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Size-induced axial band structure and directional flow of a ternary-size granular material in a 3-D horizontal rotating drum

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Differences in the material property of the granular material induce segregation which inevitably influences both natural and industrial processes. To understand the dynamical segregation behavior, the band structure, and also the spatial redistribution of particles induced by the size differences of the particles, a ternary-size granular mixture in a three-dimensional rotating drum operating in the rolling flow regime is numerically simulated using the discrete element method. The results demonstrate that (i) the axial bands of the medium particles are spatially sandwiched in between those of the large and small ones; (ii) the total mass in the active and passive regions is a global parameter independent of segregation; (iii) nearly one-third of all the particles are in the active region, with the small particles having the highest mass fraction; (iv) the axial bands initially appear near the end wall, then become wider and purer in the particular species with time as more axial bands form toward the axial center; and (v) the medium particle type exhibits segregation later and has the narrowest axial bandwidth and least purity in the bands. Compared to the binary-size system, the presence of the medium particle type slightly increases the total mass in the active region, leads to larger mass fractions of the small and large particle types in the active region, and enhances the axial segregation in the system. The results obtained in the current work provide valuable insights regarding size segregation, and band structure and formation in the rotating drum with polydisperse particles. *Published by AIP Publishing.* <https://doi.org/10.1063/1.5022861>

I. INTRODUCTION

Granular flow, which exhibits many interesting behaviors, is commonplace in both nature and industry.^{1–4} A particularly intriguing phenomenon is the inevitable segregation induced by differences in the material property (e.g., size and density) of the granular material.^{5–7} Efforts have unsurprisingly been dedicated in this regard, but the understanding of the segregation dynamics and underlying mechanisms remain incomplete.⁸ The rotating drum represents a typical apparatus for the study of granular behavior from a fundamental research perspective to practical application in industry, because of the simple geometry and wide range of flow patterns displayed depending on the operating condition.⁹ Specifically, the flow patterns in the rotating drum can be categorized into six regimes, namely, sliding, slumping, rolling, cascading, cataracting, and centrifuging.¹⁰ An in-depth understanding of the segregation behavior in a simple apparatus like the rotating drum will help to link the fundamental insights into granular flow with improving practical operations. For example, radial segregation has been reported to result in poor contact between the gas phase and the smaller particles in the radial

core, while axial segregation in inconsistent product quality,¹¹ such poor contact between the excipient and active ingredient in the pharmaceutical industry leads to ineffective and even possibly drugs with adverse effects.¹²

During the past several decades, extensive experimental activities focused on the segregation phenomenon of granular flow in the rotating drum have been conducted. The experimental work by Gupta *et al.*¹¹ in a three-dimensional rotating drum with binary-size mixtures showed that a necessary though not sufficient condition for axial segregation was a difference in the free surface angles of the two constituents. Baumann *et al.*¹³ experimentally studied the size segregation of a binary-size mixture in a two-dimensional rotating drum and found that segregation persisted even if the two constituents were very similar. With respect to the axial bands, Hill *et al.*¹⁴ experimentally studied the evolution of the axial bands in the rotating drum and found that the underlying mechanisms for the pattern evolution may originate in the bulk of the material beneath the avalanching surface. Furthermore, Choo *et al.*¹⁵ experimentally studied the initial growth and saturation of patterns of axial segregation of a binary-size granular mixture in a rotating drum and found that the wavelength of the axial band was largely independent of the rotation rate. By experimentally tracking the trajectories of differently sized particles, Ding *et al.*¹⁶ studied the granular segregation in the transverse

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plane of a rotating drum and reported that both monodisperse and binary-size mixtures exhibited active and passive regions for the rotating drum operating in the rolling regime. Kuo *et al.*¹⁷ experimentally studied the effects of operating parameters (e.g., fill level and particle size ratio) on the axial bandwidth of a binary-size mixture in the rotating drum and revealed that (i) the bandwidth dimensionalized with respect to the diameter of small particles decreased with the increase of the fill level and (ii) the dimensionless bandwidth exhibited a minimum value at a specific size ratio of rigid particles. Considering radial and axial segregation simultaneously, Kuo *et al.*¹⁸ experimentally found that the axial and radial segregation patterns were coupled within the bed, leading to new patterns different from the axial band and radial core patterns like the “cross” pattern, the “band-core-in-core” pattern, and other geometric patterns. The experimental work of Juarez *et al.*¹⁹ for binary-size particles concluded that the bandwidth for both the small and large particles scaled with the drum diameter. Beyond binary-size mixtures, Alizadeh *et al.*²⁰ experimentally tracked the particle trajectory and observed similar velocity profiles and residence times for monodisperse and polydisperse systems. The experimental work of Tilo *et al.*²¹ found that the unidirectional flow between the axial bands is driven by small differences in the size of the small beads at the band edges. Recently, Windows-Yule *et al.*¹² highlighted that the axial segregation phenomenon cannot be explained by a single mechanism.

Complementary to the experimental approach, numerical modeling has been a popular tool in the past two decades due to the advancement of computational capacity. The two key approaches for modeling particulate flow are the two-fluid model (TFM)²² and the discrete element method (DEM)^{23–25} which are different in terms of the scale at which the particles are resolved. Because DEM provides better resolution with respect to tracking the motion of each particle, the study of segregation behavior in granular flow has largely relied on DEM despite the much greater computational load required. By means of the DEM, Dury and Ristow²⁶ numerically studied the segregation dynamics of a binary-size mixture in the rotating drum and found that size segregation occurs even for small differences in particle sizes for a drum operating in the continuous flow regime. Subsequently, Rapaport²⁷ numerically demonstrated that the results can qualitatively reproduce the axial segregation features observed experimentally for a partially filled rotating drum containing a binary-size mixture. Taberlet *et al.*²⁸ reported both experimental and DEM simulation results on the size segregation of a binary-size mixture, indicating that a smooth velocity transition between the segregated small and large particles exists in the radial direction, and the axial segregation pattern is strongly influenced by radial segregation. Then, Chen *et al.*^{29,30} found using DEM that the mechanism triggering the axial band formation is the axial flow due to friction at the end walls. Alizadeh *et al.*³¹ found that Young’s modulus and static friction coefficients are influential parameters on the particle dynamics in the DEM simulation of a rotating drum operated in the rolling regime.

