Discrete Element Modelling of Particulate Flow in Die Filling and Powder Transfer

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Summary

In this thesis, numerical investigation of die filling and powder transfer within discrete element method framework is presented. The main focus of the work is to explore the contribution of die filling and powder transfer processes towards the density variation of the powder mass before compaction. The numerical investigations are carried out to provide alternative solutions in understanding die filling and powder transfer mechanisms because of the lack of theoretical and experimental solutions in the two fields. Validation of the code used was successfully carried out by comparing simulation results with the existing results of powder flow experiments conducted in controlled environment which imitate realistic industrial settings. The effects of shoe kinematics, punch kinematics, contact parameters, modelling parameters, die geometry, die orientation, and shoe volume on die filling and powder transfer have been identified. It has been confirmed that multiple passes, multiple shoe columns and powder shifting can improve powder packing. The die fill is found to decrease with the increase in friction and cohesion. On the contrary, it increases with the increase of damping. The combination of slow shoe speed during filling and slow punch speed during transfer is found to result in homogeneous powder packing inside the die. The research has also successfully integrated die filling and powder transfer in one continuous sequence in a three dimensional setting.

Simulation works have also been performed on the Variable Aperture Flowmeter to evaluate the effects of particle composition on critical aperture and angle of repose, and to determine powder flow rate. Investigations were also conducted on the bridging phenomena which conclude that bridging for monodispersed circular particles stops when the orifice is set at 5.5 particle width. The result however may change with different values of contact parameters and particle properties. Numerical study performed has shown that the discrete element method is capable of reproducing several key phenomena observed in die filling and powder transfer processes and to some extent capable of characterising powder flow in a simulated variable aperture flowmeter.

Contents

Chapter 1

Introduction

Contents

1.1 The Powder Metallurgy Path

Particulate materials have been picking up pace in material consumption because of the huge advantages Powder Metallurgy (PM) has to offer. One of the evidences is that the granular media is ranked "second, behind water, on the scale of priorities of human activities and endeavours" [Duran, 2000]. They are commercially important in applications as diverse as engineering, pharmaceuticals, chemical industry, food production, mining, agriculture, and energy production. Global powder metallurgy production covering all sectors is estimated to exceed $43 billion a year [IPMD, 2009]. However, a lot of their properties are poorly understood and their flow properties may be affected by numerous physical, chemical and environmental variables. In order to explore the behaviour of particulates, experimental studies have been and are being conducted but numerical simulation is increasingly seen as an economical and practical means to comprehend them. Ristow [1998] stated that "Since a complete description for the dynamics of granular materials is still in its infancy, numerical simulations are very valuable and sometimes even necessary to determine the static and dynamical properties in granular systems". The powder metallurgy industry increasingly uses modelling to study particulate flow and to identify process parameters instead of relying totally on trial and error in experiments [Schneider, 2002]. With smarter algorithms and new advancement in computer technology, more complex particle geometries and process parameters can be taken into consideration to create better precision in modelling and simulations of particulate matters, at higher speeds. Due to the massive growth in particle related industries, any additional understanding of particulate behaviours would contribute to a large improvement in process control and optimisation, reliability, and efficiency.

