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A numerical study of the segregation phenomenon of lognormal particle size distributions in the rotating drum

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Granular materials are mostly polydisperse, which gives rise to phenomena such as segregation that has no monodisperse counterpart. The discrete element method is applied to simulate lognormal particle size distributions (PSDs) with the same arithmetic mean particle diameter but different PSD widths in a three-dimensional rotating drum operating in the rolling regime. Despite having the same mean particle diameter, as the PSD width of the lognormal PSDs increases, (i) the steady-state mixing index, the total kinetic energy, the ratio of the active region depth to the total bed depth, the mass fraction in the active region, the steady-state active-passive mass-based exchanging rate, and the mean solid residence time (SRT) of the particles in the active region increase, while (ii) the steady-state gyration radius, the streamwise velocity, and the SRT in the passive region decrease. Collectively, these highlight the need for more understanding of the effect of PSD width on the granular flow behavior in the rotating drum operating in the rolling flow regime. *Published by AIP Publishing.*
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I. INTRODUCTION

Granular flow is extremely prevalent both naturally and industrially. A fundamental understanding of the physics underlying granular flow has been the subject of extensive research efforts.^{1–3} In the practical operation, such as in the chemical, mining, metallurgical, polymer, and pharmaceutical industries, the co-existence of particles with a range of particle properties (e.g., diameter, shape, density, friction coefficient) inevitably leads to segregation among the different species (e.g., the Brazil nut effect) and also gives rise to different transport coefficients compared to monodisperse systems.⁴ This impacts the physical or chemical processes that require uniform heating or chemical reaction and thereby adversely affects the quality of the final product.^{5,6} Knowledge of the segregation phenomenon and especially the intrinsic mechanisms underlying this phenomenon is critical not only for fundamentally understanding the profound physics but also for improving the quality of the final product and process optimization.^{7–9} Therefore, the segregation of granular materials has drawn increasing attention, particularly in the rotating drum, which is a simple geometry but exhibits meaningful and complex behaviors as the operating parameters change.¹⁰ For instance, as the rotating speed changes, the granular flow behavior can be categorized into six flow regimes,¹¹ each of which is affected by segregation differently.

Over the past few decades, experimental work has been dedicated to study the segregation of the particles in the

rotating drum, with regard to the particle motion,¹² effect of drum geometry,¹³ axial band structure,¹⁴ dynamical evolution of segregation,¹⁵ segregation of particles differing in both size and density,¹⁶ segregation patterns,^{17,18} effect of operating parameters on segregated band width,¹⁹ coarsening of the axial band,²⁰ pattern scaling,²¹ axial band scaling,²² diffusion,²³ radial segregation of ternary mixtures,²⁴ long-term coarsening,²⁵ and competing segregation mechanisms.²⁶ Based on these experimental efforts, valuable conclusions with respect to the granular segregation in the rotating drum have been obtained. Ding *et al.*²⁷ conducted experiments on the rotating drum, and their results demonstrated that the bed structure of a binary-size granular mixture is similar to that of mono-sized particles. Newey and Ozik¹⁴ experimentally studied the segregation behavior of the ternary-size granular material and found that the axial segregation was such that smaller particles formed bands within bands of larger particles. Khan *et al.*¹⁵ reported on the dynamical evolution of segregation by using digital imaging. Jain *et al.*¹⁶ experimentally studied the segregation structure of particles differing in both size and density and found that either radial streaks or the conventional core of small particles can occur depending on the particle size ratio. Charles *et al.*²¹ demonstrated that the growth rate of bands decreased as the drum diameter decreased, while Juarez *et al.*²² observed that the coarsening rate is not logarithmic when the volume fraction of small particles is very low or high. Alizadeh *et al.*²⁸ experimentally investigated the mixing and segregation of the particles and proposed a model to predict the residence time of the solids in the rotating drum. The experimental work of Finger *et al.*²⁵ demonstrated that the stripe stability in the rotating drum can be controlled by adding a small percentage of different-sized particles.

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On top of the experimental results, the numerical study of the segregation dynamics in the rotating drum via discrete element method (DEM)²⁹ is becoming more and more popular due to the improvement of the computational algorithm and the advancement of computational hardware during the past two decades. By means of DEM, Rapaport³⁰ numerically studied the axial segregation behavior in a horizontal rotating drum with the bidisperse granular mixture. They found that the different sizes of particles segregated into bands perpendicular to the axis. Furthermore, Rapaport³¹ modeled the segregation behavior of the binary-size granular material in the rotating drum. Large differences in axial velocity are found to exist between different-sized particles in the numerical work of Taberlet *et al.*³² performed by means of DEM. Using DEM, Arntz *et al.*³³ numerically explored the segregation characteristics of a binary-size granular material in the rotating drum. They observed that the extent of segregation increases with volumetric fill fraction. To study the mechanisms related to axial segregation, Chen *et al.*³⁴ numerically modeled the segregation of a binary-size granular material in the rotating drum and proposed the onset mechanism of axial band formation of the solid phase. The numerical work conducted by Arntz *et al.*³⁵ using the DEM explored the influence of the particle properties on the segregation behavior of bidisperse granular beds in the rotating drum. To assess the accuracy of the DEM-based model, Alizadeh *et al.*³⁶ simulated a mixture consisting of particles of four sizes in a rotating drum.

Most studies on granular segregation and the associated intrinsic mechanisms in the rotating drum have focused on binary-size mixtures, despite the continuous particle size distributions (PSD) being ubiquitous and the reported difference in behaviors between the two polydispersity types.^{37–41} This is primarily due to the significant increase in the computational expense because of (i) the increase in the number of particle species with a wide PSD, (ii) the smaller time step needed for resolving the motion of small particles, and (iii) the additional computation costs.⁴ In view of the widespread prevalence of the continuous PSD in the natural and industrial processes, it is of both academic and practical relevance to have an in-depth understanding of the flow behavior and the associated segregation of the various species. Thus, based on the discrete element method (DEM), the current work is targeted at exploring the flow behavior and segregation dynamics of the particles with lognormal PSDs in the rotating drum operated in the rolling flow regime, which is the most commonly operated regime in industrial operations as it provides superior mixing and heat transfer.⁴² This represents the first systematic study on the characteristics of continuous PSDs in the 3-D rotating drum. First, the overall segregation phenomenon is described, followed by the analysis of the total kinetic energy and gyration radius. Next, the entire rotating drum is geometrically divided into the active and passive regions by the active-passive interface, which is identified as positions with zero streamwise velocities. Then, the particle-scale behavior of the various particle sizes is quantitatively evaluated to understand the flow behavior in each region. Additionally, the effect of the distribution width of lognormal PSDs with the same arithmetic mean particle diameter on the flow behavior is discussed. Finally, the segregation structure and also the varying mass fractions

axially of different particle diameters are evaluated to unravel the axial segregation phenomenon of the lognormal PSD.

