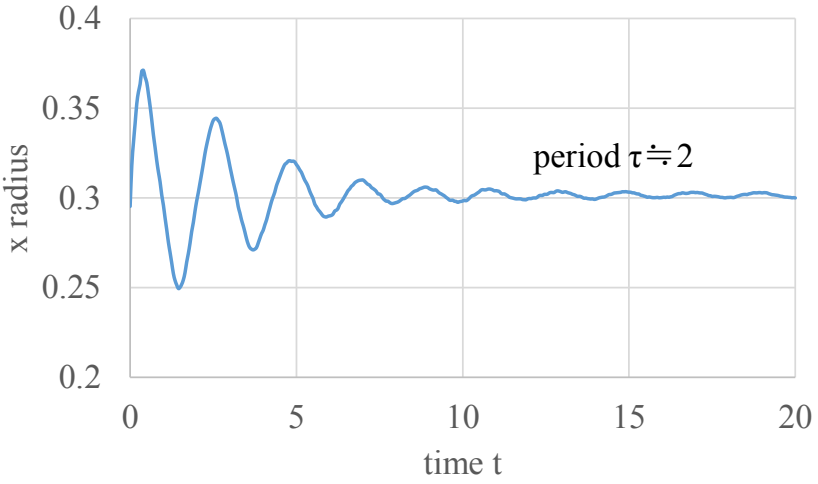

Figure 3: History of x radius of the oscillating droplet

3.2 Capillary pressure

According to the Young-Laplace equation [4], the relation between the radius of the equilibrium droplet and the pressure inside the droplet is given as

$$P_{in} = \frac{\sigma}{R} \tag{13}$$

To estimate the surface tension from this equation, the equilibrium droplets having various radiuses R=0.1, 0.2, 0.3, 0.4, 0.5 are calculated. Since the raw pressure value suffered from the numerical fluctuation, the spatial-averaging and time-averaging were conducted to know the inner pressure of the droplets. In the spatial-averaging, the pressure calculated by Eq. (6) is averaged after extracting the particles near the surface. In the time-averaging, the spatial-averaged pressure was averaged in the time range of 1.0 after equilibrium is reached. The relation between $1/R$ and the averaged pressure P_{in} is shown in Figure 4. From the figure and Eq. (13), an approximate surface tension σ=0.037 was obtained.

Figure 5 shows the potential energy with respect to the surface tension term. The potential only located on the surface while almost no potential was observed in the fluid bulk. It implies that the force acts only on the surface and does not cause the unrealistic pressure rise which was observed in the surface tension calculation using pairwise potential [5].

