Poster Session

2021 KNS Autumn meeting

Numerical Simulation on Spreading and Impact Behavior of a Single Droplet Using Smoothed Particle Hydrodynamics

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Research Background : Liquid Droplet Impact

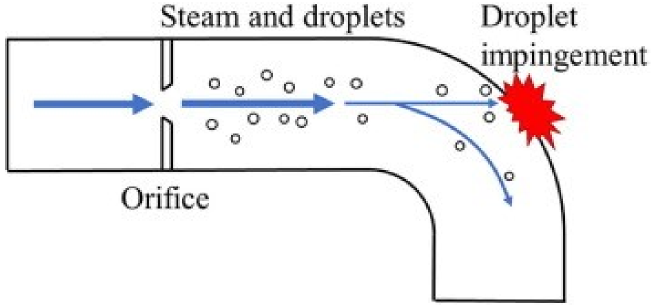
◆ Motivation

- Most of nuclear reactors use coolant in liquid phase and the liquid might break up into small droplets in many components in nuclear power plants.
- The impact of these droplets into the solid wall is considered as one of the main causes of the degradation in nuclear piping. [Harold (2011)]
- The pipe failure due to liquid impingement erosion account for a relatively small propotion compared to other phenomena, but show increasing tendency. [Bengt O.Y, 2017]

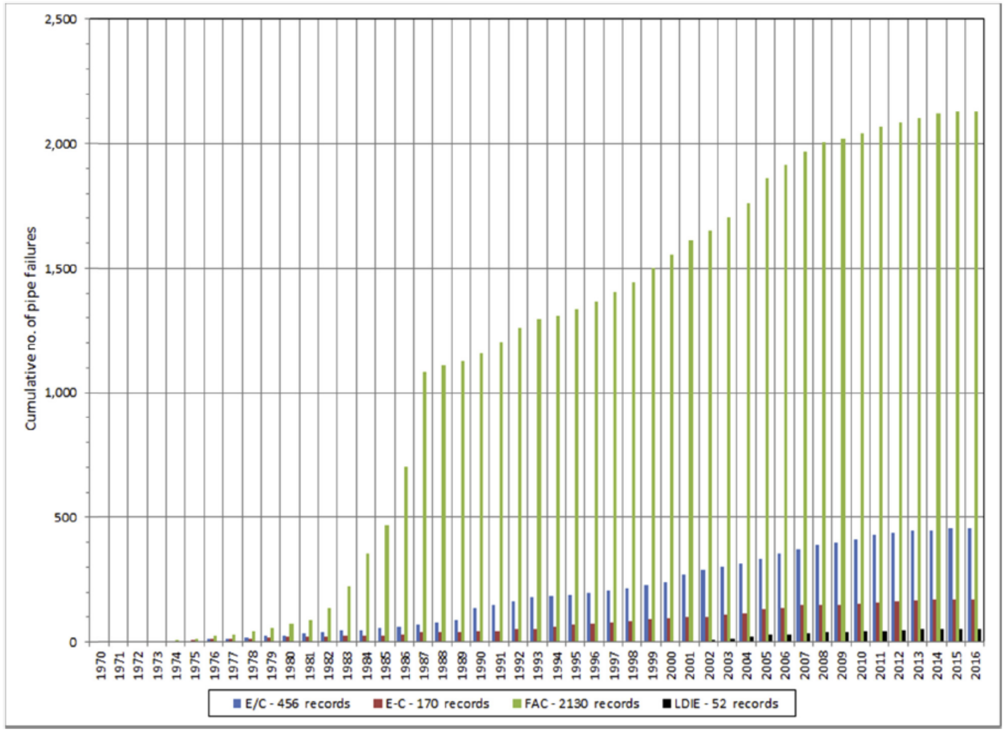
Chemical corrosion
Flow-accelerated corrosion (FAC)

Mechanical erosion
Cavitation
Flashing erosion
Liquid impingement erosion
Solid particle erosion

Classification of issues with pipe damage
[Harold (2011), Transaction of ASME]



Liquid Impingement Erosion (LIE)
[Fujisawa et al, 2016]



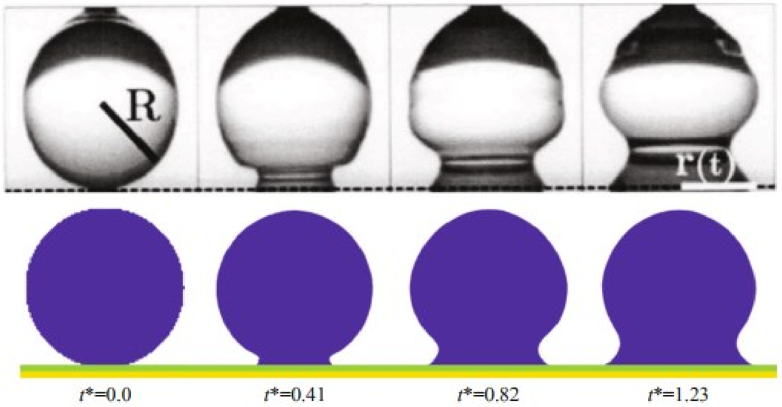
Data on pipe failures attributed to flow-assisted degradation in USA
[Bengt O.Y, 2017]

