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濡れ性のマルチスケール解析に向けたメソスケール粒子シミュレーション

Meso-scale particle simulation toward malti-scale analysis for wettng

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1. Introduction

In microgravity, surface tension becomes dominant. It leads to various issues. For example, the liquid fuel forms a thin film across tank walls. However, this film can also rupture, resulting in “dry-out,” where the surface becomes exposed. This uneven fuel distribution can reduce the performance of the fuel supply system and potentially cause engine failure. This fuel supply issue is related to "wetting", which describes how easily a droplet spreads on a solid surface. Therefore, an accurate model of wetting is crucial for controlling fuel behavior. The wetting is affected by micro-scale phenomena. An extremely thin film called “precursor film” is observed at the edge of the liquid drop. In the vicinity of this film, a localized force known as “disjoining pressure” acts to keep the film thickness constant. This force determines the stability or rupture of the liquid film. The disjoining pressure model shown in Eq. (1) can represent wetting at equilibrium1).

$$\begin{aligned}\Pi &= B\left[\left(\frac{h_*}{h}\right)^n - \left(\frac{h_*}{h}\right)^m\right],\\ B &= \frac{(n-1)(m-1)}{h_*(n-m)}\sigma(1-\cos\theta_e) \approx \frac{(n-1)(m-1)}{2h_*(n-m)}\sigma\theta_e^2,\end{aligned} \tag{1}$$

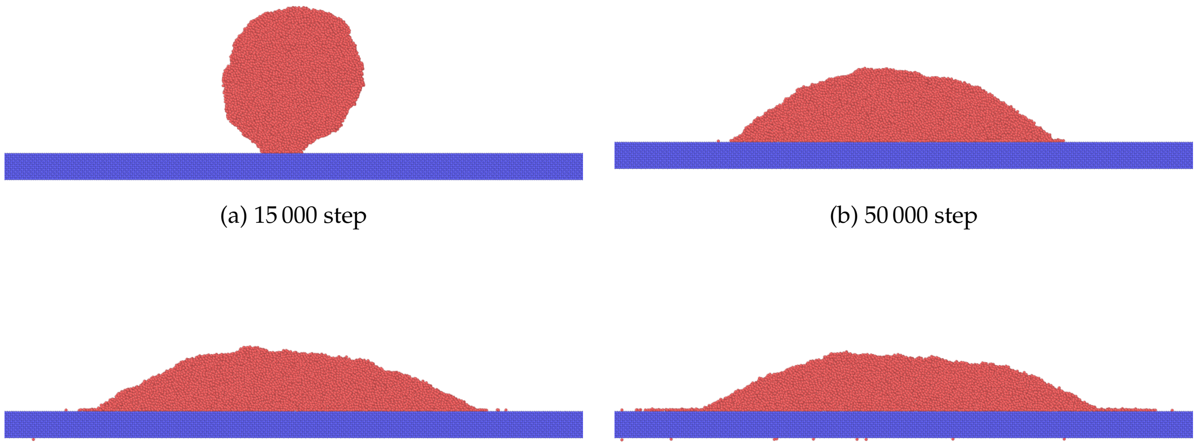
where h, h_*, θ_e and σ respectively represent the film thickness, precursor film thickness, equilibrium contact angle, and surface tension coefficient. However, this model includes empirical parameters, n and m. This study aims to determine these parameters without experiment.

2. Approach

In our approach, we first calculate the film thickness distribution near the contact line using many-body Dissipative Particle Dynamics (mDPD) simulations. The empirical parameters, n and m, are then determined by a data assimilation method.

2.1. mDPD

In the mDPD simulation, we obtained an equilibrium thickness distribution when a water droplet spreads on the solid surface. This simulation was performed using LAMMPS. In this study, all units are non-dimensional, using particles as the fundamental reference unit. We assume a single particle has a radius of 0.1 µm and set the other parameters such that the density of water becomes 1 at room temperature. The simulation box dimensions were 120, 2, and 60 in the x, y, and z directions, respectively. First, a droplet was created as 8500 particles within a cylinder of radius 15 and relaxed for 10 000 steps. A substrate of thickness 5 was created. Particles of substrate were arranged as an FCC structure. The substrate was moved to touch the droplet. After the spreading of the droplet reached equilibrium, a thickness distribution was obtained from the average over 100 000 steps.



(a) 15 000 step (b) 50 000 step

(c) 100 000 step (d) 300 000 step

Figure 1. Snapshots of simulation of the droplet spreading on solid substrate by many-body Dissipative Particle Dynamics.

2.2. Data-assimilation

To estimate the parameters n and m, we employed a data-assimilation method based on Physics-Informed Neural Networks (PINNs). PINNs is a machine learning framework proposed by Raissi et al.2). In this method, a Neural Network (NN) can work as a prediction approximator because the NN was trained in a governing equation. Furthermore, a loss between observed data and prediction is added. Because parameters in the equation are updated to minimize loss, parameters can be determined to fit observed data. In this study, the following governing equation Eq. (2) was trained by PINNs.

$$\frac{\partial h}{\partial t} = -\frac{\partial}{\partial x}\left[\frac{\sigma h^3}{3\mu}\frac{\partial^3 h}{\partial x^3} + \frac{h^3}{3\mu}\frac{\partial \Pi}{\partial x}\right] = 0, \tag{2}$$

where x, t, μ, Π respectively represent coordinate, time, viscosity coefficient and disjoining pressure. This equation is derived from Navier-Stokes equation and disjoining pressure model by lubrication approximation method.

3. Result

The process of spreading the droplet is shown in **Fig. 1**. In equilibrium shown **Fig. 1**(d), precursor film of approximately thickness 0.2 is observed and contact angle is 32.28°. This precursor film and the low contact angle indicate that a high-wetting condition was successfully reproduced.

Comparison of the thickness distribution between that predicted by the data-assimilated model and mDPD is shown in **Fig. 2**. The result of the data-assimilated model successfully captures the feature of the mDPD result. The resulting parameters were $n = 4.721$ and $m = 1.002$. Previous studies have reported parameter pairs for (n, m) such as $(3, 2)$, $(4, 3)$ and $(9, 6)$. The values determined by this study are similar in order of magnitude. However, our result suggests a smaller disjoining pressure than that of previous research, because the difference between n and m indicates the strength of the disjoining pressure.

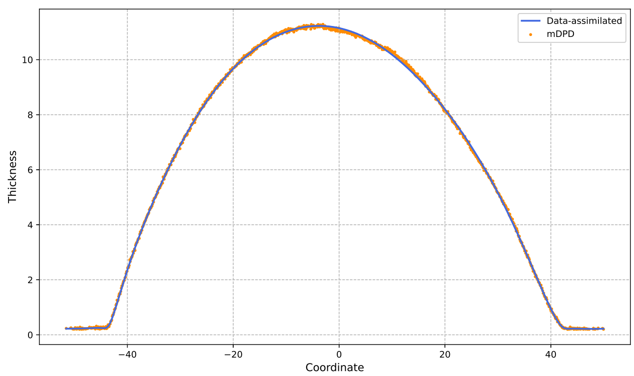


Figure 2. Comparison between the result of data-assimilated model and mDPD.

Acknowledgments

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