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AN INVESTIGATION INTO THE IMPACT OF PARTICLE PROPERTIES ON FLOW BEHAVIORS

ZHAO YA

SCHOOL OF CHEMICAL AND BIOMEDICAL ENGINEERING

2020

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PROPERTIES ON FLOW BEHAVIORS

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**AN INVESTIGATION INTO THE IMPACT OF
PARTICLE PROPERTIES ON FLOW
BEHAVIORS**

ZHAO YA

School of Chemical and Biomedical Engineering

A thesis submitted to the Nanyang Technological University

in partial fulfillment of the requirement for the degree of

Doctor of Philosophy

2020

STATEMENT OF ORIGINALITY

I hereby certify that the work embodied in this thesis is the result of original research, is free of plagiarised materials, and has not been submitted for a higher degree to any other University or Institution.

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SUPERVISOR DECLARATION STATEMENT

I have reviewed the content and presentation style of this thesis and declare it is free of plagiarism and of sufficient grammatical clarity to be examined. To the best of my knowledge, the research and writing are those of the candidate except as acknowledged in the Author Attribution Statement. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

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Chew Jia Wei

AUTHORSHIP ATTRIBUTION STATEMENT

This thesis contains material from 3 papers published in the following peer-reviewed journals in which I am listed as an author.

Chapter 3 is published as Y. Zhao, S. Yang, L. Zhang and J.W. Chew. DEM study on the discharge characteristics of lognormal particle size distributions from a conical hopper. *AIChE Journal*, 64 (4), 1174-1190 (2018). DOI: <https://doi.org/10.1002/aic.16026>.

The contributions of the co-authors are as follows:

- Prof Chew provided the initial project direction and edited the manuscript drafts.
- I designed the simulation, analyzed the data, and prepared the manuscript.
- Dr Yang provided valuable suggestions and assisted in the simulation.
- The manuscript was revised by Dr Yang and Dr. Zhang.

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- Prof Chew suggested the research area and edited the final manuscript drafts.
- I designed the model, performed the simulation, analyzed the data, and prepared the manuscript drafts.

- The manuscript was revised by Dr Yang and Dr Zhang.

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- I designed the model, performed the simulation, analyzed the data, and prepared the manuscript drafts.

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- I designed the experiment and conducted the experiment.
- Mr. Dahiphale assisted in the experiment and collection of the data.
- Dr. Tan assisted in the surface modification on glass beads.
- Prof Wang provided the electrometer and Faraday Cup and revised the manuscript.

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NOMENCLATURE

A_p	actual surface area of the particle (m ²)
A_s	surface area of a sphere with the same volume as the given particle (m ²)
Ar	Archimedes number (-)
a	half-length of the superquadric particle along the x-axis (m)
b	half-length of the superquadric particle along the y-axis (m)
$C_{smaller\ aspect\ ratio}$	The normalized number-based concentration of the smaller aspect ratio (-)
C_{large}^*	normalized concentrations of large particles (-)
C_{small}^*	normalized concentrations of small particles (-)
C_{large}^T	ratio of large particles in the total number of particles (-)
C_{small}^T	ratio of small particles in the total number of particles (-)
c	half-length of the superquadric particle along the z-axis (m)
D	the diameter of the pipe (m)
D_0	diameter of the hopper orifice (m)
D_{ref}	the reference pipe diameter of 50 mm (m)
d	particle diameter (m)
d_i	diameter of the large or small particles (m)
d_p	the diameter of the particle (m)
$d_{p,mass}$	the mass mean particle diameter for binary mixtures (m)
d_{50}	50 th percentile of the cumulative mass-based particle size distribution (m)
$(dP/dz)_0$	pressure gradient across the particle bed (Pa/m)

d_{VM}	De Brouckere mean diameter (m)
e	restitution coefficient (-)
$\mathbf{F}_{c,ij}^n$	normal contact force (N)
$\mathbf{F}_{c,ij}^t$	tangential contact force (N)
$\mathbf{F}_{d,ij}^n$	normal damping forces (N)
$\mathbf{F}_{d,ij}^t$	tangential contact forces (N)
f_N	frequency distribution for lognormal (mm ⁻¹)
$\mathbf{M}_{n,ij}$	torques between particles i and j determined by normal force (N·m)
$\mathbf{M}_{t,ij}$	torques between particles i and j determined by tangential force (N·m)
$\mathbf{M}_{r,ij}$	torque between particles i and j determined by rolling friction (N·m)
N	total particle number (-)
N_{large}	local number of large particles (-)
$N_{smaller\ aspect\ ratio}$	number of particles with the smaller aspect ratio (-)
N_{small}	local number of small particles (-)
N_{Total}	local total number of all particles (-)
n_1	blockiness parameter (-)
n_2	blockiness parameter (-)
$\mathbf{g}$	gravity acceleration (m/s ²)
G	shear modulus (Pa)
H	particle bed height in the cylindrical section (0.422 m)
h	height in the cylindrical section assessed (m)
I_i	inertia moment of particle i (kg/m ²)
K	number of particles (-)
m_i	mass of particle i (kg)
$\mathbf{n}$	unit vector in normal direction (-)
$\mathbf{Q}$	quaternion (-)
Q_{ij}	order tensor (-)
R	cylindrical radius of hopper (0.12 m)

Re_p^*	Reynolds number (-)
r	radial position assessed (m)
t	time (s)
Δt	time-step (s)
U_{pu}	the minimum pickup velocity (m/s)
$U_{pu,original}$	the minimum pickup velocity of the original particles without the surface modification (m/s)
V	volume fraction (-)
$\mathbf{V}$	translational velocities (m/s)
V_p	volume of the particle (m ³)
v_r	radial particle velocity (m/s)
v_z	vertical particle velocity (m/s)
W	mass discharge rate (kg/s)
W_0	outlet width (m)
x	x-axis in three-dimensional coordinate system (-)
x_i	the mass fraction of the species (-)
y	y-axis in three-dimensional coordinate system (-)
Y	Young's modulus (Pa)
z	z-axis in three-dimensional coordinate system (-)
δ	deformation (m)
ν	Poisson's ratio (-)
σ	standard deviation (-)
μ	mean diameter (m)
ρ_p	particle density (kg/m ³)
μ_s	particle sliding friction coefficient (-)
ω	angular velocities (rad/s)
ω_r	radial particle angular velocity (rad/s)
ω_z	vertical particle angular velocity (rad/s)
ε	particle bed voidage (-)
ε_d	flowing void fraction of the particles (-)
ν	Poisson's ratio (-)
σ	standard deviation (m)

μ	arithmetic mean of the particle diameter (m)
μ_f	the viscosity of the fluid (m/s)
ρ_b	bulk density (kg/m ³)
ρ_f	the density of the fluid (kg/m ³)
ρ_g	gas (air) density (kg/m ³)
ρ_p	particle density (kg/m ³)
φ	sphericity of particle (-)
ℓ^n	unit vector along the major axis of the non-spherical particle n (-)
δ_{ij}	Kronecker delta function (-)
α	ratio of the height of the highest particle in the arch from the line joining the two outermost particles of the arch to half the distance between the outermost particles of the arch (-)

SUMMARY

The particulate system is very common in nature and in industry. The studies on the flow behaviors in the hopper and horizontal pneumatic conveying, which are quite common equipment to process the particles in application reveal the complicated dynamic behaviors due to the interactions between the individual particles and the interactions with surrounding gas and wall. The recent development in computational the motion and effect of a large number of small particles codes and computing capabilities enable detailed study of interactions between the particle and the wall and inter-particles, hence advancing mechanistic understanding of the particle dynamic behaviors. The impact of particle properties (i.e., particle polydispersity, particle size, particle shape, particle density, and friction coefficient) on the discharge characteristics (i.e., discharge rate, particle velocity, segregation, packing, collision force) are studied. Analysis of hopper flow with spherical particles of lognormal particle size distributions (PSDs) (Chapter 3 – 5) showed (i) the hopper discharge rate decreases with the increase of PSD width and the fluctuations of the discharge rate increase as the PSD width, which is correlated to the performance of particle velocity, particle angular velocity, and the collision force. However, the well-known Beverloo correlation predicts the discharge rates of lognormal PSDs poorly; (ii) the size-segregation increases as PSD width increases; (iii) To reduce the jamming probability, the PSDs width (σ/μ), the friction coefficient, and the initial fill height can be reduced, but not changes with the particle density. The study of hopper flow with non-spherical particles (Chapter 6 and 7) revealed: (i) For the monodisperse systems, particle shape is the dominant factor dictating discharge rate, compared to other

factors like aspect ratio, preferential orientation and packing; (ii) Regarding the binary-size mixtures, while the discharge rates are still dictated by particle shape, the positive correlation between discharge rate and solid volume fraction or mean aspect ratio is clear; (iii) As for the binary-shape mixtures, the discharge rates are similar for all twelve mixtures, reflecting a surprising lack of shape effects, which in turn means the negligible impact of solid volume fraction, aspect ratio and segregation extent; (iv) In the lognormal PSDs systems, the discharge rates decrease and further jamming as PSD width (σ/μ) increases and the particle angularities increases. The packing of the hopper is associated with the PSD width and shape of the particles. Finally, the influences of initial particle charge on the minimum pickup velocity in the pneumatic conveying are evaluated (Chapter 8). The experimental results found (i) for the particle initial charge range investigated (-10 to 10 nC), U_{pu} increased monotonically with particle initial charge; (ii) the well-acknowledged correlation mis-predicted U_{pu} by up to 10% for monodisperse systems and up to 40% of binary-size systems. This underscores the necessity to account for particle initial charge in such correlations, particularly for polydisperse particle systems.

Keywords: hopper flow; discrete element method (DEM); lognormal particle size distribution (PSD); PSD width; binary mixtures; non-spherical particle; discharge rate; segregation; jamming; packing; minimum pickup velocity (U_{pu}); particle charge; pneumatic conveying

Chapter 1. Introduction

1.1. Background

Flows involving solid particles is very common in nature and in wide-ranging industries. The dynamic behavior of particles is quite complicated. That attributes to the complicated interactions between the particles and the interactions with the surrounding material [1]. Recognizing and understanding the dynamic behavior of particulate systems and the underlying mechanisms with regards to the interactions is important to produce the results that can be generally used. Therefore, granular systems have become an important research focus for these years in worldwide.

1.1.1. Hopper flow

Hoppers are extensively used in the storage and discharge of particles in wide-ranging industries, hence, the design and the flow behavior within the hoppers have unsurprisingly received much attention [2-4]. Despite being a simple apparatus, the granular flow behavior within the hopper is non-trivial, with complex dynamical behaviors like fractal-like stress chains, convection, nonlinear waves, and so on are still not well understood to date [5, 6]. Considerations which have contributed to the understanding of such granular flow behavior include pressures due to static and impact loads [2], critical arching width [7, 8], transitions between steady flow states [4, 9], among others. To advance such knowledge, the hopper provides a simple yet practical case study,

thereby influences of particle properties [10-14] and the configuration of hopper [15-18] on the discharge behavior have been studied.

1.1.2. Horizontal pneumatic conveying

Pneumatic transport of granular material, which is applied to the chemical industry, pharmaceutical industry, and agricultural industry is a common operation.[19, 20] The process can be fully automated, which is flexible, economical and environmentally friendly. The transportation processes of pneumatic transport can be divided into two modes including dense and dilute phase conveying. The dense phase conveying is a preferred method for dealing with solids. The dilute phase conveying, in which a suspension is performed by particles in the gas, which is a stable mode. This mode has lower fluctuations and excursions in gas pressures [21].Therefore, to operate optimality, control easily, and decrease the damage, the understanding of the different flow regimes in pneumatic conveying of particles is a key issue for industrial applications.

1.2. Motivation and objectives

1.2.1. Overall objectives

The system consisting of particles is quite common worldwide and the dynamic behaviors of the particles are very complicated due to the complex interactions between individual particles and their interactions with surrounding gas and wall [1]. As both the hopper and pneumatic conveying are very common to the storage, discharge, and transport of the particles in industries, proper particle properties

are essential in the flow behaviors so that the most effective methods for processing the particles can be adopted.

The overall objective of the present research is to investigate the effect of different particle properties on the flow behavior in two process systems dealing with particles, which are hoppers and the horizontal pneumatic conveying as shown in Figure 1.1. Particles exist in the polydisperse form (i.e., mixture of various sizes and/or shapes, such as binary or continuous particle size distribution system) and various particle shapes (i.e. sphere, ellipsoid, cylinder, and cuboid) widely both in nature and industries. Also, charges are often accumulated on the surface of particles under certain circumstances. These should be investigated to understand the advantages and disadvantages on the flow behavior and to improve the storage, the discharge, and the conveying of the systems for further.

Figure 1.1. Flow chart of this thesis work.

1.2.2. Hopper flow with spherical particles

The objectives of the study on the hopper flow with spherical particles are:

- To determine the impact of lognormal PSD width on the hopper discharge characteristics, namely, the discharge rate, the overall PSD and the mean particle diameter, and also local particle velocities and size-segregation.
- To assess if the available correlations can predict the discharge rate of lognormal PSD well and relate the discharge rate to other particle behaviors (i.e., radial and vertical velocity (v_r and v_z), radial and vertical angular velocity (ω_r and ω_z), and collision force (F)) to provide an explanation for the varying discharge rates resulting from the different PSD widths.
- To evaluate the jamming probability of the hopper with the coupling effects of PSD width and friction coefficient, particle density, and fill height to the hopper.

1.2.3. Hopper flow with non-spherical particles

The objectives of the study on hopper flow with non-spherical particles are:

- To investigate the solid volume fraction of the packed bed, the particle orientation, the discharge rate, the number of residual particles after discharge and the segregation extent of six different non-spherical constituent particles (namely, two ellipsoids, two cylinders and two cuboids, with the same volume but different aspect ratios) and the binary mixtures of them.
- To further look into the flow behaviors (i.e., packing of the particles initialed in the hopper, the discharge rate for different particle systems, the jamming formed during the discharge, the segregation with the discharge, the force networks performed before the discharge, and the residues presented at the

end of discharge) affected by the lognormal particle size distribution (PSD) of non-spherical particles (namely, ellipsoids, cylinders and cuboids).

1.2.4. Particle initial charge on minimum pickup velocity (U_{pu}) in pneumatic conveying

- To understand the influence of particle initial charge on minimum pickup velocity for monodisperse and binary-size particles with different particle initial charges ranging between -10 and 10 nC.
- To explore if the well-established correlations for predicting U_{pu} can be used for the range of particle initial charges.

1.3. Structure of the thesis

This thesis comprises nine chapters:

Chapter 1 provides an overview of the background of current research and research objectives planned to be achieved.

Chapter 2 provides a comprehensive literature review, including the granular flow in hoppers and pickup velocity in the horizontal pneumatic conveying.

Chapter 3 investigates the impact of spherical particles with lognormal PSD widths ranging between 10% and 70% with the same mean particle diameter of 5 mm on the discharge characteristics in the hopper.

Chapter 4 attempts to reveal the relationship between the discharge rate to other particle behaviors (i.e., radial and vertical velocity (v_r and v_z), radial and vertical

angular velocity (ω_r and ω_z), and collision force (F)) to provide an explanation for the varying discharge rates resulting from the spherical particles with different PSD widths between 10% and 70% and the same mean particle diameter of 5 mm.

Chapter 5 assesses the jamming probability of the hopper with the spherical particles of the effects of PSD width from 10% to 50% with the same mean particle diameter of 10 mm, coupled with friction coefficient, particle density, and fill height to the hopper.

Chapter 6 discusses the flow behaviors of six different non-spherical constituent particles (namely, two ellipsoids, two cylinders and two cuboids, with the same volume but different aspect ratios) and the binary mixtures of them.

Chapter 7 is dedicated to understanding the flow behaviors affected by the lognormal PSD of non-spherical particles (namely, ellipsoids, cylinders and cuboids) with the same aspect ratio.

Chapter 8 aims at understanding the influence of particle initial charge on minimum pickup velocity for monodisperse and binary-size particles with different particle initial charges ranging between -10 and 10 nC.

Chapter 9 summarizes the key conclusions and major findings of the study and provides perspectives for future works.

Chapter 2. Literature review

2.1. Particle flow in hoppers

The hopper is commonly employed in many industries to store and discharge particles, such as in the pharmaceutical, chemical, and food industries, mainly because of their capacity to enhance flow conditions for particles [22-24]. To achieve a smooth and reliable discharge rate [25-27], prevent the jamming/arching phenomenon [28-30] and understand the segregation [10, 31, 32] in hoppers have been attracting much attention in worldwide for a long time. Many experimental and numerical works have been conducted to investigate the particle dynamic behaviors in the hopper. The effects of the particle and hopper properties [33, 34], the particle size distributions [35-37], the pressure exerted in hoppers [38] on the discharge rate, flow pattern, and segregation are studied by experiments systematically. However, the microscopic structure in the hopper and the mechanisms governing the flow cannot be approached by experiments very well. Thus, numerical study is an effective method for this purpose [1]. Two numerical methods i.e. the finite element method (FEM) and discrete element method (DEM) are widely used, which the latter is more powerful to study the particulate behavior due to the particles can be tracked individually. Zheng et al. [39] predicted the mass discharge rate from the conical hoppers using the elastoplastic model implemented with a Eulerian FEM approach. They concluded that the influences of material properties in mass discharge rate were complex. The internal friction angle and wall friction remarkably affected the mass discharge rate in cases of steep hoppers but became comparatively small in

shallow hoppers. The DEM initially proposed by Cundall and Strack for granular material [40] provides a method of tracking each particle numerically and has been widely adopted to study dense particulate behavior. Zhu et al. [1] reviewed the studies based on DEM simulations, which have collectively shed light on particle packing, particle flow, and particle-fluid flow, and concluded that DEM is an effective method for the particle-scale understanding of granular flow behavior.

2.1.1. Particle size range

The particle properties of various particle size ranges which have been reported include the monodisperse [41, 42], binary-size mixtures [10, 43] and multi-size mixtures [44, 45]. In the monodisperse system, Yu and Saxén [42] demonstrated that particle velocities are almost the same throughout the hopper excluding the exit area. For the binary mixtures, Ketterhagen et al. [46] found when the fine mass fraction is 5%, the binary system has the greatest segregation. Moreover, the segregation intensity decreases with the increase of the mass fraction of fines or decrease of the particle diameter ratio of the coarse to the fine. Anand et al. [15] also got a conclusion for binary mixtures, which is the discharge rate increases with the increase of the mass fraction of fines. As for ternary-size mixtures, Yu and Saxén [37] concluded that a lower fraction of fine particles shows the less extent of segregation compared to a high fraction of fine particles. Additionally, the extent of segregation is reduced by decreasing the particle diameter ratio of coarse to fine decreases, which agrees with the result of Ketterhagen et al. [46]. Gundogdu et al. [35, 36] conducted the experiment of continuous PSDs in the conical hopper and concluded that the discharge rate

predicted by the Beverloo correlation for polydisperse powders are successfully represented by an effective mean diameter, which is the 50% weight mean diameter. However, the continuous PSDs systems with the same means but different widths exhibit distinctly different behaviors [47-55]. The inclusion of particle properties like PSD into observation is important, especially since the particles in the hoppers are unavoidably polydisperse.

2.1.2. Particle shape

Particle shape has a significant impact on the particle flow behaviors from the hopper. Many researchers contributed to the study of the impact of particle shape on hopper flow behaviors [12, 56-64]. Especially at the micro-mechanical level, the flow dynamics such as the discharge rate and its quality [65, 66] and packing density [67, 68] are heavily dependent on the particle shape [56]. The spherical particles as the ideal particles processed in the hopper are widely studied in previous works. However, the non-spherical particles are more common and more complicated. Langston et al. [65] ran the simulation in a two-dimensional (2D) hopper and found that the discharge rate of disc-shaped particles is 40% faster than the spherical particles, which is possibly due to the lower resistance to the particle alignment yielded by the flow. It contrasts to the result of increasing the angularity of the particles reduces the discharge rates from the hopper by up to 28% in the three-dimensional (3D) hopper by Cleary and Sawley [12, 69]. They also concluded the elongated particles discharged 30% lower than for spherical particles. Similarly, Höhner et al. [5, 14] found the discharge rate decreases as the angularity of the particle increases, and the flow resistance of polyhedral particles is greater than spherical particles. Fraige et al. [67] illustrated

the non-spherical particles is lower than the spherical particles and the packing of non-spherical particles is denser than the spherical by comparing the cubic particles with the spherical particles. Gui et al. [32-34] analyzed the particles with different shapes and found compared to the spherical shape, the cubic particles have the additional motion resistance. The particle shape also has significant influence in the binary mixtures system. Wang et al. [66] revealed the discharge rate decreases as the increase of the sharp planes or vertices of the particles by assessing the binary mixtures of sphere and cylinder, sphere and cube, and cylinder and cube. Yu et al. [70] illustrated that both the binary mixtures of spherical and non-spherical particles can be described by the Westman equation which displays the relationship between the porosity and the volume fractions of binary mixtures. Wang et al. [71] found flowability is reduced due to the greater resistance by the more angular of the particle. Yu and Saxén [63] illustrated although the particle shape affects the discharge rate and the continuity of the flow, the size segregation is affected by the particle shape slightly. However, Alizadeh et al. [38] conducted experiments for binary mixtures and illustrated that segregation is driven by the difference in particle shape. Govender et al. [72] numerically investigated the polydisperse polyhedral particle and found the discharge time of the polydisperse particle is between that of the larger size particle and the smaller size particle. In conclusion, previous studies have given some insights into the shape factor of non-spherical particles. However, the influence of the width of the lognormal PSD of non-spherical particles on flow behaviors is not yet understood.

2.1.3. Hopper geometry

The function of buffering to regulate flow variation and operational instability was more often used provided by the hopper as a link of the unit operations in the applications [33]. Therefore, the design of the hopper should be reliable control and the understanding of the dynamic behavior of particle flow, the principles underlying particle flow in the hopper is essential. The characteristics of the flow affected mainly by factors of hopper configurations and particle properties. With regards to hopper designs, numerous works were conducted on conical hoppers [42, 43, 46], wedge-shaped hoppers[32, 73], and rectangular hoppers [15, 74]. Balevičius et al.[75] investigated different hopper geometries, namely, space-wedged, plane-wedged, and flat-bottomed and concluded the discharge rate influenced by the geometry significantly. Ketterhagen et al. [9] revealed the hopper shape factors including the wall angles and small wall friction angles critically affect the flow mode. The mass-flow regime transited to the funnel-flow regime by increasing either or both of them. Abatzoglou et al. [76] demonstrated the variations in local segregation is linked to the average velocity and axial and radial velocity distributions affected by the hopper geometry.

2.1.4. Discharge rate

The discharge rate is one of the most important consideration for the hopper flow. The Beverloo correlation [77] and the modified correlations by many researchers are widely used to predict discharge rates of the hoppers. Many works were done to develop the Beverloo correlation for various kinds of particles. The most

widely accepted Beverloo correlation is first proposed by Beverloo et al. [77] and expressed as:

$$W = C\rho_b g^{1/2}(d_0 - kd_p)^{5/2} \quad (2-1)$$

for predicting the discharge rate of the mono-sized particles discharged from a hopper with the flat bottom and circular orifice. W is the average discharge rate from the hopper, C and k are the empirical coefficients, ρ_b is the bulk density of the particle, g is the gravitational acceleration, d_0 is the diameter of the hopper orifice, and d_p is the particle diameter. Williams [26] indicated that the correlation should be modified considering the air drag on the particles for the finer ones ($d \leq 500 \text{ }\mu\text{m}$). Moreover, Spink and Nedderman [13] found the prediction value of the Beverloo correlation for finer particles ($50 \text{ }\mu\text{m} \leq d \leq 500 \text{ }\mu\text{m}$) is about twice as the measured values in the experiment, but the relationship between the discharge rate and particle size is right. Considering the significant effect of particle shape on the discharge rate, the Beverloo correlation was further incorporated with the shape parameters [35]. The empirical constant k in the correlation was found increases as the increase of the angularity of the particle inside the hopper [78]. César et al. [79] also demonstrated the flow parameters from Beverloo's equation are correlated with the shape parameters by the experimental study for the correlations between discharge rate parameters and the shape of the particles. A recent work [80] explored the impact of orifice shape on the flow rate by methods of experiment and simulation to demonstrated the results agree well with a modified Beverloo's formula.

With regards to non-monodisperse particle systems, the Beverloo correlation was extended to binary mixtures [27] and polydisperse mixtures [35, 36]. Tüzün et al. [81, 82] predicted the discharge rate of the binary mixtures from the hopper by a modified form of the Beverloo equation successfully. The Beverloo correlation was further developed by Humby et al. [27] based on the experimental work of Arteaga and Tüzün [10] for the binary mixture systems as:

$$W = C\rho_b g^{1/2} (W_0 - Z')^{5/2} \quad (2-2)$$

where $Z' = (2.1939d_{VM} - 0.0009)$ is the modified parameter for the binary mixtures that is linked to the particle size distribution of the mixture, where $d_{VM} = \sum_i x_i d_i^4 / \sum_i x_i d_i^3$ is the De Brouckere mean diameter that is a function of the number fraction x_i and diameter d_i of particle i .

For the polydisperse systems, Gundogdu put forward the Beverloo correlation should consider the pressure gradient generated by the self-entrained gas to a modified form [35]:

$$W = C\rho_b \sqrt{g + \left(\frac{dP}{dz}\right)_0 \frac{1}{\rho_b}} (d_0 - kd_{50})^{5/2} \quad (2-3)$$

where d_{50} is the median mass-based diameter, $(dP/dz)_0 = \left(\frac{150}{\frac{\rho_g U_{mf} d_p}{(1-\varepsilon_d)\mu_g}} + \right.$

$\left. 1.75 \right) \frac{\rho_g U_{mf}^2}{d_p} \frac{1-\varepsilon_d}{\varepsilon_d^3} + \rho_g g$, in which, U_{mf} is the minimum fluidization velocity of

the particles, ρ_g is the gas density, ε_d is the void fraction of the particles, and μ_g is the dynamic gas viscosity. He also [83] measured the discharge rate under

different positive pressure differences and observed the corresponding solids discharge regimes and by the experiment in a conical hopper and revealed the relationship between the positive pressure ΔP and the discharge regime.

2.1.5. Jamming phenomenon

Although most of the hoppers are designed to discharge particles, the jamming may occur to terminate the flow by arching of particles near the outlet [30]. Therefore, in order to prevent the disadvantage of the jamming/arching, the arching structure [84, 85] and methods to avoid jamming/arching are studied [28, 86, 87]. Previous studies [84, 88-90] gained a better understanding of various aspects of jamming by simplifying the three-dimensional hopper to two-dimensional (2D) hopper. To et al. [90-92] illustrated that the jamming probability is related to the ratio orifice diameter to particle diameter by characterizing the arches formed due to the jamming. Janda et al. [93] determined that the critical size of the hopper outlet, below which the jamming exists by the experiment on particle jamming phenomenon during the discharge. Guariguata et al. [89] analyzed the geometrical properties of the arches detailly by conducting experiments in a two-dimensional hopper, and had the conclusions of (i) the shape of the arch is not affected by the ratio of the hopper outlet size to the diameter of the spherical particle, (ii) the ratio of the width of the arch (i.e., the distance between the two outermost particles of the arch structure) to the height of the arch (i.e., the distance between the highest particle of the arch and the line of width) close to 1, and (iii) static friction is significant in the arch formation. Lou [94] illustrated that the influence of particle properties (coefficient of restitution and friction) on jamming is non-negligible for smaller openings, but

can be neglected for hoppers with large openings. Lin and Fang [95] unveiled that the jamming probability decreases with the increase of the particle aspect ratio for smaller hopper outlet orifices, but increases as the particle aspect ratio increases for the hoppers of with gentler slopes by the experimental investigation on the discharge characteristics of ellipsoid particles in a 2D hopper. Longjas et al. [96] used force analysis to present three flow regimes, i.e., the jam-free continuous flow, the transitory flow, and an N -dependent jammed state by evaluating the jamming probability of mixed disk-shaped particles in a 2D hopper. In reality, the observation of the jamming phenomenon extended to 3D hoppers is meaningful. Desmond and Franklin [97] analyzed the jamming in a 3D hopper and revealed two important factors to determine the jam tendency with rod-shaped particles are hopper size and particle aspect ratio. Pournin et al. [98] obtained the function for median jamming diameter (which is the hopper opening diameter for 0.5 of jamming probability) and particle diameter by investigating the effect of friction and boundary condition, and illustrated the jamming formation comes after the concentric particle rings. To avoid jamming, vibration is one of the most effective ways [28, 87, 99]. Janda et al. [87] presented discharge behavior with the vibration and pointed out that the discharge rate increased with the vibration amplitude significantly. Mankoc et al. [28] concluded a similar result that the discharge rate is increased by vibration due to the increasing number of particles discharged between one jam after another jam obviously. Mondal and Sharma [100] put forward the design of two adjacent openings for hoppers instead of one opening can avert the jamming by observing via a numerical study.

2.1.6. Size segregation

Segregation is a typical characteristic of particle flow with polydisperse particles, like, binary mixtures, ternary mixtures, and continuous PSD. Yu and Saxén [37] concluded that the filling method is more important than the other factors which affect the intensity of segregation and suggested to pay more attention to the initial state of the hopper. Regarding binary-size mixtures, Ketterhagen et al. [46] illustrated the segregation intensity increases as the ratio of coarse particle diameter to the fine and unveiled when the fine mass fraction is 5%, the hopper has the greatest extent of segregation. For ternary-size mixtures, Yu and Saxén [37] concluded that the segregation intensity is smaller for a lower fraction of fine particles and the extent of segregation decreases with the decrease of particle diameter ratio of coarse to fine, which is consistent with the result in binary mixtures [46]. Zhao et. al. [101] numerically studied the impact of the lognormal PSD on the hopper discharge behaviors and found the extent of the segregation increases with the increase PSD width (the ratio of the standard deviation to the mean particle diameter).

2.2. Minimum pickup velocity (U_{pu}) in pneumatic conveying

Pneumatic conveyors are extensively used to transport various solid particles in a gas stream in the chemical industry, agricultural industry and pharmaceutical industry due to the low maintenance, low energy cost, ease of automation and control amenability [102, 103]. These industries have established a large number of applications of it, but the apparatus is often run based on empirical correlations, rather than scientific principles. Hence, to understand the principle in a

mechanistic way is important to operate the pneumatic conveying efficiently. The transportation processes of pneumatic transport including two modes, dense and dilute phase conveying. The former is a preferred method for dealing with solids and the later is a stable mode in which a suspension is performed by particles in the gas and has lower fluctuations and excursions in gas pressures [21]. There are many factors, like pressure, moisture, affecting the operation of the pneumatic conveying system. Particularly, the gas velocity used in pneumatic conveying influences the performance of the system and the efficiency. The proper conveying velocity can avoid the issues of sedimentation and clogging when the gas velocity is below the necessary (the minimum conveying velocity) and particle attrition, pipe erosion, and energy cost when the gas velocity is too much higher than the necessary [20, 104-108]. Therefore, it is important to identify the critical velocities to operate the pneumatic conveying systems.