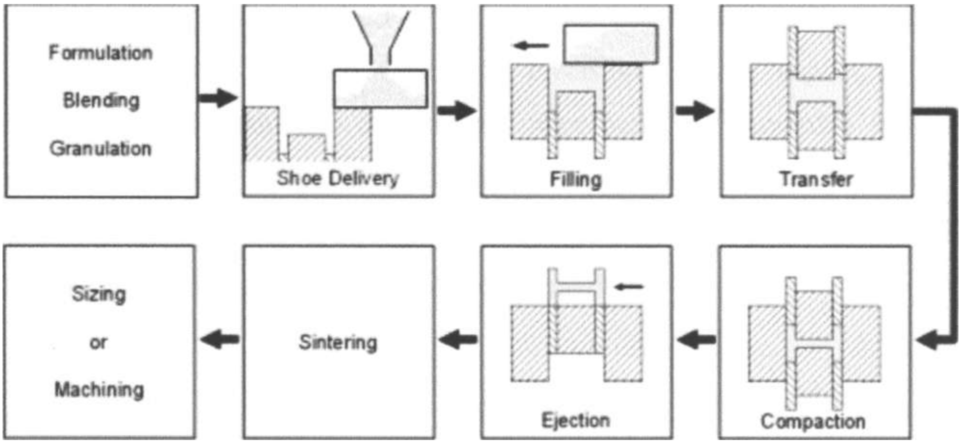

Figure 1.1 A typical processing route for a multilevel component manufactured from powder [Cocks, 2004],

Powder metallurgy is a continually and rapidly evolving technology embracing most materials in the form of metals, metallic alloys, inter-metallic compounds, ceramics, ceramic powders and ceramic compounds in a wide variety of material shapes. Figure 1.1 summarises the production stages in the powder metallurgy process. The process begins with mixing of elemental or alloy powders, followed by die filling, transfer of powder within the closed die cavity, compaction of the powder mixture, ejection of the compacted components and finally sintering of the resultant shapes in a controlled atmosphere furnace at high temperatures below the material's melting point in order to bond the particles together. Parts with specific properties, homogeneous structure and consistent* behaviour can be produced by properly mixing particulates of different materials to cater for a wide range of applications [EPMA, 2008]. Refinements can also be tailored into the properties of mechanical parts.

Powder technology is known as a superior way of producing high quality components for various applications since the last 20 years [MPIF, 2008]. It offers a lot of advantages over other metalworking technology. It minimises time and energy spent in machining processes. The powder compaction cycle which normally runs at 20 to 25 strokes per minute makes it suitable for high volume production [Rodiger, 2000]. Material utilisation in excess of 95% can be achieved and parts can be produced with close dimensional tolerance [EPMA, 2004]. Compaction process within powder metallurgy produces good surface finishing with controlled porosity. The high precision forming capability of powder metallurgy allows the production of near net shape parts with complex features which makes it an extremely energy efficient process. Furthermore, the resulting sintered components can still be heat treated for increased strength, or hardened, machined, and plated just like components manufactured by other methods.

Figure 1.2 shows a few high precision engineering products produced using the powder metallurgy process. Machining them would have been very complicated, costly, time consuming and would result in a lot of scrap especially with high volume production. Since almost all metals can be granulated [German, 1994], powder metallurgy permits a wide variety of alloy systems. PM components are currently replacing a wide range of casting, forging and machined components in the automotive industry [Wu et al., 2006]. Figure 1.3 shows the diverse classification of powder metallurgy application.

Figure 1.2 Oil pump rotor parts produced by powder metallurgy techniques [PPMI, 2008].