II. NUMERICAL DESCRIPTION

In view of the negligible influence of the slow-moving gas in the rotating drum, the motion of a specific particle i with mass m_i and moment of inertia I_i is acknowledged to be governed by Newton's second law. The governing equation for its translational motion can be formulated as

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_{j=1}^{N_c} \mathbf{F}_{c,ij} + m_i \mathbf{g}, \quad (1)$$

where $\mathbf{v}_i$ is the translational velocity, t is the time instant, N_c is the total particle-particle and particle-wall collision number, $\mathbf{F}_{c,ij}$ is the collision force between the colliding pair, and $\mathbf{g}$ is the gravitational acceleration.

The rotational motion of this particle can be described by the following equation:

$$I_i \frac{d\omega_i}{dt} = \sum_{j=1}^{N_c} \mathbf{M}_{ij}, \quad (2)$$

where ω_i represents the rotating velocity and $\mathbf{M}_{ij}$ is the torque generated between the colliding pair.

In the rotating drum, rapid granular motion results in intensive collisions between neighboring particles. Thus, the so-called soft-sphere model²⁹ is adopted to handle the frequent collisions between particles. Specifically, the colliding force ($\mathbf{F}_{c,ij}$) due to particle-particle or particle-wall interaction can be divided into the normal ($\mathbf{F}_{cn,ij}$) and tangential ($\mathbf{F}_{ct,ij}$) force components. The normal colliding force is evaluated based on the normal relative distance (δ_n) and normal relative velocity ($\mathbf{v}_n$) as

$$\mathbf{F}_{cn,ij} = k_{n,ij} \delta_{n,ij} \mathbf{n} + \gamma_{n,ij} \mathbf{v}_{n,ij}. \quad (3)$$

Here, $\mathbf{n}$ is the normal unit vector, k_n and γ_n stand for, respectively, the normal stiffness coefficient and the normal damping coefficient, which can be calculated as

$$k_{n,ij} = \frac{4}{3} Y^* \sqrt{R^* \delta_{n,ij}}, \quad (4)$$

$$\gamma_{n,ij} = 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_{n,ij} m^*}, \quad (5)$$

where Y^* is equivalent Young's modulus ($\frac{1}{Y^*} = \frac{(1-\nu_i^2)}{Y_i} + \frac{(1-\nu_j^2)}{Y_j}$), R^* is the equivalent radius ($\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j}$), β is the damping ratio ($\beta = \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}}$), S_n is the normal stiffness ($S_{n,ij} = 2Y^* \sqrt{R^* \delta_{n,ij}}$), and m^* is the equivalent mass ($\frac{1}{m^*} = \frac{1}{m_i} + \frac{1}{m_j}$).

The tangential colliding force $\mathbf{F}_{ct,ij}$ evaluated from the tangential relative displacement (δ_t) and tangential relative velocity ($\mathbf{v}_t$) can be formulated as

$$\mathbf{F}_{ct,ij} = k_{t,ij} \delta_{t,ij} \mathbf{t} + \gamma_{t,ij} \mathbf{v}_{t,ij}, \quad (6)$$

where $\mathbf{t}$ stands for the tangential unit vector. The tangential stiffness coefficient (k_t) and the tangential damping coefficient (γ_t) are calculated from its material property as

$$k_{t,ij} = 8G^* \sqrt{R^* \delta_{n,ij}}, \quad (7)$$

$$\gamma_{t,ij} = 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_{t,ij} m^*}, \quad (8)$$

where G^* and S_t are, respectively, the equivalent shear modulus ($\frac{1}{G^*} = \frac{2(2+\nu_i)(1-\nu_i)}{Y_i} + \frac{2(2+\nu_j)(1-\nu_j)}{Y_j}$) and the tangential stiffness ($S_{t,ij} = 8G^* \sqrt{R^* \delta_{n,ij}}$).

When sliding occurs between colliding pairs, the tangential colliding force is evaluated based on Coulomb's friction law as

$$\mathbf{F}_{ct,ij} = -\mu_p |\mathbf{F}_{cn,ij}|, \quad (9)$$

where μ_p is the friction coefficient.

III. NUMERICAL SETTINGS

A. Geometrical configuration and particle size distribution

The particles studied in the current work are spherical glass particles with a particle density of 2500 kg/m^3 . The diameters follow number-based lognormal particle size distributions (PSDs), formulated as follows:

$$f_{\text{lognormal}} = \frac{1}{x\sigma\sqrt{2\pi}} \exp \left[-\frac{(\ln(x) - \mu)^2}{2\sigma^2} \right], \quad (10)$$

where x is the particle diameter, μ is the arithmetic mean particle diameter that is chosen as 3 mm in this study, and σ is the standard deviation. Four PSD widths, defined as the ratio of the standard deviation to arithmetic mean particle diameter (σ/μ), in the range of 0.1 – 0.7 are studied, as shown in Fig. 1(a). For the same volumetric fill percentage of 35% (i.e., particle bed height of 0.0909 m), the total number of

particles investigated is $424\,626$, $341\,953$, $269\,117$, and $213\,457$ for PSD widths (σ/μ), respectively, of 0.1 , 0.3 , 0.5 , and 0.7 , which correspond to respective masses of 16.21 kg , 16.28 kg , 18.32 kg , and 18.93 kg . The slight increase in the total mass with increasing PSD width reflects a more closely packed system due to the wider range of particle sizes⁴³ [Fig. 1(a)]. The diameters of generated particles span two orders-of-magnitude from 0.0001 m to 0.011 m , with the resolution being diameter gaps of 0.0001 m . The initial status of the rotating drum is a homogeneous packed bed formed with the accumulation of falling particles randomly generated in the whole domain. Then, the rotating drum starts to rotate with a rotational speed of 11.6 rpm in the rolling flow regime.

Figure 1(b) presents the instantaneous snapshot of particles in the rotating drum, which is a 3-D horizontal cylinder rotating around its central axis, for the PSD width of 0.7 at the time instant of $t = 4 \text{ s}$. The diameter of the drum is 0.24 m , and the length of the rotating drum is 0.72 m . The Cartesian coordinates x - y - z are adopted with the coordinate $(0, 0, 0)$ at the drum center, with the y -axis opposite to the gravitational acceleration, the z -axis aligned with the drum axis, and the x -axis perpendicular to the y -axis and z -axis. Furthermore, another local coordinate system (x^* - y^*) is chosen to evaluate the streamwise velocity (i.e., the velocity component parallel to the particle bed surface) of the particles with x^* and y^* being parallel and perpendicular to the granular bed surface, respectively. In Fig. 1(b), the non-uniform distribution of the different particle sizes due to size-induced segregation is clear.

