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Effect of particle wettability on particle-particle adhesion of colliding particles through droplet

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ABSTRACT

In wet granulation processes, a liquid bridge formed between particles is not static but dynamic due to continuous motion of the particles. Therefore, understanding of the particle-particle adhesion by a dynamic liquid bridge is an important issue. We here conducted a direct numerical simulation of the particle-particle adhesion by a dynamic liquid bridge. The particle-particle adhesion of two colliding particles through a droplet on a particle surface was simulated. In particular, effect of particle wettability on a critical velocity for the particle adhesion (i.e., adhesiveness of the two colliding particles) was investigated. It was found that the critical velocity for the particle adhesion non-monotonically changed with the particle wettability. The critical velocity exhibited a local maximum with an increase in the contact angle, while the static liquid bridge force monotonically decreases with an increase in the contact angle. We revealed that a combined effect of the liquid bridge deformation and instantaneous liquid bridge force results in the non-monotonic dependence on the particle wettability.

1. Introduction

Wet granulation processes, in which particles are agglomerated by a binder liquid, are widely used in many areas such as pharmaceutical, food and chemical industries. Physical properties of the agglomerated particles determine quality of the final products. Therefore, understanding of how the agglomerated particles are formed from primary particles is very important. The particle-particle collision mediated by a binder liquid and subsequent particle-particle adhesion by the liquid bridge is the most fundamental phenomenon in the wet granulation. Thus, elucidation of mechanisms for the particle-particle adhesion by the liquid bridge is essential to deepen understanding of the wet granulation and would open up new directions in wet granulation technologies.

In an actual wet granulation process, the particles are moving, resulting in deformation of the liquid bridge. This means that the liquid bridge is not static but dynamic. Numerous theories and analytical models about the liquid bridge adhesion have been reported [1–5]. However, these conventional theories and analytical models cover the static liquid bridge and thus cannot explain the particle-particle adhesion by the dynamic liquid bridge. We have recently developed a numerical simulation model for the particle-particle adhesion by the dynamic liquid bridge. The simulation results showed good agreement with experimental results, confirming validity of our simulation model [6]. By using this simulation model, effects of many critical parameters such as particle colliding velocity and physical properties of particle and liquid can be directly analyzed.

Particle-particle adhesion by the dynamic liquid bridge can be affected by various factors, including physical properties of the particle and liquid, mode and intensity of the particle-particle collision. Among these factors, particle wettability is a critical factor seriously affecting quality of the granules [7,8]. In the pharmaceutical industry, use of poorly water-soluble (hydrophobic) drugs is recently increasing [9,10]. Therefore, understanding of effect of the particle wettability on the particle adhesion by the dynamic liquid bridge is an important issue for rational design of the wet granulation of hydrophobic powder formulations.

The particle wettability is evaluated by the contact angle between the particle and liquid. Some experimental studies on effect of the contact angle on wet granulation characteristics have been reported [8,11–13]. Saleh and Guigon [8] investigated the particle growth rate of powders with different contact angles in the fluidized bed granulation. However, effect of the contact angle on the particle-particle adhesion by the dynamic liquid bridge at the primary particle scale cannot be quantitatively analyzed by the experimental approaches.

Effects of the contact angle on the static liquid bridge force and rupture distance of the liquid bridge have been analyzed by theoretical approaches [3,14,15]. Mikami et al. [3] proposed mathematical models for the static liquid bridge force and rupture distance as a function of liquid bridge volume, contact angle and separation distance by solving the Young-Laplace equation. In accordance with their models, the liquid bridge force monotonically decreases and the rupture distance increases with an increase in the contact angle. However, effect of the particle wettability on the particle-particle adhesion by the dynamic liquid bridge cannot be explained by the conventional models.

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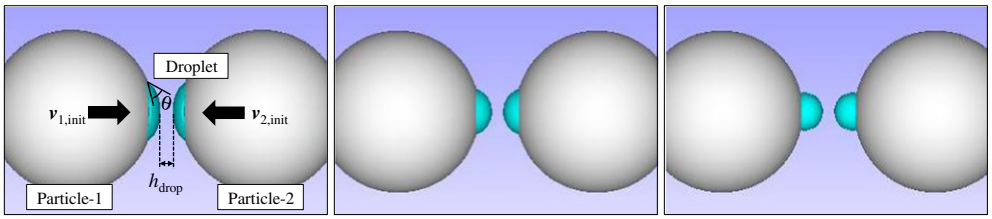

(a) $\theta = 30$ deg (b) $\theta = 60$ deg (c) $\theta = 90$ deg

Fig. 1. Initial conditions at various contact angles.

In this study, effect of the particle wettability on the particle adhesion by the dynamic liquid bridge was numerically analyzed. The particle adhesion between two colliding particles mediated by a binder droplet was simulated by solving motions of the three phases including particle, gas, and liquid. In particular, effect of the particle wettability on a critical velocity for the particle adhesion was investigated and role of the wettability in the particle adhesion by the dynamic liquid bridge was discussed.