Introduction

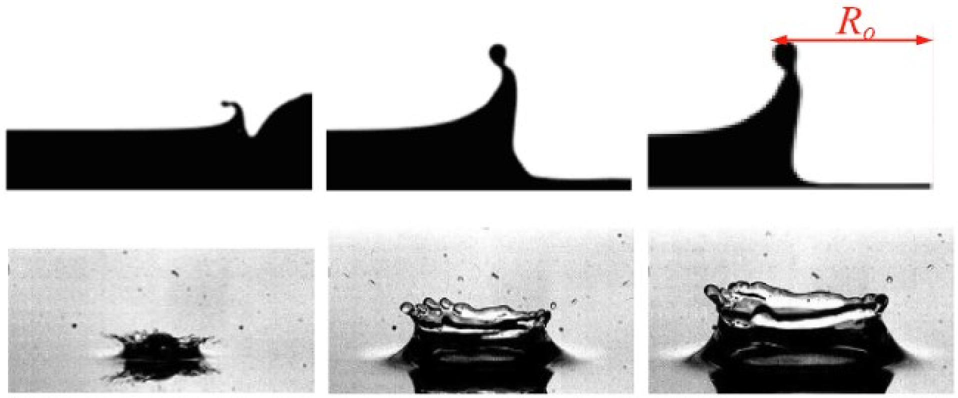
Research Background : Liquid Droplet Impact

◆ Motivation

- The majority of experimental studies have focused on the effect of various factors on the single droplet-surface collision phenomena, including the physical properties of droplet, velocity, collision angle, wetting characteristics, surface rigidity and etc. In addition, some experiments have been performed on multi-droplet or in form of jet.
- In order to illustrate the detailed information on droplet during the initial impact process such as the pressure, shape variance, distribution of secondary droplets which is still difficult in experimental studies, the numerical studies have been performed.
- Various numerical methods are adopted, which includes both mesh-based and mesh-free methods. The representative models of each method are **MPS (moving-particle semi-implicit)** and **VOF (volume of fluid)** [Zhang et al, 2020].
- **Numerical simulations of liquid droplet-surface collision are numerously performed, but the 3-dimension Lagrangian-based multi phase simulation which include surface tension modeling are very rare.**



Droplet spreading using MPS
[Guo et al., NED(2020)]



Comparison between Experiment & Simulation by CLSVOF method
[Chen et al., ANE(2020)]

Research Purpose

◆ Research purpose

- In this study, the Smoothed Particle Hydrodynamics which is the representative mesh-free CFD method is used to simulate droplet-surface collision.
- The pairwise force model is adopted to model the surface tension and wetting dynamics. The model is verified for various numerical conditions.
- Various droplet-surface collision phenomena are simulated and validated with experimental/theoretical prediction. The 3D single/multi phase simulations are conducted and compared.

Smoothed Particle Hydrodynamics (SPH)

◆ Smoothed Particle Hydrodynamics (SPH) [Monaghan, 1994]

- SPH is a **Lagrangian-based computational methods** for fluid simulation.
- The system of fluid is represented by a Lagrangian node which has individual property.
- The governing equations are solved in discretized form over the neighboring particles within **support domain**.

◆ SPH approximation

$$f_i(r) = \int_j f_j W(r_{ij}) dV_j = \sum_j f_j W(r_{ij}) \frac{m_j}{\rho_j}$$

$$(\nabla A)_i = \rho_i \sum_j m_j \left(\frac{A_i}{\rho_i^2} + \frac{A_j}{\rho_j^2} \right) \nabla W_{ij}$$

$$(\nabla \cdot \vec{v})_i = \rho_i \sum_j m_j \left(\frac{\vec{v_i}}{\rho_i^2} + \frac{\vec{v_j}}{\rho_j^2} \right) \cdot \nabla W_{ij}$$

◆ Governing equations for hydrodynamic problem

- Continuity equation

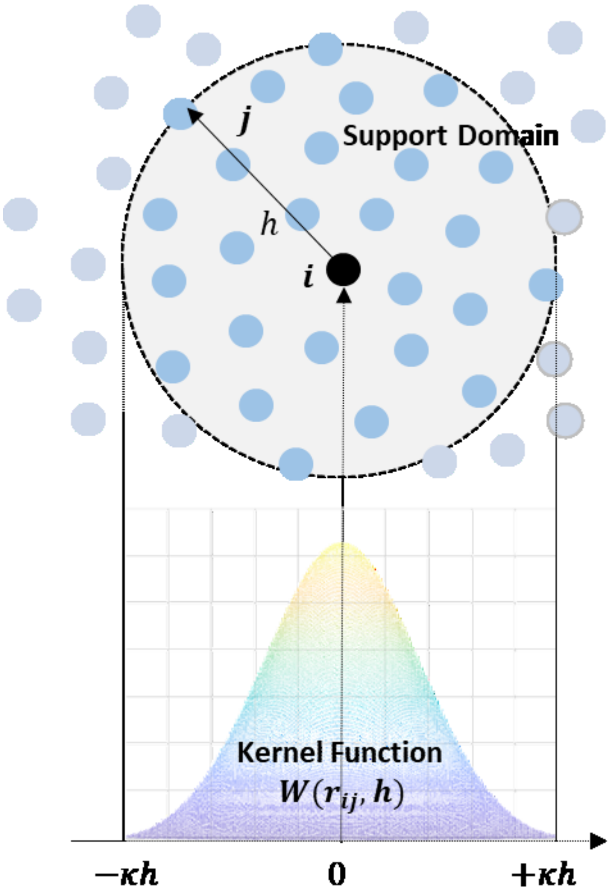
$$\frac{D\rho}{Dt} + \rho(\nabla \cdot v) = 0$$