Despite much knowledge gained to date from the experimental and numerical reports on the granular segregation

phenomenon, most have focused on binary-size mixtures, which may have limited applicability to the prevalent polydisperse size distributions, since behavioral differences between binary-size mixtures and polydisperse size distributions have been clearly observed in fluidized bed systems.^{32–35} To attempt to bridge this gap, this study is targeted at a ternary-size mixture, which would advance the collective knowledge on binary-size mixtures by shedding light on the effect of an additional component on segregation. Past studies have provided some understanding on the ternary-size mixture in heap formation,³⁶ sandpile,³⁷ hopper^{38,39} and vibrated systems.⁴⁰ The highlights include the observations that small, medium, and large grains are layered from the bottom to the top in the heap formation,³⁶ and that the ratios of the repose angles of the three particle types significantly influence the pattern formation in a sandpile.³⁷ Furthermore, ternary granular mixtures have practical significance too, e.g., the gasification of rice husk can be improved by adding silicon sand and coal;⁴¹ the performance of the iron-making blast furnace can be improved by charging the fine particles on top of the medium particles to avoid undesired percolation, and large particles to the furnace center to form a strong central gas flow with smooth solid burden discharging;³⁹ the ternary diethylamine–chloroform–methanol mixture in the separation and distillation industry that gives the unusual univolatility curve.⁴² For the rotating drum, ternary-size mixtures received comparatively less attention than binary-size mixtures, although one of the first reports on the axial segregation phenomenon nearly 80 years ago in the rotating drum was based on a ternary-size limestone mixture.⁴³ By means of DEM, Rapaport⁴⁴ numerically studied the axial segregation of a ternary mixture in a rotating drum and found that the axial band formation is such that the medium-size particles tend to be located between the bands of small and large particles. The experimental work by Hajra and Khakhar⁴⁵ demonstrated that the ternary mixtures consisting of particles of different size and density segregate depending on whether the driving forces due to size and density complement or oppose each other. The DEM work on a ternary-size mixture in a 2-D rotating drum performed by Pereira and Cleary⁴⁶ indicated that the segregation between the large and small particles is increased by the presence of the medium particle type. Despite the understanding to date on granular segregation in the ternary-size mixture, questions that remain unaddressed include details regarding the segregation progression, the band structure, the axial dispersion and the dynamical response of the different particle types to segregation.

Accordingly, this work is targeted at (i) elucidating the role of the medium-size particle type in the axial band dynamics and (ii) evaluating if the axial segregation phenomenon of the ternary-size system is similar to that of the binary-size system with respect to both the active and passive regions. The current work numerically simulates the motion of the ternary-size granular mixture in a three-dimensional rotating drum operating in the rolling flow regime to study the dynamical segregation behavior, the band structure, and formation by means of the discrete element method (DEM). Specifically, the rolling flow regime characterized by the co-existence of the active and passive regions is widely adopted in the industry since it provides for good mixing behavior and enhanced heat transfer

performance,⁴⁷ making the current study meaningful and valuable for the design, operation, and even the optimization of the system in the practical operation. The overall dynamical segregation behavior of the three particles types is first analyzed, followed by quantification of the segregation intensity. Then, the spatial distributions of the mass of each particle type in both the transverse and axial direction are investigated. Finally, the axial directional flow of each particle type underlying the axial band formation and dynamics is examined.

II. NUMERICAL METHODS

In the current work, the trajectory of every particle is tracked by means of the discrete element method (DEM) in the Lagrangian framework. For each particle, the governing equations for its translational and rotating motions are based on Newton's second law after obtaining the force experienced. Due to the large solid to gas density ratio and also the weak flow of the gas phase, the total force exerted on a particle in the current study consists of the gravity and the collisional force between the colliding particle-particle or particle-wall pair. Equations governing the motion of a specific particle can be formulated as

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

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

where m_i , I_i , $\mathbf{v}_i$, and ω_i represent, respectively, the mass, the moment of inertia, the translational, and the angular velocity of particle i ; $\mathbf{g}$, N_c , t , $\mathbf{F}_{c,ij}$, and $\mathbf{M}_{ij}$ are, respectively, the gravitational acceleration (9.8 m/s²), the total number of particles and walls colliding with the current particle, the time instant, the collision force, and the torque generated between the colliding pair of particle i and particle j .

In the current work, the particles are assumed to be rigid spherical ones that do not deform, fracture, or fragment, and thus the collision procedure between a colliding pair is modeled through the soft-sphere collision model evaluated based on material properties. For deformable particles, the finite-discrete element method (FDEM)⁴⁸ can be used. Specifically, the soft-sphere collision model initially proposed by Cundall and Strack⁴⁹ is adopted to treat the collision process, since the key feature of this model is the employment of elastic collision, viscous damping, friction, and sliding effects to simulate the collision event. Furthermore, the model can treat multiple collisions of neighboring particles in the dense granular flow, which is extremely critical for the granular motion in the current system.