To predict the minimum conveying velocity (U_{pu}) requires distinguishing the pickup mechanisms from the saltation mechanisms. Minimum pickup velocity (U_{pu}) differs from minimum saltation velocity due to the difference in the initial position of the particles. U_{pu} is defined as the minimum fluid velocity at which particles initiate to move in a constant mode without deposition in the pipe [109]. That is to say, the particles initially lie at rest on the bottom of the pipe for Minimum pickup velocity. Nevertheless, particles initially suspended for the minimum saltation velocity [106]. Compared to minimum fluidization velocity (U_{mf}) in the system of fluidization, U_{pu} in the pneumatic conveying is also the minimum gas velocity required to convey the particles and has important

applications in gas-solid flows. Nevertheless, U_{pu} is not as well understood as U_{mf} [110].

2.2.1. U_{pu} for monodisperse particles

Some researchers have studied the pickup velocity of the monodisperse particles in the pneumatic conveying. Cabrejos and Klinzing [111] proposed a technique to determine U_{pu} , which is based on visual observation. They concluded that U_{pu} decreases then increases with particle sizes increasing, which is due to cohesion of the particles decreasing in the lower particle diameter range and the inertial forces increasing in the higher particle diameter range. Furthermore, Cabrejos and Klinzing [112] developed a correlation for predicting the U_{pu} using the dimensional analysis:

$$\frac{U_{pu}}{\sqrt{gd_p}} = 0.0428 Re_p^{0.175} \left(\frac{D}{d_p} \right)^{0.25} \left(\frac{\rho_p}{\rho} \right)^{0.75} \quad (2-4)$$

where g is the gravity acceleration, d_p is the particle diameter, Re_p is the Reynolds number, D is pipe diameter, ρ_p and ρ are particle density and gas density, respectively. Then, Hayden et al. [113] studied on the monodisperse particles of Geldart groups A and C [114] and concluded that the minimum pickup velocity (U_{pu}) for the non-spherical particles is greater than the spherical particles and electrostatic force is important for the glass particles with diameters from 20 μm to 40 μm . Gomes and Mesquita [109] illustrated the U_{pu} increases as particle diameter increases agreed with the experimental finding of Cabrejos and Klinzing [111]. They also concluded U_{pu} increases with the decrease of particle sphericity and the increase of the pipe diameter. Kalman et

al. [106] investigated the Geldart groups A, B, and D for further and defined three Pickup Zones (1, 2, and 3) for classifying the particles based on the relationship between the Archimedes number (Ar) and the Reynolds number (Re_p^*). Archimedes number (Ar) is the ratio of gravitational force to viscous force and the Reynolds number (Re_p^*) is the ratio of inertial force to viscous force. The equations of the three Pickup Zones (1, 2, and 3) are as follows:

$$\text{Zone 1: } Re_p^* = 5Ar^{\frac{3}{7}} \text{ for } Ar \geq 16.5 \quad (2-5)$$

$$\text{Zone 2: } Re_p^* = 16.7 \text{ for } 0.45 < Ar < 16.5 \quad (2-6)$$

$$\text{Zone 3: } Re_p^* = 21.8Ar^{\frac{1}{3}} \text{ for } Ar \leq 0.45 \quad (2-7)$$

where Re_p^* is the particle Reynolds number modified accounting for different pipe diameters [106] and Ar is the Archimedes number.

$$Re_p^* = \frac{\rho_f d_p U_{pu}}{\mu_f (1.4 - 0.8e^{-\frac{D/D_{ref}}{1.5}})} \quad (2-8)$$

and

$$Ar = \frac{g \rho_f (\rho_p - \rho_f) d_p^3}{\mu_f^2} \quad (2-9)$$

where, ρ_f is the density of the fluid; d_p is the diameter of the particle; μ_f is the velocity of the fluid; D is the diameter of the pipe; D_{ref} is the reference pipe diameter of 50 mm; g is the gravity acceleration; ρ_p is the density of the particle. Approximately, Zone 1 is in correspondence to the larger Geldart Group

B and D particles, Zone 2 is corresponding to Geldart Group A, while Zone 3 corresponds to the highly cohesive Geldart Group C.

Figure 2.1. Three zones model of Re_p^* and Ar given by monodisperse (Kalman et al. [106]) correlations.

2.2.2. U_{pu} for binary and ternary mixtures

Goy et al. [103] studied the effect of the binary-size mixtures of spherical particles on U_{pu} . For the mixtures of particles in Zone 1, the U_{pu} increases with the increase mass fraction of larger particles. For the mixtures of particles in Zone 1 and 2, the U_{pu} decreases with the increase of the mass fraction of the larger particles, which is due to the increasing cohesive forces of particles in Zone 2. However, for the mixtures of particles in Zone 1 and 3, the U_{pu} is not affected because the inertial forces of the particles in Zone 1 are more significant than the cohesive forces of the particles in Zone 3. Kalman's equations can be applied to predict the U_{pu} of binary mixtures in Zone 1 and the mixtures of particles in Zone 1 and 2, not to the mixtures of particles in Zone 1 and 3. Recently, Anantharaman

et.al. [104] investigated the binary mixtures in gas-solid pneumatic conveying and revealed (i) the U_{pu} of binary-size mixtures is more decided by the U_{pu} of the particles with larger diameter; (ii) the U_{pu} of binary-density mixtures is more decided by the U_{pu} of the particles with larger density; (iii) the effect of particle diameter is more significant than particle density and the particle shape had a non-negligible influence on the U_{pu} . Furthermore, Tay et. al.[115] studied the pickup velocity of ternary-size mixtures. They found that the existence of smaller particles aided the entrainment of binary-size mixtures as the third species. The relationship of the Archimedes number (Ar) and the Reynolds number (Re_p^*) for binary and ternary mixtures was modified by Tay et. al.[115]:

$$Re_p^* = 20Ar^{\frac{1}{4}} \text{ for } 20 \leq Ar_{mixture} \leq 2500 \quad (2-10)$$

2.2.3. U_{pu} for polydisperse particles

A more complicated and more practical particulate system, i.e., polydisperse particles are numerically studied by Eskin et al. [116]. They revealed the particles' polydispersity is significant in the flow, which should be considered in engineering. Anantharaman et al. [110] found that U_{pu} values were surprisingly non-monotonic, which the U_{pu} decreased first and then increased with the increase of the width of the lognormal PSD. Moreover, they concluded the particles with the lower sphericity show more non-monotonic behaviors.

Chapter 3. The discharge characteristics of lognormal PSDs of spherical particles

The content of this chapter has been published under the title of *DEM Study on the Discharge Characteristics of Lognormal Particle Size Distributions from a Conical Hopper* in *AIChE Journal*, vol. 64, pp. 1174-1190, April 2018 (<https://doi.org/10.1002/aic.16026>).

Abstract

This study employs the discrete element method (DEM) to investigate the impact of the widths of lognormal particle size distributions (PSDs) with the same mean particle diameter on hopper discharge behaviors, namely, discharge rate, particle velocities, and size-segregation. Results reveal that (i) the hopper discharge rate decreases as PSD width increases; (ii) the mean discharge rates are constant with time, but the fluctuations increase as the PSD width increases; (iii) the overall size-segregation increases with PSD width; (iv) the overall mean particle diameters of the narrower PSDs do not exceed the initial mean of 5 mm, whereas that of wider ones do; (v) the relationship between PSD width and particle velocities is non-monotonic with no consistent trends; and (vi) no direct correlation exists between particle velocity and size-segregation. The results here provide valuable insights on the behavior of the prevalent polydisperse mixtures in hoppers.

Keywords: discrete element method (DEM), hopper discharge, particle size distribution (PSD), distribution width, segregation

3.1. Introduction

Hoppers are widely used in the storage and discharge of particles in wide-ranging industries; hence, the design of and flow behavior within the hoppers have unsurprisingly received much attention [2-4]. Despite the simple geometry, the granular flow behavior within the hopper is non-trivial, with complex dynamical behaviors like fractal-like stress chains, convection, nonlinear waves, and so on still not well understood to date [5, 6]. Considerations which have contributed to the understanding of such granular flow behavior include pressures due to static and impact loads [2], critical arching width [7, 8], transitions between steady flow states [4, 9], among others. To advance such knowledge, the hopper provides a simple yet practical case study, thereby effects of particle properties [10-14] and hopper configuration [15-18] on the discharge behavior have been studied.

The DEM initially proposed by Cundall and Strack for granular material [40] provides an alternative way of tracking each particle numerically and has been widely adopted to study dense particulate behavior. Zhu et al. [1] reviewed the studies based on DEM simulations, which have collectively shed light on particle packing, particle flow, and particle-fluid flow, and concluded that DEM is an effective method for the particle-scale understanding of granular flow behavior. With regards to the application of DEM for hoppers, numerous hopper designs such as conical hoppers [42], cylindrical hoppers [46], rectangular hoppers [74] and wedge-shaped hoppers [17] have been investigated. Ketterhagen et al. [9]

demonstrated that the hopper shape is a critical factor affecting the flow mode. As either or both of wall angles and small wall friction angles increase, the flow transitions from mass-flow to the funnel-flow regime. Balevičius et al.[75] found that the hopper geometry (namely, plane-wedged, space-wedged, and flat-bottomed) exerts a significant impact on the discharge velocity, which leads to the relationship between the hopper geometry and microscopic inter-particle friction. Anand et al. [15] revealed that particle-particle friction has a greater influence on the discharge rate of hopper flow than particle-wall friction. Yu and Saxen [37] concluded that, among the many factors affecting the extent of segregation, the most important one is the filling method, which suggests that the initial state prior to discharge is critical. The inclusion of particle properties like PSD into the DEM model is important, especially since the particles in the hoppers are unavoidably polydisperse. The study of various particle size ranges has been reported, including monodisperse [41, 42], binary-size mixtures [10, 43] and multi-size mixtures [44, 45]. Yu and Saxén [42] found that particles have the same velocities almost throughout the hopper except at the exit. With regards to binary-size mixtures, Anand et al. [15] revealed that the discharge rate of solid phase increases with increasing the mass fraction of fines. Ketterhagen et al. [46] assessed binary-size mixtures too. They found that the greatest extent of segregation is at the fine mass fraction of 5%, above which the segregation intensity decreases as the mass fraction of fines increases, and that the extent of segregation increases for large particle diameter ratio of coarse to fine. For ternary-size mixtures, Yu and Saxén [37] concluded that the extent of segregation reduces for a low fraction of fine particles compared to a high fraction of fine

particles, and agreed with Ketterhagen et al. [46] that reducing the particle diameter ratio of coarse to fine decreases the extent of segregation. Gundogdu et al. [117, 118] experimentally investigated the discharge characteristics of three continuous PSDs from a conical hopper, and indicated that using the 50% cumulative weight fraction as the effective mean diameter in the Beverloo equation allowed for reasonable predictions of the hopper discharge rates. Notably, although a single mean is typically provided to represent the PSD, it has been reported that continuous PSDs with the same means but different widths exhibit distinctly different behaviors [47-55].

In order to bridge the gap in the knowledge base regarding the impact of the width of PSDs with the same mean particle diameter on hopper discharge characteristics, this study uses the DEM to investigate the common lognormal PSDs. The particle systems investigated in this study have the same mean particle diameter (μ) of 5 mm, and range from a monodisperse system (i.e., particles are all of the same particle diameter) to lognormal PSDs with the ratio of standard deviation to mean particle diameter (σ/μ) of between 10 and 70%. The objective of the current study on hopper discharge is twofold: (i) to determine the impact of lognormal PSD width on the hopper discharge characteristics, namely, the discharge rate, the overall PSD and the mean particle diameter, and also local particle velocities and size-segregation, and (ii) to determine the correlation between local particle velocity and local mean particle diameter.

3.2. Material and method

3.2.1. Discrete element method (DEM)

The DEM tracks each particle in the Lagrangian framework. In granular systems, the particle motion is governed by Newton's second law, and the gas phase is neglected because of the relative stagnation and significant density difference between the gas and solid phases. The translational and rotational motion of a particle i is generally formulated per Eqs. 3-1 and 3-2, respectively:

$$m_i \frac{d\mathbf{V}_i}{dt} = \sum_{j=1}^K (\mathbf{F}_{c,ij}^n + \mathbf{F}_{c,ij}^t + \mathbf{F}_{d,ij}^n + \mathbf{F}_{d,ij}^t) + m_i \mathbf{g} \quad (3-1)$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^K (\mathbf{M}_{t,ij} + \mathbf{M}_{r,ij}) \quad (3-2)$$

where m_i is the mass of particle i , $\mathbf{V}_i$ is the translational velocity of particle i ; $\boldsymbol{\omega}_i$ is the angular velocity of particle i ; I_i is the moment of inertia of particle i ; K is the total number of particles and walls interacting with the particle i ; $\mathbf{F}_{c,ij}^n$ and $\mathbf{F}_{c,ij}^t$ are respectively the normal and tangential contact forces between particles i and j ; $\mathbf{F}_{d,ij}^n$ and $\mathbf{F}_{d,ij}^t$ are the damping forces respectively in the normal and tangential directions between particles i and j ; $\mathbf{M}_{t,ij}$ is the torque generated between particles i and j by tangential forces and $\mathbf{M}_{r,ij}$ is rolling friction torque generated between particles i and j ; and $\mathbf{g}$ and t represent respectively the gravitational acceleration and time instant. The particles are assumed to be elastic and frictional in this study, and the inter-particle interactions are defined by algorithms of classical contact mechanics, in which the normal and tangential forces between two particles are evaluated by the Hertz theory[119, 120]. The platform used in the current work is Liggghts 3.4.1.

Furthermore, the post-processing is achieved by the open-source software – ParaView 5.0.1.

3.2.2. Particle-size distribution (PSD)

The type of PSD considered in this study is the common lognormal PSD, with the following number-based frequency (f_N) distribution

$$f_N = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{(\ln(x)-\mu)^2}{2\sigma^2}\right] \quad (3-3)$$

where x is particle diameter, σ is the standard deviation of the PSD and μ is the mean particle diameter. The width of the lognormal PSD is defined here as the ratio of standard deviation to mean particle diameter (σ/μ), and the range of σ/μ values evaluated is between 10% and 70%, particularly in view of the non-monotonic segregation behavior with respect to PSD width in this range in the bubbling fluidized bed [47]. The mean particle diameter (μ) is kept constant in this study at 5 mm instead of 10 mm per that used in the experimental study of monodisperse particles in Li et al. [41], because the latter necessitated particles that are larger than one-fifth of the hopper outlet orifice diameter for the wider PSDs investigated ($\sigma/\mu \geq 50\%$), which has been reported to lead to bridging or arching by mechanical interlocking [121]. Figure 3.1 shows the different widths of the number-based PSDs researched in this study.

Figure 3.1. Number-based lognormal PSDs with a constant mean particle diameter (μ) of 5 mm and PSD widths (σ/μ) of 10, 30, 50 and 70%.

3.2.3. Simulation setup

The hopper studied is a conical hopper similar to that in the experimental study by Li et al. [41], with a cylindrical diameter of 240 mm, a total height of 500 mm, and cone height of 51.96 mm. The cone is angled at 60° and the diameter of the outlet orifice at the bottom is 60 mm. Figure 3.2 presents the schematic of the hopper filled with particles to an initial packed bed height of 474 mm. The particles studied are glass beads with a mean particle diameter (μ) of 5 mm and particle density (ρ_p) of 2460 kg/m^3 , as listed in Table 3.1 along with the other parameters adopted in the current work.

Table 3.1. Physical properties of the glass beads.

Parameter	Value
Diameter, μ (mm)	5

σ/μ (-)	10, 30, 50 and 70%
Density, ρ_p (kg/m ³)	2460
Young's modulus, Y (GPa)	0.1
Poisson ratio, ν (-)	0.25
Coefficient of static friction of particle-wall (-)	0.6
Coefficient of rolling friction of particle-wall (-)	0.05
Coefficient of restitution of particle-wall (-)	0.99
Coefficient of static friction of particle-particle (-)	0.6
Coefficient of rolling friction of particle-particle (-)	0.01
Coefficient of restitution of particle-particle (-)	0.99
Time-step, Δt (s)	2×10^{-5}

Initially, the orifice outlet at the bottom of the hopper is sealed to prevent any particle outflow. The glass beads are randomly generated in the whole domain of the hopper and allowed to settle under the gravity to a final packed bed with a height of 474 mm. Then, the seal at the orifice outlet is removed to allow the glass beads to flow outwards under the influence of gravity. To achieve the same bed height of 474 mm for all the PSD widths investigated, the number of glass beads used for the monodisperse system is 181,483, while that in the lognormal PSDs are 171,259, 145,734, 102,202 and 67,406 respectively for the widths (σ/μ) of 10, 30, 50 and 70%. The time step (Δt) used in the simulation is 2×10^{-5} s.

Figure 3.2. Schematic of the hopper initially filled to a packed bed height of 474 mm.

3.3. Model Validation

The model is validated against the experimental results of Li et al. [41]. The same monodisperse glass beads with a particle diameter (μ) of 10 mm are used. To create an initial packed bed with a height of 474 mm, 23,283 glass beads are generated in the simulation. The three-dimensional (3-D) hopper in Figure 3.2 is used in the simulation, but a semi-cylindrical one with the same dimensions is used in the experimental study [41]. Figure 3.3 shows the comparison of the bed heights between the experiment and simulation at four-time instances, namely, $t = 0$ s (Figure 3.3a), 6 s (Figure 3.3b), 12 s (Figure 3.3c) and 18 s (Figure 3.3d). At each time instance, the experimental and simulated hoppers are respectively shown on the left and right. The similar bed heights at each of the four time instances indicate similar discharge rates, which provides a preliminary validation of the model.

Figure 3.3. Comparison of the instantaneous bed height of the experimental [41] and simulated hopper at time instances of (a) 0, (b) 6, (c) 12 and (d) 18 s. The red beads in the experimental hopper represent the nine particles tracked experimentally.

To further validate the numerical model, the trajectories of the particles in the experimental and simulation studies are compared. In the experimental study [41], nine particles, which were dyed red and aligned at a bed height of 70 mm from the bed surface initially (Figure 3.3a), are tracked as the hopper emptied (Figures 3.3b-d). For the validation study, five particles are tracked via DEM. Figure 3.4 illustrates the trajectories of the five particles as they exit the hopper, with the

discrete points representing the experimental results [41] and the lines representing the simulation results. Good agreement between these two results is clear, especially in terms of the vertical trajectories higher up in the hopper. From approximately mid-height of the hopper to the discharge outlet, the slight discrepancies are presumably due to the semi-cylindrical hopper used experimentally which thereby is subjected to a greater influence from the walls, but a fully three-dimensional cylindrical hopper is used in this study [42].

Figure 3.4. Comparison of the trajectory of five tracked particles between the experiment [41] and the simulation. The boundary of the hopper is shown in grey; radial positions of 0 and 120 mm symbolize respectively the centerline and boundary of the hopper.

3.4. Results and discussion

3.4.1. Discharge rate

The discharge rate of a hopper is typically an important design consideration. Accordingly, the impact of the PSD width (σ/μ) on the discharge rate is

investigated here. Figure 3.5 illustrates the progressive mass discharged from the hopper with time as the width (σ/μ) of the lognormal PSD increases. Two key observations are: (i) the decreases in mass with time are largely linear, which indicates constant discharge rates; and (ii) the time taken to empty the hopper increases as the PSD width (σ/μ) increases, which indicates the non-negligible impact of PSD width on hopper discharge rates.

Figure 3.5. Mass discharge versus time profiles of the particle systems investigated.

Figure 3.6a displays the discharge rate versus time for the five systems with different PSD widths. Generally, agreeing with Figure 3.5, each discharge rate fluctuates around a constant value then plunges steeply to zero when the particles are depleted. Three observations are clear. First, the mass discharge rate decreases as the PSD width (σ/μ) increases. Specifically, the durations for discharging all the particles in the hopper are significantly different at 19.96 and 32.80 s, respectively, for the monodisperse system and the system with the widest lognormal PSD of $\sigma/\mu = 70\%$. Because the mass fraction of the coarser species larger than 6 mm also increases with PSD width (σ/μ), with the mass ratio of the

larger species [32]. On the contrary, since the mass fraction of finer particles smaller than 4 mm increases with PSD width (σ/μ), the results here contradict with the results for the binary mixtures, whereby the discharge rate increases as the mass fraction of the finer species increases [27]. The inability to predict the behavior of the continuous PSDs based on the available binary results is consistent with a previous study on segregation characteristics in a bubbling fluidized bed [122]. The underlying mechanism for such discrepancies is likely tied to the inter-species interactions among the multiple particle types as opposed to that between just two particle types, as evidenced by a study on ternary-size mixtures that the presence of an intermediate-sized particle type increases the segregation between the small and large particles [123]. The incomplete understanding underscores the need for more in-depth studies on such polydisperse systems. Second, the rates are approximately constant throughout the discharge process for all five particle systems, which is consistent with that for binary mixtures [124]. This indicates that the inevitable size segregation does not affect the constancy of the discharge rate throughout the hopper discharge for both the binary mixture and the continuous PSDs. Third, the fluctuation of the discharge rate increases as the PSD width (σ/μ) increases, which indicates that the outward flow of particles is smoother for the narrower PSDs. Uñac et al. [125] interpreted the fluctuations as due to repeated particle arching (which decreases discharge) and breaking of the arches (which increases discharge) during hopper discharge, and further indicated that larger particles are more likely to form arches. This sheds light on the results here, specifically in that the wider PSDs with greater mass fractions of coarser species larger than 6 mm exhibit greater

fluctuations during discharge. Multiple studies have reported on such fluctuations [18, 39, 75, 126-128], but none of them for the comparison of the different widths of PSD. Figure 3.6b further displays discharge rate versus PSD width (σ/μ), which indicates that the discharge rate decreases as PSD width increases. In particular, the decrease in the discharge rate is significant at approximately 36% when the PSD changes from a monodisperse to a lognormal PSD with σ/μ of 70%. This underscores the importance of considering PSD width (σ/μ) in the operation of hoppers.

Figure 3.6. (a) Mass discharge rate with respect to time; (b) Discharge rate with respect to PSD width (σ/μ).

3.4.2. Overall size-segregation

The significant impact of PSD width on hopper discharge rates seen in Figures 3.5 and 3.6 warrants more in-depth understanding of the associated behaviors especially in view of the ubiquity of lognormal PSDs. Therefore, this section further explores the change in PSD due to the inevitable size-segregation effects as the hopper discharges.

Figure 3.7 shows the relative particle diameter (i.e., ratio of the mean particle diameter of all the particles in the hopper at each time instant to the initial mean particle diameter of 5 mm, such that a value of 1 corresponds to a mean particle diameter of 5 mm) in the hopper with respect to time for the various PSDs, with each trendline ending at different time instants due to the varying discharge rates (Figure 3.6b). Although the PSDs have the same mean particle diameter (1), Figure 3.7 indicates that the trends are clearly different. The narrower PSDs ($\sigma/\mu \leq 30\%$) are such that the relative particle diameters do not exceed 1, whereas the wider ones ($\sigma/\mu \geq 50\%$) do, which is tied to the segregation behavior. For the monodisperse particle system, the trendline is expectedly horizontal at a relative particle size value of 1, since all the particles are of the exact same diameter. For the narrower lognormal PSDs with widths (σ/μ) of 10 and 30%, the relative particle diameter remains flat at 1 throughout most of the hopper discharge, then decreases toward the final few seconds, with a greater decrease for the PSD with $\sigma/\mu = 30\%$. This suggests the preferential segregation of the smaller particles toward the top of the particle bed as the hopper empties. Interestingly, the trends are dissimilar for the wider PSDs with $\sigma/\mu \geq 50\%$. For the intermediate lognormal PSD with a width σ/μ of 50%, the relative particle diameter increases beyond 1 gradually with time before decreasing to below 1 in the final time instants of the hopper discharge. This implies that the larger particles are retained in the hopper while the smaller particles preferentially discharge initially presumably by percolating through the larger particles; then, toward the end of the hopper discharge, the trends are more similar to that for the narrower PSDs in that the relative particle size decreases to less than 1 toward

the end of the hopper discharge. As for the widest lognormal PSD with a width (σ/μ) of 70%, the size-segregation effect is the greatest and occurs quickest. In contrast to the other PSDs, the relative particle size is above 1 throughout the hopper discharge, with the value increasing more steeply with time before decreasing toward the end of the discharge. This is presumably because the greater proportion of smaller particles (Figure 3.1) expectedly exhibit even higher tendencies to percolate through the larger particles to be preferentially discharged, although indications of the preferential segregation of the smaller particles to the top of the hopper is still present as evidenced by the decreased in the relative particle diameter in the final instants of the discharge. Therefore, Figure 3.7 indicates that the extents of the size-segregation and preferential discharge by sizes are different for the systems with different PSD widths (σ/μ), which is likely due to both the different ranges of particle sizes and the different durations over which the segregation occurred.

Figure 3.7. Relative particle size discharged with respect to time for the various PSDs. A relative particle size value of 1 correspond to a particle diameter of 5 mm, and the time instant at which the trendline ends signifies that the hopper is completely emptied.

Figures 3.8a–d further present the change in the PSDs as the hopper with initial PSD widths (σ/μ) of 10% (Figure 3.8a), 30% (Figure 3.8b), 50% (Figure 3.8c), and 70% (Figure 3.8d) empties to bed heights of 470 mm, 350 mm, and 200 mm. Clearly, the shifts in PSDs (i.e., extent of size segregation) increase as the PSD width increases. While the change in PSD during hopper discharge is negligible for the narrower PSD widths of $\sigma/\mu \leq 30\%$ (Figures 3.8a, b), the PSDs progressively shift rightwards as the hopper discharges for $\sigma/\mu \geq 50\%$ (Figures 3.8c, d). This is consistent with Figure 3.7, which shows negligible change in the relative particle diameter throughout most of the hopper discharge for the PSDs with $\sigma/\mu \leq 30\%$, but more drastic changes in the relative diameter upon the onset of hopper discharge for the wider PSDs ($\sigma/\mu \geq 50\%$) as the increased fines exhibit a greater tendency to percolate through the larger interstices between the larger particles. Because both the mass fractions of finer particles smaller than 4 mm and coarser particles larger than 6 mm increase with PSD width, the results here contradict that of binary mixtures in which the extent of segregation decreased as the mass fraction of the finer species increased [10], and also that of another study on binary, ternary and quaternary mixtures in which extent of segregation decreased as the mass fraction of coarse components increased [45]. This is likely because of the continuous range of particle sizes for the PSDs considered here leads to different interactions among the species and percolation characteristics.

Furthermore, Figure 3.9 shows the change in the representation of the different particle sizes as the hopper discharges for the four lognormal PSDs. The y-axes represent the number of particles of each size range as the hopper discharges with

respect to the initial number of particles, while the x-axes represent the mass percentage of the hopper discharged. Each sub-plot represents each of the lognormal PSDs with σ/μ ranging between 10 and 70%, while each trend represents each particle size range. The divergence of the lines increases as the PSD width increases, which indicate the extent of size-segregation increases with PSD width and agrees with Figures 3.7 and 3.8.

Figure 3.8. PSDs at particle bed heights of 474, 470, 350 and 200 mm of lognormal PSDs with σ/μ of (a) 10%, (b) 30%, (c) 50% and (d) 70%.

Figure 3.9. Number of particles of different sizes during hopper discharge normalized with respect to the initial number versus mass percentage of hopper discharged for lognormal PSDs with $\sigma/\mu =$ (a) 10%, (b) 30%, (c) 50% and (d) 70%.

Segregation indices each bounded between 0 (i.e., perfect mixing) and 1 (i.e., perfect segregation) can be used to quantify the extent of segregation. The axial and radial segregation indices are expressed as [122, 129]

$$s_{axial} = \frac{s_h - 1}{s_{h,max} - 1} \quad (3-4)$$

$$s_{axial} = \frac{s_r - 1}{s_{r,max} - 1} \quad (3-5)$$

where S_h and S_r are the actual extents of segregation expressed as

$$S_h = \frac{\langle h_{small} \rangle}{\langle h_{large} \rangle} \quad (3-6)$$

$$S_r = \frac{\langle r_{small} \rangle}{\langle r_{large} \rangle} \quad (3-7)$$

where $\langle h_{small} \rangle$ and $\langle h_{large} \rangle$ are the average dimensionless heights of, respectively, the small and large particles, while $\langle r_{small} \rangle$ and $\langle r_{large} \rangle$ are the average dimensionless radii of, respectively, the small and large particles. Here, small and large are defined, respectively, as the initial smallest number-based 15% and largest number-based 15%. Specifically,

$$\langle h_{small} \rangle = \sum_i (x_{small,i} * h_i) \quad (3-8)$$

$$\langle h_{large} \rangle = \sum_i (x_{large,i} * h_i) \quad (3-9)$$

$$\langle r_{small} \rangle = \sum_i (r_{small,i} * r_i) \quad (3-10)$$

$$\langle r_{large} \rangle = \sum_i (r_{large,i} * r_i) \quad (3-11)$$

where x_i represents the number fraction of the species in that particular axial or radial section, h_i represents the dimensionless height (with respect to the bed height) of each axial section, and r_i represents the dimensionless radius (with respect to the total radius) of each radial section. The S_{max} in Eqs. 3-4 and 3-5 is the maximum extent of segregation, which is expressed as

$$S_{max} = \frac{2x_{large} + x_{small}}{x_{large}} \quad (3-12)$$

Figure 3.10 presents the axial (S_{axial}) and radial (S_{radial}) segregation indices as the hopper discharges, which indicates that both indices increase as the hopper discharges. Regarding axial segregation, Figure 3.10a shows that S_{axial} generally increases with PSD width, with that for the wider PSDs ($\sigma/\mu \geq 50\%$) exhibiting much greater S_{axial} values while that of the narrower PSDs ($\sigma/\mu \leq 30\%$) exhibiting negligible S_{axial} values until toward the end of discharge. This agrees with Figure 3.7. The slight dip of the S_{axial} value of the lognormal PSD with $\sigma/\mu = 30\%$ below that of $\sigma/\mu = 10\%$ at about 82% of discharge is due to the transition of the bed surface from the cylinder to the cone. As for radial segregation, Figure 3.10b shows similar trends. Interestingly, the S_{radial} values of the narrowest PSD ($\sigma/\mu = 10\%$) is greater than that of the broader PSD of $\sigma/\mu = 30\%$ throughout most of the hopper discharge, which may be due to the choice of local radial region (15 mm), and designations of small (15% of smallest) and large particles (15% of largest). Nonetheless, it is clear that the broader PSDs ($\sigma/\mu \geq 50\%$) segregate much more extensively.

