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# Numerical simulation of particle–particle adhesion by dynamic liquid bridge

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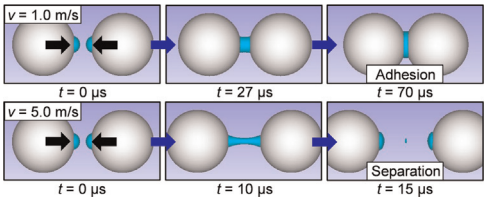
## HIGHLIGHTS

- A particle adhesion by a dynamic liquid bridge was simulated.
- Validity of the simulation model was confirmed by three verifications.
- The adhesion of particles through a droplet on a particle surface was analyzed.

## GRAPHICAL ABSTRACT

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## ABSTRACT

In powder handling processes treating wet powders (e.g. wet granulation, coating, and drying), a liquid bridge formed between particles is not static but dynamic due to continuous motion of the particles. Therefore, understanding of a particle–particle adhesion by such a dynamic liquid bridge is an important issue. We here conducted a numerical simulation of the particle–particle adhesion by the dynamic pendular liquid bridge. A computational fluid dynamics (CFD) approach with a constrained interpolation profile (CIP) method was applied to simulate a gas–liquid two phase flow, while a particle motion was calculated by taking into account the dynamic liquid bridge. To verify the simulation results, the following verifications were conducted; (i) wetting behavior of a droplet on a curved surface, (ii) static liquid bridge force between two particles, and (iii) rupture behavior of a liquid bridge with free falling of a particle. As a result, validity of the simulation results was confirmed. The particle–particle adhesion through a droplet on a particle surface was then simulated. In particular, effect of a collision velocity on a wet restitution coefficient was investigated. A velocity criterion for the particle adhesion was determined from the simulation results and compared with that estimated from an analytical model proposed by Ennis et al (1991).



## 1. Introduction

In many powder handling processes such as wet granulation, coating, and drying, powders containing a small amount of liquid are frequently processed. In such a powder, liquid bridges formed between particles can induce a particle–particle adhesion, determining quality of final products. Therefore, understanding of the particle–particle adhesion by a liquid bridge has been an important issue.

Historically, numerous studies of the liquid bridge force between particles have been conducted (e.g. Fisher, 1926; Israelachvili, 1991; Lian et al., 1993; Mikami et al., 1998; Rabinovich et al., 2005; Soulie et al., 2006). A lot of analytical models for the liquid bridge force has been proposed and confirmed to show good agreement with experimental results (e.g. Willett et al., 2000; Lambert et al., 2008). In these models proposed so far, a liquid bridge is considered as static. However, in actual powder handling processes, liquid bridges between particles can be deformed due to continuous motion of particles i.e., the liquid bridge is not static but dynamic. Therefore, in order to understand the particle–particle adhesion occurred inside the actual powder handling processes, a particle–particle

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adhesion by such a dynamic liquid bridge should be elucidated (Mazzone et al., 1987; Ennis et al., 1990).

Some experimental studies of the particle adhesion by a dynamic liquid bridge have been reported. Collision between a spherical particle and a stationary liquid film was experimentally analyzed (Kantak and Davis, 2004, 2006; Antonyuk et al., 2009; Sutkar et al., 2015). Antonyuk et al. (2009) revealed that at higher viscosity and thicker liquid layer, particle kinetic energy was more likely to be dissipated, indicating that these properties need to be large to enhance agglomeration rate. Mazzone et al. (1987) observed a rupture behavior of a liquid bridge between two particles. They found that shape of the liquid bridge was different from that under stationary condition, indicating that the analytical models for a static liquid bridge have limitations for use in the dynamic liquid bridge. Some modeling studies have also been conducted (Ennis et al., 1991; Liu et al., 2000; Balakin et al., 2013). Ennis et al. (1991) proposed a model based on a lubrication theory, in which the particle–particle adhesion by a dynamic pendular liquid bridge was simplified as an adhesion phenomenon between two particles coated with a thin liquid film. Using this model, they determined collision velocity criteria for the particle–particle adhesion. However, deformation of the liquid bridge was not taken into account in the model. Even by the experiments and the analytical modeling so far, it is still difficult to analyze the particle adhesion by a dynamic liquid bridge due to their complexities.

In such a case, a numerical simulation can be a potential approach. To simulate the particle adhesion by a dynamic liquid bridge, a solid–liquid–gas three phase flow is needed to be solved. Numerical simulations of a solid–liquid–gas three phase flow have been reported in recent years (Nishiura et al., 2008, 2010; Washino et al., 2011, 2013a, 2013b; Jain et al., 2012; Sakai et al., 2012; Sun et al., 2013). Nishiura et al. (2008, 2010) and Washino et al. (2011, 2013a, 2013b) conducted numerical simulations using a constrained interpolation profile (CIP) method (Yabe et al., 2001) to solve a gas–liquid two phase flow. Nishiura et al. (2010) simulated drying of a droplet of particle suspension in a spray drying process. Washino et al. (2013b) simulated an impingement of a droplet on a powder bed and analyzed a nucleation process in a wet granulation. Jain et al. (2012) simulated collision between a dry particle and a stationary liquid film using a volume of fluid (VOF) method. Sakai et al. (2012) and Sun et al. (2013) simulated a solid-liquid flow in a rotating cylindrical tank using a discrete element method (DEM)-moving particle semi-implicit (MPS) method. However, the particle–particle adhesion by a dynamic liquid bridge has not been investigated yet.