2. Numerical simulation model

Motions of gas, liquid, and solid should be solved to simulate the particle adhesion between two colliding particles mediated by a droplet. In this study, motions of the gas and liquid were solved by using a computational fluid dynamics (CFD) approach combined with a constrained interpolation profile (CIP) method. The particle motion was simulated by a Lagrangian approach with considering the liquid bridge force that is unsteadily changed due to deformation of the liquid bridge. Briefly, the numerical simulation model used in this study is shown below. A detailed description of the simulation model and validation of the simulation results can be found in Kan et al. [6].

2.1. Governing equations for motions of gas and liquid

Motions of the gas and liquid are described by the following governing equations:

Equation of continuity

$$\nabla \cdot \boldsymbol{u} = 0 \tag{1}$$

Equation of motion

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{1}{\rho_f}\nabla p + \frac{1}{\rho_f}\nabla \cdot \mu_f \left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right] + \boldsymbol{f}_{sf} + \boldsymbol{f}_p \tag{2}$$

Advection equation for color function

$$\frac{\partial \phi}{\partial t} + (\boldsymbol{u} \cdot \nabla)\phi = 0 \tag{3}$$

where $\boldsymbol{u}$ is the fluid velocity, t is the time, ρ_f is the fluid density, p is the pressure, μ_f is the fluid viscosity, $\boldsymbol{f}_{sf}$ is the surface tension force, and $\boldsymbol{f}_p$ is the interaction force from particle to fluid. ϕ is a color function, which is used as a parameter to discriminate two phases, i.e., the gas phase is expressed as $\phi = 0$, while the liquid phase is expressed as $\phi = 1$. Unsteady change in a gas-liquid interface was expressed by the Eq. (3). CIP method [16] was used to numerically solve the Eq. (3). A continuous surface tension (CSF) model [17] was used to calculate the surface tension force ($\boldsymbol{f}_{sf}$) in the Eq. (2). An immersed boundary (IB) method [18] was used to calculate the interaction force from particle to fluid ($\boldsymbol{f}_p$) in the Eq. (2). In the present study, the gravity was not considered, because Bond number, which is the ratio of gravity to surface tension, was $8.47 \times 10^{-5} << 1$ and influence of the gravity is negligible [19].

$\boldsymbol{f}_{sf}$ was given by the following equation [17]:

$$\boldsymbol{f}_{sf} = \frac{\sigma \kappa \nabla \phi}{\rho_f} \tag{4}$$

where σ and κ are the surface tension coefficient and the local curvature of a gas-liquid interface, respectively. The curvature was given as follows:

$$\kappa = -(\nabla \cdot \boldsymbol{n}_{lg}) \tag{5}$$

where $\boldsymbol{n}_{lg}$ is the unit normal vector at the gas-liquid interface. The surface tension force at the contact line (solid-liquid-gas interface) was also calculated by using the CSF model. At the contact line, $\boldsymbol{n}_{lg}$ is adjusted as follows:

$$\boldsymbol{n}_{lg} = \boldsymbol{n}_s \cos\theta + \boldsymbol{t}_s \sin\theta \tag{6}$$

where θ is the contact angle of a droplet or liquid bridge on a particle surface. $\boldsymbol{n}_s$ is the normal unit vector, and $\boldsymbol{t}_s$ is the tangential unit vector at the solid surface. In this simulation model, the particle wettability was considered through the contact angle θ in the Eq. (6).

2.2. Governing equation of particle motion

Translational motion of a particle can be expressed as the following equations:

$$M_p \frac{d\boldsymbol{u}_p}{dt} = \boldsymbol{F}_d + \boldsymbol{F}_{sf} + \boldsymbol{F}_{cp} \tag{7}$$

$$\boldsymbol{F}_d = -\int_{V_p} \rho_f \boldsymbol{f}_p dV \tag{8}$$

$$\boldsymbol{F}_{sf} = \int_{V_p} \sigma \boldsymbol{t}_c (\nabla\phi \cdot \boldsymbol{t}_s)(\nabla\phi_s \cdot \boldsymbol{n}_s)\, dV \tag{9}$$

$$\boldsymbol{F}_{cp} = \boldsymbol{t}_c \pi (R_p \sin\ \alpha)^2 \Delta\ p \tag{10}$$

where M_p is the mass of particle, V_p is the volume of a particle, $\boldsymbol{F}_d$ is the viscous drag force, $\boldsymbol{F}_{sf}$ is the surface tension force, and $\boldsymbol{F}_{cp}$ is the capillary pressure force. $\boldsymbol{t}_c$ and ϕ_s are the unit tangential vector at a gas-liquid

Table 1
Calculation conditions.

Particle diameter	50.0	[μm]
Particle density	1500.0	[kg/m^3]
Restitution coefficient between solid particles	1.0	[−]
Liquid density	997.0	[kg/m^3]
Liquid viscosity	0.894	[mPa·s]
Surface tension coefficient	0.072	[N/m]
Droplet volume	1150.3	[μm^3]
Contact angle	15.0–120.0	[deg]
Gas density	1.184	[kg/m^3]
Gas viscosity	1.82×10^{-5}	[Pa·s]
Time step	2.0×10^{-9}	[s]
Fluid cell size	0.813	[μm]