This section hence provides evidence that the extent of segregation generally increases monotonically with PSD width, which is tied to the decrease of discharge rates with PSD width (Figure 3.6b).

Figure 3.10. (a) Axial segregation index (S_{axial}); and (b) radial segregation index (S_{radial})

3.4.3. Particle velocity

The different discharge rates imply different velocities, which warrants a closer look at the velocity profiles. Figure 3.11 shows snapshots of the instantaneous velocity profiles and PSDs at four time instances (namely, $t = 0, 6, 12$ and 18 s) for the five particle systems assessed with the same mean particle diameter ($\mu = 5$ mm) but different PSD widths (namely, monodisperse, and lognormal PSDs with $\sigma/\mu = 10\%$ - 70%). Specifically, each column represents a specific time instant, while each row represents the system with a specific PSD. The hoppers start with the same initial packed bed with a height of 474 mm at $t = 0$ s (first column of Figure 3.11), then discharge with time. It is clear that the particle velocities throughout the particle bed increase as the hoppers discharge and the different particle sizes tend to discharge at different rates. Two interesting observations are highlighted here. First, the velocity distributions are distinctly different for the systems with different PSDs, which is presumably caused by size segregation effects. At $t = 6$ s (second column of Figure 3.11), the region of highest velocities near the discharge outlet is comparatively smallest for the widest PSD, while the velocities in the cylindrical section are higher for the monodisperse and lognormal PSD with a width of $\sigma/\mu = 10\%$. This agrees with the higher discharge rates of narrower PSD widths (σ/μ) in Figure 3.6b. At $t = 12$ and 18 s (third and fourth columns of Figure 3.11), the bed height increases monotonically with the PSD width, which affirms that the discharge rate decreases monotonically with the PSD width (σ/μ). Secondly, other than

velocities, Figure 3.11 also shows the distribution of particle sizes during the discharge, which provides a better understanding of the underlying reason for the different discharge rates. For the wider PSDs ($\sigma/\mu = 50\%$ (Figure 3.11d) and 70% (Figure 3.11e)), it appears that (i) the larger particles present at the discharge outlet presumably slow the discharge due to obstruction, and (ii) the concentration of larger particles is higher at $t = 18$ s particularly for the wider PSD widths ($\sigma/\mu = 50\%$ (Figure 3.11d) and 70% (Figure 3.11e)), which suggests that the size segregation effects lead to the delayed discharge of the larger particles, as can also be observed in Figure 3.7.

(c)

(d)

(e)

Figure 3.11. Velocity distributions at four time instances (namely, $t = 0, 6, 12$ and 18 s) of systems with five different PSDs: (a) monodisperse, (b) lognormal PSD with $\sigma/\mu = 10\%$, (c) lognormal PSD with $\sigma/\mu = 30\%$, (d) lognormal PSD with $\sigma/\mu = 50\%$, and (e) lognormal PSD with $\sigma/\mu = 70\%$.

Since the different discharge rates (Figure 3.6b) mean that the bed heights of the different particle systems are different at each time instant (Figure 3.11), it is

worthwhile to further explore the differences in the velocities. Accordingly, Figure 3.12 displays the velocity distributions for the systems with different initial PSDs at the same bed heights of 470 mm (Figure 3.12a), 350 mm (Figure 3.12b) and 200 mm (Figure 3.12c) during hopper discharge. Each row represents a bed height, while each column represents each PSD assessed. Surprisingly, at the same bed height, the velocities in the cylindrical section of the hopper trend non-monotonically with respect to the PSD width (σ/μ), which is reminiscent of the non-monotonic relationship between the PSD width and axial segregation reported before for a bubbling fluidized bed [47]. Corresponding results for binary mixtures are not available. This may be tied to the different inter-particle interactions among the different ranges of particle sizes (Figure 3.1), which leads to the behavior portrayed in Figure 3.8 in which the final relative particle size decreases then increases as the PSD width broadens. Agreeing with Figure 3.8, Figures 3.11 and 3.12 show clearly that the widest PSD ($\sigma/\mu = 70\%$) appears to have larger particles relative to other PSDs at all the heights. Collectively, Figures 3.11 and 3.12 show that the axial velocity profiles of solid phase are different for the systems with various PSD widths, which thereby cause the discharge rates (Figure 3.6) to be different too. The cross-sectional velocities are assessed next to further understand the underlying reason for the distinctive behaviors among the PSDs.

Figure 3.12. Velocity distributions at the same bed height (a) 470 mm, (b) 350 mm, and (c) 200mm for systems with different PSDs: monodisperse, lognormal PSD with $\sigma/\mu = 10\%$, lognormal PSD with $\sigma/\mu = 30\%$, lognormal PSD with $\sigma/\mu = 50\%$, and lognormal PSD with $\sigma/\mu = 70\%$.

Figure 3.13. Velocity distributions at the cone height (i.e., 52 mm). The four columns represent particle bed heights of 470 mm, 350 mm, 200 mm and 52 mm (i.e., cone height). The five rows represent the various particle distributions, namely, (a) monodisperse, (b) lognormal PSD with $\sigma/\mu = 10\%$, (c) lognormal PSD with $\sigma/\mu = 30\%$, (d) lognormal PSD with $\sigma/\mu = 50\%$, and (e) lognormal PSD with $\sigma/\mu = 70\%$.

Figure 3.13 presents snapshots of the instantaneous cross-sectional velocities and PSDs at the cone height of 52 mm for the five different initial PSDs at four particle bed heights. Specifically, each row represents each of the five PSDs, while each column represents each bed height of 470 mm, 350 mm, 200 mm and 52 mm (i.e., cone height). Expectedly, the central region where the outlet orifice exhibits higher velocities than the wall region. The demarcation of the central core of higher velocities and the radial periphery of lower velocities is more distinct for the monodisperse (Figure 3.13a) and narrow PSD width of $\sigma/\mu = 10\%$ (Figure 3.13b), whereas the regions of higher velocities are more diffuse for the wider PSDs ($\sigma/\mu \geq 50\%$; Figures 3.13d - e). As the bed empties (left to right in Figure 3.13), the velocities throughout the cross-section increase, particularly in that the central region of highest velocities enlarges and the velocities near the walls increase. Snapshots of the cross-sectional velocities and PSDs at half the cone height (i.e., 26 mm) are displayed in the Appendix (Figure 3.A1), which also agrees with the two observations here.

3.4.4. Local particle velocity and size-segregation

Figures 3.14 and 3.15 describe, respectively, the axial average velocity and average particle diameter profiles quantitatively. Each y-axis represents the

dimensionless bed height in the cylindrical section of the hopper (h/H). Specifically, h is the cylindrical height assessed and H is the initial particle bed height in the cylinder (i.e., 422 mm); it should be noted that $h/H = 0$ and 1 represent, respectively, the cone height and the initial particle bed height in the cylinder. Each x-axis represents the average particle velocity in Figure 3.14 and the average particle diameter in Figure 3.15. In each of Figures 3.14 and 3.15, the three columns depict the profiles, respectively, at dimensionless radial positions (r/R , whereby r is the radial position assessed and R is the hopper cylindrical radius of 120 mm, such that $r/R = 0$ and 1 represent, respectively, the radial center and wall) of 0, 0.5, and 1, while each row displays the profiles at a different particle bed height (namely, 470, 350, and 200 mm).

Regarding the axial velocity profiles in Figure 3.14, the trends are different at different radial positions. At the radial center (Figures 3.14a, d and g), the velocities are lower but relatively uniform higher in the bed, but increases steeply lower in the bed. Near the wall (Figures 3.14c, f and i), the velocities along the particle bed are comparatively more uniform. Two noteworthy observations with regards to the impact of PSD width on particle velocities are clear. First, the relationship between PSD width and particle velocities is generally non-monotonic with no consistent trends, which is somewhat surprising since the discharge rate decreases monotonically with PSD width (Figure 3.6). Secondly, the variations of particle velocities caused by changing the PSD width are greater lower in the bed and at the radial center (Figures 3.14a, d and g), which indicates that the phenomena in this region may have a non-negligible impact on the relationship between PSD width and discharge rate. Interestingly, the velocities

decrease monotonically as PSD width increases at $h/H < 0.1$ in Figure 3.14g, which agrees with the trend for discharge rate (Figure 3.6b), but the relationship remains non-monotonic higher in the particle bed ($h/H > 0.1$).

Figure 3.14. Dimensionless cylindrical height (h/H) versus average particle velocity. The three rows represent particle bed heights of 470 mm (a, b, c), 350 mm (d, e, f) and 200 mm (g, h, i), while the three columns represent dimensionless radial positions (r/R) of 0 (a, d, g), 0.5 (b, e, h) and 1 (c, f, i). Spatial averages are taken every 20 mm vertically and radially.

As for the axial average particle diameter profiles in Figure 3.15, expectedly, the profiles are approximately vertical lines for the monodisperse and lognormal PSD with $\sigma/\mu = 10\%$ due to the lack of size-segregation, and the axial profiles

vary increasingly with PSD width. The profiles become increasingly more contoured as the bed height decreases, which indicates that axial segregation along the particle bed becomes progressively more extensive as the hopper discharges. At taller bed heights (Figures 3.15a - c), the average particle sizes are relatively uniform along the particle bed and radial size-segregation is such that the small particles prefer the wall. At lower bed heights (Figures 3.15g - i), the axial segregation is such that the larger particles prefer to be higher up in the bed, while the radial segregation is such that the larger particles prefer the wall (which is dissimilar to that at taller bed heights). This is similar to that of the binary mixtures, in which the particles are also almost uniformly distributed initially except at the region close to the wall [32], then, the larger species increasingly dominate at the upper surface due to percolation. Interestingly, in contrast to the axial velocity profiles in Figure 3.14 whereby the axial variations are greater at the radial center, the size-segregation behavior in Figure 3.15 is such that the axial variations are greater near the wall, which suggests surprisingly a lack of correlation between the two parameters of velocity and size-segregation.

Figure 3.15. Dimensionless cylindrical height (h/H) along the particle bed versus average particle diameter. The three rows represent bed heights of 470 mm (a, b, c), 350 mm (d, e, f) and 200 mm (g, h, i), while the three columns represent radial positions (r/R) of 0 (a, d, g), 0.5 (b, e, h) and 1 (c, f, i). Spatial averages are taken every 20 mm vertically and radially.

Figures 3.16 and 3.17 describe the radial velocity and average diameter profiles, respectively, at the cone height (i.e., 52 mm). Each figure contains three sub-figures plotted with respect to the dimensionless radius of the hopper (r/R) and corresponding to three particle bed heights (namely, 470, 350 and 200 mm). In Figure 3.16, consistent with the axial velocity trends (Figure 3.14), the correlation between PSD width (σ/μ) and velocities is non-monotonic and not consistent. As for Figure 3.17, expectedly, the variation of particle diameter radially increases as the PSD width (σ/μ) increases. Three observations in Figures 3.16 and 3.17 are noteworthy. First, regardless of PSD width, the greatest radial variations of both particle velocity (Figure 3.16c) and average particle diameter (Figure 3.17c) are for the shortest particle bed. In this case, while the greatest radial variation of velocity is exhibited by the monodisperse system, the greatest radial variation of average particle diameter is by the widest PSD ($\sigma/\mu = 70\%$). This, along with the general lack of correlation between the trends in Figures 3.16

and 3.17, indicates interestingly a lack of relationship between velocity and particle size, which is consistent with the observation in Figures 3.14 and 3.15. Second, Figure 3.16 indicates that the velocities at the radial center ($r/R = 0$) increase significantly as the hopper empties, with the greatest increase of more than twofold for the monodisperse system, whereas that at the wall ($r/R = 1$) decrease. Third, Figure 3.17 shows that the average particle diameter at the wall ($r/R = 1$) is lower for the wider PSDs ($\sigma/\mu \geq 30\%$) even at the tallest bed height evaluated (Figure 3.17a), which indicates that the radial size-segregation occurs quickly once the hopper discharge starts. As the hopper empties, the average particle diameter increases for the wider PSDs ($\sigma/\mu \geq 50\%$) across the whole cross-section but less so at the wall ($r/R = 1$). This is reminiscent of the size-segregation effects in the rotating drum wherein the radial segregation is fast but axial segregation is slow [130].

Figure 3.16. Radial velocity profiles of various PSDs at the cone height (i.e., 52 mm) for particle bed heights of (a) 470 mm, (b) 350 mm and (c) 200 mm. Spatial averages are taken every 5 mm vertically and radially.

(a) (b) (c)

Figure 3.17. Radial average particle diameter profiles of various PSDs at the cone height (i.e., 52 mm) for particle bed heights of (a) 470 mm, (b) 350 mm and (c) 200 mm. Spatial averages are taken every 5 mm vertically and radially.

To further quantify the segregation phenomenon, the number fractions of small and large particles preferentially segregated to the top surface and to the hopper wall can be calculated and normalized with respect to the average number fraction in the system. These two parameters have been defined as normalized concentrations for the small (C_{small}^*) and large (C_{large}^*) particles [131]:

$$C_{small}^* = C_{small} / C_{small}^T \quad (3-13)$$

$$C_{large}^* = C_{large} / C_{large}^T \quad (3-14)$$

where C_{small} and C_{large} are, respectively, the local number fraction of small and large particles, and C_{small}^T and C_{large}^T are, respectively, the overall number fraction of small and large particles. In this study, both the axial ($C_{small,axial}^*$ and $C_{large,axial}^*$) and radial ($C_{small,radial}^*$ and $C_{large,radial}^*$) parameters are quantified, whereby the local axial number fraction reflects the region 15 mm from the top surface and the local radial axial number fraction reflects the region 15 mm from the hopper wall. Figure 3.18 illustrates $C_{small,axial}^*$, $C_{large,axial}^*$, $C_{small,radial}^*$, and $C_{large,radial}^*$ with respect to the mass percentage of hopper discharged. The greater the deviation of the values from 1, the greater the segregation is. Regarding axial segregation (Figures 3.18a, b), it is clear that the deviation from 1 increases with PSD width. Interestingly, the narrower PSDs ($\sigma/\mu \leq 30\%$) and broader PSDs ($\sigma/\mu \geq 50\%$) exhibit opposite trends. For the small particles (i.e.,

smallest 15% by number; Figure 3.18a), $C_{\text{small,axial}}^*$ becomes greater than 1 as the hopper discharges for the narrower PSDs ($\sigma/\mu \leq 30\%$) but lesser than 1 for the broader PSDs ($\sigma/\mu \geq 50\%$). This reflects the increased percolation effect associated with the broader PSDs, such that the smaller particles are discharged sooner and are almost absent for the widest PSD ($\sigma/\mu = 30\%$) toward the end of the hopper discharge. For the large particles (i.e., largest 15% by number; Figure 3.18b), $C_{\text{large,axial}}^*$ becomes slightly less than 1 as the hopper discharges for the narrower PSDs ($\sigma/\mu = 30\%$) but much greater than 1 for the broader PSDs ($\sigma/\mu \geq 50\%$), which is consistent with the increased percolation effect associated with the broader PSDs. Regarding radial segregation, Figure 3.18c shows that (i) the extent of radial segregation also increases with PSD width, and (ii) the narrower PSDs ($\sigma/\mu \leq 30\%$) exhibit opposite trends to that of the broader PSDs ($\sigma/\mu \geq 50\%$). Specifically, $C_{\text{small,radial}}^*$ increases as the hopper discharges for the narrower PSDs ($\sigma/\mu \leq 30\%$) but decreases for the wider PSDs ($\sigma/\mu \geq 50\%$). Comparing Figures 3.18c, d, the large particles segregate lesser radially than the small particles. Therefore, Figure 3.18 indicates that (i) the extents of both radial and axial segregation generally increase with PSD width; (ii) the trends of $C_{\text{small,axial}}^*$, $C_{\text{large,axial}}^*$, and $C_{\text{small,radial}}^*$ are opposite for the narrower PSDs ($\sigma/\mu \leq 30\%$) and wider PSDs ($\sigma/\mu \geq 50\%$) as the hopper discharges; and (iii) for the wider PSDs ($\sigma/\mu \geq 50\%$) with more extensive segregation, the smaller particles preferentially segregate axially to the bottom and are discharged sooner, and also radially away from the hopper wall.

Figure 3.18. Normalized concentration of (a) small and (b) large particles near the top (i.e., 15 mm from the top surface); and (c) small and (d) large particles near the hopper wall (i.e., 15 mm from the wall).

3.5. Conclusion

Despite the prevalence of continuous PSDs, its effect on hopper discharge characteristics has not been well-studied. Accordingly, this study harnesses the DEM to investigate the impact of the widths of lognormal PSDs on hopper discharge behaviors, namely, discharge rate, overall PSD and average particle size during discharge, and also local particle velocities and size-segregation during discharge. The particle systems studied have the same mean particle diameter (μ) of 5 mm and ranges from a monodisperse system to lognormal PSDs

with the ratio of standard deviation to mean particle diameter (σ/μ) of between 10 and 70%. The model was first validated by reported experimental results on a monodisperse system [41] in terms of the discharge rate and particle trajectories. Then, six noteworthy observations regarding lognormal PSDs are described as follows.

First, for the same initial bed height, the hopper discharge rate decreases as the PSD width increases, with the discharge duration of the widest lognormal PSD investigated ($\sigma/\mu = 70\%$) about 1.6 times that of the monodisperse. This contradicts with binary results that show that the discharge rate increases as the mass fraction of the finer species increases [82], and agrees with binary results that indicate that the discharge rate decreases with the mass ratio of the larger species [32]. The inability to predict the behavior of the continuous PSDs based on the available binary results is consistent with a previous study on segregation characteristics in a bubbling fluidized bed [47], and thereby underscores the need for more in-depth studies on such systems. Second, the rates for all the PSDs are constant with time, but the fluctuations increase as the PSD width increases. The constant discharge rate agrees with that of binary mixtures [124], and also with the understanding that the fluctuations increase with particle size [125] since the diameters of the largest particles increases with PSD width. Third, regarding the overall PSD during discharge, while the change in PSD is negligible for the narrower PSD widths of $\sigma/\mu \leq 30\%$, the PSDs progressively shift rightwards for $\sigma/\mu \geq 50\%$. This contradicts that of binary mixtures in which the extent of segregation decreased as the mass fraction of the finer species increased [132], and also that of another study on binary, ternary and quaternary mixtures in which

extent of segregation decreased as the mass fraction of coarse components increased [45]. Fourth, on the change in the mean particle diameter as the hopper discharges, the narrower PSDs ($\sigma/\mu \leq 30\%$) are such that the means do not exceed the initial mean of 5 mm, whereas the wider ones ($\sigma/\mu \geq 50\%$) do; this appears tied to the overall segregation behavior in which the narrower PSDs exhibit negligible shifts in PSDs as the hopper discharges whereas the wider ones do. Fifth, although the velocity profiles are distinctly different for the systems with different PSDs, the relationship between PSD width and particle velocities is generally non-monotonic with no consistent trends, which is somewhat surprising since the discharge rate decreases monotonically with PSD width. It was only at the radial center ($r/R = 0$) and lower bed heights that the local particle velocity approximately decreases as PSD width increases, which agrees with the discharge rate. Sixth, a surprising lack of correlation exists between particle velocity and size-segregation, as evident in: (i) in contrast to the axial velocity profiles whereby the axial variations are greater at the radial center, the size-segregation behavior is such that the axial variations are greater near the wall, (ii) towards the end of hopper discharge at a particle bed height of 200 mm, while the greatest radial variation of velocity is exhibited by the monodisperse system, the greatest radial variation of average particle diameter is by the widest PSD ($\sigma/\mu = 70\%$).

The contradictory results between the discharge characteristics of the lognormal PSDs studied here and that of the binary mixtures available in literature underscores the need for more in-depth understandings of the ubiquitous continuous PSDs to enhance the operation and predictive capability of hoppers

Appendix

Figure 3.A1. Velocity distributions at half the cone height (i.e., 26 mm). The four columns represent particle bed heights of 470 mm, 350 mm, 200 mm and 52 mm (i.e., cone height). The five rows represent the various particle distributions,

namely, monodisperse, lognormal PSD with $\sigma/\mu = 10\%$, lognormal PSD with $\sigma/\mu = 30\%$, lognormal PSD with $\sigma/\mu = 50\%$, and lognormal PSD with $\sigma/\mu = 70\%$.

Chapter 4. Understanding the varying discharge rates of lognormal PSDs of spherical particles

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Abstract

The focus of this study is on understanding the varying discharge rates of lognormal particle size distributions (PSDs) with the same mean particle diameter. Discrete element method (DEM) is used to simulate lognormal PSDs with the same arithmetic mean of the particle diameter of 5 mm but varying PSD widths ($\sigma/\mu = 10\%$ to 70%) in a 3D conical hopper. Four highlights are noted: (i) the Beverloo correlation and others modified to account for various particle properties predict the discharge rates of lognormal PSDs poorly, which underscores the need for more understanding on the influence of PSD width; (ii) the velocity vectors are less uniformly downwards in the hopper for the wider PSDs, which results in the slowing down of the discharge rate; (iii) the radial particle velocity, and both the radial and vertical particle angular velocity increase with PSD width throughout the first half of the hopper discharge; and (iv) the collision force magnitudes are greater for the wider PSDs, and the cross-sectional fluctuations of the collision forces at the cone height increases with PSD width. The increase of the magnitudes of these particle characteristics (namely,

radial particle velocity, angular velocity, and collision force) with PSD width underlies the decreasing hopper discharge rate.

Keywords: Discrete element method (DEM); Hopper discharge rate; Particle velocity; Lognormal particle size distribution (PSD); Collision force; Angular velocity

4.1. Introduction

Hoppers are common apparatuses for the storage and discharge of particles in various industries (e.g., pharmaceutical, chemical, and food). Despite the seeming simplicity of function, flow problems including erratic or stunted flow, dead zones, segregation, and dust explosions are prevalent [1, 133, 134]. To resolve such issues, an in-depth understanding of the mechanisms underlying the different discharge behaviors [9, 83], for example, due to different hopper configurations [17, 34, 135] and different particle properties [10, 12, 14, 27, 136], is necessary. To this end, both experimental and simulation efforts have been dedicated to investigating the discharge characteristics of hoppers [1, 35, 137, 138]. The DEM provides an effective method of tracking each particle numerically and has been widely accepted to study dense particulate behavior, which was initially proposed by Cundall and Strack [40]. Due to the dominance of collisions and significant shear in the hopper, particle-particle interactions have to be appropriately accounted for [139].

Previous DEM studies focusing on discharge behaviors in the hopper have provided some understanding on monodisperse [41, 42], binary-size mixtures [43,

46, 140] and multi-size mixtures [37, 141]. Li et al.[41] found good agreement between DEM simulation and experimental results on the particle trajectory for a high-temperature monodisperse system. Yu and Saxén [42] found that the velocity distribution is uniform except near the orifice and the static particle-wall friction is important for the flow pattern of the monodisperse flow. Rahman et al.[43] concluded that, for binary mixtures, the degree of segregation is higher in a three-dimensional system compared to a two-dimensional system and flowability is closely tied to segregation patterns. Combarros et al.[140] found that particle size has a more dominant effect than particle shape on segregation and that the critical DEM parameters in segregation simulation are static and rolling friction. Ketterhagen et al.[46] investigated the effects of the particle diameter ratio, density ratio, fines mass fraction, hopper wall angle, hopper cross-sectional shape, and the initial fill conditions of a binary-size mixture, and found that the DEM model can predict well the segregation during hopper discharge. Wu et al.[141] found that the flowability of the particles is tied to the hopper slope and the mass fraction of small particles. Yu and Saxén [37] concluded the filling method, diameter ratio of fine to coarse, wall-particle static and rolling friction, inter-particle rolling friction as well as the mass fraction of fine particles are the most important factors affecting the extent of segregation during the discharging process. Anand et al.[15, 74] further revealed that the coefficient of restitution and hopper width have negligible influence on the discharge rate, whereas friction, hopper angle, outlet width, and PSD have the more significant impact. Arteaga and Tüzün [142, 143] concluded that the discharge rates were found to increase with increasing mass fraction of fines, with the extent of this

increase being a strong function of the size ratio of the constituents. Our previous study [101] found the lognormal PSD width has a dominant influence on the discharge rate in the hopper, with the decrease in the discharge rate significant at approximately 36% when the PSD changes from a monodisperse to a lognormal PSD width (defined as ratio of standard deviation of the particle size to mean particle diameter) of 70%. The dependence of discharge rate and wall stress on particle interactions have been investigated using the discrete element model (DEM), and it was found that the proper accounting of inter-particle interactions is critical for more accurate predictions of discharge rates [135]. The effect of differential pressure (ΔP) on discharge rate in a conical hopper was experimentally studied, which indicated that increases in ΔP increased discharge rate up to a critical ΔP after which the discharge regime destabilized, and that the critical ΔP depended on hopper orifice diameter and physical properties of the particles like size distribution and particle density [83]. Recently, the discharge rate in conical hoppers was assessed using an elastoplastic model implemented with the Eulerian finite element method (FEM) approach, which demonstrated that material dilation and internal frictional angle markedly affect the discharge rate particularly for steep cones (cone angle $< 45^\circ$) [144]. Moreover, the behavior of super-quadric particles during hopper discharge was found to be such that the discharge rate always decreases with decreasing base angle or increasing blockiness, particle friction, or aspect ratio [66]. Collectively, these studies imply that particle properties like size and size distribution have a non-negligible impact on the hopper discharge rate.

The Beverloo correlation [77] represents one of the most popular for predicting hopper discharge rates, which was subsequently modified to account for varying particle properties. Because it was experimentally found that the correlation only worked well for coarser particles but not the finer ones ($d \leq 500 \mu\text{m}$), the correlation was modified based on the different momentum and drag of the particles [26]. Another group investigated finer particles ($50 \mu\text{m} \leq d \leq 500 \mu\text{m}$) and found that, although the developed correlation for discharge rates has the right relationship with particle size, it gives quantitative values about twice larger than the experimentally measured values [136]. The shape of the particles was also experimentally found to have a significant effect on the flow rate, and therefore the Beverloo correlation was further incorporated with the shape parameters [145]. A recent work [80] investigated the influence of orifice shape on the flow rate in flat-bottom hoppers numerically and experimentally and found the data can be well fitted with a modified Beverloo's formula. Also, with regards to a wider range of particle sizes, the Beverloo correlation was extended to binary-size mixtures [27] based on earlier experimental data [10] and also polydisperse mixtures by including the differential pressure gradients [35, 36].

The reports to date provide limited understanding on the granular motion of continuous PSDs, which are ubiquitous both naturally and industrially. Our recent DEM study found that the discharge rate decreases as the PSD width increases, which is tied to increasing extents of segregation but surprisingly not tied to the vertical particle velocity [101]. To obtain a more in-depth understanding, the DEM is used here to further understand the mechanisms underlying the different discharge rates of the lognormal PSDs with the same

mean diameter but different PSD widths. The specific objectives of the current study are: (1) assess if the available correlations can predict the discharge rate of lognormal PSDs well; (2) understand the impact of PSD width on the particle characteristics during hopper discharge, namely, radial particle velocity (v_r), radial and vertical particle angular velocity (ω_r and ω_z), and collision force (F); (3) armed with the understanding that the vertical particle velocity (v_z) has no direct relationship with the discharge rate [101], attempt to relate the discharge rate to these other particle behaviors to provide an explanation for the varying discharge rates resulting from the different PSD widths.

4.2. Material and method

4.2.1. Discrete element method (DEM)

In the current work, the DEM is adopted to track the motion of each particle in the Lagrangian framework. In DEM simulations, the motion of each particle is governed by Newton's second law of motion [40], with the translational and rotational motion of a particle generally formulated based on the force-displacement relationship. The equations governing the motion of each particle i are expressed as follows:

$$m_i \frac{dV_i}{dt} = \sum_{j=1}^K (\mathbf{F}_{c,ij}^n + \mathbf{F}_{c,ij}^t + \mathbf{F}_{d,ij}^n + \mathbf{F}_{d,ij}^t) + m_i g \quad (4-1)$$

$$I_i \frac{d\omega_i}{dt} = \sum_{j=1}^K (\mathbf{M}_{t,ij} + \mathbf{M}_{r,ij}) \quad (4-2)$$

where m_i , V_i , ω_i , $F_{c,ij}$, $F_{d,ij}$, g , I_i , $M_{r,ij}$, and K represent respectively the particle mass of particle i , translational velocity of particle i , angular velocity of

particle i , collision force (normal and tangential contact forces) between particle i and particle j , damping force between particles i and j , gravitational acceleration, moment of inertia of particle i , torque generated between particles i and j , and number of contacts between particle i and the neighboring particles or walls. The normal and tangential forces between two particles are evaluated by the Hertz theory [146]. The forces and torques used in the simulation are all listed in Table 4.1.

Table 4.1. The forces and torques acting between particle i and particle j .

Forces & torques	Equations
Normal contact force	$\mathbf{F}_{c,ij}^n = 4/3 Y^* (r^*)^{1/2} \delta_n^{3/2} \mathbf{n}_{ij},$
Normal damping force	$\mathbf{F}_{d,ij}^n = 2\sqrt{5/6} \beta \sqrt{S_n m^*} \mathbf{v}_{ij}^n,$
Tangential contact force	$\mathbf{F}_{c,ij}^t = 8G^* \sqrt{r^* \delta_n} \mathbf{t}_{ij},$
Tangential damping force	$\mathbf{F}_{d,ij}^t = 2\sqrt{5/6} \beta \sqrt{S_t m^*} \mathbf{v}_{ij}^t,$
Torque by tangential forces	$\mathbf{M}_{t,ij} = \mathbf{R}_{ij} \times (\mathbf{F}_{c,ij}^t + \mathbf{F}_{d,ij}^t),$
Rolling friction torque	$\mathbf{M}_{r,ij} = \mu_{r,ij} \mathbf{F}_{c,ij}^n + \mathbf{F}_{d,ij}^n \omega_{t,ij} / \omega_{t,ij} ,$

where, $1/Y^* = (1 - v_1^2)/Y_1 + (1 - v_2^2)/Y_2$, $1/r^* = 1/r_1 + 1/r_2$, $\beta = \ln(e)/\sqrt{\ln^2(e) + \pi^2}$, $S_n = 2Y^* \sqrt{r^* \delta_n}$, $1/G^* = 2(2 + v_i)(1 - v_i)/Y_i - 2(2 + v_j)(1 - v_j)/Y_j$, $S_t = 8G^* \sqrt{r^* \delta_n}$. Note that Y is Young's modulus, v is Poisson's ratio, G is shear modulus and r is particle radius.