- Momentum equation

$$\frac{D\boldsymbol{v}}{Dt} = -\frac{1}{\rho}\nabla P + \mu \nabla^2 v + \vec{f_s} + \vec{g}$$

- Equation of state

$$P = f(\rho)$$



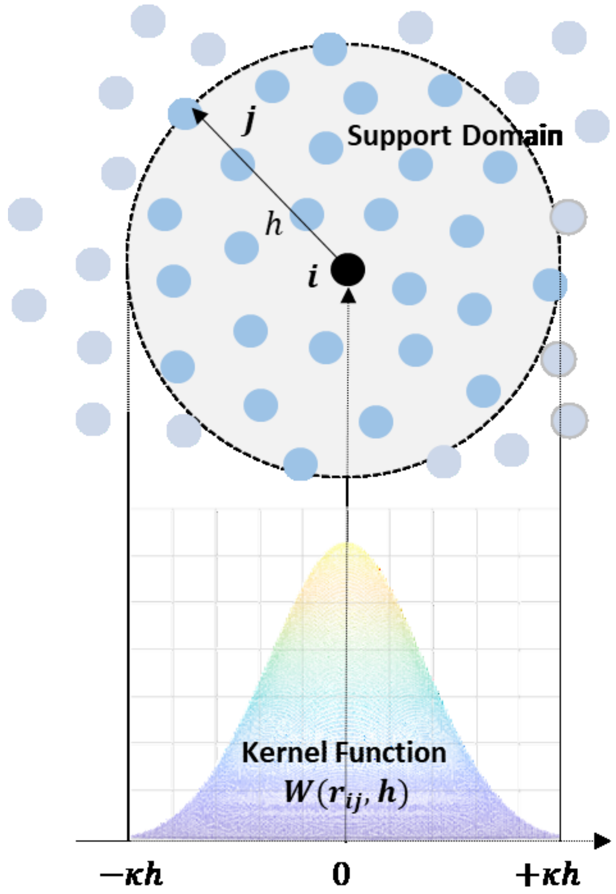
Numerical Method

Smoothed Particle Hydrodynamics (SPH)

◆ Numerical Method : SPH governing equations

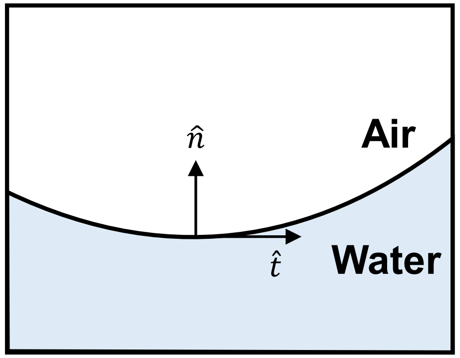
🟦 : Adopted model in this study

Mass Conservation	Density Summation		$\rho_i(r) = \sum_j m_j W_{ij}$	Mongahan(1994)
	Continuity equation		$\frac{D\rho_i}{Dt} = -\rho_i \sum_j (v_i - v_j) \cdot \nabla W_{ij} \frac{m_j}{\rho_j}$	Mongahan(1994)
Momentum Conservation	Pressure Gradient Force		$\left(\frac{D\boldsymbol{u}}{Dt}\right)_i = -\sum_j m_j \left(\frac{P_i + P_j}{\rho_i \rho_j}\right) \nabla_i W_{ij}$	Monaghan (2005)
	Laminar Viscous Force		$\left(\frac{D\boldsymbol{u}}{Dt}\right)_i = \sum_j \frac{4m_j}{\rho_i \rho_j} \frac{\mu_i \mu_j}{\mu_i + \mu_j} \frac{\vec{r_{ij}} \cdot \nabla_i W_{ij}}{\left(\lvert\vec{r_{ij}}\rvert^2 + \eta^2\right)} (\vec{u_i} - \vec{u_j})$	Morris (1997)
	Surface tension	CSF model	$\vec{f_s} = \frac{\sigma}{\rho_i} \kappa_i (\nabla c)_i$	Adami (2010)
		IPF model	$\vec{f_s} = s_{ij} cos\left(\frac{1.5\pi}{kh}\lvert r_{ji}\rvert\right) \frac{r_{ji}}{\lvert r_{ji}\rvert}$	Tartakovsky (2005)
Equation of Sate	Tait Equation		$p = \frac{{c_o}^2 \rho_0}{\gamma}\left[(\frac{\rho}{\rho_0})^\gamma - 1\right]$	Monaghan (1994)



Pairwise-Force Smoothed Particle Hydrodynamics (PFSPH)

