Granular axial band formation in rotating tumblers: a discrete element method study

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Abstract. The onset mechanism for band formation of a granular mixture in long rotating tumblers is still largely unresolved. We study this issue for axial segregation of binary mixtures having different size particles, using discrete element method simulations. Endwalls initiate axial segregation via an axial flow due to friction. The non-uniform distribution of axial velocity in the flow together with simultaneous radial segregation via percolation results in the axial flow rate of the two types of particles differing in the upstream and downstream portions of the flowing layer. Thus, small particles are driven further from the endwalls, while large particles accumulate at the endwalls. Once this occurs, a cascading mechanism begins so that other bands form due to the gradient in particle concentration near the endwalls. A small axial flow between segregated bands of small and large particles persists even after the bands are fully developed.

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1. Introduction

An intriguing property of granular media is the tendency of granular mixtures to segregate upon flow or vibration. A long horizontal rotating cylindrical tumbler that is partially filled with a mixture of particles of two sizes is often used as a canonical system to study granular mixing and segregation. Upon rotation of the tumbler, the particles segregate axially into bands rich in small or large particles.

Although first reported by Oyama [1], axial segregation has not attracted substantial attention until recent decades [2–8]. And even though several interesting properties of axial band formation, such as traveling waves and coarsening [9, 10], have been studied, the fundamental onset mechanism of axial segregation is still unclear. Hill and Kakalios [5] noted that the appearance of axial segregation strongly depends on the rotational speed, $\Omega_1$, as well as the differences in the dynamic angles of repose between the mixed and segregated phases. They also found that for a mixture of small and large glass particles, axial segregation is always initiated near endwall regions, and the bands at the endwalls are always rich in large particles [5], a result that has been confirmed by other studies [10, 11]. Alexander et al [12] found that axial segregation only occurs when the size ratio of two species is large enough; Bielenberg et al [13] noted that the size of particles relative to the tumbler diameter is also key to axial segregation; Zik et al [4] showed that the periodic modulation of tumbler diameter along the rotation axis can promote axial segregation; by studying the oscillatory dynamics for initially pre-segregated bands, Khan et al [14] found that the particle concentration along the rotation axis is closely correlated with the angle of repose of segregation bands from the initial oscillatory transient to the fully segregated state. The axial segregation is robust: it can occur in tumblers of square cross-section [10], in systems in which the interstitial fluid is a gas or a liquid [7] and in systems with a wide range of fill levels and rotational speeds [11, 15].

Owing to the complexity of the problem, theoretical progress has been limited. Savage [16] and Hill et al [5, 6] used the concept of ‘negative diffusivity’ to rationalize axial segregation, assuming that different compositions of granular mixtures have different dynamic angles of repose, which introduces an axial drift flow between segregation bands. Zik et al [4] postulated that particles with a small angle of repose have a large mobility down the axial slope, which reduces the one-dimensional (1D) mass conservation equation along the rotation axis to a diffusion equation with a ‘negative diffusivity’. To prevent particle accumulation, they assumed...
the existence of a counter axial flow. But as pointed out by Elperin and Vikhansky [17], the model is problematic because it omits the size preference in the counter axial flow. Later, another theoretical model was developed by Aranson et al [18, 19]. They coupled two 1D equations for the variation in the angle of repose and the concentration over the transverse cross-sections along the rotation axis. Although their model successfully predicts the initial axial segregation as well as band oscillation and coarsening over long times, there are still questions [14]. Moreover, the model omits the role of radial segregation, which precedes axial segregation. In fact, the bands of small particles that appear during axial segregation are locations where the radially segregated core of small particles extends to the visible free surface to appear as a band [7, 20].

Computational simulation provides a systematic approach to study the onset of axial segregation. The discrete element method (DEM) has previously been employed to study granular axial segregation in rotating tumblers. The first DEM simulation was reported by Shoichi [21] for a system with only about 1000 particles. Rapaport [22–24] used DEM to study the effects of the particle size ratio, friction coefficient and rotational speed on axial segregation in rotating tumblers. Taberlet et al [25] studied the dynamics of axial segregation bands including band oscillation and coarsening. But the focus of their computational studies was on reproducing the observed experimental phenomena; they did not investigate the fundamental onset mechanism of axial segregation or probe the flow deep into the bed of particles.

Here we address the details of the onset mechanism and extend our earlier work [26] for a minimal system that leads to five bands. Several interrelated issues are considered: the existence of axial flow between segregation bands and its nature below the surface, the mechanism of segregation and its relation to the endwalls, and the appearance of what has been interpreted as a ‘negative diffusivity’ during the development of axial segregation.