4.2.2. Simulation setup

The conical hopper studied here is similar to that in the experimental study by Li et al. [41]. Figure 4.1 shows the schematic diagram of the hopper filled with particles to an initial packed bed height of 0.474 m. The diameter of the cylindrical section is 0.240 m and the diameter of the outlet orifice at the bottom

of the conical section is 0.060 m, while the total height and cone height of the hopper are respectively 0.500 m and 0.052 m. The cone is angled at 60° to the vertical axis. The polygonal mesh is used and the hopper is divided into 700 cells. The particles are glass beads with a mean particle diameter (μ) of 5 mm and particle density (ρ_p) of 2460 kg/m^3 . Table 4.2 provides more details on the parameters used.

Figure 4.1. Geometrical description of the hopper with an initial packed bed height of 0.474 m.

Table 4.2. Details of physical parameters in the simulation.

Parameter	Value
σ/μ (-)	10, 30, 50 and 70%
Number (-)	181,483, 171,259, 145,734, 102,202 and 67,406
Density, ρ_p (kg/m^3)	2460
Initial particle bed height (m)	0.474
Cone height (m)	0.052

Diameter of cylindrical section of hopper (m)	0.24
Diameter of outlet (m)	0.06
Angle of cone (°)	60
Young's modulus, Y (GPa)	0.1
Poisson ratio, ν (-)	0.25
Coefficient of particle-wall static friction (-)	0.6
Coefficient of particle-wall rolling friction (-)	0.05
Coefficient of particle-wall restitution (-)	0.99
Coefficient of particle-particle static friction (-)	0.6
Coefficient of particle-particle rolling friction (-)	0.01
Coefficient of particle-particle restitution (-)	0.99
Time step, Δt (s)	2×10^{-5}

The number-based frequency (f_n) distribution of the common lognormal PSD investigated in this study is expressed as follows:

$$f_n = \frac{1}{x\sigma\sqrt{2\pi}} \exp \left[-\frac{(\ln(x)-\mu)^2}{2\sigma^2} \right] \quad (4-3)$$

where x , σ , and μ are respectively particle diameter, the standard deviation of the PSD and arithmetic mean particle diameter. The width of the PSDs, which is defined as the ratio of standard deviation of the PSD to mean particle diameter (σ/μ), is ranged between 10% to 70% [47]. The distribution (Eq. 4-3) is discretized such that the widest PSD is represented by 20 bins of particle diameters. The mean particle diameter (μ) is set at a smaller 5 mm instead of the 10 mm used in the experimental study [41]. This is to prevent bridging or arching caused by the presence of the larger particles in the PSDs with $\sigma/\mu \geq 50\%$ [134]. Figure 4.2 presents the PSDs investigated. The numbers of glass beads

required for an initial packed bed height of 0.474 m are 181,483, 171,259, 145,734, 102,202 and 67,406 respectively for the monodisperse system and lognormal PSDs with widths (σ/μ) of 10, 30, 50 and 70%. The detailed physical and numerical parameters are summarized in Table 4.2.

Figure 4.2. Cumulative weight fraction of particles with mono-sized, lognormal distribution with $\sigma/\mu = 10\%$, 30% , 50% , and 70% . The black dashed lines represent the 50th percentile (or median) mass-based diameter.

The protocol of the simulation is summarized as follows. Firstly, with the orifice outlet at the bottom of the hopper sealed to prevent any particle outflow, the specific number of glass beads for each targeted PSD are allowed to settle under gravity randomly in the hopper to a fixed bed height 0.474 m. Figure 4.3 displays the screenshots of the hoppers initialized with well-mixed particles of various different widths of the number-based lognormal PSDs investigated, namely, from monodisperse to lognormal PSDs with σ/μ ranging from 10 to 70%; note that the segregation indices are all zero at the start of the hopper discharge, indicating the well-mixed status [101]. Then, the seal at the orifice outlet is removed to allow the glass beads to discharge from the hopper under the influence of gravity. The

DEM model has been validated in our previous study with respect to the trajectory of the particles and the change in bed height during discharge [101].

Figure 4.3. Hoppers initialized with well-mixed particles of different PSDs: (a) monodisperse, (b) lognormal PSD with $\sigma/\mu = 10\%$, (c) lognormal PSD with $\sigma/\mu = 30\%$, (d) lognormal PSD with $\sigma/\mu = 50\%$, and (e) lognormal PSD with $\sigma/\mu = 70\%$.

4.3. Results and Discussion

4.3.1. Beverloo correlation

Figure 4.4 presents the simulation results, which show that the mass discharge rate (W) decreases as the PSD width (σ/μ) increases. This trend agrees qualitatively with two correlations [27, 36] despite some quantitative discrepancies, but disagrees with the well-known Beverloo equation [77] that instead exhibits an opposite trend. The disparity in the predictions presumably stems from the lack of consideration of polydispersity effects and warrants a closer inspection.

The most widely accepted Beverloo correlation is expressed as [77]:

$$W = C\rho_b g^{1/2}(W_0 - Z)^{5/2} \quad (4-4)$$

where W is the mass discharge rate, C is an empirical constant in the range of 0.55 and 0.65 (0.58 is used here per Mehmet and Gundogdu [36]), ρ_b is the bulk density of the packed bed of particles, g is gravitational acceleration, W_0 is the outlet width, and Z is the empty annulus width [138], which is the annulus space at the orifice through which the particle centers cannot enter and is expressed as $Z = k\mu$, where $k = 1.5$ [147] is the Beverloo constant related to the particle shape and μ is the arithmetic mean of the particle diameter. This correlation has been proposed for both the mass and the funnel flow regimes of monodisperse particles with μ larger than 0.5 mm. When applied to systems with lognormal PSDs, because the bed voidage (ε) decreases and thereby the bulk density (ρ_b) increases with σ/μ (Figure 4.5), Eq. (4-4) hence predicts that W increases with σ/μ .

Subsequently, Humby et al. [27] extended the Beverloo correlation to binary mixtures based on the experimental work of Artega and Tüzün [10]:

$$W = C\rho_b g^{1/2}(W_0 - Z')^{5/2} \quad (4-5)$$

where $Z' = (2.1939d_{VM} - 0.0009)$ is the modified parameter for the binary mixtures that is related to the particle size distribution of the mixture, where $d_{VM} = \sum_i x_i d_i^4 / \sum_i x_i d_i^3$ is the De Brouckere mean diameter that is a function of the number fraction x_i and diameter d_i of particle i . Because d_{VM} and hence Z' increases to counter the increase in ρ_b as σ/μ increases, W decreases with σ/μ . The trend surprisingly contradicts that of Beverloo et al. (Eq. (4-4) [77]).

Moreover, Gundogdu [36] explored a modified Beverloo correlation to account for the effect of the pressure gradient, as per the Ergun correlation, $(dP/dz)_0 = \left(\frac{150}{\frac{\rho_g U_{mf} d_p}{(1-\varepsilon_d)\mu_g}} + 1.75 \right) \frac{\rho_g U_{mf}^2}{d_p} \frac{1-\varepsilon_d}{\varepsilon_d^3} + \rho_g g$ (where U_{mf} and ε_d are the minimum fluidization velocity and the void fraction of the particles, respectively), to predict the discharge rate of the coarse free-flowing polydisperse powders in the conical hopper:

$$W = 0.58\rho_b \sqrt{g + \left(\frac{dP}{dz}\right)_0 \frac{1}{\rho_b}} (W_0 - kd_{50})^{5/2} \quad (4-6)$$

where d_{50} is the median mass-based diameter as shown in Figure 4.2. Because d_{50} decreases as σ/μ increases, W increases with σ/μ , so the trend agrees with Beverloo et al. (Eq. (4-4) [77]). Further applying $Z' = kd_{50} = (2.1939d_{VM} - 0.0009)$ to Eq. (4-6) gives

$$W = 0.58\rho_b \sqrt{g + \left(\frac{dP}{dz}\right)_0 \frac{1}{\rho_b}} [W_0 - (2.1939d_{VM} - 0.0009)]^{5/2} \quad (4-7)$$

Eq. 4-7 agrees quantitatively with Humby et al. (Eq. (4-5) [27]) and qualitatively with the simulations. The qualitative agreement likely stems from the perfectly spherical and non-cohesive particles are used. In summary, the simulation predicts that the average mass discharge rate decreases as the PSD width increases, which agrees with Eqs. (4-5) and (4-7) but contradicts Eqs. (4-4) and (4-6). This clearly indicates the current poor predictive capability of the performance of polydisperse mixtures, which necessitates a better understanding of the mechanisms underlying the different behaviors stemming from different

PSD widths of continuous PSDs. The subsequent sections study the impact of PSD width on the various discharge characteristics.

Figure 4.4. Discharge rates predicted by the DEM simulation and correlations by Beverloo et al. (Eq. (4-4) [77]), Humby et al. (Eq. (4-5) [27]), and Gundogdu (Eq. (4-6) and (4-7) [36]). Note that the trends for Eq. (4-6) and (4-7) are superimposed on each other.

4.3.2. Bulk density

In view of the bulk density term in the Beverloo correlation (Eq. (4-4)) causing deviation from the simulation results, the effect of the bulk density on the discharge rate should be further explored for the hoppers with lognormal PSDs. Figure 4.5 shows the bulk density as a function of the particle bed height of systems with monodisperse particles and different lognormal PSDs. The bulk density decreases as the hopper discharges. Specifically, the bulk density decreases drastically initially, then gradually decreases until a bed height of approximately 200 mm, then decreases more rapidly until the hopper empties. With respect to PSD width, the bulk density is expectedly higher for the larger PSD widths, and the difference in the bulk density values among the PSDs

remains approximately constant as the hopper discharges. On one hand, because bulk density increases but discharge rate decreases with PSD width, a negative relationship between bulk density and discharge rate is implied. On the other hand, as the hopper discharges, although the bulk density decreases, the discharge rate fluctuates around a constant value [101], which implies instead a lack of relationship between bulk density and discharge rate. The contradiction indicates that bulk density is not a dominant parameter dictating discharge rate. This is in contrast to binary mixtures, whereby the discharge rates were found to increase with increasing mass fraction of fines and thereby increasing bulk density [10]

Figure 4.5. Bulk density versus particle bed height of systems with different PSDs: monodisperse, lognormal PSD with $\sigma/\mu = 10\%$, 30% , 50% , and 70% .

4.3.3. Velocity vectors

As opposed to the flat-bottom conical hopper that has four regions (namely, plug flow zone, transition zone, converging flow zone, and stagnant zone [148]), the conical hopper angled at 60° to the vertical axis investigated here does not have a stagnant zone during hopper discharge, as seen in the velocity profiles in Figure

4.6. Specifically, Figure 4.6 illustrates the velocity vectors at the radially central plane at the bed heights of 470 mm, 350 mm and 200 mm for systems with different PSDs. For all the five particle systems of different polydispersity, Figure 4.6 shows the plug flow in the upper part, converging flow in the bottom part, and a transition region between them. In the plug flow zone, the particle trajectories are predominantly downwards except at the near-wall regions. In the converging flow zone, the particles flow towards the orifice, with the maximum velocities at the orifice outlet. As the hopper discharges and the particle bed height decreases, the plug flow zone is clearly reduced. It should be noted that the velocity profile of the narrower PSD widths ($\sigma/\mu \leq 10\%$) in Figure 4.6 is consistent with that reported previously for approximately monodisperse spherical particles [148-150]. Regarding the effect of PSD width, throughout the hopper discharge, the particle trajectories become more chaotic (i.e., less uniformly downwards) in the lower half of the hopper as the PSD width increases, which likely slows the discharge.

Monodisperse $\sigma/\mu = 10\%$ $\sigma/\mu = 30\%$ $\sigma/\mu = 50\%$ $\sigma/\mu = 70\%$

(a)

(b)

(c)

Figure 4.6. Instantaneous velocity vectors at the radially central plane and at the particle bed heights during discharging of (a) 470 mm, (b) 350 mm and (c) 200 mm for systems with different PSDs: monodisperse, lognormal PSDs with $\sigma/\mu = 10\%$, 30% , 50% and 70% .

4.3.4. Radial particle velocity (v_r), radial particle angular velocity (ω_r) and vertical particle angular velocity (ω_z)

In view of the lack of a direct relationship between PSD width and vertical particle velocity (v_z) [101], which fails to provide an explanation for the negative correlation between PSD width and discharge rate, the other velocities during hopper discharge are explored here. Figure 4.7 shows dimensionless cylindrical height (h/H , whereby h and H are the cylindrical height assessed (i.e., without the cone) and initial particle bed height in the cylindrical section of 422 mm) versus mass-average particle radial velocity (v_r), with each row representing the profiles when the particle bed height in the hopper is at 470, 350 and 200 mm, and each column reflecting dimensionless radial positions (r/R , whereby r is the radius assessed and R is the cylindrical radius of 120 mm) of 0, 0.5 and 1. In general, the radial particle velocities (v_r) (i) tend to increase with PSD width (σ/μ), with the increases being greater lower in the hopper; (ii) increase and decrease towards the wall (i.e., as r/R increases) respectively higher and lower in the hopper; (iii) are more uniform axially near the wall than at the radial center ($r/R = 0$). Analogous to Figure 4.7, Figure 4.8 illustrates the radial particle angular velocity (ω_r) of the different lognormal PSD widths at three particle bed heights and three radial positions during hopper discharge. The trends between Figs. 4.7 and 4.8 are rather similar, except that, due to friction with the wall, the radial particle angular velocities (ω_r) higher in the hopper have significantly greater magnitudes (Figs. 4.8c and f). The radial profiles (i.e., with respect to the dimensionless radius (r/R)) of the radial particle velocity (v_r) and radial particle

angular velocity (ω_r) at the cone height (i.e., 52 mm from the orifice of the hopper) when the particle bed height is 200 mm is further shown in Figure 4.A1.

Figure 4.7. Dimensionless cylindrical height (h/H) versus average radial particle velocity (v_r). The three rows represent particle bed heights of 470 mm (a, b, c), 350 mm (d, e, f) and 200 mm (g, h, i), while the three columns represent dimensionless radial positions (r/R) of 0 (a, d, g), 0.5 (b, e, h) and 1 (c, f, i). Spatial averages are taken every 20 mm vertically and radially.

The vertical particle angular velocity (ω_z) is further evaluated to assess a possible link with the decreasing discharge rate with increasing PSD width. Figure 4.9 illustrates the vertical particle angular velocity (ω_z) profiles, which indicates that the vertical particle angular velocity (ω_z) generally increases with PSD

width (σ/μ), and is consistent with the trends for both radial particle velocity (v_r ; Figure 4.7) and radial particle angular velocity (ω_r ; Figure 4.8). It should be noted that the profiles of the monodisperse system agree with a reported study also on monodisperse particles, in which both the velocity and angular velocity are small throughout the hopper other than at the exit [42]. Comparing the magnitudes of ω_r and ω_z in Figs. 4.8 and 4.9 reveal that particle rotation is more significant in the radial rather than vertical direction.

Figure 4.8. Dimensionless cylindrical height (h/H) versus average radial particle angular velocity (ω_r). The three rows represent particle bed heights of 470 mm (a, b, c), 350 mm (d, e, f) and 200 mm (g, h, i), while the three columns represent

dimensionless radial positions (r/R) of 0 (a, d, g), 0.5 (b, e, h) and 1 (c, f, i). Spatial averages are taken every 20 mm vertically and radially.

Figure 4.9. Dimensionless cylindrical height (h/H) versus average particle vertical angular velocity (ω_z). The three rows represent particle bed heights of 470 mm (a, b, c), 350 mm (d, e, f) and 200 mm (g, h, i), while the three columns represent dimensionless radial positions (r/R) of 0 (a, d, g), 0.5 (b, e, h) and 1 (c, f, i). Spatial averages are taken every 20 mm vertically and radially.

Interestingly, the correlation between PSD width and radial particle velocity (v_r) or radial particle angular velocity (ω_r) or vertical particle angular velocity (ω_z) is largely monotonically positive, which is in contrast to the lack of a direct relationship between PSD width and vertical particle velocity (v_z) [101]. Figure

4.10 summarizes the average of the four velocities, namely, v_r , v_z , ω_r and ω_z , during hopper discharge. Regarding the radial particle velocity (v_r), Figure 4.10a shows that the rate of increase of v_r with respect to hopper discharge percentage decreases as the PSD width increases. Specifically, v_r and ω_r increase gently as the discharge progresses for the first 80% of the hopper discharge (i.e., when the particle bed level is above the cone height of 51.96 mm), during which the values are greater for the wider PSDs; then the increase becomes steeper towards the final 20% of the discharge (i.e., when the particle bed level is below the cone height), during which the peak v_r value is the greater for the narrower PSDs while the peak ω_r values are similar among the PSDs. Concerning v_z (Figure 4.10b), it is only in the final 40% of hopper discharge that a negative correlation between PSD width and the v_z magnitude becomes clear. As for the particle angular velocities, Figs. 4.10c and 4.10d respectively indicate that the radial (ω_r) and vertical (ω_z) trends are similar. It should be noted that Yu and Saxén [42] concluded that the motion of monodisperse particles in the hopper is strongly influenced by angular velocity. Both ω_r and ω_z decrease as the hopper discharges for the widest PSD ($\sigma/\mu = 70\%$), but increase at increasing rates as the PSD width decreases for the narrower and monodisperse ones ($\sigma/\mu < 70\%$). Collectively, it is clear that the PSD width has a non-negligible impact on the various velocities throughout the hopper discharge. Whereas the relationship between the hopper discharge rate and v_z is unclear (Figure 4.10b), the discharge rate is clearly negatively correlated with the magnitudes of v_r , ω_r , and ω_z during the first 50% of the hopper discharge (Figs. 4.10a, c, and d).

Figure 4.10. Effect of PSD width during hopper discharge on (a) average radial particle velocity (v_r); (b) average vertical particle velocity (v_z); (c) average radial particle angular velocity (ω_r); and (d) average vertical particle angular velocity (ω_z).

4.3.5. Collision force (F)

Based on the recognition that hopper discharge represents a collision-dominated flow, the difference in collision forces among the lognormal PSD widths is examined to further understand the mechanisms underlying the different discharge rates. Particle-particle and particle-wall collisions are inextricably linked to the various particle velocities [139], as elucidated above.

The contour plots of overall collision force (F) of the monodisperse and lognormal PSDs of four different PSD widths at the cone height (i.e., 52 mm from the discharge orifice) when the particle bed heights are 470 mm, 350 mm and 200 mm are depicted respectively in Figs. 4.11, 4.12 and 4.13. Three observations are clear: (i) the overall collision force (F) increases as the PSD width (σ/μ) increases, which indicates the more extensive collisions among the wider range of particle diameters; (ii) F is non-uniform collision across the cross-section, with the highest magnitudes tending to be closer to the radial center rather than wall; and (iii) F generally decreases as the hopper discharges, with the peaks becoming broader with discharge. In particular, the increased collision force (F) with PSD width suggests that the collisions become more extensive as the range of particle diameters increases, and the collisions, in turn, impede hopper discharge.

Figure 4.11. Contour plots of the overall collision force (F) at the cone height (i.e., 52 mm from the discharge orifice) when the particle bed height is 470 mm during hopper discharge: (a) monodisperse, (b) lognormal PSD with $\sigma/\mu = 10\%$, (c) lognormal PSD with $\sigma/\mu = 30\%$, (d) lognormal PSD with $\sigma/\mu = 50\%$, and (e) lognormal PSD with $\sigma/\mu = 70\%$.

Figure 4.12. Contour plots of the overall collision force (F) at the cone height (i.e., 52 mm from the discharge orifice) when the particle bed height is 350 mm during hopper discharge: (a) monodisperse, (b) lognormal PSD with $\sigma/\mu = 10\%$, (c) lognormal PSD with $\sigma/\mu = 30\%$, (d) lognormal PSD with $\sigma/\mu = 50\%$, and (e) lognormal PSD with $\sigma/\mu = 70\%$.

Figure 4.13. Contour plots of the overall collision force (F) at the cone height (i.e., 52 mm from the discharge orifice) when the particle bed height is 200 mm during hopper discharge: (a) monodisperse, (b) lognormal PSD with $\sigma/\mu = 10\%$, (c) lognormal PSD with $\sigma/\mu = 30\%$, (d) lognormal PSD with $\sigma/\mu = 50\%$, and (e) lognormal PSD with $\sigma/\mu = 70\%$.

Figs. 4.14 and 4.15 describe the mass-averaged radial collision force (F_r) and vertical collision force (F_z) with respect to dimensionless cylindrical height (h/H) at three particle bed heights (namely, 470 mm, 350 mm and 200 mm) and three dimensionless radial positions ($r/R = 0, 0.5$ and 1). It has been reported that larger collision forces exist in both the vertical direction and horizontal direction at the hopper bottom to support the particles in the top part [148]. In this study, the trends of the radial and axial profiles are similar in terms of greater collision forces lower in the hopper, and the positive correlation between PSD width and

collision force. The increase of the forces in both directions (i.e., F_r and F_z) with PSD width, despite the discharge rates decreasing with PSD width, suggests that the random collisions among the particles are linked to slower discharge. In terms of collision force magnitudes, F_r magnitudes are somewhat surprisingly greater than F_z , especially lower in the hopper and nearer the radial center (first two columns of Figs. 4.14 and 4.15). This indicates that although the hopper discharge is in the vertical direction, the collision forces are more dominant in the radial than the vertical direction. The radial profiles (i.e., with respect to the dimensionless radius (r/R)) of the radial collision force (F_r) and axial collision force (F_z) at the cone height (i.e., 52 mm from the orifice of the hopper) when the particle bed height is 200 mm is further shown in Figure 4.A2.

Figure 4.14. Dimensionless cylindrical height (h/H) versus average radial collision force (F_r). The three rows represent particle bed heights of 470 mm (a, b, c), 350 mm (d, e, f) and 200 mm (g, h, i), while the three columns represent dimensionless radial positions (r/R) of 0 (a, d, g), 0.5 (b, e, h) and 1 (c, f, i). Spatial averages are taken every 20 mm vertically and radially.

Figure 4.15. Dimensionless cylindrical height (h/H) versus average vertical collision force (F_z). The three rows represent particle bed heights of 470 mm (a, b, c), 350 mm (d, e, f) and 200 mm (g, h, i), while the three columns represent dimensionless radial positions (r/R) of 0 (a, d, g), 0.5 (b, e, h) and 1 (c, f, i). Spatial averages are taken every 20 mm vertically and radially.

Figure 4.16 illustrates the overall collision force as the hopper discharges for the various PSDs, which indicates that (i) F declines rapidly initially before becoming relatively constant for the rest of the discharge, which is similar to the

evolution of the discharge rate as the hopper discharges [101]; and (ii) the F magnitudes increase with PSD width. Figs. 4.11 - 4.16 thus lead to the consistent conclusion that the increased collisions as the range of particle diameters increase with PSD width impede hopper discharge, which provides mechanistic insights into the decreasing discharge rate with PSD width.

Figure 4.16. Overall collision force (F) with the discharge of monodisperse and lognormal PSD with $\sigma/\mu = 10\%$, 30% , 50% and 70% .

4.4. Conclusions

In view of the ubiquity of continuous PSDs in both natural and industrial granular flow, this study aims at getting a better mechanistic understanding of the negative correlation between PSD width and discharge rate, based off a previous study that indicated that, although size-segregation increases with PSD width, no direct relationship exists between PSD width and vertical particle velocity [101]. By means of DEM, the particle velocities and collision forces of lognormal PSDs with the same arithmetic mean particle diameter (3 mm) but varying PSD widths in a 3-dimensional (3-D) hopper are examined. The model has been validated

against experimental data [41] with respect to discharge rate and particle trajectory [101]. The following results are worth noting:

1. The existing correlations, including both the well-acknowledged Beverloo correlation [77] and others modified to incorporate the effect of polydispersity [27, 36], either predict discharge rate trends with respect to PSD width that is opposite to one another or disagrees quantitatively. This highlights the lack of adequate understanding of the effect of PSD width, despite the prevalence of continuous PSDs.
2. Bulk density appears not to be a dominant parameter influencing the discharge rate. All the five particle systems of different polydispersity exhibit plug flow in the upper part, converging flow in the bottom part, and a transition region between them. Throughout the hopper discharge, the particle trajectories become more chaotic especially in the lower half of the hopper as the PSD width increases, which likely slows the discharge.
3. The radial particle velocity (v_r), and both the radial and vertical particle angular velocities (ω_r and ω_z) generally increase as the PSD width increases throughout the first half of the hopper discharge, before the trend reverses towards the end of the hopper discharge. Such a monotonic relationship between PSD width and these three particle velocities (namely, v_r , ω_r , ω_z) is in contrast to that for the vertical particle velocity, which has no direct relationship with PSD width presumably due to the influence of gravity in the same direction.
4. The radial and vertical collision forces (F_r and F_z) versus the dimensionless height trends are similar to that for the particle velocities (i.e., v_r , ω_r , ω_z). The

collision force magnitudes are greater for the wider PSDs throughout the hopper discharge, which contrasts with that for particle velocities (i.e., v_r , ω_r , ω_z) whereby the greater magnitudes associated with the wider PSDs only last for the first half of the hopper discharge. Also, the cross-sectional fluctuations of the collision force at the cone height increase as the PSD width increases.

5. The increase v_r , ω_r , ω_z , F_r and F_z as the lognormal PSD width increases underlies the decreasing hopper discharge rate with PSD width. This relationship indicates that the increased magnitudes of these parameters impede particle flow out of the hopper orifice and thereby slows the hopper discharge. Also, the increased fluctuations of the cross-sectional collision force at the cone height with PSD width underlies the increased fluctuations of the discharge rates with PSD width that was reported earlier [101].

The results emanating from this study provide a better understanding on the mechanisms underlying the different hopper discharge rates stemming from changes in the PSD width, and are expected to be valuable not only towards better operation of the hopper that inevitably contains a range of particle diameters but also the development of better correlations to enhance the predictive capability of hopper discharge.

Appendix

Figure 4.A1. (a) Radial particle velocity (v_r) and (b) radial particle angular velocity (ω_r) versus dimensionless radius (r/R) of various PSDs at the cone height (i.e., 52 mm from the discharge orifice) for particle bed heights of 200 mm. Spatial averages are taken every 5 mm vertically and radially.

Figure 4.A2. (a) Radial collision force (F_r) and (b) vertical collision force (F_z) versus dimensionless radius (r/R) of various PSDs at the cone height (i.e., 52 mm from the discharge orifice) for particle bed heights of 200 mm. Spatial averages are taken every 5 mm vertically and radially.

Chapter 5. Effect of PSD of spherical particles on Jamming

The content of this chapter has been published under the title of *DEM Study on the Effect of Particle-Size Distribution on Jamming in a 3D Conical Hopper* in *AIChE Journal*, vol. 65, pp. 512–519, November 2018 (<https://doi.org/10.1002/aic.16483>).

Abstract

Despite the advancement on the understanding on the unwelcome phenomenon of hopper jamming, the influence of the particle size distribution (PSD) width of the ubiquitous continuous PSDs remains unknown. Accordingly, this study investigated using discrete element method a range of PSD widths ($10\% \leq \sigma/\mu \leq 50\%$) of lognormal PSDs with a constant mean particle diameter of 10 mm in a three-dimensional hopper. Results indicate that, although the monodisperse particles of 10 mm diameters do not jam, the wider PSDs ($\sigma/\mu \geq 30\%$) jam. The flatter arches and higher mass-averaged force that are linked to the denser packing of wider PSDs underlie the propensity to jam. To reduce the jamming probability, the friction coefficient and initial fill height can be reduced, but not changes in particle density. The results here highlights that the mean particle diameter alone is an insufficient parameter to predict jamming and the impact of PSD width is non-negligible.

5.1. Introduction

The hopper is a critical unit operation not only of academic interest for its simple configuration yet complex granular flow behavior, but also commonplace in wider-ranging industries (e.g., chemical, pharmaceutical, food, energy) [22-24]. The particulate flow characteristics is of key importance for smooth operation and structural durability [57, 151]. In particular, the common problems that plague granular materials like arching, dead zone, segregation are also inevitable in hoppers [1, 121, 133]. Although hoppers are designed to discharge particles, a detrimental phenomenon termed ‘jamming’ occurs, whereby the particles form an ‘arch’ near the outlet and discharge is terminated [30].

To date, both numerical and experimental approaches have been adopted to understand the jamming phenomenon [84, 152, 153], including the arching structure [84, 85] and means to avoid jamming/arching [28, 86, 87]. Past studies tended to focus on the two-dimensional (2D) hopper for simplicity, resulting in a more in-depth understanding of the various aspects of jamming [84, 88-90]. To et al. [90-92] characterized the arches formed upon jamming and revealed the relationship between jamming probability and the ratio of orifice diameter to particle diameter. Janda et al. [93] presented experimental results on jamming during the discharge of grains, and determined that a critical size of the outlet orifice existed above which there was no jamming. Guariguata et al. [89] carried out experiments in a two-dimensional silo to analyze the geometrical properties of the arches in detail, and concluded that (i) the ratio of the outlet orifice size to the diameter of the spheres did not affect the arch shape, (ii) arches tended to

exhibit an aspect ratio (i.e., height of the arch from the line joining the two outermost particles of the arch to the distance between the two outermost particles of the arch) close to 1, and (iii) static friction had a dominant influence on arch formation. Lou [94] illustrated that the influence of particle properties (e.g., friction, coefficient of restitution) is negligible for hoppers with large outlet orifices, but become important for smaller orifices. Lin and Fang [95] experimentally investigated the discharge behavior of elliptical particles in a 2D hopper, and unveiled that the probability of jamming increases with the increase of the particle aspect ratio for the hoppers with gentler slopes, but reduces as the aspect ratio increases for smaller hopper outlet orifices. Longjas et al. [96] evaluated the probability of jamming of mixed disk-shaped particles in a 2D hopper using force analysis, and elucidated the presence of three likely flow regimes, namely, the jam-free continuous flow, the transitory flow, and an N -dependent jammed state. Tang et al. [88] developed a model that provides a good description of flows in a 2D hopper filled with non-cohesive particles. Desmond and Franklin [97] explored the jamming phenomenon in a three-dimensional (3D) cylinder and found the hopper size and particle aspect ratio are important factors to determine the tendency of rod-shaped particles to jam in response to the local perturbation. Pournin et al. [98] investigated the effect of friction and boundary condition on the median jamming diameter (i.e., the orifice diameter for which the jamming probability is 0.5) as a function of particle diameter (in the case of bidisperse particles, a volume-average mean was used), and pinpointed the formation of concentric particle rings as an essential precursor to jamming.

