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Effect of Young's modulus on DEM results regarding transverse mixing of particles within a rotating drum

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ABSTRACT

The use of a Young's modulus lower than its true value is commonly adopted in numerical studies based on the discrete element method (DEM), in order to reduce the computational costs. However, the sensitivity of the DEM results to the value of Young's modulus is poorly understood. In this paper, we present a study on the relationship between the Young's modulus and DEM results, where the transverse mixing of particles within a rotating drum in rolling regime was considered. The values of E_0, $0.01E_0$, $0.001E_0$, $0.0007E_0$, $0.0005E_0$, and $0.0001E_0$ were employed in the model, where E_0 was the true value of the Young's modulus of the particle. The results reveal that Young's modulus makes considerable effects on the motion behaviour of individual particle during collision. However, these effects have little contribution to the mixing of a granular bed which is the cumulative effect of the motion of all individual particles. The explanation for this is that the mixing contribution from self-diffusion owing to the random collisions of particles is negligible compared to the one from the shearing effect of particles. For Young's modulus ranging from E_0 to $0.001E_0$, the simulated mixing results are comparable to each other, and all agree well with the experimental results. However, a significant reduction occurs to the mixing rate of the granular bed with E ranging from $0.0007E_0$ to $0.0001E_0$ owing to the decrease in the shearing effects of particles, and this change is transitional rather than developmental. The effects of the drum rotation speed and filling level on the relationship between Young's modulus and particle mixing is not observed. It is proposed that there is a critical value between $0.001E_0$ and $0.0007E_0$, above which the effect of Young's modulus on the mixing of the bed is ignorable and reliable simulation results can be obtained. Therefore, there exists a lower limit for using adjusted Young's modulus to reduce the computational costs.

1. Introduction

Particulate materials are extensively employed in the chemical, metallurgical, food, mineral, ceramic, and pharmaceutical processing industries. A common device utilized to handle particulate materials for various purposes is the rotating drum. Particle mixing in the transverse section of a rotating drum, which is a dominant type of mixing in drum compared to mixing in axial direction [1], is a fundamental operation closely linked to drying [2], heating [3], and granulating processes [4]. The underlying kinematics of mixing is difficult to study due to the complexity of particle flow, regardless of the geometrical simplicity of the drum. Depending on the operation condition, six flow regimes have been identified for describing the particle motion in a rotating drum [5,6]: slipping, slumping, rolling, cascading, cataracting, and centrifuging regimes. These regimes, except for slipping and centrifuging, are closely interconnected with the process of mixing in the drum [7]. Next, the motion of rolling, which is characterized by the combination of an active layer located at the top of the bed and a passive layer at the bottom of the bed, is the most critical regime for the purpose of mixing [8,9]. Controlling the granular flow regime is considerably important for analyzing the mixing behaviour of particles in a drum. However, the mixing phenomenon of particulate materials is still not well understood due to the complex dynamic behaviour involved in the rotating drum, although considerable efforts have been conducted for handling this issue in the past decades.

In the investigation of particle mixing in a rotating drum, there is an unavoidable difficulty in the measurement of particle flow owing to the opacity of the particulate solids. For this problem, both experimental techniques and numerical simulations were developed for studying particle mixing at a microscopic scale. For instance, experiments conducted under quasi-two-dimensional drum were considered as the most immediate approach for investigation the transverse mixing process of a granular bed [10]. In order to achieve greater detail, non-invasive measuring methods have been employed for monitoring the mixing process of particles in three-dimensional drum, such as magnetic resonance

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imaging (MRI) [11], positron emission particle tracking (PEPT) [12], radioactive particle tracking (RPT) [13], and optical imaging processing (OIP) [8]. Among these methods, the PEPT can conduct the measurement of trajectory for positron-emitting tracer particles but cannot determine concentrations; MRI and RPT are well suitable for revealing the mixing statement of particles but are not suitable for being conducted outside specialized laboratory conditions; OIP has shortage in presenting flowing messages within a granular bed, although it is one of the most common methods used in the studies owing to its advantages of relative simplicity, low costs, and flexible adjustment of the drum size [14–16]. Apart from using nonintrusive techniques, numerical simulation methods have progressed to investigate this subject such as discrete element method (DEM) which was originally proposed by Cundall and Strack [17]. The DEM technique has already been proven to be efficient in providing insight into the phenomena occurring in a granular bed as well as detailed flowing information and contact forces of particles which are difficult to acquire experimentally [18–20]. Subsequently, significant number of researchers have adopted this technique for investigating the mixing behaviour of granules in a rotating drum [21].

However, the main drawback of the DEM technique for analyzing particulate system is the computational costs, which are extremely high owing to the inherent algorithm of the DEM technique for solving motion equations between particles. Therefore, the studies are typically restricted to systems containing a small number of particles or in two-dimension. The most direct method to overcome this limitation is to employ adjusted values of particle properties instead of their real values for the DEM model, particularly for the parameter of Young's modulus, in order to avoid long computation time [18,22]. Based on the principle of determining the time step for the DEM calculation [23,24], the time step adopted for a certain type of particle is inversely proportional to the square root of Young's modulus. If a smaller value of the Yong's modulus is used for the DEM model, the time step in the numerical integration will be increased, and then the real computation time can be reduced. This is certainly common in literatures regarding mixing process of particles within rotating drum [3,7,25,26]. Therefore, it is essential to investigate how the mixing of particles within the drum is affected by the value of Young's modulus. Although the contact forces and motion equations between particles, are theoretically affected by the value of Young's modulus, which causes a deviation in the mixing performance of a granular bed, DEM result obtained by some researchers agree well with experimental observations by adopting the adjusted Young's modulus. Considerable less effort has been devoted to investigate why acceptable DEM results can be acquired when incorrect particle properties are used. Alizadeh et al. [15] recently conducted a discussion about this issue where dimensionless motion equations of particles in the DEM model were analysed. They reported that the dimensionless motion equations of individual particles are nearly unaffected by Young's modulus, and therefore, acceptable simulation results can be obtained in the DEM model with false Young's modulus. However, in their studies, the time variable t in the particle motion equation is not coincident with the one in the mixing index of the bed, hence, such conclusion might require further discussion. In addition, the appropriate range for adjusting Young's modulus is unclear if a lower value is employed for reducing the DEM computation costs, where acceptable simulated mixing results can be obtained.

