Powder Technology 302 (2016) 100–107

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

Time step criteria in DEM simulation of wet particles in viscosity dominant systems

Kimiaki Washino *, Ei L. Chan, Koki Miyazaki, Takuya Tsuji, Toshitsugu Tanaka

Mechanical Engineering Department, Osaka University, Suita, Osaka 565-0871, Japan

ARTICLE INFO

Article history:
Received 21 April 2016
Received in revised form 2 August 2016
Accepted 10 August 2016
Available online 14 August 2016

Keywords:
Wet particle flow
DEM
Liquid bridge
Viscous force
Time step criteria

ABSTRACT

Discrete element method (DEM) has been applied to simulate particulate flows with wet particles by taking into account the liquid bonding forces between particles. However, there is only limited work available in literature which applies DEM to simulate wet particles with highly viscous liquid. In this paper, the currently used DEM framework is assessed and the limitations are revealed for simulations of wet particles with highly viscous liquid in terms of the time step required for stable simulations, i.e. the time step decreases with increasing liquid viscosity. Semi-empirical time step criteria based on the viscous force decay time are proposed which determine the stable time step limit for given simulation conditions.

1. Introduction

Particulate processes are frequently encountered in many industries, including chemical, pharmaceutical and food industries. In such processes, liquid is sometimes added to powder for various reasons. A typical example is wet agglomeration where liquid binder is added to fine powder to produce particle agglomerates bonded with liquid bridge forces in order to improve the powder flowability and prevent the generation of dust [1]. Especially in detergent manufacturing processes, liquid with ultra-high viscosity is added to improve the performance of detergent [2] where the viscosity is >1000 times larger than that of water. However, when highly viscous liquid is used, it is difficult to disperse liquid into powder due to the strong viscous forces exerted on powder particles, and the poor and non-uniform liquid dispersion could deteriorate the quality of final products [3]. However, the complex interaction between liquid and particles makes it difficult to fully understand these processes by experiment.

Discrete element method (DEM) [4] has been widely used over the past decades to simulate particulate flow. In DEM, the equation of motion for each particle is solved to collect information at individual particle level, which is extremely difficult to achieve by experiment. Especially when the particles are relatively coarse and spherical, it is proven that DEM can successfully provide results comparable to experimental observations [5,6,7].

An increasing number of researchers are also trying to apply DEM to simulate wet particle behaviour by taking into account liquid bonding forces, namely capillary and viscous forces [8,9,10,11] since even a small amount of liquid can significantly influence the powder flow behaviour [8]. In their work, it is assumed that liquid bridges are symmetric and exist only in the pendular state [12], i.e. a bridge is formed between a pair of particles and/or between a particle and wall. Although it is possible to determine the capillary force by numerically solving the Young-Laplace equation, it is more common to use explicit capillary force models implemented in DEM due to the computational efficiency. Several capillary force models are available in literature [8,13,14,15,16], and the results are largely comparable [17].

A pioneering work to incorporate the viscous force into DEM was reported by Lian et al. [9]. In their work, the normal component of the viscous force is given by the Adams and Perchard model [18], which is the analytical solution of the Reynolds lubrication equation, whilst the tangential component is given by the Goldman model [19] which is derived from the numerical solution of the Stokes equation. Although these are valid only for sufficiently small inter-particle separation distance, many researchers used these models in DEM [20,21,22]. Liu et al. [23] used the normal viscous force model proposed by Pitois et al. [24] which takes into account liquid bridge volume. Although these simulation results are reasonably good when compared with experiments, at least qualitatively, these pieces of work are mostly limited to the case when liquid viscosity is low, e.g. water, in which the capillary force is dominant. To the best of the authors' knowledge, there is no DEM work in literature which considers a liquid bridge with high viscosity.

DEM is an extremely computer intensive method and some simulations may take several months or more to complete. Therefore, it is

* Corresponding author.
E-mail address: washino.k@mech.eng.osaka-u.ac.jp (K. Washino).

http://dx.doi.org/10.1016/j.powtec.2016.08.018
0032-5910/

important to set an appropriate time step. Simulations may become unstable if the time step is too large. On the other hand, using unnecessarily small time step makes it difficult to finish simulations within a reasonable time scale. Typically in DEM with dry particles, the time step is determined to resolve the collision event [5,7]. When the viscous force is taken into account, the time step must also resolve the "viscous force driven event", otherwise the simulation becomes unstable as shown later in Section 3. This means that there is an additional time step constraint when simulating viscous force dominant system. However, no time step criteria for viscous force driven event can be found in literature and the time step in such system is usually determined based on the trial-and-error.

The final goal of this work is to develop a framework to perform DEM simulation of wet particles in a system where the liquid viscous force is dominant or important. The present paper is focused on assessing the currently used DEM framework and revealing its limitations especially in terms of the time step and simulation stability. Time step criteria required for stable simulation are derived by monitoring the total kinetic energy in particles settling simulations.

