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Numerical investigation on the influence of air flow in a die filling process

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ABSTRACT

Die filling is an important manufacturing process that is widely involved in material science and technology in chemical engineering. Application of numerical technologies is desired in optimizing a die filling process. The Discrete Element Method (DEM) is widely used to simulate granular flows in die filling. However, the existing DEM has a problem regarding the computation of air flow in a moving shoe system, even though the DEM is coupled with computational fluid dynamics (CFD). This is because that the simulation of a gas-solid flow with a moving boundary requires an extremely complex algorithm. In order to solve this problem, The Advanced DEM-CFD method is proposed to calculate granular particles interacting with air meanwhile during the whole die filling process. In the Advanced DEM-CFD method, a compact algorithm is employed to simulate a gas-solid flow in a moving boundary system, where wall boundary is modeled by Signed Distance Function and Immersed Boundary Method for solid phase and fluid phase. Validation tests are performed to show the adequacy of the Advanced DEM-CFD method. The results show that the simulations well agree with the experiments, and hence our numerical approach is adequate to reproduce actual die filling processes.

1. Introduction

Die filling is an important manufacturing process in material science and technology in chemical engineering. The fundamental components of a die filling system includes a die, a shoe and a table, along which the shoe containing millions of fine particles can move to the deposition area and formulate particles under the gravity [1,2]. The formulation of the particles is during the filling procedure and they are shaped into a rigid pile inside the die, during which the particles interacting with air and arbitrary geometry is happening all the time. Such kind of a gas-solid flow is examined and studied frequently in pharmaceuticals and powder metallurgy [3,4] in order to improve the quality and efficiency among the relative applications by re-evaluating the properties of the particles, devices as well as the products. A growing attention has been paid on these processes to decide the efficiency of a die filling system [5] by evaluating the states of the system at different collapsed time points. Nevertheless, it is extreme time-consuming and economically unviable for sensitivity studies of a die filling system. New geometries are changeful since adjusting to a better condition is based on a huge number of tests and experiments. It is desirable that the optimization of a die filling process is able to be realized by using 3D modeling and numerical method. The development and application of computational modeling becomes important to accomplish the study of the powder behavior during die filling process.

The Discrete Element Method (DEM) [6] is effective for reproducing particle movements. It is governed by the equation of Newton's second law of motion, in which the external forces with particles and wall boundary are physically accounted. Nowadays the DEM is applied in many fields [7], *e.g.*, pneumatic conveying [8], a fluidized bed [9–13], a packed bed [14], a blender [15]. Since the Signed Distance Function (SDF) [16] was developed to present the wall boundaries by setting a scalar field, complex shape vessel could be simulated by the DEM [17–19]. Consequently, the DEM has been applied to various industrial systems.

As far as application of the DEM to the die filling is concerned, the DEM simulations were performed without air flow and under simple systems. In previous study [20], the air flow was simulated in limited area in die-filling as thus the gas-solid flow could not be simulated completely in the whole processes. In recent studies [21,22], complex shape die was employed, where the wall boundary was modeled by meshes. Very recently, complicated die geometries could be created easily by introducing the new

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technology such as SDF into the DEM (DEM/SDF) [23]. Adequacy of the DEM/SDF was proved through validation tests in die-filling. On the other hand, the DEM/SDF could not simulate the air flow, since solid-fluid interaction model was not introduced into in the DEM/SDF model. Very recently, the authors' group developed a new solid-fluid interaction model [24], where the SDF was combined with the Immersed Boundary Method (IBM) [25,26]. In this method, wall boundary conditions of fluid phase could be simulated by the IBM, where local volume fraction was evaluated based upon the SDF. In an actual die filling system, modeling of granular flow involving air flow, moving shoe system and arbitrary shaped die is required. By using existing numerical simulation techniques, those actual conditions could not be simulated in die filling system. A gas-solid flow in die filling is facing the requirement of a more advanced modeling method. In order to solve this problem, the Advanced DEM-CFD method is newly developed, where the combination of the SDF and IBM is introduced into the DEM-CFD method. Adequacy of the Advanced DEM-CFD method is proved through validation tests in this study.

2. Numerical modeling

2.1. Solid phase

The Advanced DEM-CFD method was applied to perform a simulation of a gas-solid flow in die-filling. The solid phase was modeled by the DEM. In the DEM, the motion of every single particle is governed by Newton's second law of motion as,

$$m\frac{d\boldsymbol{v}}{dt} = \sum \boldsymbol{F_C} + \boldsymbol{F_d} - V_s\nabla p + \boldsymbol{F_g} \tag{1}$$

$$I\frac{d\boldsymbol{\omega}}{dt} = \boldsymbol{T} \tag{2}$$

where m, $\boldsymbol{v}$, t, $\boldsymbol{F}_C$, $\boldsymbol{F}_d$, V_s, P, $\boldsymbol{F}_g$, I, $\boldsymbol{\omega}$ and $\boldsymbol{T}$ represent the mass of the particle, translational velocity of the particle, time, contact force, drag force, particle volume, pressure, gravitational force, moment of inertia of the particle, rotational velocity of the particle and torque, respectively. According to the equation, the total force acting on the particles is composed of the contact force between particles, drag force interacting with the fluid, force due to pressure gradient and gravitational force. The contact force can be divided into two directions, normal and tangential as the equation shows,

$$\boldsymbol{F}_C = \boldsymbol{F}_{C_n} + \boldsymbol{F}_{C_t} \tag{3}$$

where subscript n and t represent the normal and the tangential component. Normal component of the contact force is modeled using a spring and a dashpot, and expressed by

$$\boldsymbol{F}_{\boldsymbol{C_n}} = -k\boldsymbol{\delta_n} - \eta\boldsymbol{v_n} \tag{4}$$

where k, η, $\boldsymbol{\delta_n}$ and $\boldsymbol{v_n}$ represent spring constant, damping coefficient, displacement and the relative velocity of solid particles in normal direction. The damping coefficient is acquired based on the energy dissipation,

$$\eta = -2(\ln e)\sqrt{\frac{mk}{\pi^2 + (\ln e)^2}} \tag{5}$$

where e represents the restitution coefficient.