In the current work, the collision force between colliding particles is decomposed into the tangential ($\mathbf{F}_{ct,ij}$) and normal ($\mathbf{F}_{cn,ij}$) components along, respectively, the tangential and normal directions of the colliding pair. The equations for evaluating the colliding force can be formulated as

$$\mathbf{F}_{c,ij} = \mathbf{F}_{cn,ij} + \mathbf{F}_{ct,ij}, \quad (3)$$

$$\mathbf{F}_{cn,ij} = k_{n,ij} \delta_{n,ij} \mathbf{n} + \gamma_{n,ij} \mathbf{v}_{n,ij}, \quad (4)$$

$$\mathbf{F}_{ct,ij} = \min\{(k_{t,ij} \delta_{t,ij} \mathbf{t} + \gamma_{t,ij} \mathbf{v}_{t,ij}), \mu \mathbf{F}_{cn,ij}\}, \quad (5)$$

where $\mathbf{n}$ and $\mathbf{t}$ stand for, respectively, the normal unit vector and the tangential unit vector. When the sliding occurs between the colliding particles, the friction coefficient μ is adopted to evaluate the tangential collision force. The stiffness coefficient (k) and the damping coefficient (γ) can be determined from Young's modulus Y , Poisson ratio ν , and the restitution coefficient e as follows:

$$k_{n,ij} = \frac{4}{3} Y^* \sqrt{R^* \delta_{n,ij}}, \quad (6)$$

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

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

$$\gamma_{t,ij} = 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_{t,ij} m^*}, \quad (9)$$

where β is the damping ratio ($\beta = \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}}$); Y^* , G^* , R^* , and m^* are the equivalent Young's modulus of the solid phase ($\frac{1}{Y^*} = \frac{(1-\nu_i^2)}{Y_i} + \frac{(1-\nu_j^2)}{Y_j}$), the equivalent shear modulus of the solid phase ($\frac{1}{G^*} = \frac{2(2+\nu_i)(1-\nu_i)}{Y_i} + \frac{2(2+\nu_j)(1-\nu_j)}{Y_j}$), the equivalent radius of a particle ($\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j}$), and the equivalent mass of a particle ($\frac{1}{m^*} = \frac{1}{m_i} + \frac{1}{m_j}$), respectively; and S_n ($S_{n,ij} = 2Y^* \sqrt{R^* \delta_{n,ij}}$) and S_t ($S_{t,ij} = 8G^* \sqrt{R^* \delta_{n,ij}}$) are, respectively, the normal and tangential stiffness.

To track the velocity and position of the particles, the governing equations of solid motion have to be integrated with a time step. The choice of the time step hinges on the balance between a large time step giving rise to inaccurate predictions of the flow process and a small time step needing too much computational resource and time. In the current work, the time step is chosen based on the criterion that it should be smaller than the critical characteristic time,⁵⁰ which has a relationship with the particle properties (i.e., the density ρ_p , the radius R , Young's modulus Y , and Poisson ratio ν) and can be formulated as

$$t_r = \frac{\pi R}{0.1631\nu + 0.8766} \sqrt{\frac{2\rho(1+\nu)}{Y}}. \quad (10)$$

III. COMPUTATIONAL SETUP

Figure 1 presents the geometrical configuration of the three-dimensional rotating drum studied in the current work.

FIG. 1. The geometrical configuration of the three-dimensional rotating drum investigated in the current work.

The simulation is carried out in the Cartesian coordinate system with the origin denoted as the geometry center of the cylinder, the y -direction being opposite to the gravitational acceleration, the x -direction being perpendicular to the y -direction in the transverse plane, and the z -direction being along the drum length and perpendicular to both the x - and y -directions. The drum diameter in the transverse plane (x - y) and the length along the axial direction (z) are 0.24 m and 0.72 m, respectively. The rotating speed of the drum around its axis is 11.6 rpm (i.e., 5.1724 s per revolution), which classifies it under the rolling regime. This rotating speed is chosen to be the largest of the four different rotating speeds studied in the experimental work of Alizadeh *et al.*,²⁰ for diminishing the solid residence time in both the active and passive region, enlarging the solid circulation rate of the granular phase,⁵¹ and enhancing the axial flow,⁵² so as to achieve axial segregation within a shorter physical time in view of the substantial computing load of DEM.

The particles studied in the current work have a density of 2500 kg/m³. The ternary-size granular mixture consists of particles with three different particle diameters (d_p), namely, 6 mm (large), 4.5 mm (medium), and 3 mm (small). A total number of 20 676, 49 015, and 165 430 large, medium, and small particles are involved in the current work, which gives a mass ratio of these three particle types as 1:1:1. Initially, all the particles are randomly generated in the whole domain then allowed to fall freely to form an initially well-mixed packed bed with a volumetric fill level of 35% in the rotating drum; the fill level of 35% is similar to that in Alizadeh *et al.*,^{20,31} in which only one fill level was reported. To reduce the computational time, a total of 32 cores are run in parallel to track the particle motion at a time step of 1×10^{-6} s, which is smaller than the critical time step (i.e., 4.05×10^{-5} s for the smallest particle diameter of 3 mm) from Eq. (10).⁵⁰ The simulation is run on our computing cluster, in which each node consists of 2 Intel Xeon E5-2660 CPUs and a total number of 32 GB RAM. The total simulation time is 280 physical seconds, which corresponds to nearly 54.1 revolutions of the rotating drum and took a computational time of 82 days. Details related to the particle property and numerical settings are listed in Table I.

TABLE I. Details regarding the physical and numerical parameters adopted in the current simulation.