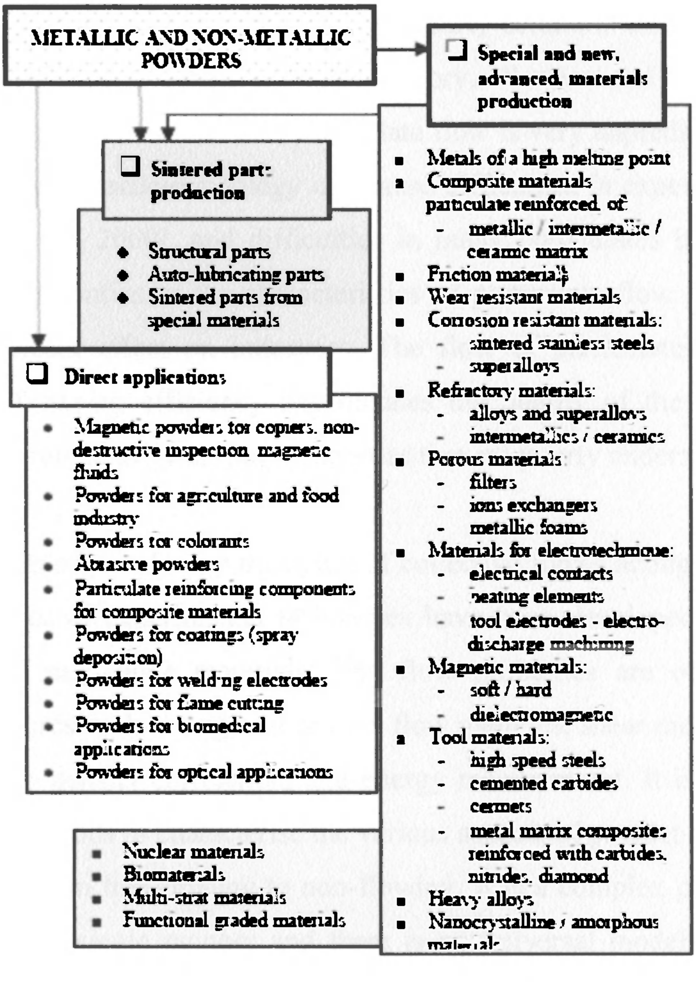

Figure 1.3 Classification of powder applications [Orban, 2004].

1.2 Particulate Flow

Particulate flows can be found in silos and hoppers during filling and discharging, in transport systems, mills, particle mixers, grinders, drilling process, shot-peening process, excavation, fluidised bed and powder classifiers. The flow properties of particulates depend upon the combined effects of a large number of physical and environmental variables.

Particle variables that can influence powder behaviour are particle size, packing density, composition, size distribution, shape, surface texture, cohesiveness, friction, surface coating, wear or attrition characteristics, propensity to electro-static charge, and the ability to recover from compaction. To add to the complexity of the flow properties, external factors such as flow rate, humidity, temperature, aeration, container surface and shape effects, transportation experience, loading history, vibration and compaction condition can also affect the powder. As a result, particulate flow is very unpredictable and non-uniform. The complexity of particle rheology can cause difficulties in experimentation and analysis [Tordesillas et al., 2000], and difficulties in many particulates handling and processing activities. Uncertainties in the characteristics of particulate flow if remain unsolved will have a significant effect on industries. The flow of particulates during manufacturing affects manufacturing efficiency and dictates the quality of the end product yet many industries still rely heavily on flow properties that are poorly understood.

Flow properties of powder are the result of collective forces acting on individual particles. A large number of experimental techniques have been developed to determine the flow behaviours of particulate materials. The flow properties are often characterised with physical measures such as angle of repose, flow methods, shear methods, compact strength correlation, tap density correlation, and energy measurement. It is often necessary to use multiple test methods to characterise the various aspects of powder flow. The flowability of powder spans from free-flowing to non-flowing. It is a complex parameter that cannot be described with a single number and there is no universal model in existence to predict powder flow behaviour in every situation.

Particulates may exhibit the properties of solids, liquids, or gases but they are not like solid, nor liquid, nor gas. The grains remain close to each other at low energy level but at a higher energy level, contacts between particles become less frequent and they become fluidised. At an even higher energy level, contacts between particles become highly infrequent and they can even enter a gaseous state. The transitions between these three states have created many particulate flow phenomena that trigger a lot of related research within manufacturing and natural environments.

1.3 Numerical Modelling of Particulate Flow

Numerical modelling has become a valuable tool in the study of different phenomena occurring at micro-mechanic scale in granular materials. Discrete element simulation is widely applied in particulate flow because it offers a lot of advantages. It allows access to information which would be very difficult or impossible to measure in a physical experiment such as instantaneous force distributions, three dimensional concentration, density distribution of particulates, flow profiles, etc. It also offers the possibility of isolating certain parameters within the flow to study the effect of other parameters of interest. With the help of modelling, material and process parameters can be identified so that metallurgical components can be produced more efficiently.

Discrete element modelling relies on the physical and material properties of individual particles and the surfaces with which they interact. Direct interaction of particles plays an important role in the flow mechanics of particulates. Simulations require precise numerical models and massive computational power. The state-of-the-art computer technology available today offers the possibility to simulate realistic three-dimensional particulate systems with complex particle shapes and specific properties at a relatively low cost.