B. Numerical settings and model validation

For the granular mixture studied, the particle properties are chosen based on the experimental and numerical data of Alizadeh *et al.*²⁸ Specifically, Young's modulus and the Poisson ratio are $1.0 \times 10^8 \text{ Pa}$ and 0.24 , respectively. The restitution coefficients between particle-particle and particle-wall collision pairs are, respectively, 0.97 and 0.85 , and the corresponding particle-particle and particle-wall friction coefficients are chosen to be 0.3 and 0.35 . To obtain the velocity and position of each particle at each time instant, the governing equations [Eqs. (1) and (2)] for the translational and rotational motion are explicitly integrated with an appropriate time step, which should be smaller than the Rayleigh time t_r ,⁴⁴

$$t_r = \frac{\pi d}{2(0.1631\nu + 0.8766)} \sqrt{\frac{2\rho_p(1+\nu)}{Y}}, \quad (11)$$

where d and ρ_p are, respectively, the diameter and density of a particle. The estimated Rayleigh time based on the smallest diameter in the current work (namely, 0.0001 m) is $1.35 \times 10^{-6} \text{ s}$; thus, the time step is chosen to be $1 \times 10^{-6} \text{ s}$ in the simulation. Furthermore, the detecting distance for building the neighboring list of the potentially colliding particles or walls for a specific particle is chosen to be 1.5 times the largest particle diameter. Each test case was run with a total number of 32 CPUs in parallel for a total of 200 physical seconds.

FIG. 1. (a) Number-based frequency of PSDs of different PSD widths (σ/μ) ranging between 0.1 and 0.7 investigated in the rotating drum and (b) 3-D illustration of the investigated rotating drum, which shows the instantaneous distribution of the various particle sizes in a lognormal PSD with a mean particle diameter (μ) of 3 mm and PSD width (σ/μ) of 0.7 at the time instant of $t = 4 \text{ s}$, with R_p (mm) standing for the particle radius.

Regarding the numerical validation, the crucial flow characteristics of monodisperse particles (i.e., all particles are of the exact same particle diameter) with the same particle properties in the rotating drum of the same geometry have been simulated and compared to the experimental data of Alizadeh *et al.*²⁸ Good agreement with respect to the dynamical angle of repose, the thickness of the active region, the time-averaged streamwise velocity of the particles, and the time-averaged radial velocity of the particles perpendicular to the bed surface was achieved.⁴⁵ Based on the successful validation of the model, the current work further enlarges the drum length to twice that of the previous one⁴⁵ and also uses particle sizes that follow lognormal distributions, while all the other parameters are kept the same.

C. Mapping of particle-scale information to the Eulerian framework

In the current work, mapping the particle-scale information of the granular material to the Eulerian framework is necessary to understand the local distribution of a specific property of the particles (e.g., the streamwise velocity). Similar to our previous work on the monodisperse system,⁴⁵ the whole rotating drum is enclosed by a cubic geometry of 24 cm $\times$ 24 cm $\times$ 72 cm ($x \times y \times z$). It is then divided into smaller cells with sizes of 3 mm, 3 mm, and 12 mm along the x , y , and z directions, respectively. After that, the mapping is carried out as follows. First, the Eulerian grid cell i where a particle j is located in is detected. Second, the instantaneous velocity ($U_{i,t}$) and angular velocity ($\omega_{i,t}$) of the particles in this grid i are evaluated by the mass-weighted averaging of the instantaneous velocities of all the N_p particles in the current grid i ,

$$U_{i,t} = \frac{\sum_{j=1}^{N_p} m_j v_{i,j}}{\sum_{j=1}^{N_p} m_j} \quad (i = x, y, z), \quad (12)$$

$$\omega_{i,t} = \frac{\sum_{j=1}^{N_p} m_j \omega_{i,j}}{\sum_{j=1}^{N_p} m_j} \quad (i = x, y, z), \quad (13)$$

where m_j is the mass of particle j , $v_{i,j}$ is the instantaneous translational velocity of particle j , and $\omega_{i,t}$ stands for the angular velocity of particle j . Second, the time-averaged particle velocity in this Eulerian grid i is evaluated by averaging all the instantaneous particle velocity,

$$U_i = \frac{\sum_{t=1}^{N_t} U_{i,t}}{N_t} \quad (i = x, y, z), \quad (14)$$

$$\omega_i = \frac{\sum_{t=1}^{N_t} \omega_{i,t}}{N_t} \quad (i = x, y, z), \quad (15)$$

where N_t represents the total number of samples.

IV. RESULTS AND DISCUSSION

A. Segregation behavior of the lognormal PSD

To qualitatively overview the dynamical segregation phenomenon in the rotating drum with a wide lognormal PSD of $\sigma/\mu = 0.7$, Fig. 2 illustrates the instantaneous distribution of

FIG. 2. Instantaneous distributions of the different particle diameters of a lognormal PSD with a PSD width (σ/μ) of 0.7 in the rotating drum: the central ($z/Z = 0$) slice at $t = 4$ s (a), 40 s (c), and 200 s (e) and the end-wall ($z/Z \sim 1$) slice at $t = 4$ s (b), 40 s (d), and 200 s (f).

the various particle diameters in the axial central slice ($z/Z = 0$) and end-wall slice ($z/Z \sim 1$) of the rotating drum at several time instants. In general, four aspects regarding the segregated granular flow behavior can be observed: First, a nearly flat particle bed surface is constructed in the system, which is similar to the typical flow behavior of the granular material in the rolling flow regime.⁴⁵ Second, in both the central and end-wall slices, the size-segregation of the particles is such that the smallest and largest ones are in the radial core and periphery, respectively, while the intermediate ones are in between. The radial segregation phenomenon can be attributed to the percolation effect for particles of different sizes, whereby the random motion within the active region constantly opens up interstitial voids that small particles are statistically more likely to fill into than larger ones.⁴⁶ Third, the dynamic angles of repose of the particles evaluated in both slices are nearly constant with time. Fourth, compared with the central slice, the particle distribution in the end-wall slice is different in that progressively more of the larger particles accumulate at the end-wall due to axial segregation.

B. Quantification of segregation dynamics

Figure 3 displays the mixing index (a), gyration radius (b) of each particle diameter range for the widest lognormal PSD (i.e., $\sigma/\mu = 0.7$), average gyration radius (c), along with the total kinetic energy (d) of the entire drum, which indicates the non-negligible impact of the PSD width despite the PSDs having the same arithmetic mean diameter.