Drum geometry	
Diameter (m)	0.24
Axial length (m)	0.72
Rotating speed (rpm)	11.6
Solid property	
Density (kg/m ³)	2500
Diameter (mm)	6.0, 4.5, and 3.0
Young's modulus of granular material (Pa)	1.0×10^8
Poisson ratio of granular material (-)	0.24
Restitution coefficient between particle-particle pair (-)	0.97
Restitution coefficient between particle-wall pair (-)	0.85
Friction coefficient between particle-particle pair (-)	0.30
Friction coefficient between particle-wall pair (-)	0.35

The selection of the particle properties is based on the numerical work of Alizadeh *et al.*,⁵⁰ in which the sensitivity of the DEM results to these parameters adopted is discussed. In the current work, similar to the numerical parameters adopted in the literature,^{31,53,54} the Young's modulus is chosen to be smaller than the experimental data for the purpose of elongating the duration of a collision pair and thus allowing for a larger time step.³¹ The Poisson ratio is chosen to be the same as the experimental data reported by Alizadeh *et al.*³¹ The restitution coefficient between the particle-particle and particle-wall collision pair is adopted based on the data reported in the literature⁵⁵ and the experimental measurement,³¹ respectively. Moreover, the friction coefficient between the particle-particle interaction pair is selected following the parameters adopted in the literature,⁵⁴ while the friction coefficient between the particle-wall interaction pair is chosen to be 0.35, which follows the suggestion of Alizadeh *et al.*³¹

The model validation has been conducted in our previous report.⁵⁶ Specifically, the validation is achieved by comparing the numerical results obtained for a 3-D rotating drum consisting of monodisperse particles ($d_p = 3$ mm) with experimental results.²⁰ Figure 2 presents the comparison of the numerical result and experimental data²⁰ of the time-averaged streamwise (i.e., parallel to the particle bed surface) velocity of the solid phase (U_{sx^*}). Clearly, the radial distribution (along the AB line in the inset figure) of U_{sx^*} obtained numerically shows the same trend as the experimental one,²⁰ specifically in that U_{sx^*} linearly increases in both the active and passive regions. Moreover, quantitative agreement is also observed. In addition to the radial distribution of U_{sx^*} , the angle of repose in the central region and end-wall region, the active region depth, and the time-averaged radial velocity of the particles also agree well with the experimental data;²⁰ more details can be found in our previous work.⁵⁶ Collectively, the numerical results agree well quantitatively with the experimental data,²⁰ confirming the reliability of the model and the corresponding numerical parameters. Compared with our previous report,⁵⁶ the same particle properties and numerical settings as the validated model⁵⁶ are used in this work, except that a ternary-size

FIG. 2. Comparison of the time-averaged streamwise velocity of the solid phase (U_{sx^*} , m/s) along the radial direction (AB line in the inset) in the rotating drum with monodisperse particles of 3 mm. The inset figure represents the vector plot of the time-averaged velocity (U_s , m/s) in the central axial slice of the rotating drum.⁵⁶

mixture and a longer drum (twice as long) are examined. Specifically, the ternary-size mixture consists of three different particle diameters, namely, 3 mm, 4.5 mm, and 6 mm; coarser constituents are chosen to reduce the total number of particles and thereby the computational resources required.

IV. RESULTS AND DISCUSSION

A. Overall size-segregation

For the binary-size mixture, the numerical work of Chen *et al.*³⁰ has presented some information regarding the internal segregation structure of the rotating drum. However, no information on the spatial evolution of the internal segregation structure of the ternary-size granular mixture is available. To illustrate the overall segregation dynamics of the mixture in the rotating drum, the iso-surfaces denoting positions with mass

fractions of 0.5 for the large (red), medium (green), and small (blue) particles are presented in Figs. 3(a), 3(c), 3(e), 3(g), and 3(i) at progressing time steps. Furthermore, the corresponding instantaneous snapshots of the particle distribution at each time instant are displayed in Figs. 3(b), 3(d), 3(f), 3(h), and 3(j). Initially within 4 s [Figs. 3(a) and 3(b)], radial segregation is already apparent, at least in part due to the kinetic sieving effect (i.e., small particles enter the interstices of the large particles),⁵⁷ which results in the size-induced radial segregation of the small particles toward the radial center [Fig. 3(b)] and large particles toward the radial periphery [Fig. 3(a)]. Comparing Figs. 3(b) and 3(d), it is clear that the small particles are present at the bed surface at $t = 4$ s [Fig. 3(b)] but are scarce at $t = 20$ s [Fig. 3(d)], which indicates that radial segregation is incomplete at 4 s. At $t = 20$ s, a radial core of small particles spans the entire drum length [Fig. 3(c)] and few small particles are present in the radial periphery of the drum

FIG. 3. 3-D illustration of the dynamical segregation behavior of the ternary-size granular mixture in the rotating drum. Iso-surface with a threshold mass fraction of 0.5 for all the three different particle types at the time instant of 4 s (a), 20 s (c), 40 s (e), 200 s (g), and 280 s (i), where the red, green, and blue represent the large, medium, and small particles, respectively. The corresponding instantaneous distribution of the three particle types are presented in $t = 4$ s (b), $t = 20$ s (d), $t = 40$ s (f), $t = 200$ s (h), and $t = 280$ s (j), where the red, green, and blue similarly represent the large, medium, and small particle types, respectively.

