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Three-dimensional axial dispersion dynamics of granular flow in the rolling-regime rotating drum

Shiliang Yang [a], Kun Luo [b], Jia Wei Chew [a,c,*]

[a] School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore 637459, Singapore
[b] State Key Laboratory of Clean Energy Utilization, Energy College, Zhejiang University, Hangzhou 310027, PR China
[c] Singapore Membrane Technology Center, Nanyang Environment and Water Research Institute, Nanyang Technological University, Singapore 637141, Singapore

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ABSTRACT

The dispersion characteristics of the granular material frequently encountered in many chemical industries play an important role in the system operation since it is related to the solid residence time, and thus further influence the heat and mass transfer behavior of the whole process. To shed some light, the discrete element method (DEM) is employed here to study a three-dimensional rotating drum, with the key focus being the axial dispersion characteristics of the solid phase. Our results prove the natural existence of a preferential channel for axial dispersion spanning the entire drum length, which provides insights on the region where the most extensive axial segregation effects are expected. Furthermore, we show that the axial solid dispersion coefficients adhere to normal frequency distributions in the active region, passive region and the entire drum. Also, increasing the rotating speed enhances while increasing the fill level diminishes the axial dispersion intensity in the system. Collectively, the results here provide new and valuable insights on the axial dispersion characteristics in the rotating drum, which is useful for the further understanding and optimization of the system.

1. Introduction

Due to its ubiquity, the granular flow has gained much attention from both academia and industry for unraveling the intrinsic mechanisms and process optimization [1–3]. However, the inherent complexity of granular flow makes a fundamental understanding of such dynamic behaviors fraught with difficulties and remains a major challenge in the physics community to date particularly when compared with that of fluid flow [4,5]. No constitutive law is available for granular flow the way that the Navier-Stokes equations are used to describe the classical fluids [6–8]. Science magazine has listed the fundamental mechanism governing granular flow as one of the 125 unanswered questions at the beginning of 21st century [9].

The rotating drum is a conventional granular flow reactor used in many chemical processes (e.g., cement, metallurgical, pharmaceutical, food processing, and waste treatment industries) due to its ability to handle particles with wide size distributions and operate in wide-ranging flow regimes [10]. The granular flow behavior in the rotating drum has drawn the attention of the physics community due to the rich physical phenomena, like the formation of a central core of small particles due to radial segregation, appearance of radial segregation before axial segregation, avalanching dynamics, coarsening behavior and moving bands of segregated particles along the axial direction [5], with characteristic time scale between 10^{-4} and $10^{4}\ \omega^{-1}$ orders-of-magnitude [10,11]. The significance of the rotating drum with respect to both the associated physics and the industrial relevance makes an in-depth understanding of the particle dynamics vital for not only providing insights into its fundamental mechanism but also the scale-up of the system. To date, reports on granular flow in the rotating drum have spouted on irregular and cohesive particle flow [12,13], mixing and heat transfer [14–16], particle flow [17,18], wet particles [19], radial and axial segregation [20–22], axial dispersion [23,24], and band dynamics [25,26]. In particular, the dispersion of the solid phase plays a critical role as it is related to solid residence time and segregation, which are tied to the heat and mass transfer involved in the practical process. Unfortunately, the nature of the frequency distribution of the solid dispersion coefficients remains controversial due to the contradicting results among various experimental and numerical studies.

Two approaches are available to evaluate the solid dispersion characteristics in granular flow, namely, the macro and micro methods [27]. In the macro approach, an initial pulse of tracked material is injected into the bed, then the change of the concentration profile along the drum length with time is monitored to determine the axial dispersion behavior. Based on the macro approach, the experimental work conducted by Rao et al. [28] studied the effects of the solid hold-up, particle size and rotating speed on the axial dispersion coefficient of the solid phase in the rotating drum. Also via the macro approach, Khan and Morris [29] experimentally studied the axial solid dispersion

* Corresponding author at: School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore 637459, Singapore.
E-mail address: JChew@ntu.edu.sg (J.W. Chew).

