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Original Research Paper

Contact force model including the liquid-bridge force for wet-particle simulation using the discrete element method

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ABSTRACT

The handling of wet particles in chemical engineering is often difficult because cohesive forces acting on wet particles cause particulate aggregation and the adherence of devices, unlike what occurs under a dry condition. The liquid-bridge force is introduced to the discrete element method in the investigation of the behavior of wet particles. However, existing numerical modeling has problems from the viewpoint of the effect of cohesion in contact states. Specifically, the cohesive force is treated as a constant value for contact states. This means the effect of the cohesive force is not only dependent on the spring constant in the discrete element simulation but is also frequently overestimated. To solve this problem, the present study developed a numerical contact model considering quantitatively the effect of the cohesive force in contact states and validated the model for a pan pelletizer. The behaviors and cascading angles of wet particles in simulation and experiments were in good agreement and the validity of the contact model was thus demonstrated. The present numerical contact model is thus a promising model for the numerical simulation of wet particles.

1. Introduction

The handling of wet particles is frequently encountered in chemical engineering processes such as mixing and granulation [1,2]. In powder processes, raw particles such as particles of soil and mineral ore often contain water. In addition, a liquid binder is added onto particles to increase contact and interaction between liquid and particles in agglomeration and/or granulation processes. The presence of a liquid such as a binder or moisture affects the behavior of wet particles. Accordingly, unlike dry particles, wet particles often form particulate aggregates and/or are responsible for the adherence of devices. Because of these complex phenomena, it is difficult to control and understand the behavior of wet particles in industrial processes. Wet particles have therefore been intensively investigated in efforts to improve their handling.

The liquid-bridge force is a dominant force acting on wet particles because the cohesive capillary force owing to the formation of liquid bridges between two adjacent particles can be stronger than gravity. Various theoretical and empirical studies have evaluated the cohesive capillary force. Although various theoretical formulas have been proposed and validated experimentally [3–5], knowledge of the effect of liquid bridges is still limited and approaches of improving wet particle handling are still largely empirical.

Numerical simulation has recently been demonstrated to be a promising approach of better comprehending the effect of the liquid-bridge force. Various numerical approaches have greatly improved our understanding of the complex phenomena of particle systems by providing detailed information that has been difficult to obtain in experiments. At the macro scale, the discrete element method (DEM) [6] has been widely employed to particulate systems. Because the DEM calculates the behavior of particles according to Newton's second law of motion, it is easy to introduce additional physics models such as that for the cohesive force [7–9]. Therefore, the DEM that considers the cohesive force has been applied to wet-particle systems in an investigation of the flow behaviors of particles in a rotating drum and fluidized bed [10–13].

The present study focused on the modeling of a liquid bridge and contact forces during particle collisions in a DEM simulation, particularly taking into account the effect of the adhesion force in the contact states. Although many numerical studies have proposed the modeling of liquid-bridge forces, the existing numerical modeling of the liquid-bridge force has problems in terms of the effect of adhesion. Specifically, existing numerical modeling has

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Nomenclature

m	particle mass (kg)
$\boldsymbol{v}$	particle velocity (m/s)
I	inertial moment of particle (kg m^2)
T	torque (J)
$\boldsymbol{F}$	eternal force (N)
$\boldsymbol{F}_g$	gravitational force (N)
$\boldsymbol{F}_{cp}$	capillary force (N)
$\boldsymbol{F}_{co}$	contact force (N)
$\boldsymbol{F}_{ec}$	elastic-cohesive force (N)
$\boldsymbol{F}_e$	elastic force (N)
$\boldsymbol{F}_d$	damping force (N)
R	reduction radius (m)
r	particle radius (m)
V	volume of liquid bridge (m^3)
V_i	volume of liquid that one particle contains (m^3)
V_{total}	volume of all liquid added into a system (m^3)
N	number of particles in a system
N_i	coordinate number of particle i
h	distance between particles or a particle and a wall (m)
H_o	thickness of liquid thin film (m)
H_r	rupture distance of liquid bridge (m)
S_i	surface area of particle i (m^2)
S	stiffness (N/m)
G	shear modulus (Pa)
E^*	reduced Young's modulus (m^2/N)
E	Young's modulus (m^2/N)
a	contact radius (m)
a_0	equilibrium radius (m)
e	restitution coefficient (–)
w	adhesion work (J/m^2)
Greek letters	
$\boldsymbol{\omega}$	angular velocity (rad/s)
γ	surface tension (N/m)
θ	contact angle (rad)
ν	Poisson ratio (–)
σ	surface energy (J/m^2)
δ	overlap (m)
Subscripts	
n	normal component
t	tangential component
L	liquid phase