To quantify the extents of radial and axial size-segregation, the mixing index Γ reported by Remy *et al.*⁴⁷ is employed in the current work,

$$\Gamma = \frac{\zeta}{\zeta_{mix}}, \quad (16)$$

where ζ and ζ_{mix} are, respectively, the instantaneous mixing degree of the system and the mixing degree of a well-mixed system. In order to calculate the mixing degree ζ , the whole bed is divided into smaller cells. Specifically, the rotating drum is enclosed by a cube with dimensions of 24 cm, 24 cm, and 72 cm along the x , y , and z directions, respectively, and then divided into cubic cells of the same dimensions of 12 mm along all the three directions. As compared with the cubic cells adopted for evaluating the time-averaged solid velocity, coarser cubic cells are used for calculating the mixing index to include more particles and thereby reduce the otherwise large fluctuations in the instantaneous mixing index. The number fraction of each particle diameter range in all the cells can be then evaluated and thereby ζ formulated as

$$\zeta = \sum_{i=1}^M (n^i \sum_{j=1}^{N_k} c_j^i \ln c_j^i), \quad (17)$$

where n^i , c_j^i , N_k , and M represent the particle number in the cell i normalized with respect to the total particle number in the whole drum, the number fraction of species j normalized

with respect to the total particle number of the cell i , the total number of species (i.e., number of different particle diameter ranges assessed) considered in the system, and the total cells adopted to divide the whole system, respectively. Therefore, the mixing index Γ ranges from 0 for a completely segregated system to 1 for a well-mixed system.

Figure 3(a) illustrates the evolution of the mixing index of the whole drum to monitor the change in the extent of segregation with time, which shows similar trends for all four PSD widths. Specifically, the mixing index (Γ) of each system decreases rapidly over the first 25 s because of the fast radial segregation and then decreases slowly due to the slow axial segregation. As the PSD width increases, the mixing index (Γ) decreases less, which implies that the extent of segregation decreases monotonically as the PSD width increases.

To better understand the radial re-distribution of particles due to radial size-segregation, the gyration radius of the solid phase can be analyzed. Specifically, the gyration radius of a particle is defined as the distance between this particle and the radial center (i.e., $x = y = 0$) of the corresponding transverse plane. Figure 3(b) presents the evolution of the mean gyration radius of each particle diameter range in the rotating drum for the widest PSD ($\sigma/\mu = 0.7$). The distinct radial preference of each particle diameter range is clear. Upon drum rotation, the fast radial segregation gives rise to rapid variations of the gyration radius of the different particle diameters within the first 25 s, with the gyration radius decreasing for the particles smaller than the mean and increasing for the particles larger than the mean. To further understand the segregation behavior, the average gyration radius in the whole drum, which is obtained by averaging the gyration radii of all the particles in the system, is depicted in Fig. 3(c). Similar to Fig. 3(a), the trends among the four PSDs are similar in terms of the more

FIG. 3. Evolution of various characteristics related to the dynamical segregation of lognormal PSDs with different PSD widths in the rotating drum: (a) mixing index, (b) gyration radius of each particle diameter range for the lognormal PSD with a PSD width (σ/μ) of 0.7, (c) average gyration radius, and (d) total kinetic energy.

rapid decrease in the first 25 s due to the reason of the fast radial segregation, whereby the smaller particles preferentially segregate radially to the radial center while the larger ones to the radial periphery. Comparing the different PSD widths, it is clear that the gyration radius decreases as the PSD width (σ/μ) increases, which is because of the greater number fraction of small particles in the wider lognormal PSDs that tend to be at the radial center. In contrast to Fig. 3(a) in which the mixing index continues to decrease with time on account of the slow axial segregation, Fig. 3(c) indicates that the gyration radius remains relatively constant after the initial decline, demonstrating that the subsequent axial segregation exerts limited influence on the radial profile.

In view of the re-distribution of different-sized particles throughout the rotating drum induced by the size-segregation phenomenon, the dynamic response of the total kinetic energy of all the particles in the whole system warrants a closer look. The total kinetic energy of the entire system is evaluated by the summation of the instant kinetic energy ($\frac{1}{2} \sum_{i=1}^{N_{total}} m_i v_i^2$) of all the particles (N_{total}) in the system, as shown with respect to time in Fig. 3(d). For each PSD, the total kinetic energy of all the particles in the whole system rapidly spikes initially and then remains nearly constant thereafter, affirming that the total kinetic energy is a global parameter, which is nearly independent of the size-induced segregation in the rotating drum. The lowest steady-state value for the narrowest PSD ($\sigma/\mu = 0.1$) is tied to the lowest mass of particles in the drum.

C. Streamwise velocity and active-passive interface

Figure 4(a) presents the contour plot of the time-averaged particle streamwise velocity (U_{sx}^*) of the widest lognormal PSD ($\sigma/\mu = 0.7$) in the axial central slice ($z/Z = 0$) of the rotating drum, which requires understanding not just with respect to the segregation phenomenon but is also needed for the continuum modeling of the surface flow.⁴⁸ The quantification of the time-averaged streamwise velocity in the local coordinate system (x^*-y^*) is the same as that adopted in our previous work,⁴⁵

$$U_{sx}^* = \frac{\sum_{i=1}^{N_t} (U_{x,i} \cdot \cos(\theta) - U_{y,i} \cdot \sin(\theta))}{N_t}, \quad (18)$$

where $U_{x,i}$ and $U_{y,i}$ stand for, respectively, the particle velocity along the x and y directions, evaluated through Eqs. (11) and (12), and θ is the dynamic angle of repose. Figure 4(a) shows that the particles higher in the particle bed rapidly fall downwards with positive streamwise velocities (U_{sx}^*), whereas those lower in the particle bed move much slower with negative streamwise velocities (U_{sx}^*). This agrees with the well-acknowledged co-existence of the active and passive regions with obviously different flow behavior in a rotating drum running in the rolling flow regime. The mixing, heat transfer, and reaction mostly occur only in the faster-moving active region,⁴² which warrants a closer look at the effect of the different segregation behaviors among the lognormal PSDs of different PSD widths in each region and thereby necessitates means to demarcate the two regions. The locations with particle streamwise velocities (U_{sx}^*) of zero are identified as the active-passive interface, which are points at which the positive streamwise velocities in the active region transitions to the negative velocities in the passive region.^{36,42} The black line in Fig. 4(a) denotes the active-passive interface for the widest lognormal PSD ($\sigma/\mu = 0.7$).

Figure 4(b) illustrates the streamwise velocities (U_{sx}^*) of the four lognormal PSDs of different widths, along with that for the monodisperse particles⁴⁵ and binary-size⁴⁹ mixtures. The trends among the different PSD widths and monodisperse and binary-size systems are similar in that the streamwise velocity (U_{sx}^*) gradients are largely linear in each region, and steeper in the active region than in the passive, which agrees with that previously observed for monodisperse systems.^{36,45} Among the different particle systems, the U_{sx}^* magnitudes are more similar in the active region than those in the passive region, which agrees with experimental results.²⁸ Moreover, the monodisperse system has the greatest U_{sx}^* , while the widest PSD ($\sigma/\mu = 0.7$) exhibits the least U_{sx}^* at the same y^* positions. Among the PSDs, (i) the PSD width has a greater impact on the streamwise velocities (U_{sx}^*) in the active region than that in the passive region, specifically in that the U_{sx}^* magnitudes decrease as the PSD width increases, and (ii) the bed height increases as the PSD width increases. Since the heat transfer behavior mainly occurs in the active region (e.g., the thermal efficiency has been shown to be proportional to the mixing zone⁵⁰ due to the high shear rate⁵¹), it is meaningful to explore the effect of the PSD width on the active region depth, which

FIG. 4. (a) Contour plot of the time-averaged particle streamwise velocity (U_{sx}^* , m/s) of the widest lognormal PSD ($\sigma/\mu = 0.7$) in the central axial slice ($z/Z = 0$) in the rotating drum and (b) effect of the PSD width on the streamwise velocity (U_{sx}^*) with respect to the bed depth. The vertical dotted line denotes the active-passive interface, and the horizontal dotted line represents the particle bed surface of the widest lognormal PSD ($\sigma/\mu = 0.7$).