◆ Surface Tension Modeling



- **Dynamic Boundary Condition (fluid-fluid)**

$$p_{\text{water}} - p_{\text{air}} - \sigma\kappa = 2\mu_{\text{water}}\widehat{n_k}\left(\frac{\partial u_k}{\partial n}\right)_{\text{water}} - 2\mu_{\text{air}}\widehat{n_k}\left(\frac{\partial u_k}{\partial n}\right)_{\text{air}}$$

$$\mu_{\text{air}}\left(\widehat{t_i}\left(\frac{\partial u_i}{\partial n}\right) + \widehat{n_k}\left(\frac{\partial u_k}{\partial s}\right)\right)_{\text{air}} - \mu_{\text{water}}\left(\widehat{t_i}\left(\frac{\partial u_i}{\partial n}\right) + \widehat{n_k}\left(\frac{\partial u_k}{\partial s}\right)\right)_{\text{water}} = \frac{\partial \sigma}{\partial s}$$

<Two representative surface tension models in SPH>

- **CSF (Continuum Surface Force)**

The CSF approach recasts surface tension from a boundary value problem to a **volume force that can be imposed within some small distance of an interface. [Brackbill (1990)]**

$$F_{sv}(x) = \sigma\kappa(\boldsymbol{x})\frac{\nabla\tilde{c}(\boldsymbol{x})}{[c]}$$

- **IPF (Intermolecular Potential Force)**

The IPF approach **inherently generate the surface tension at an interface via pairwise forces** between particles of fluid. (called non-local model) **[Tartakovsky (2005)]**

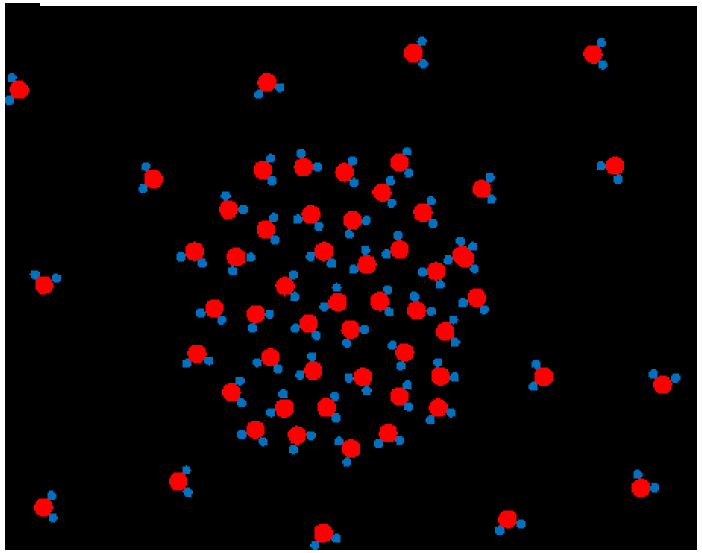
$$f_i = -m_i\langle\frac{du}{dt}\rangle_i = \sum_j f_{ij}$$

Pairwise-Force Smoothed Particle Hydrodynamics (PFSPH)

◆ PFSPH

- In microscopic scale, the anisotropic molecular structure induce the anisotropic stress near the interface and the certain amount of energy must be added to increase the surface area by a unit length, which is the mechanical definition of surface tension.

- Bringing idea from microscopic origin of surface tension, **PFSPH induces surface tension using inter-particle forces which can be thought as a coarsened form of the molecular forces. [Tartakovsky and Panchenko 2005; 2016]**



Microscopic origin of surface tension

$$\sigma_{\alpha\beta} = \int_{-\infty}^{+\infty} [T_\tau(z) - T_n(z)]\, dz$$

- **Hardy formula**
  - stress term in many-body system (from Molecular dynamics)

$$T_k(\mathrm{z}) = -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} f_{ij} \otimes (r_j - r_i) \int_0^1 \widetilde{\psi_\eta}\left(\mathrm{x} - s r_i - (1-s) r_j\right) ds$$

$$f_{ij} = -m_i m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right) \nabla_i W(r_i - r_j, h) + s_{ij} cos\left(\frac{1.5\pi}{kh}|r_{ji}|\right)\frac{r_{ji}}{|r_{ji}|}$$

$$\sigma_{\alpha\beta} = f(s_{\alpha\beta})$$

- Linear relationships between microscopic parameter and macroscopic surface tension are derived.

Numerical Method

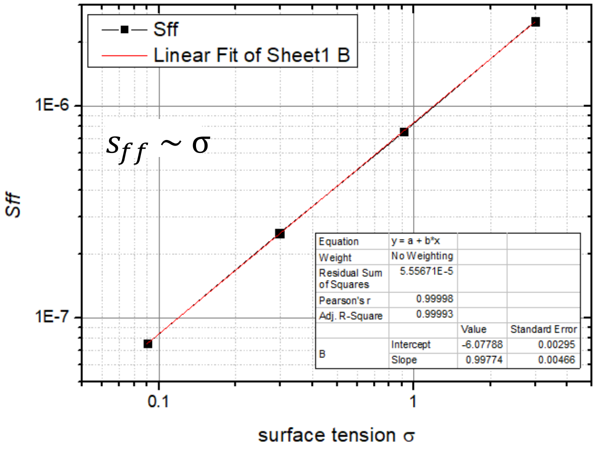
Pairwise-Force Smoothed Particle Hydrodynamics (PFSPH)

◆ PFSPH

<Single phase modeling (without air) >

- With single phase, the surface tension is calculated by the Rayleigh frequency of a oval droplet.