2. Model description in DEM

2.1. Governing equations

The main focus of the present work is a viscous force dominant system, i.e. the capillary force is negligible compared to the viscous force. In such a system, the motion of wet particle i can be governed by the following equations of motion for translation and rotation:

$$m_i\dot{\boldsymbol{v}}_i = \sum_j \left[\boldsymbol{F}^n_{c,ij} + \boldsymbol{F}^t_{c,ij} + \boldsymbol{F}^n_{v,ij} + \boldsymbol{F}^t_{v,ij}\right] + m_i\boldsymbol{g} \tag{1}$$

$$I_i\dot{\boldsymbol{\omega}}_i = \sum_j \left[\boldsymbol{r}_i \times \boldsymbol{F}^t{}_{c,ij} + \boldsymbol{F}^t{}_{v,ij}\right] \tag{2}$$

where m is the particle mass, I the particle moment of inertia, $\boldsymbol{v}$ the particle velocity, $\boldsymbol{\omega}$ the particle angular velocity, $\boldsymbol{F}_c$ the contact force, $\boldsymbol{F}_v$ the liquid viscous force, $\boldsymbol{g}$ the gravitational acceleration vector and $\boldsymbol{r}$ is the vector from the centre of particle i towards the centre of particle j with its magnitude being equal to the radius of the particle. The superscripts n and t indicate the normal and tangential components respectively.

2.2. Contact force model

The normal and tangential contact forces, $\boldsymbol{F}^n_c$ and $\boldsymbol{F}^t_c$, are calculated using the well-known Hertz-Mindlin model. The detailed description of the contact force model and its implementation in DEM can be found in literature [25,26,27].

2.3. Viscous force models

The normal viscous force is proportional to the relative translational velocity of the particles and can be written in a generic form as:

$$\boldsymbol{F}^n_v = -C^n\boldsymbol{v}^n_r \tag{3}$$

where C^n is the damping coefficient related to the liquid viscosity, and

$$\boldsymbol{v}^n_r = (\boldsymbol{v}_r \cdot \boldsymbol{n})\boldsymbol{n} \tag{4}$$

$$\boldsymbol{v}_r = \boldsymbol{v}_i - \boldsymbol{v}_j \tag{5}$$

Here $\boldsymbol{n}$ is the unit normal vector from the centre of particle i towards the centre of particle j. Several models are available in literature to evaluate C^n. Adams and Perchard [18] gave C^n from the analytical solution of Reynolds lubrication equation as:

$$\frac{C^n = 6\pi\mu\bar{r}^2}{S} \tag{6}$$

where μ is the liquid viscosity, S is the separation distance between particles (see Fig. 1) and $\bar{r} = r_i r_j/(r_i + r_j)$ is the reduced particle radius. Pitois et al. [24] assumed a cylindrical bridge shape and proposed the following correction to Eq. (6) as:

$$\frac{C^n = 6\pi\mu\bar{r}^2\left[1-\left(1+V/\pi\bar{r}S^2\right)^{-\frac{1}{2}}\right]^2}{S} \tag{7}$$

where V is the volume of the liquid bridge.

The tangential viscous force is proportional to both the relative translational and rotational velocities and can be written in a generic form as:

$$\boldsymbol{F}^t_v = -\left(C^t_T\boldsymbol{v}^t_r + C^t_R\boldsymbol{\omega}_r \times \boldsymbol{n}\right) \tag{8}$$

where C^t_T and C^t_R are the coefficients related to the liquid viscosity, and

$$\boldsymbol{v}^t_r = \boldsymbol{v}_r - \boldsymbol{v}^n_r \tag{9}$$

$$\boldsymbol{\omega}_r = r_i\boldsymbol{\omega}_i + r_j\boldsymbol{\omega}_j \tag{10}$$

Goldman et al. [19] proposed the following expressions for C^t_T and C^t_R:

$$C^t_T = 6\pi\mu\bar{r}\left(\frac{\frac{8}{15}\ln\bar{r}}{S+0.9588}\right) \tag{11}$$

$$C^t_R = 6\pi\mu\bar{r}\left(\frac{\frac{2}{15}\ln\bar{r}}{S-0.2526}\right) \tag{12}$$

These are obtained from the numerical solution of the Stokes equation and valid only when S is sufficiently small. Goldman et al. [19] also proposed the following expression which is valid for large S:

$$\frac{C^t_R = 6\pi\mu\bar{r}}{8\left(\frac{\bar{r}}{S+\bar{r}}\right)^4\left(\frac{1-\frac{3}{8}\frac{\bar{r}}{S+\bar{r}}}{}\right)} \tag{13}$$

The viscous forces calculated by the above equations tend to infinity as the separation distance approaches to zero. The minimum separation distance, $S_{\min}$ is introduced to keep the forces in finite ranges. Similar treatments can be found in literature [20,28,29]. Note that this

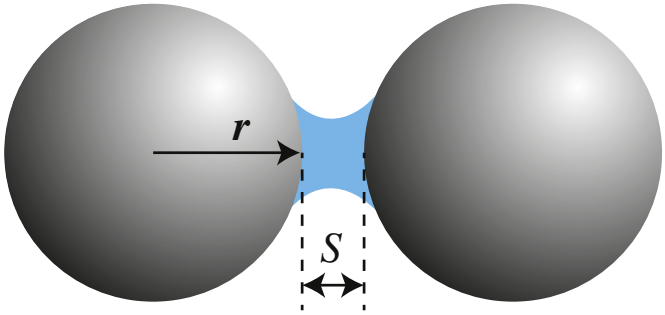

Fig. 1. Liquid bridge formed between two particles.