We here conducted a numerical simulation of the particle–particle adhesion by a dynamic liquid bridge. A computational fluid dynamics (CFD) approach with a CIP method was applied to simulate the gas–liquid two phase flow. Motion of a solid particle was calculated by taking into account the dynamic liquid bridge force. Some validations were initially conducted to verify the simulation results. The particle–particle adhesion between two colliding particles by the dynamic liquid bridge was then simulated. In particular, effect of a collision velocity on a wet restitution coefficient between particles was investigated.

## 2. Numerical simulation model

### 2.1. Governing equations of gas–liquid two phase flow

The governing equations of a gas–liquid two phase flow were given by equations of continuity and motion, and advection equation for color function as follows:

*Equation of continuity*

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

*Equation of motion*

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

*Advection equation for color function*

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

where $\boldsymbol{u}$, $t$, $\rho_f$, $p$, $\mu_f$, $\boldsymbol{f}_{sf}$, $\boldsymbol{f}_p$ and $\boldsymbol{g}$ are the fluid velocity, time, fluid density, pressure, fluid viscosity, surface tension force, interaction force from particle to fluid, and gravity, respectively. $\phi$ is a color function, which is a parameter to distinguish phase of the fluid; i.e., $\phi = 1$ means the liquid phase, while $\phi = 0$ means the gas phase. Unsteady motion of a gas–liquid interface was tracked to solve the Eq. (3). To numerically solve the Eq. (3), a CIP method (Yabe et al., 2001) was adapted. The fluid density and viscosity in a fluid cell were given as follows:

$$\rho_f = \phi\rho_l + (1-\phi)\rho_g \tag{4}$$

$$\mu_f = \phi\mu_l + (1-\phi)\mu_g \tag{5}$$

where $\rho_l$, $\rho_g$, $\mu_l$ and $\mu_g$ are liquid density, gas density, liquid viscosity, and gas viscosity, respectively.

The surface tension force ($\boldsymbol{f}_{sf}$) in the Eq. (2) was calculated by a continuous surface force (CSF) model (Brackbill et al., 1992). In the CSF model, the surface tension force ($\boldsymbol{f}_{sf}$) was given as follows:

$$\boldsymbol{f}_{sf} = \frac{\sigma\kappa\nabla\phi}{\rho_f} \tag{6}$$

where $\sigma$ is the surface tension coefficient and $\kappa$ is the local curvature of a gas–liquid interface. The curvature was calculated by the following equation:

$$\kappa = -(\nabla \cdot \boldsymbol{n}_{lg}) \tag{7}$$

where $\boldsymbol{n}_{lg}$ is the unit normal vector at the interfaces. Using the CSF model, the surface tension force at the solid–liquid–gas interface on a solid particle was also calculated. When a droplet is in equilibrium with the solid surface at a contact angle $\theta$ (Fig. 1), the unit normal vector ($\boldsymbol{n}_{lg}$) at the solid–liquid–gas interface is defined as follows:

$$\boldsymbol{n}_{lg} = \boldsymbol{n}_s \cos\theta + \boldsymbol{t}_s \sin\theta \tag{8}$$

where $\boldsymbol{n}_s$ and $\boldsymbol{t}_s$ are the unit normal and tangential vectors at the solid surface, defined as follows:

$$\boldsymbol{n}_s = \frac{\nabla\phi_s}{|\nabla\phi_s|} \tag{9}$$

$$t_s = \frac{\nabla\phi - (\boldsymbol{n}_s \cdot \nabla\phi)\boldsymbol{n}_s}{|\nabla\phi - (\boldsymbol{n}_s \cdot \nabla\phi)\boldsymbol{n}_s|} \tag{10}$$

where $\phi_s$ is a volume fraction of the solid in a fluid cell. In this simulation model, the wetting on a solid surface was taken into account through the contact angle ($\theta$), which was preliminary set as a calculation condition, and $\boldsymbol{n}_{lg}$ defined by the Eq. (8) was used to calculate the curvature ($\kappa$) at the solid–liquid–gas interface.

The interaction force from particle to fluid ($\boldsymbol{f}_p$) in the Eq. (2) was calculated by an Immersed Boundary (IB) method proposed by Kajishima and Takiguchi (2002). In the IB method, the interaction force from particle to fluid ($\boldsymbol{f}_p$) was given as follows:

$$\boldsymbol{f}_p = \frac{\varphi_s(\boldsymbol{u}_p - \boldsymbol{u}_f)}{\Delta t} \tag{11}$$

where $\boldsymbol{u}_p$ and $\boldsymbol{u}_f$ are particle and fluid velocities.