1.4 Aim of the Work

Each and every step in the powder metallurgy process contributes to the quality of the final product. In order to manufacture consistent and uniform products, each step of the PM process must be fully understood [Wu et al. (a), 2003]. Coube et al. [2005] also emphasised the importance of understanding all stages of powder manufacturing process including how the steps combine to produce the density distribution in the green part. The goal of this work is to contribute to such knowledge by carrying out numerical study to identify the factors that contribute to density variation during die filling and powder transfer.

Density variations in a green compact can lead to property variations in green or sintered parts, component distortion, shrinkage, and shape changes upon sintering [AEAT, 2001]. Since the physical and metallurgical properties of powder metallurgical components are closely related to their final density, one of the major requirements in powder metallurgy is to minimise density variations throughout powder components after compaction. The die filling from a shoe may contribute to the density gradient by introducing voids into the powder mass creating an inhomogeneous packing. Poor flowing powder may not fill the die in the time available. Sections with narrow apertures may not be completely filled. The subsequent transfer process then changes the initial packing creating shear zones which can also introduce voids in some area of the powder mass [Wu et al. (a), 2003]. Density variations may also occur throughout final pressed and sintered parts as a result of friction between powders and die during compaction, and from the shearing and deformation mechanisms that distribute the densification process throughout the powder mass [Bagley et al., 1998].

The main aim of this research work is to design, perform and analyse simulations on particulate flow with the following objectives:

1. to investigate the influence of contact parameters on particle packing.

2. to determine how the details of the powder delivery and powder transfer systems, influence the way in which powder packs inside the die.
3. to create a three dimensional modelling of die filling and powder transfer as one continuous sequence.
4. to characterise powder flow using simulated Variable Aperture Flowmeter.*

In general, all of these objectives have been achieved. The current work initially investigated the application of a Variable Aperture Flowmeter (VAF) to characterise powder. The VAF is a new development in powder measurement technique and a convenient tool which caters for the measurement of non-flowing powder. It characterises powder through flow rate, angle of repose, critical aperture, and the apparent density. The critical apertures and the angle of repose of various particle geometries were determined using a simulated VAF. The investigation into the VAF also included the study of flow rate measurement.

The discrete element method (DEM) code for the current research work was validated against experimental results from AEAT [2001], a part of MODNET project. MODNET and DIENET are two EU funded Thematic Network projects that were run by the EPMA [2008]. A parametric study was conducted in this research to identify the effects of friction, cohesion, damping, shoe volume and contact penalties on flow and particle packing. The design of the setup selected for the experiments took into consideration the shoe kinematics, the mechanism of multiple passes, the die geometry, particle packing, and powder circulation. Analysis was conducted with the application of image processing technique. The outcome of this study was put to the test in an experiment which had successfully produced an optimised density in powder filling.

The research further investigated die filling and powder transfer which focussed particularly on the contribution of the shoe speed, die orientation, particle volume, die geometry, multiple passes, multiple sectioned die shoe, particle shape and flow type on the density distribution. The novelty of this research work includes the combined three dimensional modelling of die filling and powder transfer in a complex geometry die system. The basic three dimensional setup can be further integrated with various shoe and die kinematics.

1.5 LAYOUT OF THE THESIS

The layout of the thesis following the current chapter is presented as follows:

1.5.1 Chapter 2: Literature Review

The chapter provides a review on particle flow problems and the factors that affect flow, followed by the issue of density variation in powder metallurgy processes. It also covers previous studies of Discrete Element Method, and also the recent development in experimental and simulation works on die filling and powder transfer.

1.5.2 Chapter 3: Mathematical Background

The chapter details the formulation of interaction laws and kinematics of particles involving disks, ellipses, spheres and ellipsoids.

1.5.3 Chapter 4: Variable Aperture Flowmeter

The chapter explores the characterisation of powder by the use of simulated Variable Aperture Flowmeter. It includes the determination of critical aperture, angle of repose, and flow rate.