TABLE I. Influence of the PSD width on the particle bed depth and the depth of the active region at $x^* = 0$.

PSD width (σ/μ)	0.1	0.3	0.5	0.7
Bed surface position (y^* ; m)	-0.0300	-0.0312	-0.0240	-0.0180
Active-passive interface position (y^* ; m)	-0.0317	-0.0626	-0.0580	-0.0570
Bed depth (m)	0.0900	0.0888	0.0960	0.102
Active region depth (δ ; m)	0.0317	0.0314	0.0340	0.0390
Fraction of active region depth with respect to the bed depth (%)	35.20	35.36	35.42	38.20

is the distance between the active-passive interface and particle bed surface. Although there exist several correlations for evaluating this important parameter that factors in various relevant operating parameters (e.g., drum diameter, rotating speed, and fill level),^{27,28} the PSD width has never been considered although the effect is acknowledged to be significant.^{38,52–54} Accordingly, Table I lists the numerical results related to the bed depth and active region depth of the lognormal PSDs with different PSD widths at $x^* = 0$ of the rotating drum. In general, the depth of the active region is nearly 30%–40% of the bed depth. As the PSD width (σ/μ) increases, the bed depth decreases and then increases while the active region depth decreases and then increases, the non-monotonic behavior of which is reminiscent of the similarly non-monotonic extent of segregation with respect to the PSD width in a bubbling fluidized bed.⁵⁴ On the other hand, the fraction of active region depth with respect to the bed depth increases monotonically with the PSD width, with the monodisperse system exhibiting a smaller depth than the narrowest PSD,⁴⁵ which suggests that the widest PSD ($\sigma/\mu = 0.7$) is the most efficient due to the greatest proportion of the active region. The varying depths emphasize the need to account for the PSD width in the

development of correlations for the active region depth to enhance the accuracy of predictions.

Furthermore, the effect of the PSD width on the active-passive interface positions at the axial central slice ($z/Z = 0$) and end-wall slice ($z/Z \sim 1$) is illustrated in Fig. 5. Regardless of the PSD width, the active-passive interface is smooth across the whole drum length. The influence of the PSD width is such that the height of the interface increases with the PSD width, which is in part due to the greater extents of the inter-species momentum transfer among the greater range of particle diameters. By geometrically separating the whole drum into the active and passive regions, the detailed behaviors of the particles of various particle diameter ranges can be extracted and evaluated.

Figure 6 presents the change of the horizontal velocity (U_x , m/s) with the time of the various particle diameter ranges of the widest PSD ($\sigma/\mu = 0.7$) investigated, which indicates clearly that the U_x magnitudes differ among the different particle diameters in both the active and passive regions. The instantaneous U_x of a specific particle diameter range is computed as the mass-average of all the particles in the range in each region. While the U_x magnitudes are expectedly larger

FIG. 5. Effect of the PSD width on the active-passive interface at the (a) axial central slice ($z/Z = 0$) and (b) end-wall slice ($z/Z \sim 1$). The inset in (a) represents the active-passive interface across the drum length of the widest lognormal PSD ($\sigma/\mu = 0.7$).

FIG. 6. Evolution of the horizontal velocity (U_x , m/s) of the various particle diameter ranges of the widest PSD ($\sigma/\mu = 0.7$) investigated: (a) active region and (b) passive region.

TABLE II. Effect of the PSD width on the mass-averaged translational (U) and rotational (ω) particle velocities in the active region.

PSD width (σ/μ)	U_x (m/s)	U_y (m/s)	U_z (m/s)	ω_x (deg/s)	ω_y (deg/s)	ω_z (deg/s)
0.1	0.177	0.0910	0.0237	17.02	16.76	21.55
0.3	0.167	0.0887	0.0239	15.25	15.09	19.25
0.5	0.160	0.0894	0.0256	13.37	13.22	16.82
0.7	0.153	0.0875	0.0274	12.43	12.16	15.61

TABLE III. Effect of the PSD width on the mass-averaged translational (U) and rotational (ω) particle velocities in the passive region.

PSD width (σ/μ)	U_x (m/s)	U_y (m/s)	U_z (m/s)	ω_x (deg/s)	ω_y (deg/s)	ω_z (deg/s)
0.1	0.0769	0.0556	0.005 00	4.50	4.82	5.80
0.3	0.0760	0.0553	0.005 73	4.56	4.85	5.86
0.5	0.0751	0.0573	0.006 28	4.00	4.19	5.22
0.7	0.0735	0.0572	0.007 05	3.85	3.98	5.04

in the active region, the trends of the different particle diameter ranges are similar in both regions. Specifically, in both regions, the U_x magnitudes of the smaller and larger particles, respectively, decrease and increase with time within the first 25 s because of the fast radial segregation and then become relatively constant with time which reflects the negligible influence of axial segregation. The steady-state U_x magnitudes increase monotonically with the particle diameter in both regions. The decreased U_x of the smaller particles is due to the radial segregation to the radial core that is in the slower-moving passive region, whereas the increased U_x of the larger particles is due to the radial segregation to the radial periphery, part of which is in the faster-moving active region. Moreover, Tables II and III present the effect of the PSD width on the mass-averaged translational (U) and rotational (ω) particle velocities in the active and passive regions, respectively. Compared to the monodisperse system,⁴⁵ the lognormal PSDs lead to reduced translational (U) and rotating (ω) velocities in both the active and passive regions. As the PSD width increases, most of the velocities, namely, U_x , U_y , ω_x , ω_y , and ω_z , in both regions decrease, with the exception of U_z that increases in both regions.