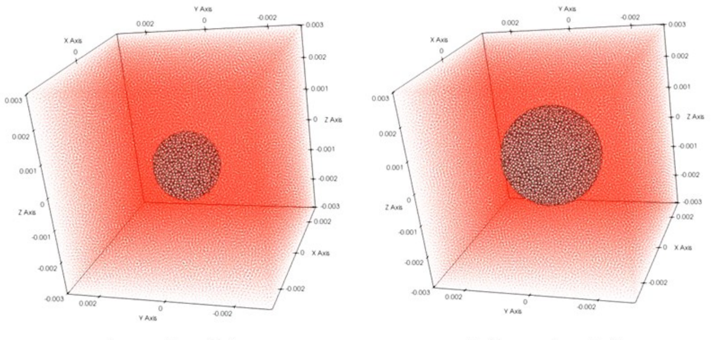
$$T_{2D} = 2\pi\sqrt{\frac{R^3\rho}{6\sigma}} \quad for\ \ 2D \qquad\qquad T_{3D} = \pi\sqrt{\frac{R^3\rho}{2\sigma}} \quad for\ 3D$$



- The PFSPH theory is based on the multi phase simulation. Different coefficient with theory is shown with single phase but, the linear relationship is shown.
- In single phase simulation the surface tension is calibrated.

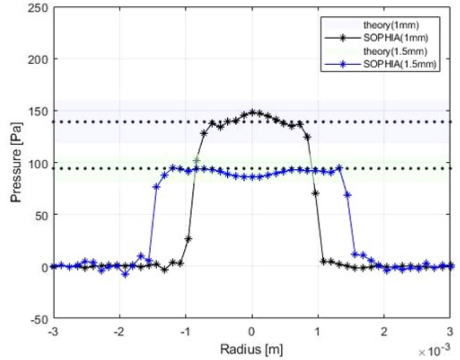
<Multi phase modeling (with air) >

<CSF model>

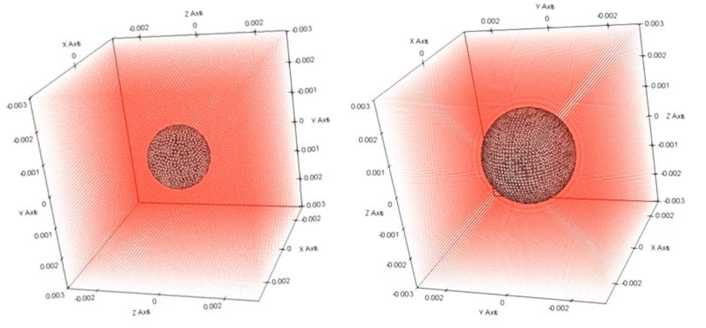


1mm droplet

1.5mm droplet

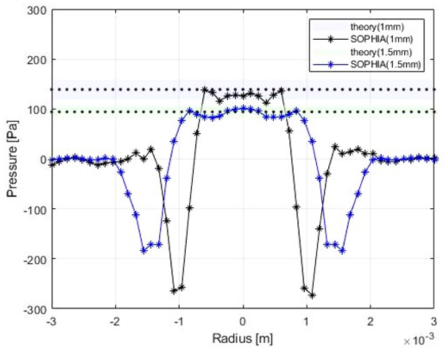


<IPF model>



1mm droplet

1.5mm droplet



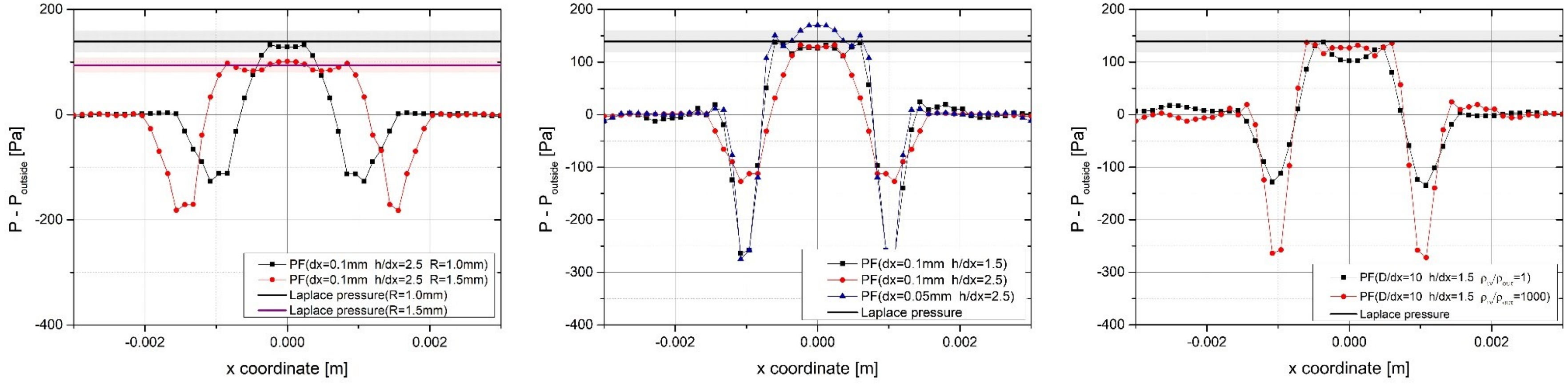
- With multi phase, the surface tension is calculated by the pressure difference.
- The difference between theoretical prediction is shown to be within 15%.
- Unlike the CSF model, a large pressure feature is shown in IPF model due to its microscopic origin.