2. Numerical method

The DEM uses an explicit, constant time step to integrate Newton’s second law to describe the translational and rotational motion of individual ‘soft’ particles. The linear-spring dashpot force model [27–30] is used here to calculate the normal force between two contacting particles. The normal force consists of two parts: a normal elastic spring force and a normal viscous damping force such that \( F_{ij}^n = [k_n \alpha - 2\gamma_n m_{eff}(V_{ij} \cdot \hat{r}_{ij})] \hat{r}_{ij} \), where \( \alpha \) and \( V_{ij} \) are the particle overlap and relative velocity of two contacting particles \( i \) and \( j \); \( \hat{r}_{ij} \) represents the unit vector in the direction between particles \( i \) and \( j \); and \( m_{eff} = m_i m_j / (m_i + m_j) \) is the reduced mass of the two particles. \( k_n \) and \( \gamma_n \) characterize the stiffness and damping of the granular materials and are related to the collision time \( \Delta t \) and restitution coefficient \( e \) [28, 30]. A tangential force model without a memory effect [22, 23, 25, 31] is used: \( F_{ij}^t = -\min(|\gamma_t V_{ij}^t|, |\mu F_{ij}^n|) \text{sign}(V_{ij}^t) \), where \( V_{ij}^t \) is the relative tangential velocity of two particles, and \( \gamma_t \) is the tangential damping coefficient. The memory-effect model, which uses the accumulated tangential displacement between two contacting particles [28, 30], was not used because it is more time-consuming and provides similar results to the simpler force model [31]. We use the Verlet algorithm [28, 32] to update the positions and velocities of particles.

We consider the specific case of a partially filled tumbler, as shown in figure 1. The diameter of the tumbler is \( D = 2R = 0.08 \) m; the length of the tumbler is \( L = 2D = 0.16 \) m;
equal volumes of small and large particles of radii 0.001 and 0.002 m fill 20% of the tumbler volume; gravitational acceleration is $g = 9.8 \text{ m s}^{-2}$; particle properties correspond to glass (density $\rho = 2500 \text{ kg m}^{-3}$, restitution coefficient $e = 0.97$ [28]). To provide an initial random mixture of particles, the two species are initially represented by mass points randomly distributed in the tumbler without any gravitational force; then the radii of the particles grow until they reach the required size; next, the gravitational acceleration is applied allowing the particles to settle to the lower portion of the horizontal tumbler. Excess particles above a flat top surface are removed, leaving about 13 800 particles in the simulation. To avoid a close-packed structure, the particles have a normal size distribution with a variance of $(0.1d)^2$, where $d$ is the particle diameter. The friction coefficients between particles and between particles and walls are set to $\mu = 0.6$; in order to save computer time, the collision time is $\Delta t = 10^{-3} \text{ s}$, consistent with previous simulations [25] and sufficient for modeling hard spheres [33, 34] based on similarity to preliminary results for $\Delta t = 10^{-4} \text{ s}$. The integration time step is $\Delta t/40 = 2.5 \times 10^{-5} \text{ s}$ to meet the requirement of numerical stability [28]. The rotational speed is $\Omega = 3.14 \text{ rad s}^{-1}$ (0.5 rot s$^{-1}$), unless otherwise noted. The curved cylindrical wall and two endwalls of the tumbler are modeled as geometrically smooth surfaces, which are assumed to have infinite mass and infinite radius (for the endwalls) for the calculation of the collision force between mobile granular particles and the walls. As shown in figure 1, the coordinate system has its origin in the center of the tumbler with the $x$-axis along the streamwise direction, the $y$-axis normal to the free surface and the $z$-axis along the tumbler axis. The corresponding velocities are $u$, $v$ and $w$. Using this coordinate system, the surface of the flowing layer would theoretically be at $y = -0.0195 \text{ m}$ for a 20% fill level if the surface is perfectly flat and no dilation is introduced during flow.

To quantitatively study the flow, the computational domain is divided into bins in the $x$-, $y$- and $z$-directions. Local flow properties are obtained by averaging values for all particles in each bin. Unless otherwise noted, to obtain statistically meaningful results, the averaging time is 2 s (one tumbler rotation). As indicated in figure 1, $Q_{up}$ and $Q_{down}$ refer to the axial flow rate of particles in the upstream and downstream sections, respectively, of the combined flowing layer and bed of particles.
3. Axial segregation with endwalls

3.1. Segregation structure

Figure 2 shows the top surface of large green and small red particles in their initial mixed condition. The accompanying video demonstrates the evolution of band formation on the top surface over the first 50 rotations of the tumbler. The endwall bands of large green particles form quickly, while the band of large green particles in the middle of the tumbler develops more slowly. The segregation is imperfect but distinct.

The evolution of the spatially averaged volume concentration profile is shown in figure 3 for small particles, $\langle C_s \rangle$, and large particles, $\langle C_l \rangle$, along the axis of rotation $z$, where $\langle \rangle$ denotes the cross-sectionally averaged values. The concentrations deviate from the initially well-mixed state very quickly as large particles begin to accumulate near the endwalls within 1 rotation (figure 3(a)). Here, $t = 0$ is the time at which the particles start to flow downward in the streamwise direction after the dynamic angle of repose is reached. After several rotations, as shown in figure 3(b), axial segregation is evident near the endwalls ($z = \pm 0.08$ m). This is consistent with the experimental observations [5, 10, 11] that bands near endwalls appear first and that they are rich in large particles. At the same time, adjacent bands rich in small particles appear. Axial segregation is evident along the entire length of the tumbler after 20 rotations, figure 3(c), with a third band of large particles appearing at the axial center of the tumbler ($z = 0$). Within 50 rotations, the segregation pattern reaches a ‘steady’ segregated state (figure 3(d)), although the positions and concentrations of bands randomly fluctuate very slightly with time. We put ‘steady’ in quotes since the initial transient in which bands form has ended. No merging of bands is evident up to 200 rotations in these simulations. This is not surprising given that this is a relatively short tumbler and that band merging typically occurs in experiments after $O(100)$ rotations and sometimes even much later [11].