To avoid jamming, one effective way is by vibration [28, 87, 99]. Janda et al. [87] observed that the discharge rate significantly increased with the vibration amplitude. Mankoc et al.[28] concluded that vibration increased the size of the avalanches (i.e., amount of particles discharged between two continuous jams) markedly. Garcimartín et al.[99] found that larger outlet orifice sizes weakened the arches that clog due to the external vibration. Mondal and Sharma [100] observed via simulations that, for a small ratio of orifice diameter to particle diameter, having two adjacent outlets averts the jamming caused by a single outlet. Collectively, past studies have shed some light on the jamming phenomenon. However, although continuous PSDs are ubiquitous both in nature and industry, and thus are very likely found in hoppers, the effect of PSDs on hopper jamming is not yet understood.

Accordingly, this study targeted at evaluating the jamming probability of lognormal PSDs with the same mean diameters but different PSD widths. The arch structures for the jammed systems were assessed qualitatively and quantitatively, then the forces in the hopper were quantified and related to jamming. Then, the effects PSD width coupled with friction coefficient, particle density and fill height were assessed.

5.2. Material and method

5.2.1. Discrete element method (DEM)

The DEM is an increasingly popular tool to enhance the understanding of particulate flow behavior [1, 40]. In DEM simulations, the motion of each particle

is described by Newton's second law, and the equations for the translational and rotational motions of individual particles are expressed as

$$m_i \frac{d\mathbf{V}_i}{dt} = \sum_{j=1}^K (\mathbf{F}_{c,ij}^n + \mathbf{F}_{c,ij}^t + \mathbf{F}_{d,ij}^n + \mathbf{F}_{d,ij}^t) + m_i \mathbf{g} \quad (5-1)$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^K (\mathbf{M}_{t,ij} + \mathbf{M}_{r,ij}) \quad (5-2)$$

where m_i is the particle mass of particle i , $\mathbf{V}_i$ and $\boldsymbol{\omega}_i$ respectively represent the translational velocity and the angular velocity of particle i , $\mathbf{F}_{c,ij}$ and $\mathbf{F}_{d,ij}$ respectively represent collision forces (includes both normal and tangential contact forces) and damping forces between particle i and particle j , I_i is the moment of inertia of particle i , $\mathbf{M}_{r,ij}$ is the torque generated between particle i and particle j , $\mathbf{g}$ is the gravitational acceleration, and K represents the number of contacts between particle i and the neighboring particles or walls. The Hertz theory is used to evaluate the normal and tangential forces between two particles [119, 120]. The open-source platform, LIGGGHTS, is used in present study for the 3D DEM simulations.

5.2.2. Simulation setup

Figure 5.1 shows the geometry of the conical hopper studied here, which is of the same dimensions as that experimentally used by Li et al. [41]. The total height of the conical hopper is 0.500 m, with a cone height of 0.052 m. The diameter of the cylindrical portion and the diameter of the outlet orifice at the bottom of the conical section are respectively 0.240 m and 0.060 m. The cone is angled at 60° to the vertical. The particles are glass beads with particle diameters of between 10 to 17 mm. The particle density (ρ_p) studied ranges from 1000 to 3500 kg/m³.

The friction coefficient ranges from 0.1 to 0.9, and the initial fill height ranges from 50 to 474 mm. The relevant parameters used in this study are summarized in Table 5.1.

The procedure is as follows. The orifice outlet at the base of the hopper is sealed, and the targeted number of glass beads is generated in the hopper randomly and allowed to free-fall under the influence of gravity. Then, the cover sealing the orifice outlet is removed and the particles are discharged under gravity. The DEM model has been validated with experimental results in our previous study with respect to the trajectory of the tracked particles and the instantaneous bed height during discharge [101].

Figure 5.1. Schematic of the 3D hopper simulated.

Table 5.1. Details of numerical and physical parameters used in this study.

Parameter	Value
σ/μ (%)	10, 20, 30, 40 and 50
Density, ρ_p (kg/m ³)	1000, 1500, 2000, 2460, 3000 and 3500
Fill height, H (m)	0.474, 0.4, 0.35, 0.3, 0.25, 0.2, 0.15, 0.1 and 0.05
Young's modulus, Y (GPa)	0.1
Poisson ratio, ν (-)	0.25
Coefficient of particle-wall static friction (-)	0.6
Coefficient of particle-wall rolling friction (-)	0.05
Coefficient of particle-wall restitution (-)	0.99
Coefficient of particle-particle static friction (-)	0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8 and 0.9
Coefficient of particle-particle rolling friction (-)	0.01
Coefficient of particle-particle restitution (-)	0.99
Time step, Δt (s)	2×10^{-5}

5.2.3. Particle-size distribution (PSD)

The The number-based frequency distribution (f_n) of the common lognormal PSD investigated in this study is expressed as follows:

$$f_n = \frac{1}{x\sigma\sqrt{2\pi}} \exp \left[-\frac{(\ln(x)-\mu)^2}{2\sigma^2} \right] \quad (5-3)$$

where x is the diameter of the particle, μ is the arithmetic mean diameter and σ is the standard deviation of the PSD. The mean particle diameter (μ) studied is 10 mm, which is the same as the monodisperse particle diameter used in the

experiments carried out by Li et al. [41]. The width of the PSDs, which is defined non-dimensionally as the standard deviation of the PSD normalized with respect to the arithmetic mean diameter of particles (σ/μ), ranges from 10% to 50%. The lower bound is different from the monodisperse particles due to the presence of smaller and larger particles, while the upper bound such that the ratio of the largest particle diameter to orifice diameter is less than 0.5 (since larger ratios have been reported to cause jamming [90]). Figure 5.2 illustrates the various number-based lognormal PSDs, with widths (σ/μ) ranging from 10% to 50%, investigated here.

Figure 5.2. Number-based lognormal PSDs with the same mean particle diameter (μ) of 10 mm and PSD widths (σ/μ) ranging from 10 to 50%.

5.3. Results and Discussion

5.3.1. Particle diameter

Figure 5.3 illustrates the evolution of the mass discharged from the hopper for monodisperse particles with diameters ranging from 10 to 17 mm. The initial particle bed heights for the monodisperse systems are all filled to 0.474m. The

friction coefficient and the particle density are 0.6 and 2460 kg/m³, respectively. The slopes of the plots are constant during discharge, indicating constant mass discharge rates. As the particle diameter increases up to 14 mm, the mass discharge rate decreases. For particle diameters of 15 mm and above, the mass remains constant with time because of jamming, which means that the discharge is halted. Some discharge occurs for the particle diameters of 15 and 16 mm, but none for the largest particle diameter investigated of 17 mm. The critical diameter for jamming in this case is 15 mm, which is a quarter of the hopper outlet orifice diameter (i.e., 60 mm) and is consistent with an earlier report by Fayed and Otten [121]. Furthermore, four more runs are performed for each monodisperse system with particle diameters between 10 and 17 mm to understand the jamming probability. Figure 5.4 indicates that the probability of jamming for particle diameters of 13 mm and below is 0, increases to 40% when the particle diameter is increased to 14 mm, and further to 100% for particle diameters of 15 mm and above are 100%.

Figure 5.3. Evolution of the mass discharged from the hopper for the monodisperse particles with diameters between 10 and 17 mm.

Figure 5.4. Jamming probability of the monodisperse systems with particle diameters between 10 and 17 mm. The initial bed height, friction coefficient, and particle density are 0.474 m, 0.6, and $2460 \text{ kg}\cdot\text{m}^{-3}$, respectively. The solid line is fitted by B-Spline.

5.3.2. PSD width

In our previous study, it was demonstrated that the mass discharge rate of the hopper decreases with PSD width (σ/μ), although no jamming was observed because of the smaller mean particle diameter (μ) investigated of 5 mm [101]. To shed light on the effect of PSD width on jamming, lognormal distributions of various PSD widths (σ/μ) but with the mean particle diameter (μ) of 10 mm are studied.

Analogous to Figure 5.3, Figure 5.5 shows the evolution of the mass discharged from the hopper for the various PSD widths from an initial packed particle bed height of 0.474 m. The friction coefficient and the particle density are 0.6 and 2460 kg/m^3 , respectively. For the narrower PSD widths of $\sigma/\mu \leq 20\%$, the hopper discharges fully, with the slightly wider PSD expectedly discharging slightly slower [101]. For the broader PSD widths of $\sigma/\mu \geq 30\%$, discharge

only occurs within the first second (Figure 5.5b) before jamming occurs, which is associated with the presence of larger particles (Figure 5.2). Interestingly, jamming does not happen for the PSD with $\sigma/\mu = 20\%$ despite it having particles larger than 15 mm (i.e., the critical jamming diameter; Figure 5.3), whereas a modest increase in the fraction of particles larger than 15 mm for the PSDs with $\sigma/\mu \geq 30\%$ causes severe jamming within the first second of discharge. Two plausible reasons are described as follows, though it is beyond this effort to conclude definitively which is more dominant in causing jamming. First, the proportions of particles larger than 15 mm, which is the critical diameter for jamming for monodisperse systems, are greater for PSDs with widths of $\sigma/\mu \geq 30\%$, which at least in part underlie the existence of jamming. Figure 5.2 indicates that, although the frequencies of particles larger than 15 mm particles are more similar for PSDs with widths of $\sigma/\mu \geq 30\%$, that for the PSD width of 20% rapidly plunges beyond 15 mm. Secondly, the increasing range of particle sizes for wider PSDs implies increasing differences between the largest and smallest particles, which range from 1.9 to 10.3 for the PSD widths investigated. The wider range of particles and thereby denser packing may also increase the likelihood of jamming. Analogous to Figure 5.4 that evaluates jamming probability vs. particle diameter of monodisperse systems, Figure 5.6 assesses jamming probability vs. PSD width of lognormal PSDs with the same mean particle diameter of 10 mm. Clearly, the jamming probability is 0 for lognormal PSDs widths of $\sigma/\mu \leq 20\%$, increases to 20% for the intermediate PSD width of $\sigma/\mu = 30\%$, and then to 100% for PSD widths of $\sigma/\mu \geq 40\%$.

Figure 5.5. Evolution of the (a) mass discharged and (b) mass discharge rate from the hopper with time for lognormal PSDs with the same mean particle diameter (μ) of 10 mm and PSD widths (σ/μ) between 0% and 50%. The initial bed height, friction coefficient, and particle density are 0.474 m, 0.6, and 2460 kg·m⁻³, respectively.

Figure 5.6. Jamming probability vs. lognormal PSD widths. The lognormal PSDs have the same mean particle diameter (μ) of 10 mm and PSD widths (σ/μ) between 10 and 50%. The initial bed height, friction coefficient, and particle density are 0.474 m, 0.6, and 2460 kg·m⁻³, respectively. The solid line is fitted by B-Spline.

The arching structures of monodisperse systems have been well-studied in previous studies [89, 93], but not for lognormal PSDs. Figure 5.7 depicts the

arches for the jammed monodisperse system with μ of 15 mm (recall that monodisperse systems with smaller particles do not jam), and that of lognormal PSDs with μ of 10 mm. A previous study has reported that the relationship between the ratio of the outlet orifice diameter to the particle diameter (R) and the average number of particles forming the arch ($\bar{n}$) can be expressed as follows [89]:

$$\bar{n} = 1.41 + 1.15R \quad (5-4)$$

Equation 5-4 implies that the number of particles forming the arch increases as the particle diameter decreases. Per Eq. 5-4, the $\bar{n}$ values are 6.0 and 8.3 respectively for the monodisperse system ($\mu = 15$ mm) and lognormal systems ($\mu = 10$ mm), which agree quite well with the integral values obtained via DEM of respectively 7 and 8 (Figure 5.7). This implies that the number of particles per arch, below which jamming does not occur, is related to the ratio R .

Apart from the number of particles that arches comprise of, another parameter characterizing arching is ratio of the height of the highest particle in the arch from the line joining the two outermost particles of the arch to half the distance between the outermost particles of the arch (α) [89, 91]. While the α value for the monodisperse system with a μ of 15 mm is 0.70, that of the lognormal PSDs are 0.69, 0.58 and 0.39 for the PSD widths (σ/μ) of respectively 30, 40 and 50%. The decreasing α value with PSD width implies that flatter arches, which is linked to the denser packing of wider PSDs, increases the tendency to jam.

(a) Monodisperse

(b) $\sigma/\mu = 30\%$ (c) $\sigma/\mu = 40\%$ (d) $\sigma/\mu = 50\%$

Figure 5.7. Particle arching structure in the radial center of the 3D hopper outlet for the various particle systems studied. All the lognormal PSDs have similar mean particle diameters (μ) of 10 mm, whereas the monodisperse has $\mu = 15$ mm since smaller diameters do not jam.

Figure 5.8 displays the mass-averaged forces (i.e., collision and gravitational forces) of the whole hopper and of only the cone portion for the various PSDs investigated before the particles start to discharge from the hopper. Clearly, the mass-averaged force increases with PSD width, which suggests that the forces have the same tendency as the jam increases with the increase of the PSD width. In particular, the discrepancy between the forces in the whole hopper and in the cone only increases with PSD width, which implies that the increased concentration of the forces in the cone is tied to the jamming of the hopper.

Figure 5.8. Mass-averaged force just before discharge of the whole hopper and the cone portion only of the monodisperse and lognormal PSDs, all with $\mu = 10$ mm.

5.3.3. Friction

The friction coefficient of the particles has been shown to affect the tendency to jam [98], with higher coefficients increasing the jamming tendency [90], because a wider range of jamming configurations is allowed by the higher frictions due to the significant role of tangential forces in the stability of the particulate system [98]. In view of the prevalence of continuous PSDs, this study assessed the

combined effect of friction coefficient and PSD width. Recall that, with a friction coefficient of 0.6 (Table 5.1), lognormal PSDs with widths of $\sigma/\mu \geq 30\%$ exhibit jamming (Figure 5.5). Accordingly, Figure 5.9 presents the trends of how much the friction coefficients have to be reduced to avert jamming for the lognormal PSDs with the initial packed particle bed height of 0.474 m and constant particle density of 2460 kg/m³. For the widest PSD ($\sigma/\mu = 50\%$) evaluated, jamming is inevitable. On the other hand, for the relatively narrower PSDs of $\sigma/\mu = 30$ and 40%, the jamming probability can be reduced by reducing the friction coefficient. Clearly, the wider the PSD is, the lower the friction coefficient has to be for the smooth discharge of the hopper.

Figure 5.9. Jamming probability with respect to the friction coefficient (ranging from 0.1 to 0.9 mm) for lognormal PSD widths (σ/μ) between 30% and 50%. The initial packed bed height is constant at 0.474 m and particle density at 2460 kg·m⁻³. The solid line is fitted by B-Spline.

In order to further understand the impact of the friction coefficient (c_f) on a lognormal PSD, Figure 5.10 displays the evolution of the mass discharge and mass discharge rate from the hopper for the lognormal PSD with an intermediate

width (σ/μ) of 30% for one trial. At the lower friction coefficients (c_f) of less than 0.5, the hopper fully discharges with the discharge being faster for the lower c_f value. On the other hand, at the higher coefficients (c_f) of 0.5 and above, the jamming happens within one second, with the jamming occurring sooner as the c_f value increases.

Figure 5.10. Evolution of (a) mass discharged from the hopper and (b) mass discharge rate for the PSD width (σ/μ) of 30% and friction coefficients (c_f) ranging from 0.3 to 0.7. The initial packed bed height is constant at 0.474 m and particle density at $2460 \text{ kg}\cdot\text{m}^{-3}$.

5.3.4. Particle density

Figure 5.11 shows the coupled effect of PSD width and particle density (ρ_p) on hopper discharge. The initial packed particle bed height is 0.474 m and friction coefficient is 0.6. Clearly, for all the systems, particles remain stuck in the hopper, indicating that the change in density does not alleviate jamming and that PSD width has a more dominant effect than particle density in the parameter space investigated.

Figure 5.11. Mass discharged from the hopper at various particle densities (ρ_p ; ranging from 1500 – 3500 kg/m³) with respect to time for the lognormal PSDs with widths (σ/μ) of (a) 30%, (b) 40% and (c) 50%. The initial packed bed height is constant at 0.474 m and friction coefficient at 0.6.

5.3.5. Fill height

The initial fill height of the hopper can be adjusted to mitigate jamming, with the probability of jamming known to increase as the number of particles increases [154]. Figure 5.12 illustrates the probability of jamming for the wider PSD widths in the range of initial fill heights between 50 and 500 mm. The jamming probability for the lognormal PSD width (σ/μ) of 30% generally increases (up to a maximum of 40%) as the fill height increase from 50 mm to 474 mm. For

the PSD width (σ/μ) of 40%, the jamming probability increases to 100% when the fill height is above 100 mm. Whereas, jamming is inevitable even with the lowest fill height investigated of 50 mm for the widest PSD (σ/μ) of 50%, it can be averted by lowering the fill heights for the PSDs with widths (σ/μ) of 30 and 40%.

Figure 5.12. Jamming probability with respect to the initial particle fill height (ranging from 50 to 474 mm) for PSD widths (σ/μ) between 30 and 50%. The friction coefficient is constant at 0.6 and particle density at $2460 \text{ kg}\cdot\text{m}^{-3}$. The solid line is fitted by B-Spline.

For a closer look at the coupled effect of PSD width and fill height, Figures 5.13a, b describe, respectively, the mass left in the hopper and mass discharge rate with time for the lognormal PSD with width (σ/μ) of 30% at various fill heights (H ; ranging from 200 to 474 mm). In the absence of jamming for the fill heights of equal to or less than 300 mm, the hopper discharges completely at similar rates. However, for fill heights of 350 mm and above, the higher the fill height is, the slower the occurrence of jamming is.

Figure 5.13. (a) Mass left in the hopper and (b) mass discharge rate with respect to time for the lognormal PSD with width (σ/μ) of 30% at various initial fill heights (H) ranging from 200 mm to 474 mm.

5.4. Conclusions

Because the effect of PSD width of continuous PSDs on hopper jamming is important but not yet understood to date, this study employed DEM to shed some light. Armed with the understanding that monodisperse particles with diameters of 10 mm do not cause hopper jamming, lognormal PSDs with a constant mean particle diameter of 10 mm and PSD widths (σ/μ) ranging between 10% and 50% were investigated.

The following results are worth highlighting. First, introduction of polydispersity increases jamming probability. Specifically, the wider PSDs ($\sigma/\mu \geq 30\%$) of the same mean diameter results in hopper jamming. Second, the characterization of the arch indicates that the α value decreases with PSD width. It appears that wider PSDs give flatter arches, which could underlie the increased jamming tendency. Third, the mass-averaged force in the hopper increases with PSD width, which implies that higher forces could be tied to the increased tendency to jam.

Fourth, the wider the PSD is, the lower the friction coefficient has to be for the smooth discharge of the hopper. Fifth, the change in particle density in the range investigated does not alleviate hopper jamming by the wider PSDs. Sixth, to avert jamming, the initial fill height can be lowered, though even a slight fill height still causes jamming for the widest PSD.

The results obtained in this study provide new insights on hopper jamming, notably in that the mean particle diameter alone is an insufficient parameter to predict jamming. This underscores the non-negligible impact of PSD width on the jamming behavior during hopper discharge, and thereby emphasizes the need for further studies to better design and operate such systems.

Chapter 6. Hopper discharge behaviors of binary mixtures of non-spherical particles

The content of this chapter has been accepted under the title of *DEM Study on Hopper Discharge Behaviors of Binary Mixtures of Non-Spherical Particles* in *AIChE Journal*.

Abstract

This study is aimed at unveiling the influence of binary mixtures of non-spherical particles on hopper discharge behavior, which remains poorly understood. The discrete element method (DEM) is employed to simulate seven particle types (namely, a sphere, two ellipsoids, two cylinders and two cuboids) with the same volume. Seven monodisperse systems, three binary-size and twelve binary-shape mixtures are assessed. For the monodisperse systems, particle shape is the dominant factor dictating discharge rate, compared to other factors like aspect ratio, preferential orientation and packing. Regarding the binary-size mixtures, while the discharge rates are still dictated by particle shape, the positive correlation between discharge rate and solid volume fraction or mean aspect ratio is clear. As for the binary-shape mixtures, the discharge rates are similar for all twelve mixtures, reflecting a surprising lack of shape effects, which in turn means the negligible impact of solid volume fraction, aspect ratio and segregation extent.

Keywords: binary mixtures; discrete element method (DEM); superquadric particle; discharge rate; segregation

6.1. Introduction

The hopper is commonly encountered in many applications, such as in the pharmaceutical, chemical, and food industries, for the storage and discharge of particles [22, 24, 155, 156]. Correspondingly, the understanding of the principles underlying particle packing and flow in the hopper has been the focus of many studies, due to the importance of the flow characteristics for the design and operation of the hopper [14, 157]. Many factors (e.g., hopper geometry [9, 75, 80, 158-160], particle properties [10, 57, 101, 161-164], and flow conditions [74, 83, 165]) may affect the flow dynamics. The focus of this study is on particle shape, which has been shown to have a significant influence on the particle flow behaviors [56, 166-168].

Past studies have adopted both numerical [65, 71, 169] and experimental [14, 33] approaches to investigate the impact of particle shape on the hopper system. Cleary and Sawley [12, 56] investigated the effect of particle shape on shear flow and hopper discharge by the DEM, revealing that the discharge rate of elongated particles is 30% lower than spherical particles and non-spherical particles are harder to shear. Höhner et al. [14, 57] conducted both experiments and simulations, and concluded the mass flow rate from the hopper reduces as the angularity of the particle increases, and the flow resistance of polyhedrals is larger than spheres. Gui et al. [59-61] simulated the discharge rates of the particles with different shapes, concluding that the cubic shape has additional motion resistance compared to the spherical shape. Soltanbeigi et al. [58] explored the mechanical characteristics of multi-spherical and superquadric

particles by DEM, and concluded that (i) the heap profile in the angle of repose test is affected by the properties of angularity in superquadric and multi-sphere particles considerably; and (ii) particle shape influences shear strength, porosity and mode of motion, but has lesser influence on the mass flow rate in hopper discharge.

In binary systems, particle shape has also been shown to have significant impact. Ng et al. [64] researched on the coupled effect of particle shape and fines content on the behavior of binary mixtures, and found that particle shape has more influence on the peak shear strength than fines content. Yu and Saxén [63] demonstrated that particle shape has little effect on size segregation, but the continuity of the flow is affected when the shape becomes more complex. Alizadeh et al. [62] studied experimentally that segregation is driven by the difference in particle shape in a binary mixture. Collectively, past studies have given some insights into the binary mixtures of non-spherical particles. However, what remains unknown is whether binary-size and binary-shape mixtures of non-spherical constituent particles exhibit different hopper discharge behaviors.

In order to bridge the gap in the knowledge with regards to the impact of the different binary mixtures on hopper discharge, this study harnesses the DEM to investigate six different non-spherical constituent particles, namely, two ellipsoids, two cylinders and two cuboids, with the same volume but different aspect ratios. Three binary-size and twelve binary-shape mixtures, along with seven monodisperse systems, are assessed. The solid volume fraction of the packed bed, the particle orientation, the discharge rate, the number of residual particles after discharge and the segregation extent are evaluated systematically.

6.2. Material and method

6.2.1. Representation of a superquadric particle

The superquadric method is used for representing the non-spherical particles. It was developed by expanding the quadric surface and has been widely used to describe particles with convex and concave shapes. Each superquadric particle investigated in this work is described with the following equation [170]:

$$f(x, y, z) = \left(\left| \frac{x}{a} \right|^{n_2} + \left| \frac{y}{b} \right|^{n_2} \right)^{\frac{n_1}{n_2}} + \left| \frac{z}{c} \right|^{n_1} - 1 = 0 \quad (6-1)$$

where a, b and c respectively stand for the half-length of the superquadric particles along the x , y and z axes; and n_1 and n_2 are the blockiness parameters governing the curvature of the particle surface. An ellipsoid is obtained for $n_1 = n_2 = 2$, a cylinder is obtained if $n_1 \gg 2$ and $n_2 = 2$, and a cuboid is obtained if $n_1 = n_2 \gg 2$. By modifying these five parameters, many types of non-spherical particles can be accurately represented [170].

This study assesses seven types of particles (namely, one sphere, two ellipsoids, two cylinders and two cuboids), each of which is described by Equation 6-1. Figure 6.1 displays the seven particles and their dimensions, while Table 6.1 lists the parameters used to describe the particles. Sphericity (φ) is calculated using the definition by Wadell [171] based on the ratio of the surface area of a sphere with the same volume as the given particle (A_s) to the actual surface area of the particle (A_p):

$$\varphi = \frac{A_s}{A_p} = \frac{\pi^{\frac{1}{3}}(6V_p)^{\frac{2}{3}}}{A_p} \quad (6-2)$$

where V_p is volume of the particle and A_p is the surface area of the particle.

Specifically, (i) each particle has the same volume of $5.24 \times 10^{-7} \text{ m}^3$ and particle density (ρ_p) of 2460 kg/m^3 ; (ii) the sphere is such that $a = b = c = 5 \text{ mm}$, and (iii) for the ellipsoid, cylinder and cuboid, one species of each shape is such that $a = b = 4 \text{ mm}$, and the other is such that $a = b = 6 \text{ mm}$. The aspect ratio is calculated as the ratio of c (the half-length of the superquadric particles along the z -axis) to a (the half-length of the superquadric particles along the x -axis). In particular, the sphere has an aspect ratio of 1, and the species of each shape that is more disk-like has a smaller aspect ratio. For the binary mixture, a representative volume-based mean aspect ratio ($\overline{c/a}$) was calculated, as expressed in Table 6.3. The three types of particles (i.e. Ellipsoid3, Cylinder3 and Cuboid3) with larger aspect ratio ($c/a > 4$) are further shown in Figure A6.1 and Table A6.1.

$$n_1 = n_2 = 10$$

(f)

(g)

Figure 6.1. Three-dimensional superquadric particles investigated: (a) Sphere, (b) Ellipsoid1, (c) Ellipsoid2, (d) Cylinder1, (e) Cylinder2, (f) Cuboid1, and (g) Cuboid2.

Table 6.1. Details of parameters of superquadric particles with similar volumes used in this study.

	a (mm)	b (mm)	c (mm)	n_1	n_2	aspect ratio (c/a)	sphericity
Sphere	5	5	5	2	2	1.00	1.00
Ellipsoid1	4	4	7.81	2	2	1.95	0.96
Ellipsoid2	6	6	3.47	2	2	0.58	0.97
Cylinder1	4	4	5.21	10	2	1.30	0.87
Cylinder2	6	6	2.32	10	2	0.39	0.78
Cuboid1	4.03	4.03	4.03	10	10	1.00	0.81
Cuboid2	6	6	1.82	10	10	0.30	0.68

6.2.2. Governing equations for particle motion

The DEM proposed by Cundall and Strack is an extensively used method to describe the flow behavior of each particle in the granular flow system [1, 40]. In DEM, the motion of every particle is governed by Newton's second law, and the rotational motion and translational motion of each individual particle can be formulated as follows:

$$I_i \frac{d\omega_i}{dt} = \sum_{j=1}^K (\mathbf{M}_{n,ij} + \mathbf{M}_{t,ij} + \mathbf{M}_{r,ij}) \quad (6-3)$$

$$m_i \frac{d\mathbf{V}_i}{dt} = \sum_{j=1}^K (\mathbf{F}_{cn,ij} + \mathbf{F}_{ct,ij}) + m_i \mathbf{g} \quad (6-4)$$

where, $\mathbf{F}_{cn,ij} = k_{n,ij} \delta_{n,ij} \mathbf{n} + \gamma_{n,ij} \mathbf{v}_{n,ij}$ (6-5)

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

in which, m_i is the particle mass, $\mathbf{V}_i$ and ω_i are the translational and angular velocity, $\mathbf{F}_{cn,ij}$ and $\mathbf{F}_{ct,ij}$ are collision forces along the normal and tangential directions, I_i is the moment of inertia, $\mathbf{M}_{n,ij}$ and $\mathbf{M}_{t,ij}$ are the torques between particles determined by normal force and tangential force if the normal force doesn't pass through the centroid of the non-spherical particles, $\mathbf{M}_{r,ij}$ is the torque generated by rolling friction, $\mathbf{g}$ is the gravitational acceleration, K represents the number of contacts of the particle i with the neighboring, $\mathbf{n}$ and $\mathbf{t}$ are respectively the unit vectors along the normal and tangential directions of a colliding pair. Moreover, k and γ are stiffness and damping coefficients can be calculated on the basis of the material properties and overlap distance as shown in Table 6.2. Specifically, when calculating the equivalent R^* , the radius of each particle is evaluated based on the curvature of the contacting point of this particle. The friction coefficient μ is adopted to limit the friction force when sliding occurs between the colliding pair. The Hertz theory is applied to evaluate the normal and tangential forces between particles [119, 120].

Table 6.2. Equations adopted to calculate the stiffness and damping coefficients of the particles. [172]

Normal stiffness coefficient ($k_{n,ij}$)	$k_{n,ij} = \frac{4}{3} Y^* \sqrt{R^* \delta_{n,ij}}$
Tangential stiffness coefficient ($k_{t,ij}$)	$k_{t,ij} = 8 G^* \sqrt{R^* \delta_{n,ij}}$
Normal damping coefficient ($\gamma_{n,ij}$)	$\gamma_{n,ij} = 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_{n,ij} m^*}$
Tangential damping coefficient ($\gamma_{t,ij}$)	$\gamma_{t,ij} = 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_{t,ij} m^*}$
Where the related variables are evaluated as	
$\beta = \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}}$, $S_{n,ij} = 2 Y^* \sqrt{R^* \delta_{n,ij}}$, $S_{t,ij} = 8 G^* \sqrt{R^* \delta_{n,ij}}$, $\frac{1}{Y^*} = \frac{(1-\nu_i^2)}{Y_i} + \frac{(1-\nu_j^2)}{Y_j}$, $\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j}$, $\frac{1}{m^*} = \frac{1}{m_i} + \frac{1}{m_j}$, $\frac{1}{G^*} = \frac{2(2+\nu_i)(1-\nu_i)}{Y_i} - \frac{2(2+\nu_j)(1-\nu_j)}{Y_j}$	

To simulate irregular particles via DEM, local coordinates with axes chosen to be the principal axes of inertia are applied to model the rotational motion of the particles. Quaternions, which quantify the orientation of the non-spherical particles and thus the instantaneous direction of a specific particle can be evaluated, are commonly used for determining the rotational motion of the particles [66, 173, 174]. More details about the particle-particle and particle-boundary contact detection algorithm can be found in references [66, 175-178].