Pairwise-Force Smoothed Particle Hydrodynamics (PFSPH)

◆ PFSPH

<Multi phase modeling>

- The IPF model is validated with various numerical conditions. [(a) radius, (b) spatial/smoothing resolution, (c) density ratio]



(a) (b) (c)

- The static modeling on adhesion force with solid is also validated with theoretical prediction and showed the difference within 20%.

$\theta_{theory} = 30°$
$\theta_x = 24.8°$
$\theta_y = 30.0°$

$\theta_{theory} = 60°$
$\theta_x = 57.4°$
$\theta_y = 60.5°$

$\theta_{theory} = 90°$
$\theta_x = 88.8°$
$\theta_y = 87.9°$

$\theta_{theory} = 120°$
$\theta_x = 114.2°$
$\theta_y = 117.1°$

$\theta_{theory} = 150°$
$\theta_x = 141.3°$
$\theta_y = 138.7°$

Droplet Surface Interaction

◆ SPH simulation conditions

- Three cases are selected for validation on modeling wetting dynamics of droplet-surface collision.
    - Droplet-surface spreading on dry surface
    - Droplet collision to the dry surface
    - Droplet collision to the wet surface

Results

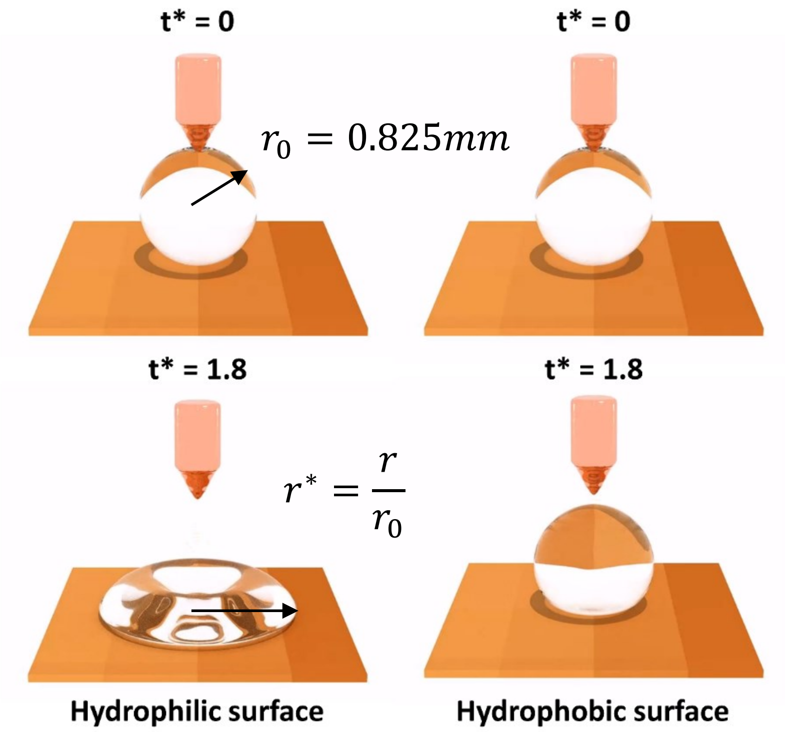
Droplet Spreading on the solid surface

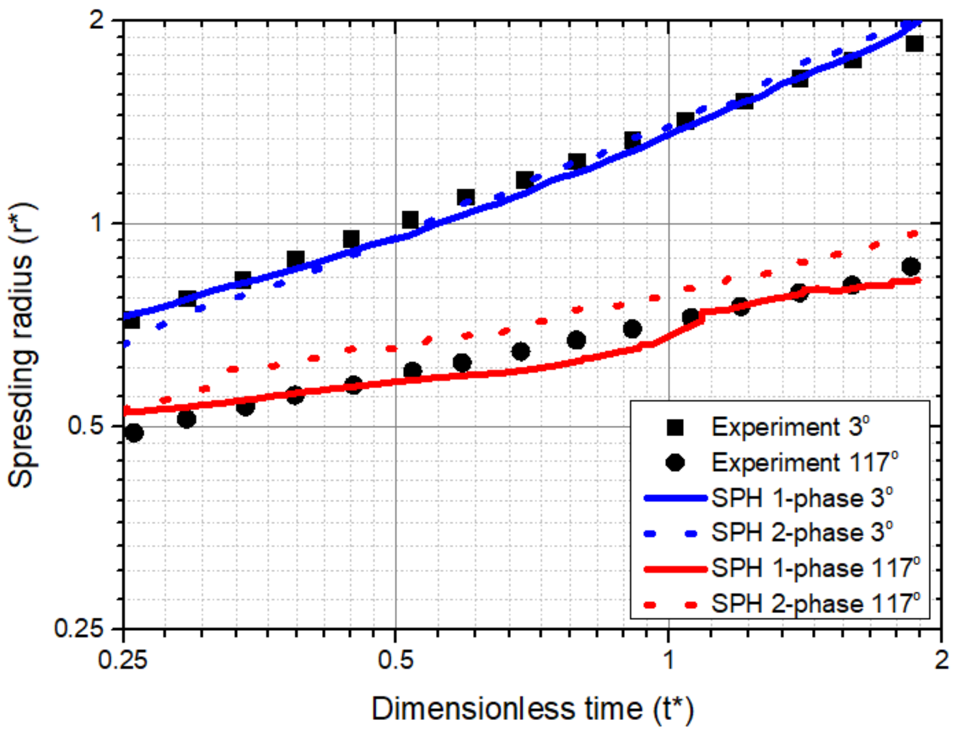
◆ Droplet Spreading on the hydrophilic/hydrophobic solid surface