Although magnetic resonance imaging (MRI) measurements have shown the outline of the radial segregation core of small particles during axial segregation [20], numerical
Figure 3. Evolution of the cross-sectionally averaged species concentrations along the axial length at different times: (a) initial segregation (0–1 rotations), (b) intermediate segregation (4–5 rotations), (c) further segregation (20–21 rotations) and (d) full segregation (49–50 rotations). □, concentration of small particles, ⟨Cs⟩; ◦, concentration of large particles, ⟨Cl⟩.

simulations can provide additional information about the internal structure of the axial segregation bands. Figure 4 shows slices at different axial positions at two representative times: initial axial segregation (1 rotation) and full axial segregation (50 rotations). As observed in experiments [7, 15, 20], radial segregation starts very early and continues for the entire course of axial segregation. The band of small particles at \( z = -0.04 \) m is a consequence of the expansion of the radial core of small particles to the free surface. At steady state, these bands of small particles are relatively pure, although there are still a few large particles present at the periphery of the tumbler and in the flowing layer. The band of large particles at the mid-length of the tumbler (\( z = 0 \) m) is much less pure than the band of small particles at steady state. The large particles generally surround a core of small particles, but continually mix and re-segregate in the flowing layer. Between bands at \( z = -0.02 \) and \( z = -0.06 \) m the particles are less segregated. Although both types of particles are initially present near the endwalls (\( z = -0.07 \) and \( z = -0.08 \) m), the larger particles dominate near the endwalls at steady state.
The internal structure of the segregation can be captured by means of iso-surfaces of small and large particle number densities, $n_s$ and $n_l$, as shown in figure 5 for three representative times. The iso-surfaces are shown side by side, but in reality the green iso-surface (large particles) overlays the red iso-surface (small particles). Early in the segregation process at 4–5 rotations, the core of relatively pure small particles is completely enclosed within the iso-surface of large particles, and it extends along the entire axial length of the tumbler. Later, at 20–21 and 49–50 rotations, the small particles still extend over nearly the entire length of the tumbler except right at the two endwalls. Bulges in the red iso-surface (small particles) protrude beyond the green.
Figure 5. Structures of small and large particle volumes at different times as represented by isosurfaces of the number density of particles. (a) Small particle volume, \( n_s \geq 8 \times 10^7 \) particles \( \text{m}^{-3} \); (b) large particle volume, \( n_l \geq 5 \times 10^6 \) particles \( \text{m}^{-3} \).

iso-surface if the iso-surfaces are overlaid. The dumbbell-shaped red iso-surface for small particles is similar to that observed experimentally when the interstitial fluid is index matched to large clear particles [7]. The two lobes correspond to the two bands of small particles, and the narrow portion at the center of the tumbler is where the radial core of small particles is surrounded by a band of large particles (figure 5(b)). The large particles also surround the narrow core of small particles near the two endwalls (figure 5(b)).

3.2. Axial velocity field during axial segregation

The free surface and subsurface flow fields for the mixture (both particles species) at four representative times are illustrated in figure 6. Each plot consists of the contours of the absolute value of the axial velocity and streamtraces obtained from the integration of the streamwise \((u)\) and axial \((w)\) velocities. Due to the slight variation in the dynamic angle of repose along the length of the tumbler and dilation during flow, the ‘free surface’ measurements are actually at a plane at \( y = -0.02 \text{m} \), just below the top surface.

As conjectured by Savage [16] and Hill et al [5], convective axial flow indeed occurs during the development of axial segregation bands, and this axial flow strongly depends on the evolution of the species concentration distribution in the system. As axial segregation begins, shown in figure 6(a), the axial flow field at the free surface of the bi-disperse system is similar to that for a mono-disperse system [30, 35, 36]. Axial flows are associated with each endwall; particles near the endwalls move away from the endwall in the upstream portion of the flowing

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Figure 6. Evolution of the velocity field on the free surface at $y = -0.02 \text{ m}$ and below the surface at $y = -0.025 \text{ m}$. Black curves are streamtraces from the integration of streamwise velocity ($u$) and axial velocity ($w$). The boundary of the flowing layer, defined as the locus of points where the streamwise velocity changes from negative to positive, is shown as a dotted curve for $y = -0.025 \text{ m}$. Color contours represent the levels of absolute value of the axial velocity ($w$). (a) Initial segregation (first 0–1 rotation), (b) intermediate segregation (4–5 rotations), (c) further segregation (20–21 rotations) and (d) full segregation (49–50 rotations).

layer and then move back in the downstream portion. The origin of this endwall-related axial flow has been explained in terms of mass conservation [30, 35, 36]. Streamwise flow of particles in the transverse slices nearest the endwalls is slowed by the frictional endwalls. Since all of the particles in the solid body rotation portion of any slice of the tumbler must pass through the flowing layer, the only way to conserve mass while accommodating the reduced streamwise
velocity and the thinner flowing layer \[30\] near the endwalls is for these particles to flow axially away from the endwall in the upper portion of the flowing layer and then back toward the endwall in the downstream portion.