1.5.4 Chapter 5: Validation and Parametric Study

This chapter covers simulation works to duplicate existing experimental results involving three cases of die filling and one case of powder transfer for the purpose of validating the code to be used for the investigation of die filling and powder transfer. The chapter then covers a parametric study designed to observe and identify the effect of contact parameters, shoe volume and simulation parameters on the results of powder filling.

1.5.5 Chapter 6: Die Filling and Powder Transfer

The work on die filling investigates the flow behaviour of powder from a die shoe into a simple die and a stepped die, while observing the effects of shoe kinematics, die orientation and powder volume on powder packing. The shoe kinematics involves multiple passes and various shoe speeds. Simulation of die orientation effect involves a Modnet die and a Dienet die that are set back to back to capture two different die orientations. Parallel and orthogonal three dimensional (3D) die orientations are also investigated. The powder volume effect simulation work involves the filling of a Modnet and a Dienet die, again set back to back in a continuous setup. The combined die filling and powder transfer works are conducted in 2D and finally extended into a 3D.

1.5.6 Chapter 7: Conclusion and Recommendations

The chapter highlights the novelty achieved and how the work contributes to the advancement of die filling and powder transfer research in particular, and the powder research community as a whole. Finally some future works to be done in this area are addressed.

1.5.7 Appendices

Appendix A contains geometric construction to support Chapter 4 while Appendix B supports image analysis in Chapter 6.

Chapter 2

Literature Review

Contents

2.1 Introduction

Powders are inherently unstable in relation to their flow performance despite their wide application in industries. This is because of their micromechanical behaviour which is inherently discontinuous and heterogeneous [Oda and Iwashita, 1999], Bates [1999] found that any changes in operating condition, equipment geometry, material and variables of operation can change even the properties of free flowing powders. Jaeger [1996] reported that it is difficult to achieve reproducibility of granular flow behaviour since each configuration has its unique properties Bertrand [2005] wrote, "Due to the complex nature and the multifaceted flow of granular materials, only partial understanding of the mechanisms governing the processes involved in the development and manufacturing of granular products is available". Therefore, a systematic understanding of particulate behaviour, flow properties and tooling mechanics is necessary to comprehend, predict and control the flow of particulate materials. Before proceeding to the work in the thesis it is appropriate to review the most relevant literature. This chapter investigates some of the particulate flow phenomena and the models used to study them.

2.2 Flow Problems

Poor flow of powders has detrimental effects in final powder metallurgy products and it increases operating costs. Flow problems always occur when particles flow through containers, and mechanical parts. Among the most common ones are arching, ratholing, flooding, flow rate limiting problem, and segregation which often occur in hopper and silo flow.

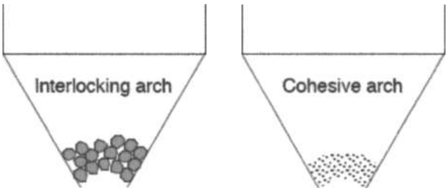

Figure 2.1 Interlocking arch and cohesive arch in a silo [Jenike, 2006].

In a hopper, a stable arch or a bridge of particulates can form above die cavities or hopper aperture which is strong enough to support the weight of the material above it causing flow stoppage. Arching can also occur during die filling. Figure 2.1 shows arch formation which is a common problem caused by interlocking particles or by cohesive particles. Beverloo et al. [1961] were among of the first to explore these mechanisms. They found that an orifice opening six times larger than particle diameter as the limit below which arching occurred. Marinelli and Carson [1992] suggested the use of a circular outlet sized about six to eight times the largest particle size to physically prevent interlocking arch.

Flow of particulate material sometimes concentrates to the centre of the solids in a silo leaving a stable stagnant zone on the sides of a hopper, a problem known as ratholing which generally occurs when the silo walls are not steep and smooth enough. A cohesive strength test can be used to determine the outlet aperture size to prevent ratholing from occurring [Dick, 2005]. Flow problems can also be caused by a sudden surge of material attempting to leave a hopper when air intermixes with falling particles. This can result in flooding which often happens when aerated fine powders start behaving like liquid and discharge uncontrollably. The aeration effect is known as fluidization. Ferrari [2002] reported that the quality of particles flow changes considerably with fluidization, and aeration was found to increase the discharge rate by more than tenfold. On the positive side, controlled aeration can be used to assist flow of particulates.