6.2.3. Simulation setup

The conical hopper studied, whose dimensions are similar to that used in the experimental work of Li et al. [41], is shown in Figure 6.3. The total height of the hopper is 0.50 m, and the diameter of the cylindrical part and the outlet orifice at the bottom of the cone portion are 0.24 m and 0.06 m, respectively, while the slope of the cone portion is 60° to the vertical. The parameters used in the simulations are summarized in Table 6.3. The particles inside the hopper is randomly generated under gravity to a fixed bed height 0.474 m initially, which can ignore the wall effects due to the satisfaction of when the ratio of equivalent particle diameter ($d_v = 0.01$ m) to container diameter ($D = 0.24$ m) is greater than 0.04, the ratio of fill height (h) to container diameter should be greater than 1 provided by Zou et al. [179]

Table 6.4 lists the fifteen binary mixtures investigated, with the volume fraction of each constituent being 0.5, which are divided into four categories. The first category contains mixtures with similar shapes but different sizes, the second

contains mixtures of ellipsoids and cylinders, the third contains mixtures of ellipsoids and cuboids, while the fourth contains cylinders and cuboids.

Figure 6.2. Schematic of the hopper.

Table 6.3. Details of numerical and physical parameters used in this study.

Parameter	Value
Particle volume (m^3)	5.24×10^{-7}
Particle density, ρ_p (kg/m^3)	2460
Hopper fill height, H (m)	0.474
Young's modulus, Y (GPa)	0.1
Poisson ratio, ν (-)	0.25
Coefficient of particle-wall static friction (-)	0.6
Coefficient of particle-wall rolling friction (-)	0.05
Coefficient of particle-wall restitution (-)	0.99
Coefficient of particle-particle static friction (-)	0.6
Coefficient of particle-particle rolling friction (-)	0.01
Coefficient of particle-particle restitution (-)	0.99
Time step, Δt (s)	5×10^{-5}

Table 6.4. Binary superquadric particles investigated. The volume fraction of each constituent in the hopper is 0.5.

			Mean aspect ratio ($\overline{c/a}$)
Category 1: Binary-size	Ellipsoid1	Ellipsoid2	1.27
	Cylinder1	Cylinder2	0.85
	Cuboid1	Cuboid2	0.65
Category 2: Ellipsoid + Cylinder	Ellipsoid1	Cylinder1	1.63
	Ellipsoid1	Cylinder2	1.17
	Ellipsoid2	Cylinder1	0.94
	Ellipsoid2	Cylinder2	0.48
Category 3: Ellipsoid + Cuboid	Ellipsoid1	Cuboid 1	1.48
	Ellipsoid1	Cuboid 2	1.13
	Ellipsoid2	Cuboid 1	0.79
	Ellipsoid2	Cuboid 2	0.44
Category 4: Cylinder + Cuboid	Cylinder1	Cuboid1	1.15
	Cylinder1	Cuboid2	0.80
	Cylinder2	Cuboid1	0.70
	Cylinder2	Cuboid2	0.35

6.3. Results and discussion

6.3.1. Model validation

The DEM model used here has been developed in our previous work to understand the dynamics of spherical particles in a hopper and validated against experimental results [41] with respect to the trajectories of the tracked particles [101]. This study extends the implementation to non-spherical particles represented by the superquadric equations. The model is then validated with experiments [180], which involve the random packing of 250 cylindrical particles

(each with diameter of 8 mm and length of 5.3 mm) in a cylindrical container with inner diameter of 50.6 mm and height of 130 mm. Figure 6.3 compares the packed beds between the simulation and experimental results. The simulated bed height of 53.9 mm and volume fraction of 0.615 agree well with the corresponding experimental data of 53.3 mm and 0.621 [180]. For further validation of the model, the discharge rates of the monodisperse particles, binary-size mixtures and binary-shape mixtures are compared with the well-acknowledged Beverloo correlation [77]:

$$W = C\rho_b\sqrt{g}(D_0 - kd_p)^{5/2} \quad (6-7)$$

where C and k are empirical constants, ρ_b is the bulk density of the packed particles, g is the gravitational constant, D_0 is the diameter of the hopper orifice and d_p is the particle diameter. While C depends on the hopper geometry and angle of internal friction of particles, k depends on the particle shape. Fitting the results yielded $C = 0.58$ and $k = 1.0; 1.7; 2.1; 2.5$ for spheres, ellipsoids, cylinders and cuboids, respectively, which agree with the reported ranges of C and k values [27, 77, 78, 181-183]. The simulated discharge rates and Beverloo predictions are displayed in Figures 6.7b, 6.12b and 6.19d.

Figure 6.3. Comparison of the packed bed of cylindrical particles obtained via (a) simulation and (b) experiment [180].

6.3.2. Monodisperse particles

One of the extraordinary characteristics for non-spherical particles is their orientation. Figure 6.4 shows the screenshots of the different packings of the single type of particles at the time step of 0 (i.e., right before the discharge) at the mid-height (i.e., 97 - 377 mm) of the hopper close to the wall. Clearly, the preferential orientations of the various shapes are different, with the species with larger aspect ratios (namely, Ellipsoid1 (Figure 6.4b) and Cylinder1 (Figure 6.4d)) preferentially orientated with their longest dimensions vertical, while species with smaller aspect ratios (namely, Cylinder2 (Figure 6.4e) and Cuboid2 (Figure 6.4g)) preferentially oriented with their longest dimensions horizontal. Such orientations inevitably affect their discharge from the hopper. The screenshots of the packings of three types of particles (i.e. Ellipsoid3, Cylinder3 and Cuboid3) with $c/a > 4$ at the time step of 0 (i.e., right before the discharge) at the mid-height (i.e., 97 - 377 mm) of the hopper close to the wall are further shown in Figure A6.2, which have the similar preferential orientations to Ellipsoid1 and Cylinder1.

$$n_1 = 10, n_2 = 2$$

(d)

(e)

$$n_1 = n_2 = 10$$

(f)

(g)

Figure 6.4. Screenshots of the packing of the single type of particles: (a) Sphere, (b) Ellipsoid1, (c) Ellipsoid2, (d) Cylinder1, (e) Cylinder2, (f) Cuboid1, and (g) Cuboid2 at the time step of 0 (i.e., right before discharge) at mid-height (i.e., 97 - 377 mm) of the hopper close to the wall.

Although preferential orientations of the various shapes are shown close to the wall, the particles' orientations in the whole hopper are not presented the consistent results. Figure 6.5 shows the order parameter for the whole hopper of the monodisperse systems with respect to the aspect ratio (c/a). The order parameter S , which quantifies the uniformity of alignment, is calculated by diagonalizing of the symmetric traceless order tensor $\mathbf{Q}$ to get the largest eigenvalue [184, 185].

$$Q_{ij} = \frac{3}{2N} \sum_{n=1}^N \left[\ell_i^n \ell_j^n - \frac{1}{3} \delta_{ij} \right] \quad (6-8)$$

where N is the total particle number, ℓ^n is the unit vector along the major axis of the non-spherical particle n , and δ_{ij} is the Kronecker delta function. The higher the S value is, the greater the similarity in the orientations of the particles is. In Figure 6.5, the S values are nearly zero when the aspect ratio (c/a) is close to 1, indicating that the particles' alignment is less uniform for aspect ratio (c/a) close to 1, which agrees with the relationship between the order parameter and aspect ratio in previous studies [186, 187].

Figure 6.5. Order parameter S of different types of monodisperse particles versus the aspect ratio (c/a).

Since the packing of the particles likely affects hopper discharge, the solid volume fractions of the different types of monodisperse particles are plotted against aspect ratio (c/a) in Figure 6.6. Three observations are worth noting for the aspect ratio (c/a) smaller than 2. Firstly, the solid volume fraction generally increases as the aspect ratio increases, indicating that the more disk-like particles with smaller aspect ratios exhibit looser packing. Secondly, the two species of

cuboids exhibit the least and greatest solid volume fractions, suggesting that the packing of some shapes is more sensitive to changes in aspect ratios. The highest solid volume fraction of the cuboid agrees with an earlier work [66], which attributes it to the increased contact points. Thirdly, although both the Sphere and Cuboid1 have the same aspect ratio of 1, the solid volume fraction is greater for the latter, which indicates that particle shape has a non-negligible influence on the packing. This agrees with an earlier study, which also concluded that the maximum packing ratio is different for different particle shapes [188]. Additionally, it shows much looser packing for the monodisperse particles with the aspect ratio (c/a) greater than 4.

Figure 6.6. Solid volume fraction of different types of monodisperse particles versus aspect ratio (c/a).

Regarding hopper discharge, Figure 6.7a displays the mass discharged from the hoppers of monodisperse particles with time, while Figure 6.7b further displays the discharge rate with respect to aspect ratio. Clearly, for the monodisperse systems, particle shape is the dominant factor dictating discharge rate, relative to aspect ratio (Figure 6.7b), orientation (Figure 6.4) and packing (Figure 6.6).

Firstly, the hopper discharge is the fastest for the sphere, followed by ellipsoids, then cylinders and finally cuboids. The poor flowability of cuboids has been linked to the larger contact surfaces [66, 78]. The results are consistent with previous studies that also indicate the better flowability of spheres relative to other shapes [14, 57, 66]. Wang et al. [66] indicated that the discharge rate decreases with aspect ratio, whereas the effect of aspect ratio on discharge rate seems negligible compared to the effect of particle shape in this study; this is presumably linked to the particle volume increasing with aspect ratio in the former, whereas the particle volume is kept constant here. Secondly, the fluctuations of the discharge rate are smaller for the sphere and ellipsoids, while greater for cylinders and cuboids, which has been tied to the increased collision due to the increased angularities of the particles [14, 57, 183]. The mass discharged from the hoppers with time of three types of monodisperse particles (i.e. Ellipsoid3, Cylinder3 and Cuboid3) with $c/a > 4$ are further shown in Figure A6.3. Nevertheless, jamming or arching is generated, because the elongated particles are larger than one-fifth of the hopper orifice diameter [121]. The results in Figure 6.7b show that the discharge rate of the monodisperse particles with various particle shapes in the simulation agree well with the predictions of the Beverloo correlation.

Figure 6.7. (a) Mass discharged from the hopper of the monodisperse particles with time and (b) comparison of the discharge rate between the simulation and Beverloo correlation versus the aspect ratio (c/a).

Figure 6.8 illustrates the velocity vectors at the bed heights of 470 mm, 350 mm and 200 mm for the systems with different particle shapes. Three typical regions, i.e., plug flow region, transition region and converging flow region are shown from the top of the hopper to the bottom. The velocity in the plug flow zone is smaller and more uniform than that in the converging flow zone. Only for the Sphere in Figure 6.8g, the trajectories of the particles are mainly downwards exclude near the wall in the plug flow zone, while the particles vectors are towards the center of orifice with larger velocities in the converging flow zone, which is consistent with the study by Zhu and Yu [189]. As the particle bed height decreases, the plug flow zone reduces. Notably, the chaotic particle trajectories regarding the effect of particle shape in the non-spherical particle systems in Figure 6.8a-f likely slows the discharge [183].

Figure 6.8. Instantaneous velocity vectors at the particle bed heights of 470 mm, 350 mm and 200 mm for the systems with different shape particles: (a) Ellipsoid1, (b) Ellipsoid2, (c) Cylinder1, (d) Cylinder2, (e) Cuboid1, (f) Cuboid2 and (g) Sphere.

Upon inspection of the hoppers after discharge, it was found that some hoppers are not fully emptied. Specifically, whereas the hoppers containing monodisperse Sphere, Ellipsoid1, Ellipsoid2 and Cylinder1 are discharged fully, residual particles are observed for the hoppers containing the monodisperse particles with the lower sphericity values (Table 6.1), namely, Cylinder2, Cuboid1 and Cuboid2. Figures 6.9a - c show that, in particular for the Cylinder2 and Cuboid2 particles (which have the lowest aspect ratios among the particles (Table 6.1)), the residual particles seem to be oriented with the largest faces approximately horizontal, indicating that such an orientation impedes flow, as also evident in the slower discharge rates (Figure 6.7a). It is clear that the hopper with Cuboid2 (Figure 6.9c), which has the smallest aspect ratio (Table 6.1), has the largest number of particles that remain stuck in the hopper. Figure 6.9d further illustrates the number of monodisperse particles left in the hopper versus aspect ratio, demonstrating that (i) the cuboids exhibit much greater variability than the cylinder; and (ii) the number of particles left in the hopper are similar for both Cylinder2 and Cuboid1, despite the different aspect ratios, which indicate the shape effect is more important than the aspect ratio as defined.

Figure 6.9. Screenshots of monodisperse particles left in the hopper with (a) Cylinder2, (b) Cuboid1, and (c) Cuboid2. (d) Number of monodisperse particles left in the hopper versus aspect ratio (c/a).

6.3.3. Binary-size mixtures

Figures 6.10a - c display the screenshots of the different packings of binary-size mixtures (i.e., the two constituents are of the same shape and volume, but have different aspect ratios) at the time step of 0 (i.e., right before discharge) at mid-height (i.e., 97 - 377 mm) of the hopper close to the wall. Similar to the monodisperse systems in Figure 6.4, the constituents with larger aspect ratios (namely, Ellipsoid1 and Cylinder1) tend to orientate with the longest dimensions

oriented vertically, while those with smaller aspect ratios (namely, Cylinder2 and Cuboid2) horizontally. Figure 6.10d shows the solid volume fractions of the binary-size mixtures versus mean aspect ratio ($\overline{c/a}$). Similar to the monodisperse systems (Figure 6.6), the solid volume fraction increases as the mean aspect ratio ($\overline{c/a}$) increases and the fluctuation is the greatest for the cuboids. An earlier experimental study on binary-size spherical particles indicated that the solid volume fraction increased as the size ratio increased [190], which is not the case here, thereby highlighting the importance of shape effects

Figure 6.10. Screenshots of the packing of the binary-size mixtures of (a) Ellipsoid1 + Ellipsoid2, (b) Cylinder1 + Cylinder2, and (c) Cuboid1 + Cuboid2 at the time step of 0 (i.e., right before discharge) at the mid-height (97 - 377 mm) of the hopper close to the wall. The constituent with the larger aspect ratio (c/a) is colored yellow while the other blue. (d) Solid volume fraction versus mean aspect ratio ($\overline{c/a}$).

Figure 6.11 shows the impact of mean aspect ratio ($\overline{c/a}$) of binary-size mixtures on the order parameter S in the whole hopper. The S values in hoppers with Ellipsoid1 + Ellipsoid2, Cylinder1 + Cylinder2, and Cuboid1 + Cuboid2 are in between of the values of the two constituents in a hopper, demonstrating the S value is influenced by the mixture of different particle sizes. Consistent with the results of the monodisperse particles, the S value is close to 0 when the mean aspect ratio ($\overline{c/a}$) is around 1.

Figure 6.11. Order parameter S of the binary-size mixtures of Ellipsoid1 + Ellipsoid2, Cylinder1 + Cylinder2, and Cuboid1 + Cuboid2 versus the mean aspect ratio ($\overline{c/a}$).

Figure 6.12 shows the mass discharged with respect to time from the hopper and the discharge rate versus mean aspect ratio ($\overline{c/a}$) for the three binary-size mixtures. The discharge rate in the hopper with the binary-size mixtures of Ellipsoid1 + Ellipsoid2 is the fastest, followed by Cylinder1 + Cylinder2, and then Cuboid1 + Cuboid2. The relative rates and magnitudes are similar to that of monodisperse particles (Figure 6.7a), indicating similarly the best flowability of ellipsoids and worst of cuboids. Also, the fluctuations are significantly greater for the binary mixture cuboids, which is linked to the greatest fluctuations of monodisperse cuboids (Figure 6.7b). Interestingly, although the solid volume fraction and aspect ratio correlate poorly with discharge rate for the monodisperse systems, the discharge rate increases with solid volume fraction or mean aspect ratio ($\overline{c/a}$) for the binary-size mixtures. The results in Figure 6.12b show that the discharge rates of the binary-size mixtures with various particle shapes in the simulation agree well with the predictions of the Beverloo correlation.

(a)

(b)

Figure 6.12. (a) Mass discharged from the hopper with respect to the time, and (b) the comparison of the discharge rate between the simulation and Beverloo

correlation versus the mean aspect ratio ($\overline{c/a}$) for binary-size mixtures of Ellipsoid1 + Ellipsoid2, Cylinder1 + Cylinder2, and Cuboid1 + Cuboid2.

Figure 6.13 illustrates the velocity vectors at the bed heights of 470 mm, 350 mm and 200 mm for systems of binary-size mixtures. The velocity distribution is consistent with the results for non-spherical monodisperse particles, which the magnitudes of velocities are smaller and more uniform in the plug flow zone than the converging flow zone and the particle trajectories are chaotic in these systems of binary-size mixtures.

Figure 6.13. Instantaneous velocity vectors at the particle bed heights of 470 mm, 350 mm and 200 mm for systems of binary-size mixtures: (a) Ellipsoid1 + Ellipsoid2, (b) Cylinder1 + Cylinder2, and (c) Cuboid1 + Cuboid2.

Analogous to Figures 6.9a – c for the monodisperse systems, Figures 6.14a - b display the screenshots of residual particles of binary-size mixtures of Cylinder1 + Cylinder2 and Cuboid1 + Cuboid2 at the end of the hopper discharge. The binary-size mixture of Ellipsoid1 + Ellipsoid2 is fully discharged, which is consistent with that for the monodisperse ellipsoid systems. Similar to Figure 6.9, the residual Cylinder2 and Cuboid2 (which have the lowest aspect ratios among the particles (Table 6.1)) are oriented with the largest faces horizontal, thereby impeding flow and slowing the discharge. Figure 6.14c illustrates the number of particles left in the hoppers. As with the monodisperse systems (Figure 6.9d), the cuboid system exhibits greater fluctuations and has more particles left in the hopper.

(a)

(b)

(c)

Figure 6.14. Screenshots of particles left in the hopper from the binary-size mixtures of (a) Cylinder1 + Cylinder2 and (b) Cuboid1 + Cuboid2. The constituent with the greater aspect ratio (c/a) is colored yellow while the other green. (c) Number of particles left in the hoppers of the binary-size mixtures versus mean aspect ratio ($\overline{c/a}$).

Since segregation is inevitable for binary mixtures, a closer look at such effects and the corresponding impact on hopper discharge is warranted. Most of the previous studies on binary mixtures are either for constituents with similar shape but different volumes, or different in both the shape and volume, with results indicating that the fraction of the smaller constituents decreases with discharge [62, 64, 66, 124, 190-192]. In this study, the two constituents have similar volumes and shapes, but differ in aspect ratio. The normalized number-based concentration of the constituent with the smaller aspect ratio at each time (t) is calculated by [131]:

$$C_{smaller\ aspect\ ratio,t} = \frac{(N_{smaller\ aspect\ ratio,t}/N_{total,t})}{(N_{smaller\ aspect\ ratio,t=0}/N_{total,t=0})} \quad (6-9)$$

where $N_{smaller\ aspect\ ratio}$ is the number of particles with the smaller aspect ratio, and N_{total} is the total number of all particles. Figure 6.15 presents $C_{smaller\ aspect\ ratio}$ with respect to the percentage discharge of the binary-size mixtures from the hopper. Initially (within the first 20% of hopper discharge), the $C_{smaller\ aspect\ ratio}$ values of all three binary-size mixtures remain at approximately 1, implying equal discharge of both constituents. As the discharge progresses, the $C_{smaller\ aspect\ ratio}$ values of the three binary mixtures diverges, indicating that the segregation behavior differs. Specifically, (i) the

$C_{smaller\ aspect\ ratio}$ value of the Cuboid1 + Cuboid2 mixture increases with discharge, reflecting the preferential discharge of Cuboid1 (i.e., the constituent with the larger aspect ratio), which agrees with the highest number of residual Cuboid2 (Figure 6.9d); (ii) the $C_{smaller\ aspect\ ratio}$ value of the Cylinder1 + Cylinder2 mixture decreases with discharge, reflecting the preferential discharge of Cylinder2 (i.e., the constituent with the smaller aspect ratio) before Cylinder2 becomes predominantly the residual particles at the end of the discharge (Figure 6.14b); and (iii) as for the mixture of Ellipsoid1 and Ellipsoid2, the $C_{smaller\ aspect\ ratio}$ value remains closest to 1 throughout the discharge, reflecting the least segregation extent among the three mixtures and may be tied to the highest discharge rate.

Figure 6.15. Normalized number-based concentration of the constituent with the smaller aspect ratio ($C_{smaller\ aspect\ ratio}$) with respect to percentage discharge for the binary-size mixtures of Ellipsoid1 + Ellipsoid2, Cylinder1 + Cylinder2, and Cuboid1 + Cuboid2.

6.3.4. Binary-shape mixtures

A closer look at the effect of the lesser studied binary-shape mixtures on hopper discharge is attempted here. Figure 6.16 shows the screenshots of the different packings of binary-shape mixtures at the time step of 0 (i.e., right before discharge) at the mid-height (97 - 377 mm) of the hopper close to the wall. Similar to Figures 6.10a – c, preferential orientations of the different particle shapes persist in the binary-shape mixtures.

Figure 6.16. Screenshots of the packing of the binary-shape mixtures of (a) Ellipsoid1 + Cylinder1, (b) Ellipsoid1 + Cylinder2, (c) Ellipsoid2 + Cylinder1, (d) Ellipsoid2 + Cylinder2, (e) Ellipsoid1 + Cuboid1, (f) Ellipsoid1 + Cuboid2, (g) Ellipsoid2 + Cuboid1, (h) Ellipsoid2 + Cuboid2, (i) Cylinder1 + Cuboid1, (j) Cylinder1 + Cuboid2, (k) Cylinder2 + Cuboid1, and (l) Cylinder2 + Cuboid2 at the time step of 0 (i.e., right before discharge) at the mid-height (97 - 377 mm) of the hopper close to the wall. The constituent with the greater aspect ratio (c/a) is colored yellow while the other green.

Figure 6.17 shows the impact of mean aspect ratio ($\overline{c/a}$) of binary-shape mixtures on the order parameter S in the whole hopper. Consistent with the binary-size mixtures, the S values in hoppers with Ellipsoid + Cylinder, Ellipsoid + Cuboid, and Ellipsoid + Cuboid are in between of the S values of the two constituents in a hopper. Obviously, the S values for the binary-shape mixtures decreases as the mean aspect ratio ($\overline{c/a}$) increases in the range of 0 to 2, demonstrating the S value for binary-shape mixtures is influenced by the shape and aspect ratio of the constituents in the mixtures.

Figure 6.17. Order parameter S of the binary-shape mixtures of Ellipsoid + Cylinder, Ellipsoid + Cuboid, and Cylinder + Cuboid versus the mean aspect ratio ($\overline{c/a}$).

Figure 6.18 illustrates the solid volume fraction of the various binary-shape mixtures with respect to mean aspect ratio ($\overline{c/a}$). As opposed to Figures 6.6 (monodisperse) and 10d (binary-size), the relationship between solid volume fraction and mean aspect ratio ($\overline{c/a}$) is not strictly positive, which is tied to the inter-particle contact of particles of different shapes. This highlights the importance of shape effects in hopper discharge that needs to be accounted for in the development of correlations and models.

Figure 6.18. Solid volume fraction versus mean aspect ratio ($\overline{c/a}$) for the binary-shape mixtures of Ellipsoid + Cylinder, Ellipsoid + Cuboid, and Cylinder + Cuboid.

Figures 6.19a - c display the mass discharged from the hopper with respect to time for the different binary-shape mixtures. As opposed to Figures 6.7a and 6.12a, the difference in the discharge rates among the different binary-shape systems are more insignificant, suggesting the drowning out of the particle shape effects on discharge rate by the mixing of the particle shapes. Figure 6.19d further summarizes the discharge rates of the binary-shape mixtures versus mean aspect ratio ($\overline{c/a}$), indicating that (i) the mixtures containing cuboids have larger error bars, which agree with that for the monodisperse (Figure 6.7b) and binary-size mixtures (Figure 6.12b); (ii) the mean aspect ratio ($\overline{c/a}$) has a negligible effect on discharge rate, which contradicts the trends for binary-size mixtures whereby the discharge rate increases with aspect ratio (Figure 6.12b); and (iii) all the binary-shape mixtures have similar discharge rates, which also is contrary to that for binary-size mixtures whereby different shapes give distinctly different discharge rates (Figure 6.12b). In summary, the similar discharge rates of the binary-shape mixtures are poorly correlated with solid volume fraction or aspect ratio. These underscore the different behaviors of different types of binary mixtures. Fitting the average values of $k = 1.9, 2.1, 2.3$ of the different shape particles for Ellipsoid + Cylinder, Ellipsoid + Cuboid and Cylinder + Cuboid, respectively, the results in Figure 6.19d show that the discharge rates of the

binary-shape mixtures with various particle shapes in the simulation agree well with the predictions of the Beverloo correlation.

Figure 6.19. Mass discharged from the hopper with time for the binary-shape mixtures of (a) Ellipsoid + Cylinder, (b) Ellipsoid + Cuboid, and (c) Cylinder + Cuboid. (d) Comparison discharge rate from the hopper between the simulation and Beverloo correlation with mean aspect ratio ($\bar{c}/a$) for the binary-shape mixtures.

Figure 6.20 illustrates the velocity vectors at the bed heights of 470 mm, 350 mm and 200 mm for systems of binary-shape mixtures. The velocity distribution is consistent with the results for monodisperse particles and binary-size mixtures, which demonstrates the velocity directions for non-spherical particles difference are shown always chaotic.

Figure 6.20. Instantaneous velocity vectors at the particle bed heights of 470 mm, 350 mm and 200 mm for systems of binary-shape mixtures: (a) Ellipsoid1 + Cylinder1, (b) Ellipsoid1 + Cylinder2, (c) Ellipsoid2 + Cylinder1, (d) Ellipsoid2 + Cylinder2, (e) Ellipsoid1 + Cuboid1, (f) Ellipsoid1 + Cuboid2, (g) Ellipsoid2 + Cuboid1, (h) Ellipsoid2 + Cuboid2, (i) Cylinder1 + Cuboid1, (j) Cylinder1 + Cuboid2, (k) Cylinder2 + Cuboid1, and (l) Cylinder2 + Cuboid2

Figure 6.21 depicts the residual particles remaining in the hoppers after the discharge of the binary-shape mixtures. For the Ellipsoid + Cylinder mixtures, only Ellipsoid1 + Cylinder2 and Ellipsoid2 + Cylinder2 have particles left in the hopper, which is linked to the incomplete discharge of the monodisperse Cylinder2 (Figure 6.9). Figures 6.21a and b show clearly that Cylinder2 is dominant among the residual particles. For the other two types of binary-shape mixtures, all exhibit incomplete discharge due to the presence of cuboids, since both monodisperse cuboid species do not fully discharge (Figure 6.9). Regarding

the binary Ellipsoid + Cuboid mixtures, the cuboids are the dominant residual species (Figures 6.21c - f). As for the Cylinder + Cuboid mixtures, due to the poorest flowability associated with Cuboid2 (Figure 6.9), the binary-shape mixtures containing Cuboid2 has significant residual particles (Figures 6.21h and j). Figure 6.21k further summarizes the number of residual particles versus mean aspect ratio ($\overline{c/a}$) for all the binary-shape mixtures. Clearly, the relationship between aspect ratio and extent of incomplete hopper discharge is poor, implying the consideration of shape type is necessary.

(a)

(b)

(c)

(d)

(e)

(f)

(g)

(h)

(i)

(j)

(k)

Figure 6.21. Screenshots of residue particles in the hopper with the binary-shape mixtures of (a) Ellipsoid1 + Cylinder2, (b) Ellipsoid2 + Cylinder2, (c) Ellipsoid1 + Cuboid1, (d) Ellipsoid1 + Cuboid2, (e) Ellipsoid2 + Cuboid1, (f) Ellipsoid2 + Cuboid2, (g) Cylinder1 + Cuboid1, (h) Cylinder1 + Cuboid2, (i) Cylinder2 + Cuboid1, and (j) Cylinder2 + Cuboid2. The constituent with the larger aspect ratio (c/a) is colored yellow while the other green. (k) Number of particles left in the hopper of the binary-shape particles versus to mean aspect ratio ($\overline{c/a}$).

To explore the segregation effects of the binary-shape mixtures during hopper discharge, Figure 6.22 plots $C_{smaller\ aspect\ ratio}$ versus percentage discharge, which is analogous to Figure 6.15. Since the discharge rates are similar for all binary-shape mixtures, the different segregation extents have little effect on the discharge rate. Two observations are clear. Firstly, among the three types of binary-shape mixtures, all four mixtures of Cylinder + Cuboid similarly give minimal segregation (Figure 6.22c), while those of Ellipsoid + Cylinder give the most dissimilar segregation extents (Figure 6.22a). Secondly, where Ellipsoid1, which has the largest aspect ratio, is present (Figures 6.22a and b), the $C_{smaller\ aspect\ ratio}$ value increases during discharge, indicating the preferential discharge of Ellipsoid1 that is tied to the vertical orientation.

Figure 6.22. Normalized number-based concentration of the constituent with the smaller aspect ratio ($C_{\text{smaller aspect ratio}}$) with respect to percentage discharge for the binary-shape mixtures of (a) Ellipsoid + Cylinder, (b) Ellipsoid + Cuboid, and (c) Cylinder + Cuboid.

6.4. Conclusion

Studies on the effect of particle shape on hopper flow have been reported, but the effect of binary mixtures of various particle shapes remains poorly understood. Accordingly, this study employed DEM to first study seven monodisperse particles (namely, one sphere, two ellipsoids, two cylinders and two cuboids) of different shapes but similar volume. Three binary-size and twelve binary-shape mixtures, as well as seven monodisperse systems, are investigated. The packing, discharge rate, number of residual particles, and segregation extents are assessed.

The following results are worth highlighting. For the monodisperse systems, particle shape is the dominant factor dictating discharge rate, relative to other factors like aspect ratio, preferential orientation and packing. With regards to the binary-size mixtures, (i) the relative discharge rates and magnitudes are similar to that of monodisperse particles, indicating the dominant effect of particle shape; and (ii) the discharge rate increases with solid volume fraction or mean aspect ratio, which contrasts with that of monodisperse systems whereby solid volume fraction and aspect ratio correlate poorly with discharge rate. As for the binary-shape mixtures, (i) the relationship between solid volume fraction and mean aspect ratio is not strictly positive, which contrasts with that for the monodisperse and binary-size mixtures, and is tied to the inter-particle contact of particles of different shapes; (ii) the discharge rates are very similar for all twelve mixtures, and thus poorly correlated with solid volume fraction, aspect ratio and segregation extent; and (iii) the relationship between mean aspect ratio and extent of incomplete hopper discharge is poor. The results highlight the non-negligible effect of mixtures of particle shapes (in particular, binary-size and binary-shape mixtures investigated here) on hopper discharge, which needs to be accounted for in the development of correlations and models.