D. Particle distribution characteristics in two regions

Figure 7(a) further shows the number and mass fractions of the particles in the active and passive regions for the widest lognormal PSD width ($\sigma/\mu = 0.7$) investigated, which indicates that the fractions change slightly initially but remain relatively constant with time. Due to the comparatively greater volume of the passive region, both number and mass fractions in the passive region are expectedly greater by approximately twofold. Notably, the steady-state mass fraction of the widest PSD in the active region is 28.95%, which is slightly larger than that (24.16%) of the monodisperse system⁴⁵ and also that (27.53%) of the binary-size system,⁴⁵ which indicates that the presence of a wider size distribution increases the proportion of the particles in the active region. Figure 7(b) depicts the mass fraction in the active region of each particle diameter range with respect to the total mass of each particle diameter range in the initial lognormal PSDs. Several aspects are worth highlighting: (i) the decreasing trends demonstrate that the mass fraction in the active region of each particle diameter range decreases as the particle diameter increases, which agrees with that of a binary-size mixture;⁴⁹ (ii) the mass

FIG. 7. (a) Distribution profile of number and mass fractions in the active and passive regions for the widest lognormal PSD ($\sigma/\mu = 0.7$) investigated and (b) mass fraction of each particle diameter range (with respect to the total mass of each particle diameter range in the initial PSD) in the active region for the different PSD widths. $\bar{d}_p$ stands for the mean diameter of each particle diameter range.

fraction of the largest species in each lognormal PSD in the active region is approximately 25%, regardless of the PSD width; (iii) due to the larger mass fraction of the small particles in the active region, the number fraction is greater than the mass fraction in the active region [Fig. 7(a)]; and (iv) increasing the PSD width increases the mass fraction in the active region [Fig. 7(b)], which is mainly due to the skewed nature of the lognormal PSDs [Fig. 1(b)].

E. Exchanging rate of particles between the two regions

During steady-state drum rotation, many particles dynamically exchange between the active and passive regions through the active-passive boundary. Figure 8(a) displays the evolution of the total exchanging rate. Similar to the total kinetic energy, the total exchanging rates between these two regions become nearly constant within the first 25 s, which implies that it behaves as a global parameter that is not influenced by the size-induced segregation and agrees with the observation for a binary-size mixture.⁵⁵ Increasing the PSD width increases the total exchanging rate, which is tied to the greater total mass (Sec. III). Furthermore, the exchanging rate across the interface of each particle diameter range composing the lognormal PSD is also monitored and the time-averaged value is evaluated. Figures 8(b)–8(d) present for the various particle diameter ranges the mass-based exchanging rates, the mass initial mass-based PSDs [obtained from the number-based PSDs in Fig. 1(a)], and the number-based exchanging rates, respectively. The mass-based exchanging rate [Fig. 8(b)] and total mass [Fig. 8(c)] of each particle diameter range have similar trends in that the magnitudes increase and then decrease with $\bar{d}_p$ for all lognormal PSD widths, which somewhat mimic the overall lognormal PSDs [Fig. 1(a)], and thereby indicates

that the exchanges between the two regions are closely tied to the proportion of each particle diameter range present in the whole drum. To evaluate the number-based exchanging rate, the mass-based exchanging rate [Fig. 8(b)] is normalized with respect to the corresponding mass [Fig. 8(c)] of each particle diameter range, as presented in Fig. 8(d). In contrast to the mass-based exchanging rate [Fig. 8(b)], the number-based exchanging rate [Fig. 8(d)] decreases monotonically with $\bar{d}_p$ for all PSD widths, indicating that the active-passive exchanges of the smaller particles are faster than those of the larger ones, which agrees with that for a binary-size granular mixture.⁵⁵ Regarding the effect of the PSD width, increasing the PSD width increases the number-based exchanging rate.

F. Contour plot of occupancy frequency

To further explore the extent of segregation of the lognormal PSD in the rotating drum, Fig. 9 presents the contour plot of the number-based occupancy frequency of different particle diameter ranges in the central slice ($z/Z = 0$) of the rotating drum with the widest PSD ($\sigma/\mu = 0.7$). Specifically, the occupancy frequency in a grid cell i (i.e., the Eulerian mapping grid mentioned in Sec. III) is evaluated as the ratio of the total particle number of a specific particle diameter to the total number of particles crossing this specific grid cell over the whole time range. The regular patterns in Fig. 9 are due to radial segregation. For the particle diameter range of the smallest species, namely, $d_p \in [0.1 \text{ mm}, 1 \text{ mm}]$ [Fig. 9(a)], a concentrated core is observed because of the preferential accumulation of the small particles to the radial core, and a higher frequency is also observed at the lower end of the particle bed surface due to the free-falling behavior [as similarly reflected in Fig. 2(a)]. As the particle diameter increases to

FIG. 8. Exchanges of particles across the active-passive interface: (a) evolution of the total exchanging rate, (b) mass-based exchanging rate of each particle diameter range for the different PSD widths, (c) initial mass-based PSDs, (d) number-based exchanging rate of each particle diameter range for the different PSD widths. $\bar{d}_p$ stands for the mean diameter of each particle diameter range.

FIG. 9. Contour plot of the number-based occupancy frequency in the central slice $z/Z = 0$ of the various particle diameter ranges in the widest PSD ($\sigma/\mu = 0.7$) investigated: (a) $d_p \in [0.1 \text{ mm}, 1 \text{ mm}]$, (b) $d_p \in [2 \text{ mm}, 3 \text{ mm}]$, (c) $d_p \in [4 \text{ mm}, 5 \text{ mm}]$, (d) $d_p \in [6 \text{ mm}, 7 \text{ mm}]$, (e) $d_p \in [8 \text{ mm}, 9 \text{ mm}]$, and (f) $d_p \in [10 \text{ mm}, 11 \text{ mm}]$. Each black line stands for the active-passive interface.

FIG. 10. Histogram of the probability frequency of the solid residence time (SRT) in the active region (a) and passive region (b) of the widest PSD ($\sigma/\mu = 0.7$) investigated.

$d_p \in [2 \text{ mm}, 3 \text{ mm}]$ [Fig. 9(b)] and $[4 \text{ mm}, 5 \text{ mm}]$ [Fig. 9(c)], the high frequency in the radial core diminishes and the high-frequency regions appear in between the radial core and periphery. For the larger particles of $d_p \in [6 \text{ mm}, 7 \text{ mm}]$ [Fig. 9(d)], $[8 \text{ mm}, 9 \text{ mm}]$ [Fig. 9(e)], and $d_p \in [10 \text{ mm}, 11 \text{ mm}]$ [Fig. 9(f)], they mainly concentrate in the radial periphery, with the highest frequency near the bed surface. Thus, in general, the smaller and larger particles, respectively, segregate radially to the core and periphery, which is in accordance with the experimental and numerical work on the ternary-size granular mixture in the rotating drum.^{24,56}

G. Solid residence time

The solid residence time (SRT) in each region, which determines material renewal and dispersion behavior, is critical in practical operations. For example, in the coating

process,^{57,58} this parameter strongly influences the coating time and coating uniformity and thus the quality of the coated particles in the final product. Hitherto, many efforts have been devoted to studying the influence of operating parameters (e.g., drum speed and fill level) on SRT,⁵⁸ but information regarding the effect of the width of the prevalent continuous PSDs on SRT is amiss. After geometrically separating the whole drum into the active and passive regions, the SRT in each region is evaluated. Specifically, for the particle considered,

TABLE IV. Effect of the PSD width on the residence time in the active and passive regions.