Other axial flows appear as the segregation proceeds. When two bands of small particles develop and a band of large particles appears at the center of the tumbler (consistent with the concentration profile in figure 3(c)), particles in the center band tend to flow toward the adjacent bands of small particles in the upstream portion of the flowing layer and flow back in the downstream portion, as shown in figure 6(c). As axial segregation continues from figure 6(c) to figure 6(d), these axial flows grow stronger and persist even for the middle band, which is distant from the endwalls, and even after the bands are fully formed. Particles in all three large particle bands (at \(z = 0.0, \pm 0.08\) m) flow toward the adjacent bands of small particles in the upstream portion of the flowing layer and back into the large particle bands in the downstream portion. Comparing the concentration profiles at this time (figure 3(d)) with the surface axial flow field (figure 6(d)), we find that the magnitude of the axial velocity is negligible at the center of each segregation band (around \(z = \pm 0.04\) m and \(z = 0\) m). The magnitude of the endwall-related axial flow increases as the axial segregation bands near the endwalls develop, and the maximum axial flows always occur at the interface between bands (around \(z = \pm 0.065\) m and \(z = \pm 0.02\) m).

The velocity field on a subsurface plane at \(y = -0.025\) m shows that the axial flow persists into the flowing layer, although the magnitude of axial velocity diminishes with depth, similar to the mono-disperse case \[30\]. The region with axial flow at \(y = -0.025\) m is similar to that at the free surface, except that the region in which flow occurs is smaller. The interface between negative and positive streamwise flow regions (where \(u = 0\)) in the upstream and downstream portions, a measure of the flowing layer depth, changes slightly with axial position as is the case for the mono-disperse flow. Note that the interface is a measure suggestive of the flowing layer depth, but not the actual flowing layer depth because of the rotation of the tumbler. The actual flowing layer is deeper and extends to the edge of the colored region in the figure. The streamwise length of the flowing layer (measured vertically from the upper dashed curve to the lower one) for the bands of large particles near the endwalls and at the center (around \(z = 0\) m) decreases with the development of axial segregation from figure 6(a) to figure 6(d), while the streamwise length of the flowing layer at the bands of small particles (around \(z = \pm 0.04\) m) increases slightly.

Representative snapshots of the dynamic angles of repose, based on the outline of the particles on the top surface of the flow at different axial positions, are shown in figure 7. The snapshot after 1 rotation in figure 7(a) (close to the initially well mixed state) displays a higher angle of repose near the endwalls (about \(32^\circ\) at \(z = -0.08\) m) than occurs elsewhere in the tumbler (about \(28^\circ\) at \(z = -0.04\) and \(z = 0\)). The higher dynamic angle of repose near endwalls is related to endwall friction \[37\]. With the development of segregation bands, the dynamic angle of repose at the central band of large particles becomes larger (about \(29^\circ\) at \(z = 0\) m) than that of the adjacent band of small particles (about \(27^\circ\) at \(z = -0.04\) m), as shown in figure 7(b). This difference in the angle of repose and the related axial drift flow between segregation bands has been suggested previously as an explanation of the onset of axial segregation \[5, 6\], but in this paper we will propose a different mechanism. The particle concentration and the local surface slope are in phase with each other during the whole course of axial segregation, consistent with experimental observations \[14\]. Thus, the surface slope is not an independent parameter in addition to species concentration, as has been assumed in one continuum model \[18, 19\].
Of course, these simulations offer the opportunity to directly determine the axial velocity of the two types of particles. The axial drift during the course of axial segregation at 4–5 rotations when the two bands of small particles are developing is shown in figure 8. During the development of the two bands of small particles, there is very little difference between the axial velocity profiles of the small and large particles at a position where the magnitude of axial flow is relatively large (figures 8(a) and (b)). The linearly decreasing axial velocity from the surface at \( y = -0.02 \) m through the depth of the flowing layer at \( y \approx -0.03 \) m in figure 8(b) is similar to that in a mono-disperse system [30]. The small axial velocity well below the surface is due to slippage between the particles and the wall. Experiments with a similar fill level of 1 and 2 mm glass particles in a smooth acrylic tumbler indicate that a small degree of slippage regularly occurs at the tumbler walls. The axial flow at this time occurs only near endwalls with negligible axial flow in the central portion of the tumbler, as shown in figure 8(c).

The axial flow for two axial positions between bands (\( z = -0.02 \) m and \( z = -0.065 \) m) later in the segregation process, at 20–21 rotations, is shown in figures 9(a)–(d). For both locations, the axial velocity profiles of the two particle species are again quite similar. Likewise, the axial velocities along the length of the tumbler, figure 9(e), are similar. In fact, the difference between the axial velocities of small and large particles is less than 0.003 m s\(^{-1}\) (about 10% of the maximum axial velocity) in 50% of the flowing layer.