Appendix

Table 6.A1. Details of parameters of superquadric particles with similar volumes used in this study.

	Ellipsoid3	Cylinder3	Cuboid3
a (mm)	4	4	6
b (mm)	4	4	6
c (mm)	7.81	5.21	1.82
n_1	2	10	10
n_2	2	2	10
aspect ratio (c/a)	4.63	4.64	4.19
sphericity	0.96	0.87	0.68

Table 6.A2. Number of particles simulated. Each case was simulated three times.

System	Simulation 1	Simulation 2	Simulation 3
Ellipsoid1	23815	23813	23820
Ellipsoid2	23188	23172	23196
Cylinder1	23860	24051	24033
Cylinder2	22469	22747	22751
Cuboid1	23634	24744	24111
Cuboid2	22231	22130	21614
Ellipsoid1 + Ellipsoid2	11617+11617	11629+11629	11619+11619
Cylinder1+ Cylinder2	11514+11515	11654+11653	11644+11644
Cuboid1+ Cuboid2	11909+11909	11381+11382	11164+11164
Ellipsoid1 + Cylinder1	11933+11934	11931+11931	11933+11933
Ellipsoid1 + Cylinder2	11497+11497	11487+11486	11481+11481
Ellipsoid2 + Cylinder1	11748+11749	11772+11772	11771+11770
Ellipsoid2 + Cylinder2	11417+11417	114115+11416	11506+11405
Ellipsoid1 + Cuboid1	12083+12083	12071+12070	12070+12070
Ellipsoid1 + Cuboid2	11310+11310	11320+11320	11311+11311
Ellipsoid2 + Cuboid1	11961+11961	11932+11931	11945+11945
Ellipsoid2 + Cuboid2	11199+11198	11194+11194	11201+11201
Cylinder1 + Cuboid1	12095+12095	12025+12025	12054+12054
Cylinder1 + Cuboid2	11223+11224	11296+11295	11245+11246
Cylinder2 + Cuboid1	11681+11682	11692+11692	11624+11623
Cylinder2 + Cuboid2	11437+11437	11276+11277	11275+11275

Figure 6.A1. Comparison discharge rate from hopper between all cases studied.

$$n_1 = n_2 = 2$$

$$n_1 = 10, n_2 = 2$$

$$n_1 = n_2 = 10$$

(a)

(b)

(c)

Figure 6.A2. Three-dimensional superquadric particles investigated: (a) Ellipsoid3, (b) Cylinder3, and (c) Cuboid3.

$$n_1 = n_2 = 2$$

$$n_1 = 10, n_2 = 2$$

$$n_1 = n_2 = 10$$

(a)

(b)

(c)

Figure 6.A3. Screenshots of the packing of the single type of particles: (a) Ellipsoid3, (b) Cylinder3, (c) Cuboid3 at the time step of 0 (i.e., right before discharge) at mid-height (i.e., 97 - 377 mm) of the hopper close to the wall.

Figure 6.A4. Mass discharged from the hopper of the monodisperse particles of Ellipsoid3, Cylinder3, and Cuboid3 with time.

Chapter 7. Effect of lognormal PSDs of non-spherical particles on hopper discharge characteristics

The content of this chapter has been submitted and peer-reviewed under the title of *Effect of Lognormal Particle Size Distributions of Non-Spherical Particles on Hopper Discharge Characteristics* in *Powder Technology*.

Abstract

This study focusses on the hopper discharge characteristics of lognormal particle size distributions (PSDs) of non-spherical particles (namely, ellipsoids, cylinders and cuboids). Discrete element method (DEM) is employed to understand the coupled effects of sphericity and lognormal PSD width. The results reveal that: (i) the ellipsoids with the aspect ratio of 0.9 have the most similar discharge behaviors with the spheres, but the differences increase as the PSD width increases; (ii) the packing density in the hopper increases as PSD width increases and particle sphericity decreases; (iii) regardless of sphericity, the discharge rate decreases and the jamming probability increases as the PSD width increases; (iv) for the same PSD width, the jamming probability is the greatest for cuboids and least for the ellipsoids; and (v) the lower-sphericity cylinder and cuboid have some residual particles left in the hopper upon complete discharge, and the number of residues is greater and increases with PSD width for the latter. The results provide new insights regarding the behavior of wide PSDs of non-

spherical particles in the hopper, highlighting the non-negligible impact of the coupled effect of PSD and particle non-sphericity.

Keywords: discrete element method (DEM); granular flow; superquadric method; non-spherical; lognormal particle size distributions (PSDs)

7.1. Introduction

The storage and discharge of particles require hoppers, which are unsurprisingly standard units in many industries like pharmaceutical, chemical, construction [1, 22, 73]. Although a very simple device, the flow behaviors are complex, with poor flowability and jamming (i.e., stoppage of discharge) being common problems. To develop a better understanding of the particulate flow characteristics in a hopper, extensive experimental [14, 33, 34] and numerical [17, 42, 46, 74] studies have been conducted. The impact of the material and hopper properties [33, 34], pressure imposed [38], particle size distribution [35-37] on the discharge rate, flow pattern and segregation in the hopper have been experimentally studied. However, experiments are limited in for example creating precise particle size distributions in view of the fixed sieve sizes available and unveiling the contact forces among the particles. To circumvent these, the numerical method is an effective complementary tool [1]. In particular, the DEM [40], which tracks every particle, has been widely adopted to investigate dense particulate behaviors. Past DEM studies on granular material have been proven to agree well with experiments [141, 172, 193] and empirical predictions [117, 118, 135]. This study is targeted at employing DEM to understand the

coupled effects of particle non-sphericity and particle size distribution, which are prevalent but remains poorly understood, on hopper discharge behavior.

Particle shape is well-acknowledged to significantly influence the flow dynamics [56]. For the hopper, the flow pattern [12], discharge rate and quality [65, 66], and packing density [67, 68] are all heavily shape dependent. Therefore, many attempts have been made to study the impact of particle shape of monodisperse (i.e., similar sized) particles on hopper discharge [12, 56-64]. Claery and Sawley [12, 69] concluded that the elongated particles have a discharge rate of 30% lower than spherical particles, and increasing the angularity of the particles decreases the flow rates by up to 28%. Langston et al. [65] found that the flow rate of disc-shaped particles is 40% faster than the circular particles in 2D simulations but not 3D simulations, due to the lower resistance to particle alignment in the latter. Fraige et al. [67] demonstrated cubes exhibit denser packing but lower flow properties compared to the spheres. Tao et al. [194] compared the corn-shaped and spherical particles, and showed the velocity and voidage of the former are respectively larger and smaller than the latter. Other than monodisperse systems, particle shape also shows a significant influence in binary mixtures (i.e., two different particle types). Wang et al. [71] found that the more angular particles show a greater resistance to discharge, resulting in reduced flowability is reduced, with the mixture of less angular and more angular particles demonstrating an approximately linear combination of effects. Wang et al. [66] investigated the binary mixtures of spheres and cylinders, spheres and cubes, and cylinders and cubes, and revealed the flow rate decreases as the quantity of particles with sharp planes or vertices increases. Yu et al. [70] assessed that both the binary mixtures

of spherical and non-spherical particles can be described by the Westman equation, which describes the relationship between particle properties and volume fractions of binary mixtures. Yu and Saxén [63] elucidated that size segregation is affected slightly by particle shape, but the complexity of the particle shape in the mixtures has an effect on the continuity of the flow. For the polydisperse system, Govender et al. [72] numerically investigated polydisperse polyhedral particles and found the discharge time of polydisperse particles is between that of the smaller and larger sizes. Collectively, past studies have given some insights into the effect of shape factor on hopper discharge behavior. However, the influence of the width of the lognormal particle size distribution (PSD), which is ubiquitous, of non-spherical particles on flow behaviors is not yet understood.

Therefore, in this study, we performed DEM simulations to evaluate the effect of the width of lognormal PSDs of non-spherical particles (namely, ellipsoids, cylinders and cuboids) on hopper discharge. The packing, discharge rate, jamming, size-segregation during the discharge, force network before the discharge, and residues after the discharge are systematically studied.

7.2. Material and method

7.2.1. Representation of a superquadric particle

Each non-spherical particle is described by the superquadric formula [170]:

$$f(x, y, z) = \left(\left| \frac{x}{a} \right|^{n_2} + \left| \frac{y}{b} \right|^{n_2} \right)^{\frac{n_1}{n_2}} + \left| \frac{z}{c} \right|^{n_1} - 1 = 0 \quad (7-1)$$

where a, b and c stand for the half-length of the superquadric particles along the respective principal axes; and n_1 and n_2 are the blockiness parameters that govern the edge sharpness. Many types of non-spherical particles can be modeled by modifying these five parameters [170]. For example, ellipsoids are obtained when $n_1 = n_2 = 2$, cylinders are obtained when $n_1 \gg 2$ and $n_2 = 2$, and cuboids are obtained when $n_1 = n_2 \gg 2$. The global coordinates are used for tracking the position of the particles while the local ones to model the rotational motion of the irregular particles. The exchange between the two coordinates is achieved by a transformation constructed from quaternions, which quantify the orientation of the non-spherical particles and thus the instantaneous direction of a specific particle can be evaluated [66, 173, 175].

Figure 7.1 displays the three-dimensional particles (namely, sphere, ellipsoid, cylinder and cuboid), while Table 7.1 lists the numerical parameters used to describe the particles. Note that the sphere has been studied previously [195], and is used for comparison against the non-spherical particles here. Each non-spherical particle has the same particle density (ρ_p) of 2460 kg/m^3 and aspect ratio of 0.9, which is the ratio of c to a (i.e., the ratio of the z -axis dimension to the x -axis dimension). The particle sphericity (ϕ) is defined as the ratio of the surface area of a sphere with the same volume as the particle (A_s) to the actual surface area of the particle (A_p) [171]:

$$\phi = \frac{A_s}{A_p} = \frac{\pi^{\frac{1}{3}}(6V_p)^{\frac{2}{3}}}{A_p} \quad (7-2)$$

where V_p is volume of the particle and A_p is the surface area of the particle. The sphericities of the particles investigated are listed in Table 7.1.

Figure 7.1. Three-dimensional superquadric particles studied: (a) sphere, (b) ellipsoid, (c) cylinder, and (d) cuboid.

Table 7.1. Numerical parameters used to describe the mean-sized superquadric particles of the lognormal PSDs.

Particle type	n_1 (-)	n_2 (-)	a (mm)	b (mm)	c (mm)	ϕ (-)
Sphere	2	2	5	5	5	1.000
Ellipsoid	2	2	5.179	5.179	4.661	0.998
Cylinder	10	2	4.524	4.524	4.072	0.873
Cuboid	10	10	4.174	4.174	3.757	0.805

7.2.2. Governing equations for particle motion

The particle systems are assumed to be composed a set of discrete, non-spherical, non-cohesive, frictional particles, which are tracked individually. The flow behavior of each particle in the system is described by the DEM, which was initiated by Cundall and Strack [40]. Following Newton's second law, the translational and rotational motion of each non-spherical particle are formulated as:

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^K (\mathbf{M}_{n,ij} + \mathbf{M}_{t,ij} + \mathbf{M}_{r,ij}) \quad (7-3)$$

$$m_i \frac{d\mathbf{V}_i}{dt} = \sum_{j=1}^K (\mathbf{F}_{cn,ij} + \mathbf{F}_{ct,ij}) + m_i \mathbf{g} \quad (7-4)$$

where, $\mathbf{F}_{c,ij}^n = k_{n,ij} \delta_{n,ij} \mathbf{n} + \gamma_{n,ij} \mathbf{v}_{n,ij}$ (7-5)

$$\mathbf{F}_{c,ij}^t = \min\{(k_{t,ij} \delta_{t,ij} \mathbf{t} + \gamma_{t,ij} \mathbf{v}_{t,ij}), \mu \mathbf{F}_{cn,ij}\}, \quad (7-6)$$

in which the subscript i and j stand for particles i and j , m is the mass of the particle, I is moment of inertia, $\mathbf{V}$ is translational velocity, $\boldsymbol{\omega}$ is angular velocity, $\mathbf{F}_{cn,ij}$ and $\mathbf{F}_{ct,ij}$ are collision forces along the normal and tangential directions, $\mathbf{M}_{t,ij}$ and $\mathbf{M}_{r,ij}$ are respectively the torque generated by tangential forces and rolling friction within particles i and j , $\mathbf{M}_{r,ij}$ is the torque generated by rolling friction, K is the number of contacts of the particle i with walls and the particles neighbored, g is the gravitational acceleration, $\mathbf{n}$ and $\mathbf{t}$ are respectively the unit vectors along the normal and tangential directions of a colliding pair. Moreover, k and γ are stiffness and damping coefficients can be calculated on the basis of the material properties and overlap distance as shown in Table 7.2. Specifically, when calculating the equivalent R^* , the radius of each particle is evaluated based on the curvature of the contacting point of this particle. The friction coefficient μ is adopted to limit the friction force when sliding occurs between the colliding pair. The particle in this study is considered as elastic and frictional particle, and the interactions between the particles are defined by algorithms of classical contact mechanics, in which the Hertz theory evaluates the inter-particle normal and tangential forces. [119, 120]. The simulation in this study is conducted by LIGGGHTS 3.8.0 and the post processing is achieved by ParaView 5.4.1.

Table 7.2. Equations adopted to calculate the stiffness and damping coefficients of the particles. [172]

Normal stiffness coefficient ($k_{n,ij}$)	$k_{n,ij} = \frac{4}{3} Y^* \sqrt{R^* \delta_{n,ij}}$
Tangential stiffness coefficient ($k_{t,ij}$)	$k_{t,ij} = 8 G^* \sqrt{R^* \delta_{n,ij}}$
Normal damping coefficient ($\gamma_{n,ij}$)	$\gamma_{n,ij} = 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_{n,ij} m^*}$
Tangential damping coefficient ($\gamma_{t,ij}$)	$\gamma_{t,ij} = 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_{t,ij} m^*}$
Where the related variables are evaluated as	
$\beta = \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}}, S_{n,ij} = 2Y^* \sqrt{R^* \delta_{n,ij}}, S_{t,ij} = 8G^* \sqrt{R^* \delta_{n,ij}}, \frac{1}{Y^*} = \frac{(1-\nu_1^2)}{Y_1} + \frac{(1-\nu_2^2)}{Y_2}, \frac{1}{R^*} = \frac{1}{R_1} + \frac{1}{R_2}, \frac{1}{m^*} = \frac{1}{m_1} + \frac{1}{m_2}, \frac{1}{G^*} = \frac{2(2+\nu_1)(1-\nu_1)}{Y_1} - \frac{2(2+\nu_2)(1-\nu_2)}{Y_2}$	

in which, $1/Y^* = (1 - \nu_1^2)/Y_1 + (1 - \nu_2^2)/Y_2$, $1/r^* = 1/r_1 + 1/r_2$, $\beta = \ln(e)/\sqrt{\ln^2(e) + \pi^2}$, $S_n = 2Y^* \sqrt{r^* \delta_n}$, $1/G^* = 2(2 + \nu_1)(1 - \nu_1)/Y_1 - 2(2 + \nu_2)(1 - \nu_2)/Y_2$, $S_t = 8G^* \sqrt{r^* \delta_n}$. Y is Young's modulus, ν is Poisson's ratio, G is shear modulus and r is particle radius.

7.2.3. Particle size distribution (PSD)

The PSD investigated in this study is the lognormal type, which is common in nature and industry. The number-based frequency distribution (f_n) is expressed as follows:

$$f_n = \frac{1}{x\sigma\sqrt{2\pi}} \exp \left[-\frac{(\ln(x) - \mu)^2}{2\sigma^2} \right] \quad (7-7)$$

where x is the equivalent spherical diameter, which is defined as the diameter of a sphere has the same volume as the given non-spherical particle [196], σ is the standard deviation and μ is the mean diameter of the entire particles. The mean particle diameter (μ) studied is constant at 10 mm, which is that used in the experiments for mono-sized particles conducted by Li et al. [41] and our previous numerical study [195]. The width of the PSDs, which is the ratio of the standard deviation divided by the mean particle diameter (σ/μ), ranges from 10% to 50%. The lower bound is such for distinction from monodisperse particles and the upper bound is so to prevent jamming by the largest particles (since particles more than half that of the orifice diameter are known to jam the hopper [90]).

Figure 7.2 shows the frequency of number-based lognormal PSDs against widths (σ/μ) between 10% and 50% studied.

Figure 7.2. Number-based lognormal PSDs with constant mean particle diameter ($\mu = 10$ mm) and various PSD widths ($10\% \leq \sigma/\mu \leq 50\%$) studied.

7.2.4. Simulation setup

Figure 7.3 illustrates the geometry of the hopper used in this study, which is identical to the conical hopper used in the experiment by Li et al. [41]. The hopper's is 500 mm, with a diameter of 240 mm. The cone height is 51.96 mm and the angle between the cone and the vertical wall is 60° . The diameter of the orifice is 60 mm. The other relevant numerical parameters are shown in Table 7.3. The particles are initially randomly generated under gravity in the hopper before the hopper discharge happens with a sealed orifice to a packed bed height of 474 mm, and then, the particles are flowed out from the hopper under gravity by removing opening up the orifice.

Figure 7.3. Schematic of the hopper studied.

Table 7.3. Physical and numerical parameters used in this study.

Parameter	Value
Initial packed bed height, H (m)	0.474
Poisson ratio, ν (-)	0.25
Young's modulus, Y (GPa)	0.1
Particle-wall and particle-particle static friction coefficient (-)	0.6, 0.6
Particle-wall and particle-particle rolling friction coefficient (-)	0.05, 0.01
Particle-wall and particle-particle restitution coefficient (-)	0.99, 0.99
PSD width, σ/μ (-)	10% - 50%
Time step, Δt (s)	5×10^{-5}

7.2.5. Model validation

The model used has been developed in our previous work for spherical particles in a hopper [101] and validated against experimental results [41] with respect to the particle bed heights at various discharge times and trajectories of the tracked particles [101]. This study further validates the model for non-spherical particles represented by the superquadric equations with experiments carried out by Kodam et al. [180] shown in Figure 7.4. In the experiment, 250 cylindrical particles (each with a diameter and length of 8 mm and 5.3 mm, respectively) were randomly packed in a cylindrical container with an inner diameter of 50.6 mm and height of 130 mm. The simulated bed height of 53.9 mm and volume fraction of 0.615 agree well with the corresponding experimental data of 53.3 mm and 0.621 [180]. This provides validation of model for simulating superquadric particles.

Figure 7.4. Comparison of the cylindrical particles bed packed by (a) simulation and (b) experiment [180].

7.3. Results and discussion

7.3.1. Packing

The solid volume fractions of the four different types of lognormal PSD particles are plotted against PSD width in Figure 7.5. The results for spheres are from an earlier study [195]. Three observations are worth noting. Firstly, among the particle types, the cuboids have the greatest solid volume fractions, while the spheres and ellipsoids have the least solid volume fractions. This suggests that particle shape exerts a non-negligible effect on particle packing, which in turn affects hopper discharge, and agrees with previous reports that cuboids exhibit the densest packings and that cylinders have denser packing than spheres with the same aspect ratio [66]. Secondly, different from the spherical particles of the solid volume fractions increasing with the increase of the PSD width, the packing of non-spherical particles keeps a comparably constant value for narrower PSDs (i.e. $\sigma/\mu \leq 20\%$). Then, the broader PSDs (i.e. $\sigma/\mu \geq 30\%$) exhibit denser packing due to the percolation effect, whereby the smaller particles occupy the interstices of the larger particles. This indicates the important coupled effect of particle shape and PSD width on packing and correspondingly hopper behaviors. Thirdly, the spheres and ellipsoids have the same solid volume fractions for monodisperse systems, but differ for wider PSDs, with the spheres exhibiting higher solid volume fractions at smaller σ/μ values (i.e., 10% and 20%) and the ellipsoids exhibiting higher solid volume fractions at larger σ/μ values (i.e., 30% and greater). This substantiates the important effect of both particle shape and PSD width on particle packing.

Figure 7.5. Solid volume fraction of four different types of particles with respect to PSD width (σ/μ).

7.3.2. Discharge rate

Figure 7.6 illustrates the mass discharged with time for various lognormal PSDs of spheres, ellipsoids, cylinders and cuboids with the same mean particle diameter of $\mu = 10$ mm. Similar to the earlier study [101], Figure 7.6 indicates that (i) the slopes of the trends are almost consistent, indicating the discharge rates are approximately constant during the discharge; (ii) the discharge rate reduces when the PSD width increases, which may be tied to the denser packing (Figure 7.5); and (iii) jamming occurs for wider PSDs. Three observations related to particle shapes are noteworthy. Firstly, the least constant discharge rates are exhibited by the cuboids, as reflected in the slight fluctuations of the slopes, which is consistent with the results for the monodisperse and binary mixture systems in our previous study [197]. Secondly, among the different particle shapes, jamming occurs at the narrowest PSD width for the cuboid at $\sigma/\mu = 20\%$, compared to that at 30% for the spheres, ellipsoids and cylinders. Thirdly, the

jamming behaviors differ among the particle shapes. For the sphere and ellipsoid, when jamming occurs, no discharge occurs at all. On the other hand, for the cylinder and ellipsoid, no discharge at all occurs for the widest PSDs ($\sigma/\mu \geq 40\%$) while some discharge occurs for the narrower PSDs.

Figure 7.6. Mass discharge versus time for different particle shapes: (a) sphere [195], (b) ellipsoid, (c) cylinder, and (d) cuboid.

To further evaluate the impact of lognormal PSD and particle shape on hopper discharge, Figure 7.7 presents the average discharge rates (i.e., averaged over the period before jamming occurs) versus PSD width for the four particle shapes.

The spheres and cuboids exhibit the greatest and least discharge rates, respectively, which agrees with our previous study [197].

Figure 7.7. Average hopper discharge rates of four different particle shape systems versus PSD width (σ/μ).

7.3.3. Particle velocity

Figure 7.8 presents the individual particle velocity vectors at the discharge beginning of bed heights of 474 mm for the systems with different particle shapes. The individual particle trajectories are shown by the distributions of the magnitude and the direction of the individual particle vectors. Obviously, at the beginning of discharge, the more chaotic particle trajectories happen to broader PSDs (i.e. $\sigma/\mu > 30\%$) which occurs jamming during the discharge. Notably, the chaotic particle trajectories likely not only slows the discharge [183] but also stops the discharge. The typical regions including plug flow region, transition region and converging flow region [189] are shown from the top of the hopper to the bottom for the narrower PSDs of $\sigma/\mu < 30\%$. In addition, the converging

flow zones in the narrower PSD systems for spheres and ellipsoids are more concentrated than the cylinders and cuboids.

Figure 7.8. Instantaneous velocity vectors at the discharge beginning i.e. the bed heights of 474 mm for the systems with different shape particles: (a) spheres, (b) ellipsoids, (c) cylinders, and (d) cuboids.

7.3.4. Jamming

Figure 7.6 has indicated that jamming occurs at different PSD widths for different particle shapes, which can be tied to the different packing of the particles of different shapes and PSDs seen in Figure 7.5 [195]. To better understand the transition from complete discharge to jammed hoppers, Figure 7.9 plots the jamming probability for five runs versus PSD width for the different particle shapes. The jamming probability trends for the spheres and ellipsoids are superimposed, indicating the slight change in shape has negligible impact on jamming probability, despite some differences in packing (Figure 7.5) and discharge trends (Figures 6 and 7). Similar to the spheres, the ellipsoids do not jam for smaller PSD widths of $\sigma/\mu \leq 20\%$, has a 20% chance of jamming for the PSD width of $\sigma/\mu = 30\%$, and a 100% chance of jamming for wider PSD widths of $\sigma/\mu \geq 40\%$. For the cylinders and cuboids, the jamming probability curves are shifted leftwards, reflecting greater jamming tendencies at lower PSD widths.

Figure 7.9. Jamming probability versus lognormal PSD width (σ/μ) for four different particle shapes. The solid line is fitted by B-Spline.

7.3.5. Segregation

Figure 7.10 displays the relative mean particle diameter in the hopper versus time for the various particle shapes and PSD widths. Specifically, the relative mean particle diameter is defined as the value of the mean particle diameter of the particles inside the hopper at each time instant divided by the mean particle diameter before discharge [101]. For the monodisperse and completely jammed systems, the relative mean particle diameter remains constant at 1 with time, because the particle sizes in the hopper remain exactly the same. On the other hand, for all other systems, the relative mean particle diameter changes during the discharge. In the initial part of hopper discharge, the relative mean particle diameter remains constant, indicating negligible size-segregation effects, which agrees with a previous study that indicated size segregation is only slightly affected by particle shape [63]. Then, towards the end of the discharge, the relative mean particle diameter decreases with time due to size-segregation effects, indicating the preferential discharge of the larger particles. This agrees with previous studies [101]. The slight exceeding of the value of 1 for the case of the intermediate lognormal PSD width (i.e. $\sigma/\mu = 30\%$) of the ellipsoids is similar to that for spheres [101]. Interestingly, the final relative mean particle diameters of the jammed hoppers are smaller than 1, implying the smaller particles are the ones stuck in the hopper.

Figure 7.10. Relative mean particle diameter regarding to time for three non-spherical particle systems: (a) ellipsoids, (b) cylinders, and (c) cuboids.

7.3.6. Force networks

The force network is an important characteristic of granular systems [189]. Figure 7.11 shows the normal contact forces throughout the filled hopper before discharge for the three non-spherical particle systems. The interesting observations about the force network are that (i) the forces are higher at the lower part of the hopper, which agrees with our previous study on spherical particles [183]; (ii) the forces increase with PSD width, which underlies the lower discharge rate and also jamming for wider PSDs, because of the associated restriction to movement between particles [198] due to denser packing; (iii)

noting that jamming has been reported to occur above a certain threshold force [199], it appears that the threshold differs for different particle shapes; and (iv) the forces are lower for the cuboids, despite the lowest discharge rates and highest jamming tendencies, which contradicts observation (ii). The latter two observations underscore the importance of considering shape effects.

Figure 7.11. Force networks at the initial of discharge of three non-spherical particle systems (a) ellipsoids, (b) cylinders and (c) cuboids of the monodisperse and PSD width (σ/μ) of 10% - 50%.

7.3.7. Residue

Even in the absence of clear jamming for the monodisperse and narrow PSD systems, some hoppers do not fully empty. Specifically, residual particles are observed for the hoppers containing the cylinders and cuboids, while the hoppers with the spheres and ellipsoids are discharged fully. This agrees with our previous study on monodisperse and binary mixture systems [197], and indicates increased difficulty in discharging angular particles. Figure 7.12 displays the residual particles of the cylinders and cuboids for the monodisperse and narrower PSD ($\sigma/\mu = 10\%$ and 20%) systems. Clearly, the hoppers with cuboids (Figures 12d-f) have more residues than those with cylinders (Figures 12a-c). Figure 7.13 quantifies the number of particles left in the hopper versus PSD width (σ/μ), demonstrating that (i) the cuboids consistently exhibit more residual particles and variability than the cylinders, indicating the importance of shape effects; and (ii) the number of particles left in the hopper increases with PSD width for cuboids but remains approximately the same for cylinders, indicating the significant impact of PSD width for the former but negligible impact for the latter.

Figure 7.12. Screenshots of residual cylinders and cuboids from the systems of monodisperse, lognormal PSD with $\sigma/\mu = 10\%$ and 20% .

Figure 7.13. Number of particles left in the hoppers of the cylinders and cuboids of the monodisperse system and narrower PSD widths (σ/μ) of 10% and 20% .

7.4. Conclusion

The DEM approach is adopted here to investigate the discharge behaviors of lognormal PSDs of ellipsoids, cylinders, and cuboids with the same mean particle diameter of $\mu = 10$ mm. The width of lognormal PSDs ranges between $10\% \leq \sigma/\mu \leq 50\%$. A few highlights are described as follows.

Firstly, the ellipsoids have the most similar discharge behaviors as the spheres in packing, discharge rate, jamming and segregation, but the increase of lognormal PSD width increases the differences between them. Secondly, both broader PSD width and lesser particle sphericity leads to denser packing, as evident in the cuboids with the widest PSD having the highest solid volume fraction among the systems assessed. Thirdly, regardless of particle shape, the discharge rate decreases and likelihood for jamming increases with PSD width, which is tied to the increased force chain restricting the relative movement between particles. The jamming probability is greatest for the cuboids and least for the ellipsoids at the same PSD width. Fourthly, the more angular the particles are, the greater the tendency for particles to be left in the hopper even after complete discharge. Cuboids have more residues and the amount increases with PSD width, whereas ellipsoids do not exhibit any residues.

The conclusions emanating from this work provide a better understanding on the discharge behaviors of lognormal PSDs of non-spherical particles, and are expected to enhance the design and operation of such systems.

Chapter 8. The effect of particle initial charge on minimum pickup velocity (U_{pu})

The content of this chapter has been published under the title of *The Effect of Particle Initial Charge on Minimum Pickup Velocity (U_{pu}) in Pneumatic Conveying*. Chemical Engineering Research and Design, 156, Pages 343-352, 2020. (<https://doi.org/10.1016/j.cherd.2020.02.013>)

Abstract

Pneumatic conveying experiments involving monodisperse and binary-size mixtures of glass beads with charges in the range of -10 to 10 nC have been carried out. The mass loss method was adopted, with the minimum pickup velocity (U_{pu}) determined as the minimum velocity at which entrainment occurred. Similar to previous studies on minimum fluidization velocity, the U_{pu} increased with particle initial charge for the positively charged particles (0 – 10 nC). Surprisingly, however, negatively charged particles exhibited an opposite trend such that the U_{pu} decreased with charge magnitude. Therefore, for the particle initial charge range investigated (-10 to 10 nC), U_{pu} increased monotonically with particle initial charge, and the well-acknowledged correlation mis-predicted U_{pu} by up to 10% for monodisperse systems and up to 40% of binary-size systems. This underscores the necessity to account for particle initial charge in such correlations, particularly for polydisperse particle systems.

Keywords: minimum pickup velocity (U_{pu}); particle charge; pneumatic conveying; triboelectric; binary mixture; particle size distribution

8.1. Introduction

Pneumatic conveying is extensively used in various industries, including chemical, pharmaceutical and agricultural, because of the amenability for large-scale operation, low energy cost and ease of the operation [102, 103]. The gas velocity used in pneumatic conveying is inevitably an important parameter that has to be properly controlled. A gas velocity below that necessary would cause the particles to settle and thereby result in clogging, whereas a gas velocity too much higher than that necessary would cause higher energy cost, particle attrition and pipe erosion [20, 106-108]. Therefore, it is important to identify the critical velocities to operate such pneumatic conveying systems.