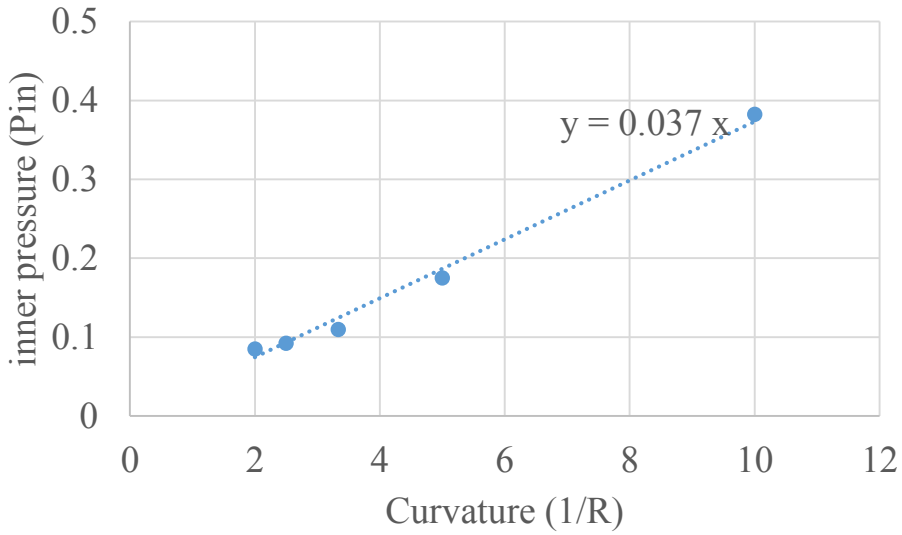

Figure 4: Relation between $1/R$ and inner pressure P_{in}

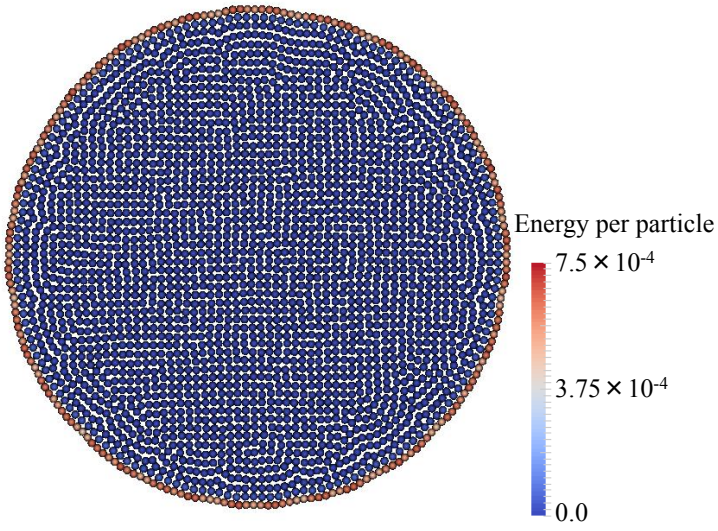

Figure 5: Potential energy with respect to the surface tension calculation

3.3 Capillary rise

The initial state of the capillary rise calculation is shown in Figure 6. The sideward boundaries are set as periodic boundaries. The walls are expressed by the red fixed particles, at which the calculations are conducted in the same manner as at the blue moving particles except for the position update. The gravity g=1.0 is given. The snapshots of the calculation

are shown in Figure 7. After the liquid rose in between walls, it reached the equilibrium state at around t=3.0. Since the relation among the elevation difference h_1-h_2, the curvatures of the surfaces $1/R_1$, $1/R_2$ and surface tension σ are given as

$$\rho g(h_1 - h_2) = \sigma\left(\frac{1}{R_1} - \frac{1}{R_1}\right) \tag{14}$$

in the equilibrium state [4], the surface tension can be estimated as σ=0.041, where h_1-h_2=0.54, R_1=0.06 and R_2=0.30 (Figure 8) were used.