### 3.3. Axial particle flux

Since the axial velocities of the two species are similar during the entire course of axial segregation, it is difficult to explain the onset mechanism of axial segregation in terms of the axial velocity field alone. Hence, it is useful to consider how the axial velocity and particle number densities combine to bring about flows leading to axial banding. Figure 10 shows the axial velocity of the mixture, the number density of small particles and large particles,
Figure 8. Comparison of the axial velocities of the two species at three representative positions during the development of axial segregation (averaged over rotation 4–5): (a) axial velocity along the streamwise direction on the free surface at $y = -0.02\,\text{m}$ and $z = -0.065\,\text{m}$, (b) axial velocity profile through the depth of the flowing layer at $x = 0.02\,\text{m}$ and $z = -0.065\,\text{m}$ and (c) axial velocity on the free surface along the axial length at $x = 0.02\,\text{m}$ and $y = -0.02\,\text{m}$. □, Axial velocity of small particles; ◦, axial velocity of large particles.

and the axial particle flux $q = w n$ (number particles $\text{m}^{-2}\,\text{s}^{-1}$) averaged over rotations 0–1 of both small and large particles on the same cross section at $z = -0.065\,\text{m}$. The axial velocity of the mixture shown in figure 10(a) represents the axial velocity of both small and large particles since they are nearly identical. The axial velocity field shown in figure 10(a) is nearly symmetric about the midpoint of the flowing layer ($x = 0\,\text{m}$). Nevertheless, the distributions of small and large particles at this cross section differ as a consequence of radial segregation (percolation), as shown in figures 10(b) and (c). Large particles are near the surface, and small particles are deep in the flowing layer. Thus, the axial flux of small particles away from the endwall in the upstream portion ($q_s > 0$) is larger than the flux toward the endwall in the downstream portion ($q_s < 0$), as shown in figure 10(d). This results in small particles being conveyed away from the endwall. The opposite occurs in the case of large particles. As shown in figure 10(e), the axial flux of large particles away from the endwall in the upstream portion ($q_l > 0$) is less than the axial flux of large particles toward the endwall ($q_l < 0$) in the downstream portion. As a result, in the upstream portion of the flowing layer where the particles are mixed, both small and large
Figure 9. Comparison of the axial velocities of the two species at five representative positions during further development of axial segregation (averaged over rotations 20–21): (a) axial velocity along the streamwise direction on the free surface at \( y = -0.02 \) m and \( z = -0.065 \) m, (b) axial velocity on the free surface along the streamwise direction at \( y = -0.02 \) m and \( z = -0.02 \) m, (c) axial velocity profile at \( x = 0.02 \) m and \( z = -0.065 \) m, (d) axial velocity profile at \( x = 0.02 \) m and \( z = -0.02 \) m and (e) axial velocity on the free surface along the axial length at \( x = 0.02 \) m and \( y = -0.02 \) m. □, axial velocity of small particles; ○, axial velocity of large particles.

Particles move away from the endwall. Small particles percolate to the lower part of the flowing layer (radial segregation) where the axial velocity back toward the endwall is less, while the large particles on the top of the layer are in a region of higher axial velocity back toward the
endwall. The result is that small particles flowing away from the endwall in the upstream portion of the flowing layer are less likely to return to near the endwall in the downstream portion; large particles flowing away from the endwall in the upstream portion are more likely to return in the downstream portion. This results in a steady increase of the degree of segregation until the steady state is reached.

This can be demonstrated more clearly by considering the axial flow rates of both particle types. The axial flow rate on every transverse slice can be divided into the upstream portion
and the downstream portion, denoted as $Q_{up,s}$, $Q_{up,l}$, $Q_{down,s}$, and $Q_{down,l}$ (m$^3$s$^{-1}$), with the subscripts $s$ and $l$ indicating small and large particles. Here we distinguish the ‘upstream’ and ‘downstream’ portions of every cross-section as the streamwise position where the sign of the axial velocity changes rather than using the center of the flowing layer ($x = 0$ m), since the interface between the negative and positive axial flow regions varies with depth. The axial flow is calculated based on the axial velocity, the number of particles, and the volume of particles in either the upstream or downstream portion. For example, 

$$Q_{up,s} = \sum_{i=1}^{k} w_{i,s} n_{i,s} S_i V_s / 0.64.$$ 

Here the index $i$ represents the summation over individual bins in the upstream portion; $w_{i,s}$ and $n_{i,s}$ are the locally averaged axial velocity (m s$^{-1}$) and the number density (number of particles m$^{-3}$) of small particles in bin $i$; $S_i$ is the section area on the $xy$-plane of bin $i$, which is a constant for the Cartesian averaging mesh used here; $V_s$ is the volume of a small particle; and 0.64 is a factor accounting for the void fraction for dense sphere packing to provide an accurate numerical value of the volume flow rate. (Although this factor is borrowed from random mono-disperse packing [38], it is valid for the mixtures of small and large particles in our bi-disperse system, since the size ratio of the two species is not so large that the small particles can occupy voids between large particles.)

Consider $Q_{up,s} + Q_{down,s}$, the net axial flow rate of small particles, which is shown in figure 11(a) for 0–1 rotations. At $z = 0.065$ m, where the boundary between the bands forms, $Q_{up,s} + Q_{down,s} < 0$, indicating that the number of small particles flowing away from the endwall in the upstream portion ($Q_{up,s} < 0$) is more than that toward the endwall in the downstream portion ($Q_{up,s} > 0$). The opposite occurs in the case of large particles, shown in figure 11(b). That is, near the left endwall ($z = 0.065$ m) $Q_{up,l} + Q_{down,l} > 0$, indicating that the number of large particles flowing away from the endwall in the upstream portion ($Q_{up,l} < 0$) is less than that toward the endwall in the downstream portion ($Q_{up,l} > 0$). Near the right end of the tumbler ($z = -0.065$ m), the situation is reversed. Hence, at both ends of the tumbler, the small particles tend to move away from the endwall on average, while the large particles tend to move toward the endwall on average, thus initiating band formation near the endwalls. As time progresses, similar differences in the axial flow of the two species occur as other bands evolve away from the endwalls. However, the net axial flow for each particle species decreases
as the bands become fully formed, and eventually the net axial flow of both species becomes negligible at steady state (50 rotations).