[Fig. 3(d)]. Simultaneously, the large particles segregate to the radial periphery and the medium segregate to in between the small and large particles [Fig. 3(c)]. At $t = 40$ s, the sandwiching of the medium particles in between the large and small becomes more obvious both radially and axially [Fig. 3(e)], which is in accordance with the previous reports.^{45,46} Axially, due to friction induced by the end walls, bands consisting predominantly of one particle type start to form, with large particles near the end-walls, followed by medium then small particles. As time progresses, the axial segregation effect becomes more evident in Figs. 3(g) and 3(h), with some small particles clearly at the bed surface where the axial bands of small particles form and large particles dominating at the end-wall [Fig. 3(h)]. At axial positions without the axial bands, the radial core of small particles is engulfed radially by the medium followed by the large particles [Fig. 3(g)]. At $t = 280$ s [Figs. 3(i) and 3(j)], the axial bands consisting almost wholly of one particle type are formed, with the distinct ones being the large ones right at the end walls followed by the medium then small, while other less distinct axial bands of small particles are seen near the axial center of the drum. The axial symmetry is clear. Comparing Fig. 3 with that of the binary-size system,⁵⁸ the additional medium particles in the ternary-size system act as a spatial barrier to segregate the small and large particles.

B. Cross-sectional size-segregation

For the rotating drum operating in the rolling regime, two regions with significantly different flow characteristics are well acknowledged, namely, the rapid descending flow in the active region and the slower rotation with the bottom wall in the passive region. The boundary between these two regions can

be identified as positions with zero streamwise (i.e., parallel to the bed surface) velocity, that is, where the particle motion changes direction.⁵⁹ The demarcation of the two regions allows for the evaluation of the characteristics in each.

Figure 4 presents the number fraction distribution plots of the large [Fig. 4(a)], medium [Fig. 4(b)], and small [Fig. 4(c)] particles in the axial center plane ($z/Z = 0$) of the rotating drum, where each black line stands for the active-passive interface. Radial segregation results in the general preferential congregation of the large [Fig. 4(a)] and small [Fig. 4(c)] particles, respectively, to the radial periphery (i.e., near the drum wall and bed surface) and core, although some small particles are present at the bed surface [Fig. 4(c)] due to the cascading of the small particles after being lifted by friction with the drum wall. As for the medium particles [Fig. 4(b)], the highest concentrations are observed to be in between those of the large and small, which is unique to the ternary-size mixture as compared to the binary-size one.⁵¹ Interestingly, while the medium particles are almost absent in the radial center dominated by the small particles, they are prominently present in the radial periphery dominated by the large particles. This indicates that the radial segregation between the small and medium particles is more extensive than that between the large and medium particles.

C. Extent of segregation

To quantitatively evaluate the overall segregation, a mixing index Γ can be defined to quantify how well-mixed or segregated the different particle types are

$$\Gamma = \frac{\zeta}{\zeta_{mix}}, \quad (11)$$

FIG. 4. Number fraction distribution of each particle type in the central slice ($z/Z = 0$) of the rotating drum, where each black line stands for the active-passive interface: (a) large particles; (b) medium particles; and (c) small particles.

where ζ and ζ_{mix} stand for the instantaneous mixing extent and the mixing extent of a well-mixed system, respectively. Hence, the mixing index Γ ranges from 0 to 1, which corresponds, respectively, to a completely segregated system and a completely well-mixed system. To evaluate the mixing extent ζ , the whole system is divided into M sample cells^{60,61}

$$\zeta = \sum_{i=1}^M (n^i \sum_{j=1}^k c_j^i \ln c_j^i), \quad (12)$$

where n^i , c_j^i , and k stand, respectively, for the number fraction of the total particles in the current sample cell i to the total particles in the whole system, the number fraction of component j to the total number in the current cell i , and the total number of species considered.

In the current work, to evaluate the mixing index (Γ), the whole drum is enclosed by a cube with dimensions of 0.24 m, 0.24 m, and 0.72 m along the x , y , and z directions, respectively, and then further divided into smaller cubic grids with equal dimensions of 12 mm on all three sides. The evolution of the mixing index (Γ) of the ternary-size granular mixture is illustrated in Fig. 5. In general, the size-induced segregation results in the continuous decrease of Γ from 1 (initially completely well-mixed) with time, with the decrease being rapid within the first 40 s due to the fast radial segregation, then subsequently more gradual due to the slower and longer lasting axial segregation. The steepest decrease in the Γ values (and thereby the highest Γ values) is between the large and small particles, which indicates the most extensive segregation, whereas the gentlest decrease (and thereby the lowest Γ values) is between the large and medium particles, which indicates the least extensive segregation. This agrees with the cross-sectional segregation plots presented in Fig. 4. Notably, the significantly lower Γ values for the large and small particles relative to those of the whole system demonstrate that the presence of the medium particle type more extensively segregates the large and small particle types, which is due to the medium particle type acting as a spatial barrier, as discussed in Fig. 4.

FIG. 5. Time evolution of the mixing index of the ternary-size mixture in the rotating drum.

For the current drum investigated, a semi-empirical law for the mixing index can be proposed, based on the observation that the mixing index (Γ) between any two constituents in the ternary mixture can be well-approximated by the corresponding diameter ratio. Specifically, at $t = 280$ s, the mixing indices (Γ) of the two constituents of medium-large, small-large and small-medium are, respectively, 0.8, 0.37, and 0.69, which are interestingly similar to the diameter ratios of, respectively, 0.75, 0.5, and 0.66. This indicates that the mixing index between any two constituents in the ternary mixture in the rolling-regime rotating drum can be approximated by

$$\Gamma_{ab} = \frac{d_a}{d_b}, \quad (13)$$

where d_a and d_b stand for the particle diameter of smaller and larger particle type of the two constituents, respectively. In view of the widespread application of the rotating drum in industrial processes, further exploration of the effects of the important operating parameters (e.g., rotating speed, particle size ratio, fill level, and drum diameter) on the mixing index, and also the validation and improvement of the semi-empirical law proposed above will be valuable for the design and optimization of the system.