In this study, the three-dimensional discrete element method was employed for simulating the transverse mixing of particulate media composed of uniform sized spheres within a rotating drum. The particle sample adopted currently was glass bean, which is one of the most widely used materials in studies. The physical properties of particles and drum related to the mixing behaviour of a granular bed were measured directly and the numerical model was validated experimentally using the optical image processing method. Then, we specifically examine the sensitivity of particle mixing to the value of Young's modulus used in DEM simulation in terms of mixing pattern, mixing rate, and particle velocities. The objective of this article is to obtain a better understanding about the relationship between DEM results and Young's modulus, when mixing of particles within a drum is considered, and then evaluate the feasibility of using the adjusted Young's modulus to reduce the computation cost.

2. Methodology description

2.1. Numerical modeling of particles

The discrete element method model proposed by Cundall and Strack [17] can predict the trajectories, velocities, and positions of all the particles by solving Newton's motion equations for each of them in the system. To model time-dependent particle motion in a rotating drum, the tree-dimensional DEM model with soft contact approach which is suitable for simulating a dense particle system [18,27] was adopted. The basic algorithm of the DEM model described in previous studies [17] will not be presented here. The key factors of modeling such as kinematics modeling of particles and time step for calculation are clarified below.

As the particulate materials used in the experimental tests were mono-dispersed glass beans, the spherical element of the DEM model was employed for presenting the particles in the drum. The total force acting on particle i with radius R_i in the system, as shown in Fig. 1, includes gravity $m_i\boldsymbol{g}$ and contact force $\boldsymbol{F}_{ij}$ (in normal direction $\boldsymbol{F}_{n,ij}$ and tangential direction $\boldsymbol{F}_{t,ij}$), accounting for the particle i-particle j interactions. The total torque on particle i is the summation of all forces with respect to it. Note that the boundary, the drum, is considered as a particle with infinite mass in the system, and the interaction of particle-boundary is similar to the particle-particle interaction. Then, the translational and rotational motions of particle i in the system can be described using the dynamic equations derived from Newton's law:

$$m_i\frac{d^2\boldsymbol{r}_i}{dt^2} = m_i\boldsymbol{g} + \sum_j\left(\boldsymbol{F}_{n,ij} + \boldsymbol{F}_{t,ij}\right) \tag{1}$$

$$I_i\frac{d^2\boldsymbol{\theta}_i}{dt^2} = -\mu_{r,ij}F_{ij}R_i\hat{\boldsymbol{w}}_i + \sum_j \boldsymbol{R}_i \times \boldsymbol{F}_{t,ij} \tag{2}$$

where $\boldsymbol{r}_i$, $\boldsymbol{\theta}_i$, m_i and I_i are the position vector, angular displacement, mass and moment of inertia of particle i, respectively; $\hat{\boldsymbol{w}}_i$is the unit angular velocity of particle i ($\hat{\boldsymbol{w}}_i = \dot{\boldsymbol{\theta}}_i/|\dot{\boldsymbol{\theta}}_i|$); and $\mu_{r,\,ij}$ is the rolling friction coefficient between particle i and j. Then the simplified Hertz-Mindlin contact force model proposed by Tsuji et al. [28], which could make a reasonably precise representation of the particle moving behaviour during collisions without increasing the computational calculation considerably [15,25,29], was employed for figuring the contact forces $\boldsymbol{F}_{n,ij}$ and $\boldsymbol{F}_{t,ij}$ owing to the plastic and elastic deformation at the contact point:

$$\boldsymbol{F}_{n,ij} = \frac{4}{3}E^*R^{*\frac{1}{2}}\delta_n^{\frac{3}{2}} - \sqrt{\frac{20}{3}}\beta\left[E^*m^*(R^*)^{\frac{1}{2}}\right]^{\frac{1}{2}}\delta_n^{\frac{1}{4}}\boldsymbol{v}^{rel}_{n,ij} \tag{3}$$

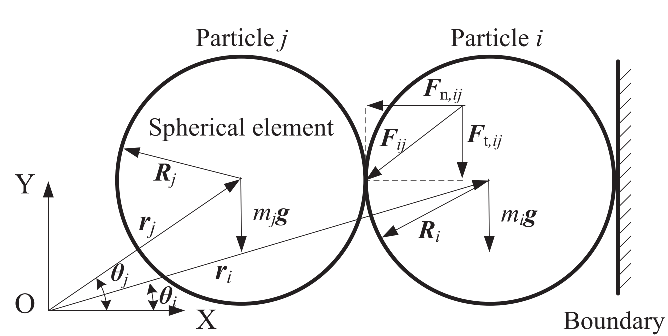

Fig. 1. Schematic of particles in contact.