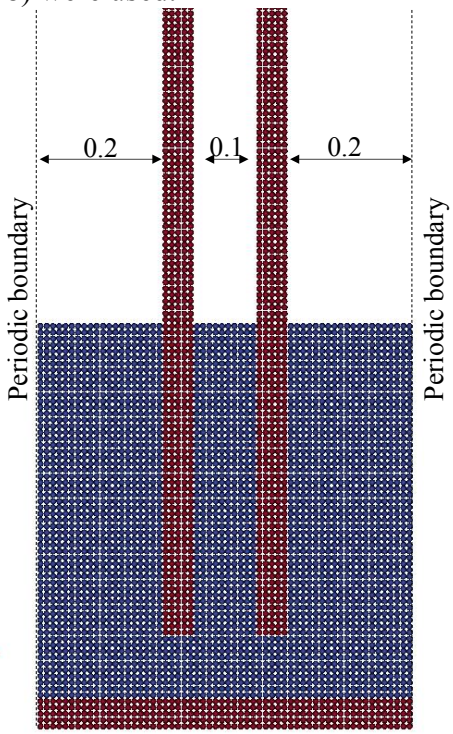

Figure 6: Initial state of the capillary rise calculation

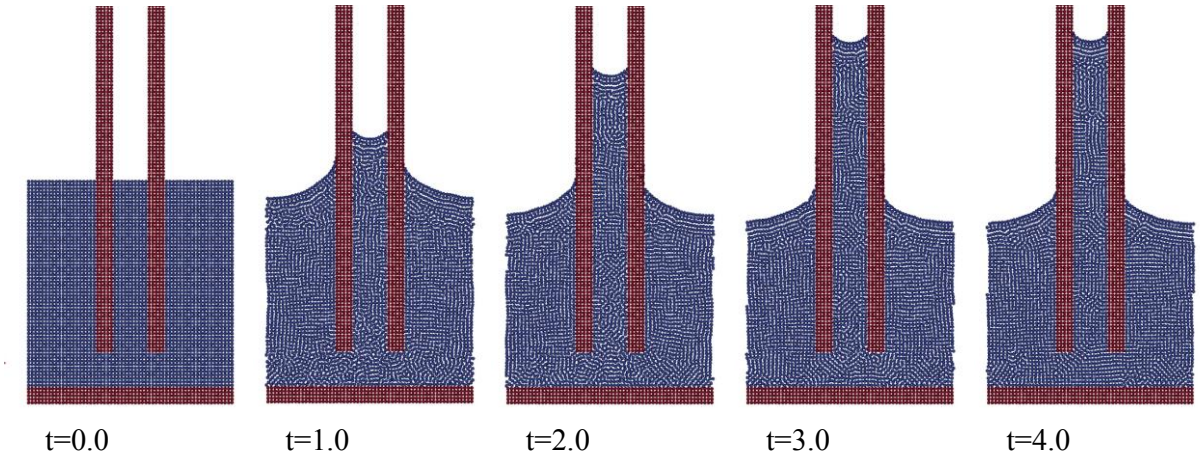

Figure 7: Capillary rise calculation

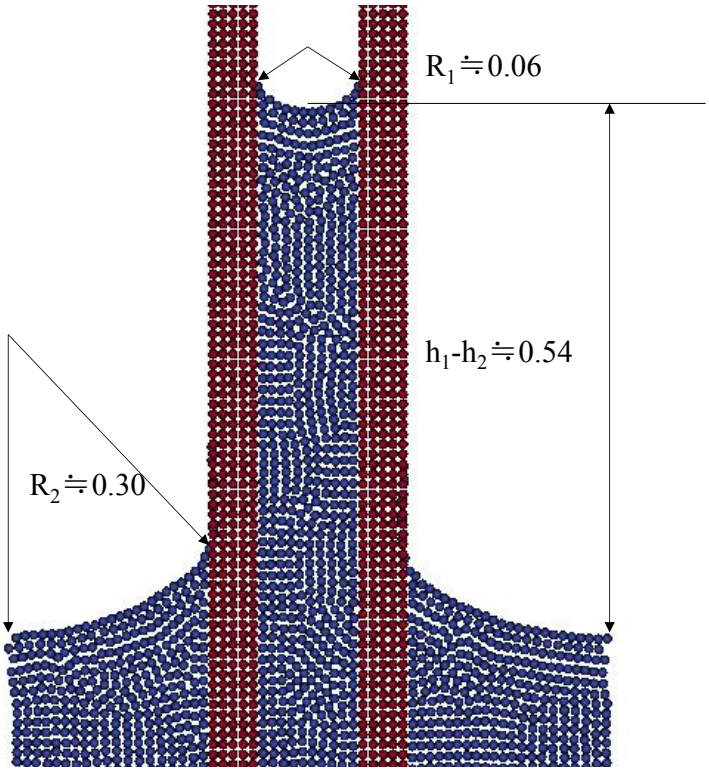

Figure 8: Length at the equilibrium state

Though the droplet oscillation calculation, the capillary pressure calculation and the capillary rise calculation, the surface tensions σ were estimated. The values obtained were not contradictory. It implies the applicability of the new surface tension calculation model using many-body potential.

4 CONCLUSIONS

A new model for surface tension calculation is developed. A many-body potential force is introduced in the context of Moving Particle Full-implicit method [7]. The new surface tension model is tested in the calculations of droplet oscillation, capillary pressure and capillary rise. Since the surface tensions estimated through each calculation are not contradictory, it is confirmed that the new model can well express surface tension in the particle method.

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