The tangential component of the contact force is given by

$$\boldsymbol{F}_{C_t} = \begin{cases} -k\boldsymbol{\delta_t} - \eta\boldsymbol{v_t} & (|\boldsymbol{F}_{C_t}| \le \mu|\boldsymbol{F}_{C_n}|) \\ -\mu|\boldsymbol{F}_{C_n}|\dfrac{\boldsymbol{v_t}}{|\boldsymbol{v_t}|} & (|\boldsymbol{F}_{C_t}| > \mu|\boldsymbol{F}_{C_n}|) \end{cases} \tag{6}$$

where μ represents friction coefficient.

The drag force acting on a solid particle is given by

$$\boldsymbol{F_d} = \frac{\beta}{1-\varepsilon}(\boldsymbol{u_f} - \boldsymbol{v})V_s \tag{7}$$

where ε, $\boldsymbol{u_f}$, and β are the void fraction, the fluid velocity and interphase momentum transfer coefficient respectively. We use Ergun [27] and Wen-Yu [28] equations to acquire the momentum exchange coefficient. The drag force of both dilute and dense gas-solid flow can be precisely computed by the model. A void fraction of 0.8 is adopted as the boundary between these two equations in the evaluation of β. The β is given by:

$$\begin{cases} \beta_{Ergun} = 150\dfrac{(1-\varepsilon)^2}{\varepsilon}\dfrac{\mu_f}{d_s^2} + 1.75(1-\varepsilon)\dfrac{\rho_f}{d_s}\left|\boldsymbol{u_f} - \boldsymbol{v}\right| & (\varepsilon \le 0.8) \\ \beta_{Wen-Yu} = \dfrac{3}{4}C_d\dfrac{\varepsilon(1-\varepsilon)}{d_s}\rho_f\left|\boldsymbol{u_f} - \boldsymbol{v}\right|\varepsilon^{-2.65} & (\varepsilon > 0.8) \end{cases} \tag{8}$$

In Eq. (8), μ_f represents the fluid viscosity, ρ_f represents the fluid density and d_s is the solid particle diameter. C_d corresponding to the drag coefficient is obtained by the following equation,

$$C_d = \begin{cases} \dfrac{24}{Re_s}\left(1 + 0.15{Re_s}^{0.687}\right) & (Re_s \le 1000) \\ 0.44 & (Re_s > 1000) \end{cases} \tag{9}$$

and the dimensionless particle Reynolds number expressed as Re_s is given by the equation,

$$\mathrm{Re}_s = \frac{\left|\boldsymbol{u_f} - \boldsymbol{v}\right|\varepsilon\rho_f d_s}{\mu_f} \tag{10}$$

2.2. Gas phase

The continuum fluid phase, or gas phase, is governed by continuity equation and Navier-Stokes equation, where local volume average technique is applied [29],

$$\frac{\partial\varepsilon}{\partial t} + \nabla\cdot\left(\varepsilon\boldsymbol{u}_f\right) = 0 \tag{11}$$

$$\frac{\partial\left(\varepsilon\rho_f\boldsymbol{u}_f\right)}{\partial t} + \nabla\cdot\left(\varepsilon\rho_f\boldsymbol{u}_f\boldsymbol{u}_f\right) = -\varepsilon\nabla p - \boldsymbol{f} + \nabla\cdot(\varepsilon\boldsymbol{\tau}) + \varepsilon\rho_f\boldsymbol{g} \tag{12}$$

where $\boldsymbol{f}$ and $\boldsymbol{\tau}$ represent the interaction between gas-solid phases and the viscous stress. $\boldsymbol{f}$ is defined according to Newton's third law of motion:

$$\boldsymbol{f} = \frac{\sum_{i=1}^{N_{grid}}\boldsymbol{F}_d}{V_{grid}} \tag{13}$$

where N_{grid} is the number of solid particles located in the local grid and V_{grid} is the cell volume. $\boldsymbol{F}_d$ is given by Eq. (7).

2.3. Wall boundary modeling

The wall boundary modeling has always been an important part in numerical simulations. In the Advanced DEM-CFD method, combination of the SDF and the IBM was employed for a moving wall boundary in die-filling. Wall boundary modeling of the Advanced DEM-CFD method is briefly addressed for solid and fluid phase as below.

2.3.1. SDF based wall boundary for solid phase

In this study, SDF was employed for creating the wall boundary. The SDF is denoted as $\phi(\boldsymbol{x})$, which is expressed as:

$$\phi(\boldsymbol{x}) = d(\boldsymbol{x})\cdot s(\boldsymbol{x}) \tag{14}$$

where $d(\boldsymbol{x})$ represents the minimum distance pointing from the surface of the geometry structure and $s(\boldsymbol{x})$ represents the sign of