PSD width (σ/μ)	0.1	0.3	0.5	0.7
SRT in the active region (s)	0.695	0.704	0.715	0.769
SRT in the passive region (s)	1.806	1.640	1.478	1.402

FIG. 11. Comparison of the mean solid residence time (SRT) of the various particle diameters in the different lognormal PSDs in the active region (a) and passive region (b). $\bar{d}_p$ stands for the mean diameter of each particle diameter range.

the residence time in a particular region is calculated as the time elapsed between the time instant at which it crosses the active-passive interface and the time instant at which it recrosses the active-passive interface. Figure 10 presents the histogram of the probability frequency of the SRT in the active and passive regions of the widest PSD ($\sigma/\mu = 0.7$) investigated, which indicates clearly the differences between the two regions. Compared to the active region [Fig. 10(a)], the SRT in the passive region [Fig. 10(b)] has a broader range of values, lower mean value, and lower peak value. In particular, the mean SRT in the passive region is 1.4 s, which is nearly two times of that in the active region and signifies that a particle spends roughly one-third of the time in the active region. Interestingly, the SRT frequency distribution in these two regions is significantly different from the corresponding ones in the rotating drum either with monodisperse particles⁴⁵ or a binary-size granular mixture,⁵⁵ which highlights the need for more understanding on such continuous PSD systems. Table IV quantifies the effect of the PSD width on SRT in the active and passive regions. Increasing the PSD width increases the SRT in the active region but reduces that in the passive one. Furthermore, regardless of the PSD width, the SRT in the passive region is nearly two or three times of that in the active region. Compared with the monodisperse⁴⁵ and binary-size⁵⁵ mixture, the continuous PSD gives rise to higher SRT values in the active region and lower SRT values in the passive region. The SRT results here thereby suggest that the existing correlations for predicting the SRT magnitudes based on the mean

diameter of the particles³⁶ would mis-predict by 10%–20% as the PSD width varies. This indicates the need for more understanding on the effect of the PSD width to improve predictive capability.

Because the different particle diameters tend to circulate along different paths in the rotating drum due to the inherent segregation (Fig. 9), the SRT associated with each particle species is investigated. Figure 11 presents the mean SRT of each particle diameter range in both the active and passive regions of the rotating drum for the four lognormal PSDs assessed. Generally, SRT increases with the particle diameter in both the active and passive regions due to the radial segregation behavior, which is similar to that of a binary-size granular material.⁵⁵ Particularly for the widest PSD ($\sigma/\mu = 0.7$) investigated, the SRT of largest particles in the passive region is nearly two times of that of the smallest particles. Clearly, increasing the PSD width enhances and diminishes the SRT in the active and passive regions, respectively.

H. Axial segregation

The size difference of the particles in the rotating drum not only induces radial segregation in the transverse plane but also axial segregation along the drum length, which was first observed in the experiments conducted by Oyama⁵⁹ in 1939, but the understanding remains incomplete to date particularly with regard to a continuous PSD. To give a vivid illustration of the internal segregation structure of the particles in the

FIG. 12. 3-D illustration of the internal segregation structure of the widest PSD ($\sigma/\mu = 0.7$) at $t = 200$ s, with red, yellow, blue, and light gray representing the iso-surfaces (i.e., positions with mass fractions of 0.5) of the particle diameter ranges of $d_p \in [0.1 \text{ mm}, 1 \text{ mm}]$, $[2 \text{ mm}, 3 \text{ mm}]$, $[4 \text{ mm}, 5 \text{ mm}]$, and $[6 \text{ mm}, 7 \text{ mm}]$, respectively.

FIG. 13. Space-time plot of the axial distribution of the mass of particles in the rotating drum of the widest PSD ($\sigma/\mu = 0.7$).

widest lognormal PSD, Fig. 12 presents the 3-D illustration of the distribution of the various particle diameter ranges evaluated at $t = 200$ s of the widest PSD ($\sigma/\mu = 0.7$) investigated. Specifically, the iso-surfaces (i.e., positions with mass fractions of 0.5) of the particle diameter ranges of $d_p \in [0.1 \text{ mm}, 1 \text{ mm}]$, $[2 \text{ mm}, 3 \text{ mm}]$, $[4 \text{ mm}, 5 \text{ mm}]$, and $[6 \text{ mm}, 7 \text{ mm}]$ are represented by red, yellow, blue, and light gray, respectively. As per the radial segregation trends seen earlier (Fig. 9), the smaller and larger particles preferentially segregate radially to the core and periphery, respectively. As for axial segregation, the iso-surfaces of each of the particle diameter range extend almost throughout the drum length, with the shortest iso-surface length for the smallest particles and the longest

for the largest because of the dominance of the largest particles at the end walls. Furthermore, the iso-surfaces of the smaller particles (red and green) are ballooned at the ends due to the enrichment of the particle diameter ranges away from the end walls as the largest particles progressively accumulate at the end walls. Similar to that for radial segregation, the intermediate-sized particles (green and blue) are in between that of the smallest and largest particles axially too. Note that the 3-D segregation trends of the other distributions [Fig. 1(a)] are similar and thus are not presented here in detail for brevity.

The radial segregation induced by the size difference leads to the re-distribution of the different particle species

FIG. 14. Space-time plot of the mass fraction with respect to the total mass in each corresponding section of the different particle diameter ranges of the widest PSD ($\sigma/\mu = 0.7$): (a) $d_p \in [0.1 \text{ mm}, 1 \text{ mm}]$, (b) $d_p \in [2 \text{ mm}, 3 \text{ mm}]$, (c) $d_p \in [4 \text{ mm}, 5 \text{ mm}]$, (d) $d_p \in [6 \text{ mm}, 7 \text{ mm}]$, (e) $d_p \in [8 \text{ mm}, 9 \text{ mm}]$, and (f) $d_p \in [10 \text{ mm}, 11 \text{ mm}]$. Note that the scale adopted for each species is different for clearer representation.

in the transverse plane, while axial segregation leads to redistribution along the axial direction. Figure 13 presents the space-time plot of the total mass of particles along the axial direction, which is similar to that of a binary-size mixture.⁶⁰ Specifically, the values are obtained by dividing the whole drum length into 36 uniform sections and summing the instantaneous mass in each section. In general, axial segregation results in the reduction of mass near the end-walls, which is mainly due to the dominance of large particles and the relative absence of smaller particles to fill the interstices. Furthermore, the slow axial segregation throughout the drum rotation duration negligibly affects the mass distribution of the particles.