- The spreading phenomenon of the droplet is validated based on the experimental results performed by Bird et al. (2008). The results are shown in figure with dimensionless spreading radius according to the dimensionless time.
- The simulation is performed both in single/multi phase and both results are well matched with experimental results. **It has been shown that the dynamic modeling of wetting behavior using pairwise force model works well in both single and multi phase.**

Numerical condition

- $\rho_l = 1000 kg/m^3$
- $\rho_g = 1 kg/m^3$
- $\mu_l = 10^{-3} Pa \cdot s$
- $\mu_g = 10^{-5} Pa \cdot s$
- $\sigma = 0.073 \mathrm{N/m}$
- Particle distance = $50 \mu m$

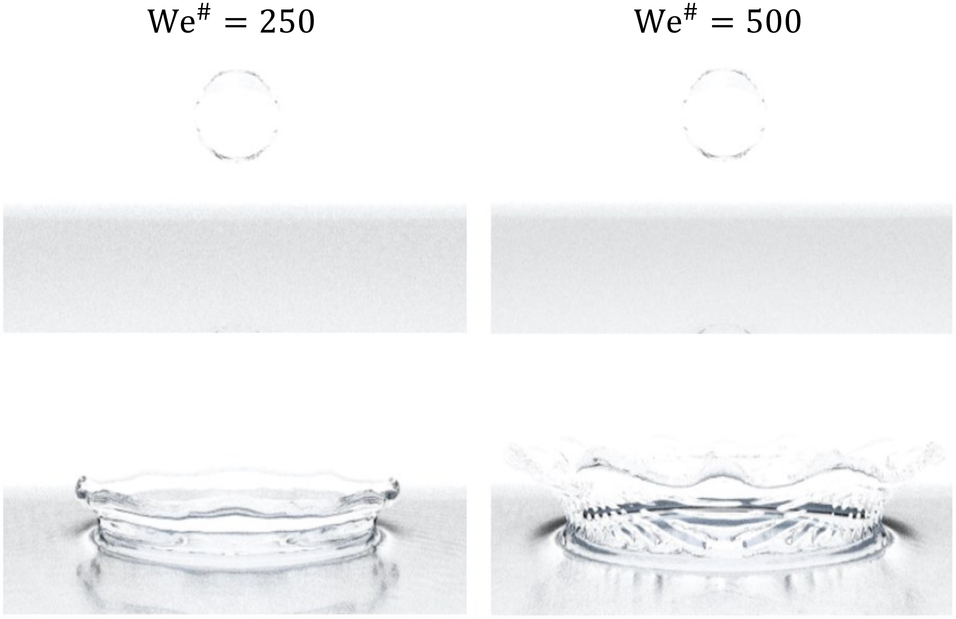


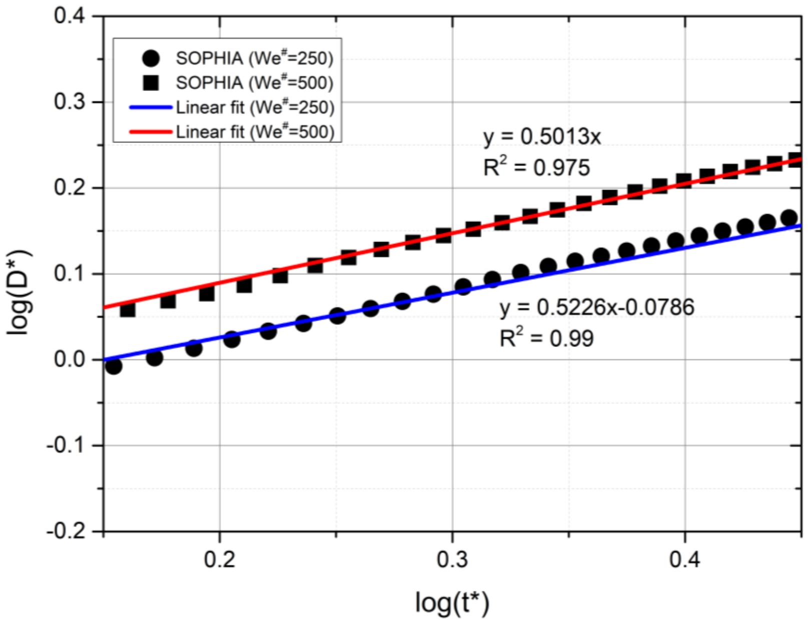


Droplet impact to the wet solid surface

◆ Droplet impact to the wet super-hydrophobic solid surface

- The droplet-wet surface collision phenomena is simulation on super-hydrophobic surface (no wetting). The thin liquid film (lamella) is generated above the water surface and spreads after the droplet splash on the wet surface.
- **The shape of the water surface at same time instant is compared to theoretical prediction and the index of dimensionless diameter of droplet are well agreed with theory.**
- In this case, the thin liquid film required super-high spatial resolution. Therefore, only the single phase simulation is performed.