This imbalance in the net flow of small and large particles can be used to qualitatively explain the onset of axial segregation, as shown in figure 12. For an initially well-mixed granular mixture, the endwall friction introduces an axial flow near the endwalls. Particles of both sizes move from region 1 near the endwall into the adjacent region 2 in the upstream portion of the flowing layer. Due to the difference in the axial flow of small particles between the upstream portion and the downstream portion, fewer small particles return from region 2 to region 1 (small solid arrow of figure 12). For mass conservation, large particles take their place (large dashed arrow). The net result is that small particles are conveyed from the region close to the endwall (1) to the adjacent region (2), leaving a band rich in large particles in region 1 and a band rich in small particles in region 2. As the concentration of small particles increases in region 2, a new axial flow is generated, from region 3 to region 2 in the upstream portion and back to region 3 in the downstream portion; again, from the imbalance of the axial flow rate for small particles in the upstream and downstream portions, this new axial flow conveys small particles from region 3 to region 2, leaving a band rich in large particles in region 3. The process continues, forming more bands in the system, eventually achieving alternating segregation bands in the entire tumbler.

Thus, it is the non-uniformity of the axial velocity field (faster near the surface of the flowing layer and slower deep in the flowing layer) and the non-uniformity of particle concentration distribution (large particles at the surface and small particles deeper at the downstream end of the flowing layer) that cause axial segregation. This explains why axial segregation only occurs when the size ratio of the two species is large enough [13] and why radial segregation is a necessary precursor to axial segregation. Weak radial segregation, when the sizes of the particles are close, does not carry small and large particles into different axial flow regions at the downstream end of the flowing layer, so axial segregation occurs very slowly, if at all.

4. Axial segregation with no endwalls

The role of the endwalls in axial band formation becomes clearer by simulating the same system with periodic boundary conditions, thus eliminating the axial flow from the frictional endwalls. Particle concentrations along the length of the tumbler over 200 rotations are shown in figure 13. Compared to the frictional endwall case (figure 3), the magnitude of the concentration

\[\text{Figure 12.} \text{ Schematic representation of the onset of axial segregation in the system near the left endwall (viewed looking at the free surface). Solid arrows: axial flow of small particles; dashed arrows: axial flow of large particles. The endwall is the left side of region 1, and the flow is from top to bottom.}\]
fluctuations remains very small and no segregation bands appear in the system after 200 rotations. Local extrema in concentration come and go over time. None grow into segregation bands. Similar results occur for frictionless endwalls. That is, no significant axial flow occurs and no bands form.

When the rotational speed is increased from $\omega = 3.14 \, \text{rad s}^{-1}$ to $\omega = 6.28 \, \text{rad s}^{-1}$ for periodic boundary conditions, some local extrema of concentration gradually evolve into segregation bands within 50 rotations, as shown in figure 14. However, not all concentration fluctuations develop into segregation bands, and the final segregation bands originate from a subset of the early concentration fluctuations (those around $z = -0.065$ m and $z = 0.005$ m in figure 14(b)). Comparing figures 13 and 14, it appears that for the same magnitude of the concentration fluctuations, a greater rotational speed promotes band formation, while a smaller rotational speed does not. This is consistent with experimental observations [5] that axial segregation only occurs at higher rotational speeds and segregated bands tend to resolve to a mixed state at lower rotational speeds.

Slices at different axial positions at two representative times (after 10 and 50 rotations) are shown in figure 15. The radial segregation exists for the entire course of axial segregation with
Figure 14. Evolution of the cross-sectionally averaged species concentrations along the axial length at different times for periodic boundary conditions with $\omega = 6.28 \text{ rad s}^{-1}$: (a) 0–1 rotation; (b) 4–5 rotation; (c) 9–10 rotation; (d) 49–50 rotation. □, concentration of small particles; ○, concentration of large particles.

a core of small particles extending through large and small particle bands at $z = 0.015 \text{ m}$ and $z = -0.065 \text{ m}$ (although the core is quite small here). As is the case with endwalls, the small particle bands are relatively pure with only a few large particles at the periphery, whereas large particle bands retain a core of small particles. Between bands ($z = -0.03 \text{ m}$), the particles are somewhat mixed, although the small particle core is evident. Snapshots of the dynamic angles of repose of small ($z = 0.015 \text{ m}$) and large ($z = -0.065 \text{ m}$) particle bands after 50 rotations are shown in figure 16. Again, the band of large particles has a higher dynamic angle of repose (about 28° at $z = -0.065 \text{ m}$) than the band of small particles (about 25° at $z = 0.015 \text{ m}$).