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of a pulse in a rotating drum using two different particle sizes. They concluded that the axial evolution of the segregated core can be described by a self-similar concentration profile whose width scale with t^{α} (where t stands for time and $\alpha \approx 0.3 < 1/2$) and thus this process is sub-diffusive. By means of magnetic resonance imaging (MRI), Fischer et al. [30] experimentally found that the pulse of small particles in a drum of large particles follows Fickian diffusion, while the pulse of large particles in a drum of small ones is sub-diffusive. On the other hand, in the micro method, the trajectory of the solid phase is tracked and the corresponding dispersion coefficients are evaluated according to the Einstein equation [31]. Via the micro approach, Parker et al. [32] experimentally tracked a radioactive tracer particle within a partially filled drum, and concluded that the axial dispersion of the solid phase is independent of the drum diameter but strongly dependent on particle size. Recently, experiments conducted by McLaren et al. [33] indicated that the solid dispersion in the rotating drum is related to the rotating speed and particle size, and follows a normal distribution.

The numerical simulation of dense granular flow using discrete element method (DEM) has increasingly become a powerful tool in the past two decades for shedding light on the intrinsic fundamental mechanisms of a variety of phenomena [34–37]. In DEM, the solid motion is resolved at the particle-scale level, with particle trajectories tracked based on integrating the governing equation of solid motion. Using DEM, Taberlet and Richard [38] tracked the concentration profile of small grains, and found that the mean-square displacement increases linearly with time, which indicates normal diffusion of the solid phase along the axial direction. This conclusion clearly contradicts with the experimental results of Khan and Morris [10], who found that this process is sub-diffusive. Third et al. [24] numerically studied the axial dispersion in the rotating drum and found the axial dispersion is dependent on particle size and drum size. In stark contrast to Parker et al. [32] and Third et al. [15], Taberlet and Richard [38] numerically found that the axial dispersion is independent of particle size. Furthermore, Third et al. [39] numerically demonstrated the normal dispersion of both large and small particles in the bi-disperse system, which contradicts with the experimental results of Fisher et al. [12]. Recently, Christov and Stone [40] concluded that the initial band width of tracked particles should be taken into account for evaluating the axial dispersion.

In spite of the slew of reports on solid dispersion trends in the literature, many fundamental questions regarding the axial solid dispersion in the rotating drum still persist. Some questions attempted in this study include: (i) is there any preferential regions for solid dispersion along the axial direction; and (ii) what are the frequency distributions of the solid dispersion coefficients in the passive and active regions of the drum. Meanwhile, all the previous experimental and numerical studies explored the mean value of the axial dispersion coefficient. As a new approach, the instantaneous dispersion of the solid phase is investigated in the current work, which provides a different perspective on the dispersion behavior via the Einstein equation [31] that is based on the particles' positions. In the present study, the DEM simulation of granular flow in a three-dimensional (3-D) rotating drum is carried out to study the axial dispersion of the solid phase. First, the spatially-resolved distribution of the axial solid dispersion coefficients in the 3-D drum is obtained to indicate the existence of a preferential channel for axial dispersion. Then, the frequency distributions of the axial solid dispersion coefficients in the active and passive regions and the entire drum are explored to determine whether the distributions are normal. Finally, the influence of the key operating parameters of rotating speed and fill level on axial dispersion is investigated.