Theoretical prediction [Yarin and Weiss (1995)]

$$\frac{D}{D_0} = kT^{\frac{1}{2}}$$

k dimensionless constant

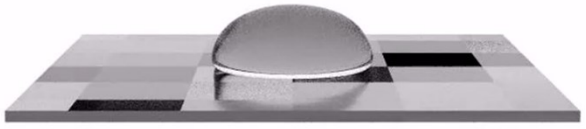
Droplet impact to the dry solid surface

◆ Droplet impact to the dry hydrophobic solid surface

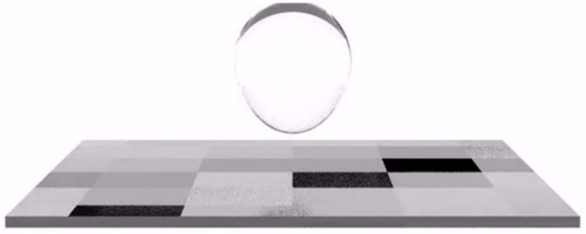
- The droplet-dry surface collision phenomena is simulation on hydrophobic and super-hydrophobic surface. The droplet motion after the collision and the spreading radius before bounce motion are compared with experimental results performed by Kim et al (2012).
- Different trend between single and multi phase is shown. **The multi phase simulations well predict the spreading radii but, the results of single phase simulations are quite deviated from the experimental results.**

Numerical condition

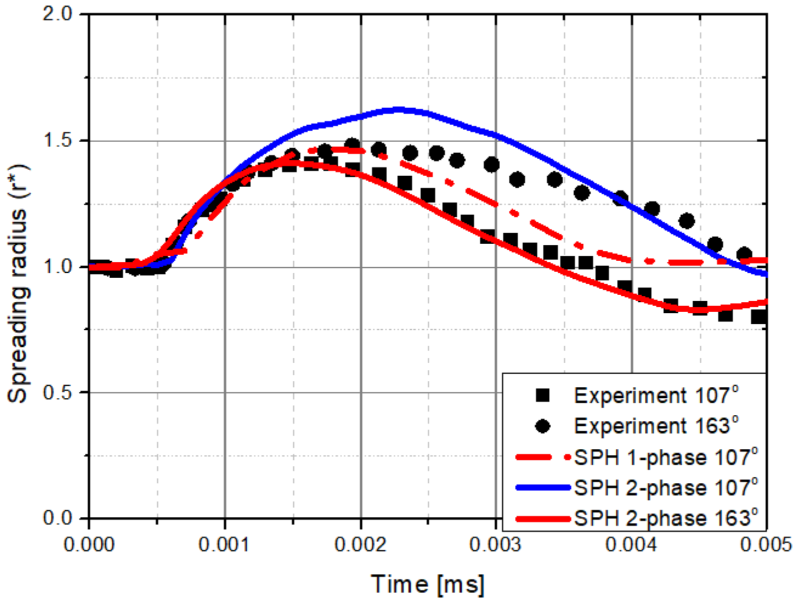
- $\rho_l = 1000kg/m^3$
- $\rho_g = 1kg/m^3$
- $\mu_l = 10^{-3}Pa \cdot s$
- $\mu_g = 10^{-5}Pa \cdot s$
- $\sigma = 0.073\mathrm{N/m}$
- Particle distance = $50\mu m$
- Initial radius $r_0 = 0.66\ mm$
- We=4.6



Hydrophobic surface (θ_{static} = 107°)



Super-Hydrophobic surface (θ_{static} = 163°)



Conclusion & Summary

- The 3-D single/multi phase Smoothed Particle Hydrodynamics method is used to analyze various droplet-surface collision phenomena. The pairwise force model is adopted to physically model the surface tension and wetting characteristics. **It has been shown that the model works well with static modeling on the fluid-fluid and fluid-solid interactions with various numerical conditions.**

- The droplet spreading behavior is simulated and the spreading kinematics are well agreed with the experimental results. **It has been shown that the model properly simulate the dynamic wetting characteristics of the droplet-solid interaction with both the single and multi phase.**

- The droplet impact to the wet wall is simulated. Due to the high resolution required by the thin lamella, only the single phase simulations are covered in this study with this case. **The single phase simulation well predicts the analytical prediction.**

- The droplet impact to the dry wall is simulated. **The multi phase simulations well predict the spreading radii but, the results of single phase simulations are quite deviated from the experimental results.** The presence of the air and difficulty in modeling contact angle hysteresis in single phase might be the reasons for the difference.

- Various droplet-surface collision phenomena are covered in this study. It has been shown that the single/multi-phase has potential on predicting the kinematics of the droplets during the collision with surface. However, some difference between the single/multi phase modeling has been shown and further study is needed with wider range of the numerical and experimental condition.

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