The averaged axial velocity fields at 49–50 rotations on the free surface ($y = -0.02 \text{ m}$) and a subsurface plane at $y = -0.025 \text{ m}$ are shown in figure 17. It is evident that, consistent with the situation for the middle band, which is distant from the endwalls in figure 6, axial flow exists between segregation bands in the case of periodic boundary conditions, although the axial velocities are lower than with endwalls. Again, the axial flow is from the band of large particles to the adjacent band of small particles in the upstream portion of the flowing layer and back to the band of large particles in the downstream portion. From the concentration profiles at this time (figure 14(d)), it is evident that the straight streamtraces always occur at the centers of the segregation bands (around $z = -0.065 \text{ m}$ and $z = 0.015 \text{ m}$), and the largest axial flows occur at
After 10 rotations

After 50 rotations

\[ z = 0.015 \text{m} \]
\[ z = -0.03 \text{m} \]
\[ z = -0.065 \text{m} \]

**Figure 15.** Snapshots of slices at different axial positions for periodic boundary conditions with \( \omega = 6.28 \text{ rad s}^{-1} \), at two different times: after 10 and 50 rotations (full axial segregation).

**Figure 16.** Difference in the dynamic angles of repose of two cross sections after 50 rotations for periodic boundary conditions with \( \omega = 6.28 \text{ rad s}^{-1} \). Blue curve: outline of the particle surface around the center of the band of small particles \((z = 0.015 \text{ m})\); green curve: outline of the particle surface around the center of the band of large particles \((z = -0.065 \text{ m})\).

the interface between bands (around \( z = -0.03 \text{ m} \) and \( z = 0.06 \text{ m} \)). The boundary of the flowing layer at the band of small particles (around \( z = 0.015 \text{ m} \)) is also wider than that of the band of large particles (around \( z = -0.065 \text{ m} \)), indicating that the flowing layer is deeper here. This is not surprising given that particles are flowing into this band from adjacent bands at the upstream portion, and mass conservation requires that all particles pass through the flowing layer. While it is evident that axial flow between bands exists even with no endwalls, its origin is unclear.
Figure 17. The velocity field at 49–50 rotations for periodic boundary conditions with $\omega = 6.28 \text{ rad s}^{-1}$: (a) on the free surface at $y = -0.02 \text{ m}$; and (b) below the surface at $y = -0.025 \text{ m}$. Black curves are streamtraces from the integration of streamwise velocity ($u$) and axial velocity ($w$); color contours represent the levels of the absolute value of the axial velocity ($w$).

When endwalls are present, the friction driving the axial flow near the endwalls initiates band formation. But bands and their associated axial flows appear away from the endwalls in this case (the middle band in figures 3 and 5), as well as when there are no endwalls at all (figures 14 and 17). The origin of these axial flows and why bands form only at higher rotational speeds deserve further investigation.

5. Concentration gradients

Returning to the case with frictional endwalls, we consider the relation between the particle concentration gradient and the axial flow. Figure 18 shows the magnitude of axial flow as axial segregation develops. Here the magnitude of the axial flow of the entire mixture in the upstream and downstream portions is represented by the absolute values of $Q_{up,mix} = Q_{up,s} + Q_{up,l}$, the total flow rate of two species in the upstream portion, and $Q_{down,mix} = Q_{down,s} + Q_{down,l}$, the counterpart in the downstream portion (where subscripts $s$, $l$ and mix refer to small particles, large particles and the mixture). Since the bands of large particles near the endwalls develop more quickly than the two bands of small particles and the center band of large particles, the averaging time used to calculate the axial flow rate is 2 s (1 rotation) early in the segregation process and 6 s (3 rotations) later in the process.

The endwall-related axial flow starts immediately with the initial rotation (figure 18(a)) and its magnitude increases as fully developed segregation is achieved (figure 18(d)). The axial flow is initially quite small at the center portion of the tumbler before the two bands of small particles and the center band of large particles appear. Since it is quite difficult to identify the upstream
Figure 18. Magnitude of the axial flow rate of the mixture in the upstream and downstream portions along the axial length averaged over four different time periods: (a) initial segregation (0–1 rotations); (b) intermediate segregation (4–5 rotations); (c) further segregation (19–22 rotations); (d) full segregation (rotations 47–50). □: magnitude of the total axial flow rate in the upstream portion, $|Q_{up,mix}|$; ○: magnitude of the total flow rate in the downstream portion, $|Q_{down,mix}|$.

and downstream portions for the small, random axial velocity, these data are indicated by dashed lines in figures 18(a) and (b). At later stages of axial segregation, local maxima in the axial flow occur at the interface between two adjacent bands (around $z = \pm 0.065$ m and $z = \pm 0.02$ m in figure 18(d)) and minima in the axial flow occur at the centers of each band (two endwalls, around $z = \pm 0.04$ m, and $z = 0$ m in figure 18(d)). Of course, the axial flow rates of the mixture in the upstream and downstream portions at all axial positions balance each other, having nearly identical magnitudes but opposite directions. The volume of particles in every slice is conserved during the development of axial segregation.