treated the cohesive force as a constant value for contact states although it has treated the cohesive force as a valuable value depending on the length of the liquid bridge for non-contact states. In the DEM, various models are available to calculate the contact force. In a simple contact model composed of a linear spring, viscous dashpot and friction slider, low spring stiffness is usually adopted to reduce the computational load [11,14,15]. However, the effect of adhesion forces is often overestimated because it depends on the spring constant in the DEM simulation. Additionally, the overestimated adhesion forces of wet particles result in erroneously high levels of particulate aggregation and adherence of devices. It is thus necessary to consider not only the non-contact states but also the contact states. In contrast, a contact model composed of a non-linear spring, viscous dashpot and friction slider is usually based on the Hertz theory. Since physical properties of particles such as Young's modules and Poisson's ratio can be easily introduced to this contact model, it is often used for the investigation of the contact mechanism of elastic spheres or particles. Thornton and Ning [16] proposed an analytical solution for the coefficient of restitution for adhesive, elastic-plastic spheres based on the concept of theoretical contact mechanics. Lian et al. [17] proposed a model that combined auto-adhesion between particles arising from van der Waals forces and the capillary force calculated from the Young–Laplace equation, and demonstrated the contact mechanics of wet agglomerates. Although this previous research focused on the contact mechanics of wet agglomerates, the applicability of this model to macroscopic behavior of wet particles was not demonstrated. Accordingly, it is necessary to develop a numerical model for wet particles considering not only the non-contact states but also the contact states.

The objective of the present study was to develop a numerical DEM model, including considering the effect of a liquid-bridge force in the contact states, to apply the model to wet particles and to demonstrate the adequacy of the model by comparing experimental data in a pan pelletizer system. To model the wet particle behavior in macro scale, a numerical contact model was introduced considering quantitatively the effect of a liquid bridge force and adhesion force in the contact state. To calculate a liquid bridge force, the theoretical formula proposed by Israelachvili [18] was adopted. To calculate a contact force, the contact mechanics based on Johnson, Kendall and Roberts (JKR) theory [19] was introduced. In this model, the normal elastic force was expressed by a non-linear spring based on Hertz contact theory. Meanwhile, the normal adhesion force was described by surface energy, Young's modulus, and the radius of the contact circle. To validate the adequacy of this model, simulation results were compared with experimental results for a pan-type pelletizer system in terms of macroscopic behavior.

2. Numerical modeling

2.1. Governing equation of particle motion

The motion of solid particles was modeled employing the DEM. In the DEM, the motion of an individual particle is calculated using Newton's second law of motion. The governing equations of the translation and the rotation are respectively

$$m\dot{\boldsymbol{v}} = \boldsymbol{F}, \tag{1}$$

$$I\dot{\boldsymbol{\omega}} = \boldsymbol{T}, \tag{2}$$

where m is the mass of a solid particle, $\boldsymbol{F}$ is the external force, I is the particle inertia, $\boldsymbol{T}$ is torque, and $\boldsymbol{v}$ and $\boldsymbol{\omega}$ are the translational velocity and rotational velocity respectively. In this study, the force working on the gravity center of a solid particle is defined as

$$\boldsymbol{F} = \boldsymbol{F}_g + \boldsymbol{F}_{cp} + \boldsymbol{F}_{co}, \tag{3}$$

where $\boldsymbol{F}_g$ is the gravitational force acting on the solid particle, $\boldsymbol{F}_{cp}$ is the capillary force acting on the solid particle, and $\boldsymbol{F}_{co}$ is the contact force including the adhesion force acting on the solid particle. The definitions and models of the capillary force and contact force are described in the following sections.

2.2. Modeling of the capillary force due to the liquid bridge

In the model constructed in this study, when a liquid bridge forms between a particle and another particle, or a particle and a wall, a cohesive force acts in the normal direction. The calculation