D. Mass distribution in the active and passive regions

Quantifying the mass distribution of the ternary-size mixture in the active and passive regions of the rotating drum provides insights regarding the mass loading in the drum and also the dynamical response of different particle types to the size-induced segregation. Figure 6(a) presents the evolution of the mass fraction of all the particles distributed in the active and passive regions. Other than the initial 20 s, the mass fractions of the particles distributed in these two regions are nearly constant with time, indicating the lack of influence by both the radial and axial segregation. This indicates that the mass fraction of all the particles in each region can be treated as a global parameter that is independent of the segregation phenomenon. Quantitatively, the mass fraction of the particles in the passive region is 72.2%, which is nearly three times of that in the active region (27.8%). Compared with the binary-size mixture,⁶² the addition of medium particle type slightly increases and decreases of the mass distribution of all the particles distributed, respectively, in the active and passive region.

Figure 6(b) presents the evolution profiles of the mass fraction of each particle type (i.e., the mass of each particle type in the region with respect to the same particle type in the whole drum) in the active region. Specifically, the evolution profiles of the mass fraction of each particle type in the passive region can be inferred. The segregation phenomena clearly influence the mass distribution of each particle type distributed in the two regions. The mass fractions of the large and small particle types are, respectively, the lowest and highest in the active region, and vice versa in the passive region due to radial segregation (Fig. 4). Notably, the change in the mass fraction is most drastic for the small particle type at the initial phase, with a steep increase in the active region and a

FIG. 6. Evolution of mass fraction in the active and passive regions: (a) all the particles; (b) each particle type in the active region.

corresponding decrease in the passive region, indicating a significant transfer of small particles from the passive region into the active region. As axial segregation ensues, the direction of transfer of the small particles reverses as the axial bands form. On the contrary, the large and medium particle types first transfer from the passive to the active regions during radial segregation, before transferring from active to passive regions during axial segregation. It should be noted that the mass fraction of the medium particles lies in between that of the large and small particles and is least affected by the segregation, which agrees with Figs. 3 and 4 in that the medium particles exhibit behaviors intermediate to that of the large and small ones.

The time-averaged mass fractions of the three particle types (related to the total mass of each particle type) distributed in the active region of the rotating drum are, respectively, 25.9%, 27%, and 30.7% for the large, medium, and small particles, which indicates that roughly one-third of the mass of each particle type lies in the active region due to its relatively lower volume. Regarding particle type, the mass fraction of each particle type in the active region is the highest for the large particle type followed by the medium particle type and finally the small particle type. In our previous work on a binary-size mixture of 3 mm and 6 mm,⁶² the time-averaged mass fractions are, respectively, 25.83% and 29.23%. Thus, compared with the binary-size mixture,⁶² the presence of the medium particle type in the ternary-size mixture slightly increases and decreases the mass fraction of, respectively, the large ($d_p = 6$ mm) and small ($d_p = 3$ mm) particle types in the active region.

E. Axial mass distribution

The above discussion unveils the effect of radial segregation on the mass distribution in the transverse plane, while the current attempts to investigate the effect of axial segregation on the spatial distribution of the three particle types in the rotating drum. Figure 7(a) presents the space-time plot of the total mass while Fig. 7(b) the quantitative axial distribution at various time instants. Specifically, this axial distribution is obtained by first dividing the axial drum length into 36 equal sections, followed by evaluating the total mass of all the particles in each section at every time instant. Figure 7(a) shows that the axial segregation phenomenon reduces the total mass near the end walls very quickly such that the total mass near the wall region ($|z/Z| > 0.9$) is smaller than the other regions [Fig. 7(b)]. The lower total mass in the end-wall region is mainly because of the extensive congregation of the large particles and the relative absence of other particle types (Fig. 7), which leads to a relatively lower packing density.⁶³ Away from the end walls ($|z/Z| < 0.9$), the total mass values are distributed relatively more uniformly axially [Figs. 7(a) and 7(b)].

To further understand the axial segregation behavior in the drum, Fig. 8 presents the space-time plots of the mass fractions of the three particle types distributed along the axial direction, while Fig. 9 quantitatively plots the axial distribution profiles of the mass fractions at several time instants. Initially, all three particle types are uniformly distributed along the drum length due to the initial homogeneous mixture. Then, axial segregation leads to obvious changes of the mass fractions of

FIG. 7. Total mass in the rotating drum versus dimensionless axial position (z/Z , where z and Z , respectively, stand for the axial position assessed and the half length of the drum such that $z/Z = 0$ and 1 refer, respectively, to the axial center and end wall): (a) space-time plot and (b) axial distribution at various time instants.

FIG. 8. Space-time plot of the mass fraction of the three particle types: (a) large particle type; (b) medium particle type; and (c) small particle type.