The axial flows strengthen until steady state and then persist. Comparing figures 18 and 3, it is evident that strong axial flows correspond to steep concentration gradients. The axial flow rate and the axial gradient of small particle concentration, $\partial \langle C_s \rangle / \partial z$, during the development of the axial segregation, are compared in figure 19. The gradient is calculated as a central finite difference except near the endwall. In the region where the frictional endwalls play no role in

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the development of the central band of large particles, the axial flow rate and the concentration gradient overlap one another when scaled with an appropriate factor. In fact, the overall shapes of two profiles along the entire length of the tumbler are similar. The axial flow in the upstream portion always has the same sign as the concentration gradient at all axial positions, and the axial positions where zeros or extrema appear coincide. Therefore, it is reasonable to conclude that, as assumed by Savage [16], the strength of the axial flow between segregation bands is proportional to the concentration gradient, that is, $Q_{up,mix} \propto \partial \langle C_s \rangle / \partial z$, at least away from the endwalls. Similar relationships occur for $Q_{down,mix}$ and $\partial \langle C_s \rangle / \partial z$ or $\partial \langle C_l \rangle / \partial z$, which is essentially a mirror image of $\partial \langle C_s \rangle / \partial z$ (not shown).

Several models of axial segregation are based on the concept of the so-called ‘negative diffusivity’ [4–6], [16, 18, 19], which is different from true granular diffusion [39–41]. To determine whether the use of a negative diffusivity model for axial segregation is warranted, we calculate the axial diffusivity of the small particles, $K$, at every axial position using Fick’s first law of diffusion: $\langle C_s \rangle (\langle w_s \rangle - \langle w \rangle) = -K \partial \langle C_s \rangle / \partial z$, where $w_s$ is the local axial velocity of small particles, and $\langle w_s \rangle = \langle C_s w_s \rangle / \langle C_s \rangle$ is the cross-sectionally averaged axial velocity. Diffusivity is plotted in figure 20 using different scales for different times during the course of the segregation. Clearly, a net negative diffusivity exists in regions where there is axial segregation: near the endwalls in figures 20(a) and (b) when bands near the endwalls develop and in the central portion in figures 20(b) and (c) when the center bands develop. When there is no axial segregation in the central portion (figure 20(a)), the diffusivity is positive at almost all axial positions of this portion, reflecting the tendency of the particles to diffusively mix in this region. The magnitude of the negative axial diffusivity for the bands near the endwalls is larger than that of the central bands. As expected, the magnitude of the diffusivity decreases with time and approaches zero at the fully developed segregated state in figure 20(d). Positive or zero diffusivity tends to occur at the centers of the segregation bands, around $z = \pm 0.04$ m in figure 20(b). For a few positions (for example $z = 0.015$ m in figure 20(b) where the denominator used to calculate the diffusivity, $\partial \langle C_s \rangle / \partial z$, is very close to zero), anomalies occur due to the randomness in the data and the problems associated with taking the derivative of noisy data. Of course, negative diffusivity is

![Figure 19. Comparison of the axial flow rate of the mixture in the upstream portion (□) and concentration gradient of small particles (○): (a) 19–22 rotations and (b) 47–50 rotations.](http://www.njp.org/)
not the physical mechanism of band formation; it is simply a convenient modeling construct that reflects the differential axial transport of the two types of particles.

6. Conclusions

We have examined the details of axial segregation in a long tumbler through an in-depth computational study of the segregation of a mixture of particles having two different sizes. Friction at the endwalls generates axial flow due to mass conservation. The two particle species move in the same direction with almost identical velocity everywhere in the system: all particles flow from the bands of large particles into the bands of small particles in the upstream portion of the flowing layer and then flow back in the downstream portion. The axial flow rates of the mixture in the upstream and downstream portions are balanced on every cross-section.

Our findings depart from the conventional mechanism suggested for axial segregation. Different angles of repose between segregated bands are observed, but the axial flow drives the axial segregation. It is the non-uniform distribution of axial velocity and species concentration on the cross-section that introduces unbalanced distribution of axial flow of individual species in the upstream and downstream portions. Small and large particles flow away from the endwall (or the center of a large-particle band) in the upstream portion, but large particles tend to flow...
back toward the endwall (or large particle band) more than small particles in the downstream portion, because percolation has carried small particles deeper into the flowing layer where the axial velocity is smaller. Although this is clearly not a diffusion process, the differential transport of small and large particles in a cross-sectional slice appears like a negative diffusivity that has been used in ad hoc models of axial segregation [4–6, 16, 18, 19].

This mechanism can also explain the results for density systems of same-size heavy and light particles [26, 42–45]. In these systems, light particles accumulate at the endwalls but no bands form. Radial segregation due to buoyancy occurs throughout the tumbler, but axial flow only occurs near the endwalls. Near the endwalls, both heavy and light particles flow away from the endwalls in the upstream portion of the flowing layer. In the downstream portion, heavy particles fall deeper into the flowing layer where the axial flow is smaller, but light particles near the surface flow back toward the endwalls to concentrate there.

Many open issues remain, including (i) a better understanding of the axial velocity field related to the frictional endwalls, the different angles of repose between adjacent bands and the resulting concentration gradients; (ii) the connection between radial segregation and axial segregation; (iii) the origin of bands away from the endwalls (middle band in figure 3) or in the case of periodic boundary conditions (figure 14); (iv) the nature of band coarsening and traveling waves [9, 10]; and (v) the influence of axial flow from other shapes of endwalls or sidewalls on axial segregation; for example, axial segregation in spherical tumblers [31, 46, 47]. In fact, the ultimate experiment would be to eliminate the endwalls altogether, perhaps with particles in a flexible toroidal tumbler that is somehow rotated about its circumferential axis.

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