Correspondingly, several studies have investigated the minimum pickup velocity (U_{pu}), which is the critical velocity at which particles start to entrain, and minimum saltation velocity (U_{salt}), which is the velocity at which critical velocity at which particles start to settle. Hayden et al.[113] found a non-monotonic relationship between particle size and U_{pu} due to the interplay between inter-particle cohesion and inertial effects. Cabrejos and Klinzing [200-202] found that the pipe diameter affected on the pickup mechanism and also that U_{pu} decreased then increased with respect to particle diameter in the range between 10 to 1000 μm . Anantharaman et al. [104, 110, 203, 204] concluded that the U_{pu} correlations developed for micron-sized particles are not applicable

for nanoparticles, and also comprehensively assessed the impact of particle sphericity and polydispersity. Gomes and Mesquita [205, 206] also compared the U_{pu} and U_{salt} values predicted by existing correlations as a function of the pipe diameter, solid mass flow rate, and particle diameter, density, and sphericity. They demonstrated that U_{pu} increases when particle sphericity decreases, and increases with pipe diameter and particle diameter. Collectively, past studies have enhanced the understanding on such critical velocities in pneumatic conveying, but a gap remains regarding the effect of particle initial charge.

Regarding the effect of particle charge on pneumatic conveying, past studies have shed some light on the resulting phenomena. Lim et al. [207] found using CFD-DEM (computational fluid dynamics coupled with discrete element method) that the presence of an electric field caused flow reversal in the dense region and forward flow in the dilute region. Yao et al. [208, 209] found that induced current, particle charge density, and equivalent current of the charged granular flow increased with decreasing flow rates during pneumatic conveying. Satoru et al. [210] analyzed the particle movement in a pneumatic conveying process under various operating conditions by DEM, and found that the electrification of particles during the pneumatic conveying process is mainly determined by the number of particle collisions against the pipe wall and vertical component of the impact velocity. The current study aimed at building on these understanding by establishing the relationship between particle initial charge and U_{pu} .

Accordingly, this study characterized the U_{pu} values of monodisperse and binary-size particles with different particle initial charges ranging between -10

and 10 nC. The specific objectives were to assess: (1) the influence of particle initial charge on U_{pu} ; (2) if charge type (i.e., positive or negative) or charge magnitude has a more dominant influence; and (3) if the well-established correlations for predicting U_{pu} can be used for the range of particle initial charges investigated.

8.2. Material and method

8.2.1. Experimental setup

The schematic of the pneumatic conveying setup for determining the minimum pickup velocity (U_{pu}), which is similar to that in earlier studies [104, 110, 204], is displayed in Figures 8.1a - b. The setup consisted of three cylindrical sections with a consistent inner diameter of 16 mm, which were made of acrylic and connected by screws on the flanges. Section A was 91 cm long, which is to ensure that the compressed air fed into the setup was fully-developed before it entered Section B. Section B was 30 cm long, and comprised of upper and lower semi-cylindrical halves. Specifically, the lower half was packed with plasticine for a length of 27 cm from the side of Section A and for a length of 0.5 cm from the side of Section C, while the length of 2.5 cm in between served as a chamber for loading the particles to be investigated. Each sample for the pneumatic conveying tests was 4 g. The air velocity value was maintained due to the constant cross-sectional area for air flow in Section B [103, 115]. The length of Section C was 83 cm to minimize exit effects.

Regarding whether the results are applicable for other pipe lengths, it should be noted that Bunchatheeravate et al. [211] found that pneumatic conveying behaviors are similar for different pipe lengths if the pipe wall and particle materials are the same, which is the case here.

Figure 8.1. (a) Schematic of the pneumatic conveying setup; (b) details of Section B; and (c) U_{pu} Mass loss versus the air velocity for the unmodified glass beads, which indicates a U_{pu} value of 5.3 m/s.

8.2.2. Material and Surface Modification

The glass beads used, which were surface-modified to confer different charges, purchased from Abrasive Engineering Pte. Ltd., Singapore. The particle density of the glass beads was 2500 kg/m³. The glass beads were classified into a narrower size range using standard-sized sieves (Cole-Parmer) and a sieve-shaker (Cole-Parmer) to obtain only the fractions between the 150 and 250 μm , 300 and 355 μm , 425 and 500 μm sieves, giving mean particle diameters (d_p) of 200, 327.5, and 462.5 μm , respectively. All particles were Geldart Group B particles [114], and the intermediate mean particle diameter of 327.5 μm was such that it was approximately the mid-value of the Geldart Group B size range.

The charge of the glass beads was modified through surface reaction, as depicted in Figure 8.2. Specifically, the glass beads were made positive by adhering (3-Aminopropyl) triethoxysilane (APTES; Sigma-Aldrich) onto the surface, and then negative by further reacting with poly (acrylic acid) (Sigma-Aldrich).

The first step was the surface activation of the glass beads. 25 g of glass beads were etched in 100 ml of 4 M sodium hydroxide (NaOH; EMD Millipore) at room temperature for 20 min. The etched glass beads were filtered and washed with deionized water (DI water) until neutralized (i.e., pH = 7). The glass beads were then dried in a vacuum oven at 100 °C for 24 h.

Regardless of whether the final charge was targeted to be positive or negative, the second step was to confer positive charge on the surface-activated glass beads. 10 g of the etched glass beads were transferred into 40 ml of ethanol (Sigma-Aldrich), and 1 ml of ammonium hydroxide (Sigma-Aldrich) and 1 ml of APTES

was added. After the slurry was stirred overnight, the glass beads were filtered (Whatman) and washed with DI water until neutralization (tested with pH paper). Finally, the glass beads that were surface-coated with APTES were dried at room temperature for 24 h. For the glass beads targeted to have positive charge, this was the final step. On the other hand, for the glass beads target to have negative charge, another step was necessary, as described as follows.

5 g of the resulting positively charged glass beads from the previous section were suspended using a magnetic stirrer in 20 ml of ethanol (Sigma-Aldrich) and 0.5 g of poly (acrylic acid) (Sigma-Aldrich) for 4 h. The particles were then filtered (Whatman) and washed with DI water until neutralization (tested with pH paper), then dried under vacuum at 80 °C for 24 h to obtain the negatively charged glass beads.

Figure 8.2. Reaction schemes for surface-modification of the glass beads for different charges: (a) positive charge, and (b) negative charge.

8.2.3. Measuring the charge density of particles

An electrometer (Advantest R8252 digital electrometer) and a Faraday cage (Advantest TR8031) were used to measure the charge density of the particles. A sample of 4 g of glass beads was characterized each time before being used for each pneumatic conveying test. The charge density of the particles was measured as follows. At first, the electrometer was zeroed. Then, 4 g of glass beads was transferred to the Faraday cage by a wooden spoon, which is a charge insulator and thereby negligibly affected the particle charges. When the electrometer value became stable, the data was recorded as the charge density.

8.2.4. Measurement of minimum pickup velocity (U_{pu})

The minimum pickup velocity (U_{pu}), which is the air velocity at which the mass loss due to entrainment is non-zero, was determined by the modified weight loss method, which obtains the mass loss curve by a higher quantity measurements of the very small weight losses, developed by Kalman et al. [106] and subsequently used in a few studies [104, 110, 204]. The procedure for the measurement of U_{pu} was as follows.

Firstly, a sample of 4 g of glass beads was loaded into the sample compartment in the lower semi-cylindrical half of Section B (Figure 8.1b) and the surface of the particle bed levelled by a plastic (insulator) stick to minimize any change in the particle charge, after which the mass of Section B was measured using a balance (Mettler-Toledo ME204; four decimal places in grams). Secondly, the flanges of Sections A, B and C were connected by screws to ensure air-tightness.

Thirdly, the compressed air was set at the desired value (starting from the lowest of the range to the tested) using the rotameter and flowed through the setup for 2 minutes [103, 110, 115, 203]. Fourthly, the air flow was shut off and the sections were disconnected in order to measure the mass of Section B. Subsequently, the third and fourth steps were repeated at higher and higher air velocities until the mass loss became significant. A mass loss curve (i.e., mass loss versus air velocity; Figure 8.1c) was then plotted, and the U_{pu} determined as the minimum air velocity that resulted in a mass loss of 0.01 g.

The procedure was repeated three times for each particle charge type.

8.3. Results and discussion

8.3.1. SEM images of the modified and unmodified particles

Figure 8.3 shows the SEM images of the unmodified, and positively and negatively charged glass beads, which were spherical. Clearly, although the particle size remained the same, the surfaces of the modified glass beads had adherents that led to the different charges. It should be noted that the thickness of the additional coats formed on the surface of the glass beads was much smaller than the diameters of micron-sized particles, which agrees with previous studies [212-215].

Survey of the lower magnification images indicate that both the unmodified and modified glass beads were dispersed as individual particles, reflecting that the surface modifications did not cause the glass beads to be cohesive.

(a)

(b)

(c)

Figure 8.3. SEM images of glass beads with a mean particle diameter (d_p) of 327.5 μm : (a) unmodified; (b) positively charged; and (c) negatively charged.

8.3.2. U_{pu} of the unmodified particles

Figure 8.1c illustrates the mass loss versus air velocity curve for the unmodified glass beads with a mean particle diameter (d_p) of 327.5 μm . The U_{pu} was determined to be 5.3 m/s, which agrees with an earlier experimental study [110]. Note that the higher variability of the mass loss values at velocities greater than U_{pu} was likely tied to size-segregation effects [104, 110], since although the samples were pre-sieved to a narrower size distribution, the glass beads were not all of the exact same size.

Furthermore, U_{pu} can be predicted based on the relationship between the modified Reynolds number (Re_p^* ; i.e., modified to account for the effect of the pipe diameter) and Archimedes number (Ar) according to the well-established Kalman et al. [106] correlation for monodisperse particle systems:

$$Re_p^* = 5Ar^{\frac{3}{7}} \text{ for } Ar \geq 16.5 \quad (8-1)$$

where

$$Re_p^* = \frac{\rho_f d_p U_{pu}}{\mu_f (1.4 - 0.8e^{-\frac{D/D_{ref}}{1.5}})} \quad (8-2)$$

$$Ar = \frac{g \rho_f (\rho_p - \rho_f) d_p^3}{\mu_f^2} \quad (8-3)$$

where ρ_f is the density of the fluid, d_p is the diameter of the particle, μ_f is the viscosity of the fluid, D is the diameter of the pipe, D_{ref} is the reference pipe diameter of 50 mm, g is the gravitational acceleration, ρ_p is the density of the

particle. This gives a U_{pu} value of 5.2 m/s, which approximately agrees with the experimental value of 5.3 m/s (Figure 8.1c).

Based off the Kalman et al. correlation [106] for monodisperse systems, another correlation has been developed for binary mixtures [115]. Eq. (8-1) was modified to give:

$$Re_p^* = 20Ar^{\frac{1}{4}} \text{ for } 20 \leq Ar \leq 2500 \quad (8-4)$$

where the d_p of the mixture is calculated by:

$$d_{p,binary} = m_1 d_{p1} + m_2 d_{p2} \quad (8-5)$$

where m stands for mass fraction.

8.3.3. Effect of positive charge

The possible change in charge before and after each test was ascertained. Figure 8.4 displays final charge versus initial charge in the range of 0 to 14 nC for the monodisperse glass beads with a mean particle diameter (d_p) of 327.5 μm . For the lower charge values of below 5 nC, the difference between initial and final charges was negligible. However, for the higher charge values of above 5 nC, the discrepancies between the initial and final charges were greater, indicating more extensive charge transfer that led to an overall charge accumulation, which is linked to the more significant contact and friction under the higher U_{pu} (Figure 8.5) [210, 216]. In view of the general agreement between initial and final charges, the U_{pu} values were correlated with the initial charges to determine the effect of charge on U_{pu} in this study.

Figure 8.4. Comparison of the charges before and after pneumatic conveying of the positively charged glass particles ($d_p = 327.5 \mu\text{m}$). The solid line represents $y = x$, while the discrete points represent the experimental results.

Figure 8.5 presents the variation of U_{pu} with particle initial charge values between 0 and 10 nC, which shows that U_{pu} increased monotonically with charge. This agrees with a previous study, in which the U_{pu} values of the glass beads were higher in the absence of an antistatic film (Larostat®, BASF) inside of the test pipe to dissipate the charges [113]. This also agrees with fluidization studies that concluded that minimum fluidization velocities increased with particle charge [217, 218].

Figure 8.5. Minimum pickup velocity (U_{pu}) versus positive charge value for the glass particles ($d_p = 327.5 \mu\text{m}$). The solid line represents a best-fit linear line ($R^2 = 0.63$), while the discrete points represent the experimental results.

8.3.4. Effect of negative charge

Analogous to Figure 8.4, Figure 8.6 shows the change in particle charges before and after each experiment for the monodisperse glass beads with a mean particle diameter (d_p) of $327.5 \mu\text{m}$. Compared to that for the positively charged particles, the discrepancies between the final and initial charges were greater for the negatively charged particles in the range between -11 and 0 nC . In particular, for the more negative charges of -2 and below, the final charge tended to be less negative than the initial charge, indicating the dissipation of charges. On the other hand, for the less negative charges of between 0 and -2 nC , charge tended to accumulate such that the final charge became more negative than the initial. This implies contradictory trends between the positively and negatively charged particles, specifically in that larger positive charge magnitudes ($> 8 \text{ nC}$) tended to accumulate charge during the pneumatic conveying (Figure 8.4), whereas larger negative charge magnitudes ($< -2 \text{ nC}$) tended to dissipate charge (Figure 8.6). The reason underlying the opposite tendency is likely tied to the positive 1 nC charge of the pipe (Figures 8.1a - b), which caused further charge buildup for the positively charged particles and charge dissipation for the negatively charged particles.

Figure 8.6. Comparison of the charges before and after pneumatic conveying of the negatively charged glass particles ($d_p = 327.5 \mu\text{m}$). The solid line represents $y = x$, while the discrete points represent the experimental results.

Figure 8.7 describes the effect of various negative charge magnitudes on U_{pu} , which shows that U_{pu} decreased as the particle initial charge became more negative. Surprisingly, this again appears to be counter to the results for the positively charged particles (Figure 8.5), specifically in that U_{pu} increased with charge magnitude for the positively charged particles, but decreased with charge magnitude for the negatively charged particles. This also seems to contradict with the increase in minimum fluidization velocity (U_{mf}) with particle charge [217, 218]. An earlier study on the U_{pu} of nanoparticles also pointed out different trends between U_{pu} and U_{mf} in that the difference between polar and apolar species was lesser in the case of the former because of the fewer number of immediate neighboring particles [203].

Figure 8.7. Minimum pickup velocity (U_{pu}) versus initial negative charge for the glass particles ($d_p = 327.5 \mu\text{m}$). The solid line represents a best-fit linear line ($R^2 = 0.71$), while the discrete points represent the experimental results.

8.3.5. Summary on the effect of charge for monodisperse glass particles ($d_p = 327.5 \mu\text{m}$)

Electrostatic charge buildup and dissipation effects have been reported to intensify with time then reach an equilibrium [208]. In this study, glass beads with larger positive charge magnitudes tended to accumulate charge during the pneumatic conveying, while those with larger negative charge magnitudes tended to dissipate charge. The scatter of data in Figures 8.4 – 8.7 reflect the greater variability associated with particle charge effects; despite the scatter, the trends are clear.

Figure 8.8 summarizes the average minimum pickup velocity (U_{pu}) versus particle initial charge spanning negative and positive charges for the monodisperse glass beads with a mean particle diameter (d_p) of $327.5 \mu\text{m}$. Surprisingly, U_{pu} increased monotonically with charge in the range of -10 to 10

nC, regardless of positive and negative charge type. This was unexpected, because earlier reports on fluidized beds indicated higher minimum fluidization velocities for charged particles [217, 218], with greater charge magnitudes conferring more extensive inter-particle repulsion and thereby behaving more similarly, so U_{pu} was expected to decrease then increase in the charge range investigated. To further explore this counter-intuitive trend, binary-size systems were evaluated.

Figure 8.8. The average minimum pickup velocity (U_{pu}) versus the particles modified with different initial charge for the glass particles ($d_p = 327.5 \mu\text{m}$).

8.3.6. Effect of charge on the U_{pu} of the binary-size mixtures

The charges of the constituents unavoidably changed upon mixing. Table 8.1 presents the charges of the constituents, and the resulting binary-size mixture (made up of 50% by mass of each) before and after the pneumatic conveying tests. Clearly, the charge of the mixture was dissimilar to that of either constituents due to tribocharging effects. Analogous to Figures 8.4 and 8.6, Figure 8.9 presents the change in the particle charges before and after each experiment for the binary-size mixtures consisting of equal masses of glass beads

with particle diameters of 200 μm and 462.5 μm . The scatter of charges for the binary systems (Figure 8.9) were greater than that for the monodisperse ones (Figures 8.4 and 8.6) due to the augmented tribocharging effects for the former because of the presence of different particle sizes[219, 220]. Moreover, as shown in Table 8.1, the charges of the two components in each mixture are quite different. The charge magnitude of the difference of the two components may affect the final charge.

Figure 8.10 shows the U_{pu} values versus charge for the binary-size mixtures. Similar to Figure 8.8, U_{pu} trended approximately linearly with charge. This reaffirms the counter-intuitive relationship of U_{pu} versus charge, even in the presence of tribocharging effects between the glass beads of disparate sizes. Therefore, in contrast to fluidization systems whereby higher minimum fluidization velocities were observed for more highly charged particles [217, 218], U_{pu} increased monotonically with charge.

Table 8.1. Example of charges (nC) of the constituents of the binary-size mixture, and the resulting mixture before and after pneumatic conveying. Each sample for the pneumatic conveying tests was 4 g.

200 μm	462.5 μm	Mixture (initial)	Mixture (final)
-6.16	-1.27	-8.38	-3.43
-3.37	-1.74	-5.63	-2.84
-4.05	-0.83	-3.88	-2.38
-4.33	0.70	-4.08	3.34
-5.46	1.85	-1.70	-4.83
-1.78	3.17	2.06	4.89
-4.84	7.65	3.34	0.77

Figure 8.9. Comparison of the charges before and after pneumatic conveying of the binary-size mixture of 50 % by mass of 200 μm and 462.5 μm glass particles. The solid line represents $y = x$, while the discrete points represent the experimental results.

Figure 8.10. Minimum pickup velocity (U_{pu}) versus initial charge value for the binary-size mixture of 50 % by mass of 200 μm and 462.5 μm glass particles. The solid line represents a best-fit linear line ($R^2 = 0.58$), while the discrete points represent the experimental results.

8.3.7. Re_p^* versus Ar

Figure 8.11 describes the relationship between Re_p^* (Eq. 4) and Ar^* (Eq. 5) for the range of charges investigated. The lines represent the correlations, while the discrete points represent the experimental data obtained in this study. For the monodisperse system, Figure 8.11a shows that the well-acknowledged correlation [106] was deficient in predicting the U_{pu} values for particles that had greater charge magnitudes, with errors of up to $\pm 10\%$. More specifically, the correlation tended to under-predict and over-predict for the U_{pu} values of respectively the positively and negatively charged particles. For the binary-size mixtures, Figure 8.11b shows that both the monodisperse correlation [106] and binary correlation [115] over-predict the U_{pu} values measured, with an error of up to 40% and with the latter giving expectedly a slightly better prediction. This ascertains the need to account for particle initial charge in the development of such correlations, particularly for non-monodisperse systems.

Figure 8.11. Re_p^* (Eq. (8-3)) versus Ar^* (Eq. (8-4)) for the range of particle initial charges investigated, with the discrete data points representing the

experimental data and the lines representing the correlations (Kalman et al.[106] for monodisperse systems and Tay et al.[115] for binary systems): (a) monodisperse; and (b) binary-size mixtures.

8.4. Conclusion

In view of the gap in the knowledge base regarding the effect of particle initial charge on the minimum pickup velocity (U_{pu}), pneumatic conveying experiments were conducted for glass beads surface-modified to resulting charges in the range of -10 to 10 nC. Monodisperse particle systems with the same particle diameter (327.5 μm) were investigated, along with binary-size mixtures composed of equal masses of 200 μm and 462.5 μm glass beads. The mass loss method was adopted [104, 110, 204].

A few key results were obtained. Firstly, monodisperse glass beads with larger positive charge magnitudes tended to accumulate charge during the pneumatic conveying, whereas those with larger negative charge magnitudes tended to dissipate charge. Due to increased tribocharging effects between the different particle sizes, the change in charges before and after pneumatic conveying were greater for the binary-size mixtures. Secondly, although U_{pu} was expected to increase with charge magnitude due to increased inter-particle repulsion, U_{pu} increased monotonically with charge in the range of -10 to 10 nC for both monodisperse and binary-size systems. This is counter to the understanding on fluidization systems whereby higher minimum fluidization velocities were observed for more highly charged particles [217, 218]. Thirdly, for the range of particle initial charges investigated here, the lack of accounting of particle initial

charges caused the well-acknowledged correlations to mis-predict U_{pu} by up to $\pm 10\%$ for the monodisperse systems and up to 40% for the binary-size mixtures. This underscores the need to factor in particle charge in such correlations, particularly for polydisperse systems. Recommended follow-up studies include (i) the coupled effects of charge and continuous particle size distribution, especially since the latter has been shown to exhibit interesting behaviors [110]; and (ii) investigation of a wider range of monodisperse particle sizes to understand if the effect of charge varies with size.

The results of this study contribute to the understanding on the impact of charged particles, and are expected to be valuable in the validation of two-fluid models and also the development of better correlations for charged particles.

Chapter 9. Conclusions and future perspectives

9.1. Conclusions

The research presented in this thesis contributed to providing insights into the flow behaviors of particles in hoppers and gas-solid horizontal pneumatic conveying. The characteristics of the particulate dynamics in hoppers (namely, discharge rate, particle velocity, segregation, packing, and jamming, etc.) was enabled by the DEM, while the minimum pickup velocity in the horizontal pneumatic conveying was characterized by the experimental weight loss method.

The hopper studies bridge the gap of discharge characteristics of lognormal particle size distributions and non-spherical particles, show the jamming probability at different situations. Thus, we obtain the methods to keep a steady state flow, avoid jamming and reduce the segregation during the discharge by controlling the particle properties in the application. The particles charged is very common, especially in dry area. The pneumatic conveying experiments bridge the gap of relationship between particle initial charge and U_{pu} and improve the knowledge on the U_{pu} to avoid improper gas velocity leading to particle clogging or particle attrition and pipe erosion. However, the current study is working on the small-scale apparatus. The factor of scale-up should be tested for the industrial application.

9.1.1. Hopper flow

In chapter 3, our study on the discharge characteristics of lognormal particle size distributions from a conical hopper concluded that the hopper discharge rate

decreases with the increase of the PSD width, with the discharge duration of the widest lognormal PSD investigated ($\sigma/\mu = 70\%$) about 1.6 times that of the monodisperse. The rates for all the PSDs are constant with time, but the extent of fluctuation increases as the PSD width increases. Regarding the overall PSD during discharge, while the change in PSD is negligible for the narrower PSD widths of $\sigma/\mu = 30\%$, the PSDs progressively shift rightwards for $\sigma/\mu = 50\%$. On the change in the mean particle diameter as the hopper discharges, the narrower PSDs ($\sigma/\mu = 30\%$) are such that the means do not exceed the initial mean of 5 mm, whereas the wider ones ($\sigma/\mu = 50\%$) do. Although the velocity profiles are distinctly different for the systems with different PSDs, the relationship between PSD width and particle velocities is generally non-monotonic with no consistent trends, which is somewhat surprising since the discharge rate decreases monotonically with PSD width. It was only at the radial center ($\sigma/\mu = 50$) and lower bed heights that the local particle velocity approximately decreases as PSD width increases, which agrees with the discharge rate.

In chapter 4, we tried to understand the varying discharge rates of lognormal particle size distributions from the hopper. This led to findings that the Beverloo correlation and others modified to account for various particle properties predict the discharge rates of lognormal PSDs poorly, which underscores the need for more understanding on the influence of PSD width. The velocity vectors are less uniformly downwards in the hopper for the wider PSDs, which results in the slowing down of the discharge rate. The radial particle velocity, and both the radial and vertical particle angular velocity increase with PSD width throughout the first half of the hopper discharge. The collision force magnitudes are greater for the

wider PSDs, and the cross-sectional fluctuations of the collision forces at the cone height increases with PSD width. The increase of the magnitudes of these particle characteristics (namely, radial particle velocity, angular velocity, and collision force) with PSD width underlies the decreasing hopper discharge rate.

In chapter 5, the study on the effect of particle size distribution on jamming was investigated, where the mean particle diameter increased two times as in the previous study of chapters 3 and 4. Results indicate that, although the monodisperse particles of 10 mm diameters do not jam, the wider PSDs ($\sigma/\mu \geq 30\%$) jam. The flatter arches and higher mass-averaged force that are linked to the denser packing of wider PSDs underlie the propensity to jam. To reduce the jamming probability, the friction coefficient and initial fill height can be reduced, but not changes in particle density. The results here highlight that the mean particle diameter alone is an insufficient parameter to predict jamming and the impact of PSD width is non-negligible.

In chapter 6, the hopper discharge behaviors of binary mixtures of non-spherical particles were unveiled by numerical simulation. For the monodisperse systems, particle shape is the dominant factor dictating discharge rate, compared to other factors like aspect ratio, preferential orientation and packing. Regarding the binary-size mixtures, while the discharge rates are still dictated by particle shape, the positive correlation between discharge rate and solid volume fraction or mean aspect ratio is clear. As for the binary-shape mixtures, the discharge rates are similar for all twelve mixtures, reflecting a surprising lack of shape effects, which in turn means the negligible impact of solid volume fraction, aspect ratio and segregation extent.

In chapter 7, the hopper flow of the non-spherical particles with the more complicated polydisperse i.e. lognormal particle size distributions was presented. The ellipsoids have the most similar discharge behaviors with the spheres in the three non-spherical particle systems. However, the increase of the PSD width (σ/μ) can deepen the gap between them. The packing of the hopper is associated to the PSD width and shape of the particles. The discharge rates of all particle shape systems decrease and further jamming with PSD width increases. The jamming probability is greatest for the cuboids and least for the ellipsoids at the same PSD width. The more angular the particles have (cuboid > cylinder > ellipsoid), the more particles left in the hopper. The results here provide new insight regarding the impact of particle shape with lognormal PSDs on the particle flow in the hopper.

9.1.2. Pneumatic conveying

In view of the gap in the knowledge base regarding the effect of particle initial charge on the minimum pickup velocity (U_{pu}), pneumatic conveying experiments were conducted for glass particles surface-modified (4 g) to resulting charges in the range of -10 to 10 nC. Monodisperse particle systems with the same particle diameter (327.5 μm) were investigated, along with binary-size mixtures composed of equal masses of 200 μm and 462.5 μm glass particles. The mass loss method was adopted [104, 110, 204].

A few key results were obtained. Firstly, monodisperse glass particles with larger positive charge magnitudes tended to accumulate charge during the pneumatic conveying, whereas those with larger negative charge magnitudes tended to dissipate charge. Due to increased tribocharging effects between the different

particle sizes, the change in charges before and after pneumatic conveying was greater for the binary-size mixtures. Secondly, although U_{pu} was expected to increase with charge magnitude due to increased inter-particle repulsion, U_{pu} increased monotonically with charge in the range of -10 to 10 nC for both monodisperse and binary-size systems. This is counter to the understanding on fluidization systems whereby higher minimum fluidization velocities were observed for more highly charged particles [217, 218]. Thirdly, for the range of particle initial charges investigated here, the lack of accounting of particle initial charges caused the well-acknowledged correlations to mis-predict U_{pu} by up to $\pm 10\%$ for the monodisperse systems and up to 40% for the binary-size mixtures. This underscores the need to factor in particle charge in such correlations, particularly for polydisperse systems.

The results of this study contribute to the understanding on the impact of charged particles, and are expected to be valuable in the validation of two-fluid models and also the development of better correlations for charged particles.

9.2. Future Perspectives

After coming up with the discharge behaviors of particles with lognormal particle size distributions, it leaves modifying the well-known Beverloo correlation for prediction of the discharge rate of the hopper with lognormal particle size distributions. However, the discharge rate of the non-spherical particles with binary mixtures agrees well with the Beverloo correlation in our study. Research could aim to consider including the PSD width in the correlation and discuss weights of the particle mean diameter, standard deviation, and PSD width.

Secondly, for the jamming in hoppers, the threshold of binary mixtures and continuous particle size distributions could be tested by numerous experiments and simulations. Moreover, the possibility of jamming of different particle size distributions could be tested also.

Thirdly, larger-scale hopper system could be used to test if the discharge behaviors including discharge rate, segregation, jamming phenomenon, etc. still keep similar results.

Fourthly, at the same particle volume, the increase of particle angularities decreases the discharge rate and increases the solid volume fraction and residues. Thereby, it would be possible to assess if the relationship could maintain the particles with more angularities.

Last but not least, for the minimum pickup velocity of charged particles in the horizontal pneumatic conveying, the charge on the glass beads could be expanded if there are more efficient methods. Furthermore, the impact of the particle initial charge with continuous particle size distributions can be tested in the future.

LIST OF PUBLICATIONS

1. Y. Zhao, S. Yang, L. Zhang and J.W. Chew, “DEM study on the discharge characteristics of lognormal particle size distributions from a conical hopper”, *AIChE Journal*, 64 (4), Pages 1174-1190, 2018.
2. Y. Zhao, R.A. Cocco, S. Yang and J.W. Chew, “DEM study on the effect of particle size distributions on jamming in a 3D conical hopper”, *AIChE Journal*, 65, Pages 512-519, 2019.
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4. Y. Zhao, Shubham Dahiphale, Yong Zen Tan, Chi Hwa Wang, Jia Wei Chew, “The Effect of Particle Initial Charge on Minimum Pickup Velocity (U_{pu}) in Pneumatic Conveying,” *Chemical Engineering Research and Design*, 156, Pages 343-352, 2020.
5. Y. Zhao, Jia Wei Chew, "DEM Study on Hopper Discharge Behaviors of Binary Mixtures of Non-Spherical Particles." *AIChE Journal*: e16254.
6. Y. Zhao, Jia Wei Chew, “Effect of Lognormal Particle Size Distributions of Non-Spherical Particles on Hopper Discharge Characteristics,” (under review).
7. S. Yang, Y. Sun, Y. Zhao and J.W. Chew, “A numerical study of the segregation phenomenon of lognormal particle size distributions in a rotating drum”, *Physics of Fluids*, 30 (5), 053301, 2018. Editor’s Pick.

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