To understand the evolution of the axial distribution of each particle diameter range due to axial segregation, Fig. 14 presents the space-time plots of the mass fraction of the various particle diameter ranges (i.e., the mass of the particle diameter range considered with respect to the total mass in each section) of the widest PSD ($\sigma/\mu = 0.7$). It should be noted that the scale adopted for each species is different for better representation in view of the different magnitudes. For the smaller particles

of $d_p \in [0.1 \text{ mm}, 1 \text{ mm}]$ [Fig. 14(a)] and $[2 \text{ mm}, 3 \text{ mm}]$ [Fig. 14(b)], axial segregation gives rise to lower mass fractions near the wall ($|z/Z| > 0.8$) and higher mass fractions away from the wall ($0.6 < |z/Z| < 0.8$) and also clear axial bands after the initial 25 s. For the intermediate particle diameter range of $d_p \in [4 \text{ mm}, 5 \text{ mm}]$ [Fig. 14(c)], the axial bands appear later at $|z/Z| \sim 0.8$ and the particles are uniformly distributed in the axial center ($|z/Z| < 0.4$). For the larger particles of $d_p \in [6 \text{ mm}, 7 \text{ mm}]$, $[8 \text{ mm}, 9 \text{ mm}]$, and $[10 \text{ mm}, 11 \text{ mm}]$ [Figs. 14(d)–14(f)], axial segregation gives rise to the enrichment and reduction of particles at the end walls ($|z/Z| > 0.9$) and the immediately adjacent sections ($0.6 < |z/Z| < 0.8$), respectively, and also axial bands in the axial center. In particular, Fig. 14(e) shows the formation of an axial band of the large particles at the axial center ($z/Z = 0$) that progressively widens with time.

In general, it is observed that (i) axial segregation starts at the onset of drum rotation, instead of after the achievement of radial segregation, which is similar to the binary-size mixture;⁶⁰ (ii) as drum rotation progresses, the axial bands of each particle diameter range become more distinct and wider, which corresponds to the progressive preferential

FIG. 15. Instantaneous axial distribution of the mass fraction of the various different particle diameter ranges of the widest lognormal PSD ($\sigma/\mu = 0.7$): (a) $d_p \in [0.1 \text{ mm}, 1 \text{ mm}]$, (b) $d_p \in [2 \text{ mm}, 3 \text{ mm}]$, (c) $d_p \in [4 \text{ mm}, 5 \text{ mm}]$, (d) $d_p \in [6 \text{ mm}, 7 \text{ mm}]$, and (e) $d_p \in [8 \text{ mm}, 9 \text{ mm}]$.

accumulation of the specific particles and thereby the growth of the bands; (iii) compared to the smaller and larger particles, the intermediate-sized particles of $d_p \in [4 \text{ mm}, 5 \text{ mm}]$ are more uniformly distributed especially in the axial center of the drum [Fig. 14(c)]; and (iv) the axial segregation trend is in accordance with the previous reported work in literature^{34,36} and has been tied to the friction induced by the end walls.^{34,36}

To quantitatively describe the dynamical segregation behavior along the axial direction, Fig. 15 presents the axial distribution profiles of the mass fraction of several particle diameter ranges at various time instants for the widest PSD ($\sigma/\mu = 0.7$) investigated. For the smaller particles of $d_p \leq 5 \text{ mm}$ [Figs. 15(a)–15(c)], axial segregation gives rise to the reduction in the mass fractions near the end walls ($|z/Z| \sim 1$) and the corresponding enrichment leading to peaks in the immediately adjacent sections ($|z/Z| \sim 0.7\text{--}0.8$), while the axial center ($|z/Z| < 0.4$) has more uniform mass fractions. For the larger particles of $d_p \geq 6 \text{ mm}$ [Figs. 15(d) and 15(e)], axial segregation results in the enrichment and reduction of the mass fractions near the end walls and the immediately adjacent sections, respectively. As the drum rotates continuously, several observations on the axial segregation phenomenon are clear: (i) the distinct peaks and troughs at $|z/Z| \sim 0.6\text{--}0.9$ corresponding to the axial bands of propagate towards the axial center; (ii) whereas the smaller [Figs. 15(a)–15(c)] and larger [Fig. 15(e)] particles progressively exhibit greater peaks and troughs, respectively, at $|z/Z| \sim 0.6\text{--}0.9$, the intermediate-sized particles exhibit both peaks and troughs in this region; (iii) several peaks and troughs in the mass fractions of the smallest particles [Fig. 15(a)] start to appear in the axial center ($|z/Z| < 0.4$). The bands will slowly coarsen with time on a time scale of $O(1000)$ revolutions.⁴⁸

V. CONCLUSIONS

Based on the discrete element method (DEM), the particle-scale dynamics of lognormal PSDs in a 3-D rolling-regime rotating drum is numerically studied to understand the effect of the PSD width on the flow characteristics of the granular material in this apparatus. The following conclusions can be obtained:

- (1) The presence of a wide range of particle diameters leads to rapid radial segregation (with the smallest and largest particles preferentially tending toward, respectively, the radial core and periphery, and the intermediate-sized particles are in between) and slow axial segregation (with the largest particles accumulating at the end walls). As the PSD width of the lognormal PSDs increases, the steady-state mixing index increases, the steady-state gyration radius decreases, and the total kinetic energy increases. Within each PSD, the steady-state gyration radius increases monotonically with the particle diameter.
- (2) The streamwise velocity (U_{sx}^*) is similar among the lognormal PSD widths and monodisperse and binary-size mixtures in the active region, but the magnitudes decrease with the PSD width in the passive region. Regardless of the PSD width, nearly 30% of the total

mass and 35% of the total number are in the active region throughout the drum rotation, and the mass fraction in the active region decreases monotonically with the particle diameter. As the PSD width increases, the fraction of the active region depth with respect to the total bed depth increases and the mass fraction in the active region increases.

- (3) The steady-state mass-based exchanging rate of the particles between the active and passive regions is nearly constant, which indicates that this parameter is independent of size-segregation and thus can be treated as a global parameter, and increases with the PSD width. Regardless of the PSD width, the trends of the mass-based active-passive exchanging rate with respect to the particle diameter mimic that of the overall lognormal PSD, while the number-based exchanging rate decreases with the particle diameter.
- (4) The mean SRT in the passive region is nearly two times of that in the active region, and the range of SRT is wider in the passive region. As the PSD width increases, the mean SRT in the active region increases while that in the passive region decreases. Regardless of the PSD width, the SRT in both the active and passive regions increases monotonically with the particle diameter. The shapes of the SRT histograms in both the active and passive regions of the lognormal PSDs are different from that of the monodisperse⁴⁵ and binary-size mixture,⁵⁵ which warrants the need to understand such continuous PSD systems.
- (5) The slow axial segregation throughout the drum rotation duration negligibly affects the mass distribution of the particles, which constantly has a lower mass at the end walls but otherwise uniform axially. The axial segregation of the largest particles to the end walls, the formation of axial bands consisting primarily of a specific particle diameter range, and the band coarsening behavior are in accordance with previous reports on non-monodisperse systems.^{34,36}

The results emanating from this work provide detailed behaviors of lognormal PSDs in a rotating drum, some of which are different from that expected from monodisperse and binary-size mixtures, which highlights the need for further understanding on such ubiquitous systems.

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