all three particle types as axial bands dominated by a single particle type form. Several key observations in Figs. 8 and 9 related to the axial segregation phenomenon are described as follows. First, although the radial segregation is clearly evident at the time instant of $t = 20$ s [Fig. 3(c)], the axial segregation is comparatively slower, as indicated by the approximately uniform axial distribution of the mass fraction of the three particle types in Figs. 8 and 9(a). In particular, only a slight increase and decrease of, respectively, the large and small particle types can be observed at the end walls ($|z/Z| > 0.9$) in Fig. 9(a), while the medium particles are not affected even at the end walls. Second, compared with the large and small particle types, the axial band formation of the medium particle type occurs later [after nearly 25 s; Fig. 8(b)]. Third, axial segregation becomes clearer at the end walls at the time instant of $t = 40$ s [Figs. 9(b) and 8], with the significantly different mass fractions between the large and small particles near the end walls ($|z/Z| > 0.8$), and the mass fraction of the medium particles deviating from the reference line also at $|z/Z| > 0.8$. The peak mass fraction values of each particle type indicate that the large particles form the most distinct (i.e., highest mass fraction) axial bands at the end walls, followed adjacently by the least distinct (i.e., lowest mass fraction) axial bands of medium particles, then axial bands of small particles. The mass fractions of these axial bands near the end walls increase with time [Figs. 9(a)–9(e)] such that the mass fractions of the large and small particles in the respective axial bands are 0.8×280 s [Fig. 9(e)], while that of the medium particles is lower at about 0.55. Third, additional bands of large and small particle types start to become distinct in the axial center region at about 100 s [Figs. 8(a), 8(c), and 9(c)], but the medium particle type does not exhibit any clear axial band in the axial center yet at this time. The alternative axial bands of large, medium, and small particles in the axial center are clear by

200 s [Figs. 8(a), 8(c), and 9(d)], and the mass fractions in the bands grow with time [Fig. 9(e)]. Fourth, the axial bands widen with time due to the progressive accumulation of each particle type with time, with the widths of each type decreasing from the end walls to the axial center. Fifth, at the end of 280 s, four distinct axial bands are formed for each particle type, as indicated by peaks with mass fractions of greater than 0.4 in Fig. 9(e). The axial bands of large particles are formed at approximately $|z/Z| = 1$ and 0.5, that of medium particles at 0.85 and 0.65, and small ones at 0.75 and 0.25. It should be noted that the axial distributions of the mass fractions of the three particle types shown in Fig. 9 are symmetrical about the central axial slice of $z/Z = 0$; this is because the wall-induced axial segregation initially starts in the end-wall regions and then propagates toward the axial central region from the two ends of the drum, which results in the symmetrical distribution pattern of the solid distribution about $z/Z = 0$. Therefore, the positions of the axial bands are such that the large particles are at the end walls, followed by the medium particles, then the small particles, then the medium, large, and finally small particles.

In general, the axial segregation initially occurs near the end walls and then progresses toward the central part of the drum with the appearance of a traveling wave pattern. For the ternary-size mixture, the bands of the large and small particle types have higher mass fractions (i.e., more distinct and purer) relative to that of the medium one. The axial bands of the medium particle type form the latest in time, and the band-widths seem to be narrower. Compared with the binary-size system,⁶² the presence of the medium particle type does not change the band number of the small and large particle types, but increases the peak mass fraction values of the bands of the small and large particle types due to the more extensive segregation as observed earlier.

FIG. 9. Comparison of the mass fraction of the three particle types distributed along the drum length at several time instants: (a) 10 s; (b) 40 s; (c) 100 s; (d) 200 s; and (e) 280 s. The black dashed line is a reference line representing a mass fraction of 0.3333.

F. Temporal mass distribution

Axial segregation results in the re-distribution of different particle types along the axial length of the rotating drum. To evaluate the dynamic evolution of the axial mass distribution of the different particle types, the whole drum is similarly divided into 36 equal sections along the axial direction, followed by evaluating the total mass of all the particles of each particle type at each time instant. In view of axial symmetry and the more prominent changes near the end walls (Figs. 8 and 9), Fig. 10 presents the evolution of the mass distributions of the three particle types in the axial regions near the end walls ($-1 < z/Z < -0.5$) of the rotating drum. Several observations worth highlighting are that (i) the mass trends are not constant but continuously evolve over the whole simulation duration due to the on-going axial segregation; (ii) axial segregation starts right from the beginning and lasts over the entire time range, instead of occurring only after radial segregation, as indicated by the change in the mass values of the large and small particles from $t = 0$; (iii) axial segregation influences the

mass distribution of the large and small particles only within a limited region ($-1 < z/Z < -0.83$) within the initial 120 s and has negligible influence on the medium particle type within the initial 80 s; and (iv) the trends of the large and small particles are opposite, and that of the medium particles mimic the large or small at different axial positions.

G. Directional flow of particles underlying the band formation

For the formation of axial bands consisting predominantly of one particle type, biased axial directional movements of the particles of different types are needed. Accordingly, the axial directions of the three particle types into each axial section are studied by first uniformly dividing the drum into 36 axial sections, followed by monitoring the total mass of each particle type being transported into each region from the left and the right. Due to the more extensive axial segregation near the end walls, the analysis is carried out in the region near the wall of $-1 < z/Z < -0.78$. Figure 11 presents the change in total

FIG. 10. Evolution of the mass of three particle types in the different axial regions ($-1 < z/Z < -0.5$) of the rotating drum: (a) large particles; (b) medium particles; and (c) small particles.