2. Mathematical model

In the current study, the solid phase is resolved at the particle-scale level. Based on the balance of the forces, all the particles are tracked in the Lagrangian framework, and the particle-scale information is updated at each time instant. In the rotating drum, due to the rapid granular flow, the effect of the gas phase on the solid motion is neglected. Accordingly, only the gravitational and collision forces of the solid phase are considered. The translational and rotational motion of the solid phase is governed by Newton's second law, as described in the following:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = \sum_{j=1}^{k} \boldsymbol{F}_{c,ij} + m_i \boldsymbol{g} \tag{1}$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{k} \boldsymbol{M}_{ij} \tag{2}$$

where m_i and I_i are respectively the mass and moment of inertia of particle i; t and $\boldsymbol{g}$ (9.8 m/s^2) are respectively the time instant and gravitational acceleration; $\boldsymbol{v}_i$ and $\boldsymbol{\omega}_i$ are respectively the translational and rotational velocity of particle i; k is the total number of particles and walls colliding with the current particle; $\boldsymbol{F}_{c,ij}$ represents the interaction force between the colliding pair of particle i and particle j or the particle with the wall; and $\boldsymbol{M}_{ij}$ represents the torque exerted on the current particle.

In the dense granular flow, the collisions among neighboring particles are predominant and strongly influence the solid motion in the system. As multiple collisions exist simultaneously in the rotating drum, the soft-sphere model originally proposed by Cundall and Strack [41], in which the spring, dashpot and slider models are utilized to mimic this process, is adopted to treat the collisions. The interaction force of a colliding pair, which can be divided into the tangential and normal components, is described as:

$$\boldsymbol{F}_{c,ij} = \boldsymbol{F}_{cn,ij} + \boldsymbol{F}_{ct,ij} = \left(k_{n,ij}\delta_{n,ij}\boldsymbol{n} + \gamma_{n,ij}\boldsymbol{v}_{n,ij}\right) + \min\left\{\left(k_{t,ij}\delta_{t,ij}\boldsymbol{t} + \gamma_{t,ij}\boldsymbol{v}_{t,ij}\right), \mu \boldsymbol{F}_{cn,ij}\right\} \tag{3}$$

where μ stands for the friction coefficient of the solid phase; the subscripts n and t stand for the variable component along respectively the normal and tangential directions; $\boldsymbol{n}$ and $\boldsymbol{t}$ represent respectively the normal and tangential units of a collision pair; δ and $\boldsymbol{v}$ are respectively the particle displacement and relative velocity of a colliding pair. The normal and tangential stiffness coefficient ($k_{n,ij} = \frac{4}{3}Y^*\sqrt{R^*\delta_{n,ij}}$ and $k_{t,ij} = 8G^*\sqrt{R^*\delta_{n,ij}}$), and the normal and tangential damping coefficient ($\gamma_{n,ij} = 2\sqrt{\frac{5}{6}}\beta\sqrt{S_{n,ij}m^*}$ and $\gamma_{t,ij} = 2\sqrt{\frac{5}{6}}\beta\sqrt{S_{t,ij}m^*}$) are evaluated from the material property of the solid phase, such as the equivalent Young's modulus $\frac{1}{Y^*} = \frac{(1-\nu_i^2)}{Y_i} + \frac{(1-\nu_j^2)}{Y_j}$, the equivalent radius $\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j}$, the equivalent mass $\frac{1}{m^*} = \frac{1}{m_i} + \frac{1}{m_j}$, and the equivalent shear modulus $\frac{1}{G^*} = \frac{2(2+\nu_i)(1-\nu_i)}{Y_i} + \frac{2(2+\nu_j)(1-\nu_j)}{Y_j}$. Details regarding the equations adopted to calculate these variables can be found in our previous study [42].

As mentioned before, there exists two approaches frequently adopted to evaluate the axial dispersion behavior of the granular material, namely, the macro approach based on fitting the transient solid concentration and the micro approach based on the particle displacement statistics [27]. Harnessing the advantage of the particle-scale information obtainable by means of DEM, the micro approach is adopted in the current work. Specifically, the Einstein equation [31] is adopted to evaluate the dispersion intensity of the solid phase. In the time interval of Δt, the axial dispersion coefficient D_i of particle i moving an axial displacement of Δz_i can be formulated as

$$D_i = \frac{(\Delta z_i)^2}{2\Delta t} \tag{4}$$

For a specific region (e.g., the whole system, the active region), the axial dispersion intensity of the solid phase is quantified by time-averaging the instantaneous dispersion coefficients of the solid phase at