mass and axial directional of each particle type in each axial section. Each of the four rows represents the axial positions of $-1 < z/Z < -0.94$, $-0.94 < z/Z < -0.89$, $-0.89 < z/Z < -0.83$, and $-0.83 < z/Z < -0.78$, while each of the three columns represent the large [(a), (d), (g), and (j)], medium [(b), (e), (h), and (k)], and small [(c), (f), (i), and (l)] particles. It should be noted that the vertical axis of Fig. 11 represents the mass transportation of a specific particle type to the left and right region, which is normalized by the initial mass of this particle type in the corresponding region. Near the left end-wall [$-1 < z/Z < -0.94$; Figs. 11(a)–11(c)], mass cannot be transferred from the left due to the physical barrier, so mass can only be transferred rightwards. In this region, the total mass of large [Fig. 11(a)] and small [Fig. 11(c)] particles continuously increases and decreases, respectively, with time, which corresponds to the congregation of large particles to form the axial band and dispelling of small particles. The variations of the large and small particles are the steepest in the first 60 s, while that of the medium particles, on the contrary, is relatively more drastic only after the first 60 s but the changes in magnitudes are minimal compared to the other two particle types. This implies extensive segregation of the large and small particles within the first 60 s, after which all three particle types partake in the less extensive axial segregation of large particles toward the end walls while medium and small particles away from the end walls. In the adjacent region of $-0.94 < z/Z < -0.89$ [Figs. 11(d)–11(f)], the particles transferred from the left region expectedly is the same as that of the particles transferred to the right region in Figs. 11(a)–11(c), but the trends of the total mass of all particle types are opposite to that in Figs. 11(a)–11(c). The decrease in the total mass of the large

particles [Fig. 11(d)] is due to the preferential movement of the large particles toward the end wall [Fig. 11(a)]. Meanwhile, the total mass of the medium particles decreases slightly initially ($t < 60$ s) due to the significant increase of small particles [Fig. 11(f)] resulting from the extensive segregation at the wall [Fig. 11(c)], but starts to increase as they become increasingly dispelled from the end wall region [Fig. 11(b)], which leads to the formation of an axial band of medium particles. As for the small particles [Fig. 11(f)], they initially ($t < 60$ s) congregate in this region ($-0.94 < z/Z < -0.89$) due to the extensive segregation away from the end wall, but the total mass starts to decrease as the rightward movement increases with time. Further from the wall at $-0.89 < z/Z < -0.83$ [Figs. 11(g)–11(i)], the mass of both large [Fig. 11(g)] and medium [Fig. 11(h)] particles decreases due to the increased transfer of the particles toward the axial center, while that of small particles increases due to the increased transfer from the wall, which leads to the formation of an axial band of small particles [Fig. 11(i)]. Still further from the wall at $-0.83 < z/Z < -0.78$ [Figs. 11(j)–11(l)], another axial band of medium particles is formed as the medium particles accumulate in this region with time, as the other two particle types get dispelled toward the axial center.

Thus, in general, the preferential axial directional movement of the different particle types underlies the formation of the axial bands. The end walls induce the preferential movement of the large particles toward the wall, thereby forming axial bands of large particles at the end walls and dispelling other particle types away from the end walls. Due to the different inertia of the different particle types leading to varying tendencies of axial motion, the axial bands of different particle types alternate among one another.

FIG. 11. Directional axial flow of the three particle types in several axial regions: the rows represent the axial positions of $-1 < z/Z < -0.94$, $-0.94 < z/Z < -0.89$, $-0.89 < z/Z < -0.83$, and $-0.83 < z/Z < -0.78$, while the columns represent the large [(a), (d), (g), and (j)], medium [(b), (e), (h), and (k)], and small particles [(c), (f), (i), and (l)]. Note that the transportation of particles to the left and right region is normalized with the initial mass of this particle type in the corresponding region.

V. CONCLUSIONS

By means of the discrete element method (DEM) to numerically simulate the granular motion of the ternary-size mixture in the three-dimensional rotating drum in the rolling regime, the dynamical segregation phenomenon, axial band formation, and the spatial redistribution of the three particle types in a ternary-size mixture are studied. Based on the numerical results, the following conclusions can be drawn:

- (1) The fast radial segregation gives rise to a radial core of small particles that span the whole drum length. Then, the slow axial segregation disrupts this channel by the formation of axial bands consisting predominantly of one particle type alternating with another particle type. The segregation of the ternary-size mixture is such that the medium particles (i) are generally sandwiched in between the large and small particles both radially and axially; and (ii) are slower to exhibit segregation relative to the large and small particles.
- (2) The fast radial segregation leads to a sharp decrease of the mixing index within the first 40 s, while the slow axial segregation causes the mixing index to gradually decrease with time. The mixing index indicates that the most extensive segregation between two particle types is between the large and small particles, while the least extensive is between the large and medium particles. This is evidenced in that the large and small particles mainly congregate in the radial periphery and core, respectively, while the medium ones are distributed comparatively uniformly in the radial periphery.
- (3) After dividing the system into the active and passive region, the total mass fractions in both regions are independent of the segregation, and thus can be treated as global parameters. Radial segregation causes more large and small particles to congregate, respectively, in the passive and active regions, while axial segregation has the opposite effect. Quantitatively, the mass of each of the three particle types in the passive region is nearly three times of that in the active region. The small particle

type has the highest mass fraction in the active region, followed by the medium and finally the large particle type.

- (4) Axial segregation leads to a reduction of the total mass of particles at the end walls due to the congregation of the large particles. The end walls initiate the axial segregation by the formation of the axial bands at the end walls, and then the existing bands widen and become purer in the specific particle type while more axial bands form toward the axial center. The non-uniform mass distribution of the three particle types and thereby the band formation is tied to axial segregation.
- (5) Alternative bands of large, medium and small particles can be found axially in a ternary-size granular mixture. As compared to the large and small particle types, the axial bandwidth and purity of the medium particles are lower for the medium particle type.
- (6) The formation of axial bands necessitates specific axial directional movement of each particle type. This is initiated at the end walls by the preferential movement of large particles toward the end walls and small particles away from the end walls, leading to the formation of axial bands of large particles at the end walls, followed by adjacent axial bands of medium particles and then axial bands of small particles.
- (7) As compared with the binary-size system, the presence of the medium particle type slightly increases the total mass in the active region, gives rise to larger mass fractions of the small and large particle types in the active region, and enhances the axial segregation in the system.

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