Flow rate limiting problems can be observed in closed die cavity filling. In this case, flow is slowed down by air entrapment by fine, low permeability powders resulting in the formation of a pressure gradient. Air at the bottom of the enclosed cavity is forced through the flowing powder. This pressure gradient acts against gravity and reduces the flow rate. This effect was studied by Wu et al. (c), [2003]. They found that this problem can be reduced by using particles with high permeability or by filling in a vacuum environment.

Another common problem in particulate flow is segregation. It is the separation of particles of different size, different density, different shape and different particle resilience. Williams [1976] identified particle size as the most important factor in the segregation of particulates. Bridgewater [1976] observed that segregation often occurs at the surface during flow where small particles tend to accumulate in the central region and larger particles can mostly be found close to the side walls due to their higher mobility [Standish, 1985]. Carson et al. [1986] reported that there are five segregation mechanisms: sifting or percolation which causes the movement of smaller particles through a matrix of larger particles; differences in particle velocity on the surface which slow down finer particles due to frictional drag slowing down their motions; dynamic effect which results in separation by dynamic characteristics such as inertia and resilience; fluidisation where finer particles retain air in their void spaces much longer in a bin discharge; and finally entrainment of particles in an air stream resulting in finer particles remaining suspended longer in an air stream. Sifting segregation tests (ASTM Standard D6940-03) and fluidization tests (ASTM Standard D6941-04) can be used to monitor the tendency of powders of different particle sizes to segregate. Jenike [2004] offers mechanical solutions to solve hopper problems. Table 2.1 lists and grades the effectiveness of the alternative solutions.

Even though flow problems can sometimes be tackled by trial and error, a more thorough and comprehensive understanding of the flow behaviour of particles is necessary to precisely address flow problems of particles in complex circumstances. Baxter et al. [2000] placed emphasis on the scientific studies of powder flow phenomena by simulation, which offers more understanding compared to problem solving by experience-based approach because of the ease of knowledge transfer from material to material and process to process.

2.3 Factors Affecting Particulate Flow

Many studies have been conducted by several workers on the effects of particle size, shape, cohesion, friction, packing condition, density and aeration on the particulate flow. The following discussion focuses on some of the factors affecting flow behaviour of particulates.

Table 2.1 The effectiveness of mechanical solution in hopper flow problems. [Jenike 2004].

	Problem				
Solution	**Arching**	**Ratholing**	**Flooding**	**Rate Limiting**	**Segregating**
Hopper Modification;					
Liner	Good	Good	Good	Poor	Good
Transition Hopper	Good	Good	Good	Fair	Good
Expanded Flow	Good	Good	Good	Poor	Poor
Larger Outlet	Good	Fair	Poor	Good	Poor
Inserts					
Inverted Cone	Poor	Fair	Fair	Poor	Fair
Hopper-In-Hopper	Good	Good	Good	Poor	Good
Pup Tent	Poor	Fair	Poor	Poor	Poor
Feeder Modifications					
Mass-Flow Screw	Good	Good	Good	Good	Fair
Mass-Flow Bel: Interface	Good	Good	Good	Good	Fair
Vented Rotary Valve	Good	Poor	Poor	Good	Poor
Flow-Aid Devices					
Air Cannon	Good	Fair	Poor	Poor	Poor
Vibration	Fair	Fair	Poor	Poor	Poor
Agitation	Good	Good	Fair	Poor	Fair
Aeration					
Air Permeation	Poor	Poor	Poor	Good	Poor
Fluidization	Good	Fair	Good	Good	Poor

2.3.1 Particle Shape

Particle shape contributes significantly to the shear strength of granular assembly and determines where the material will fail. Particle size, shape, size distribution and shape distribution can also significantly affect the packing density of a system. Figure 2.2 shows the qualitative descriptors to categorise the many existing shapes of particles. Large spherical particles with smooth surfaces flow better compared to smaller spherical ones.

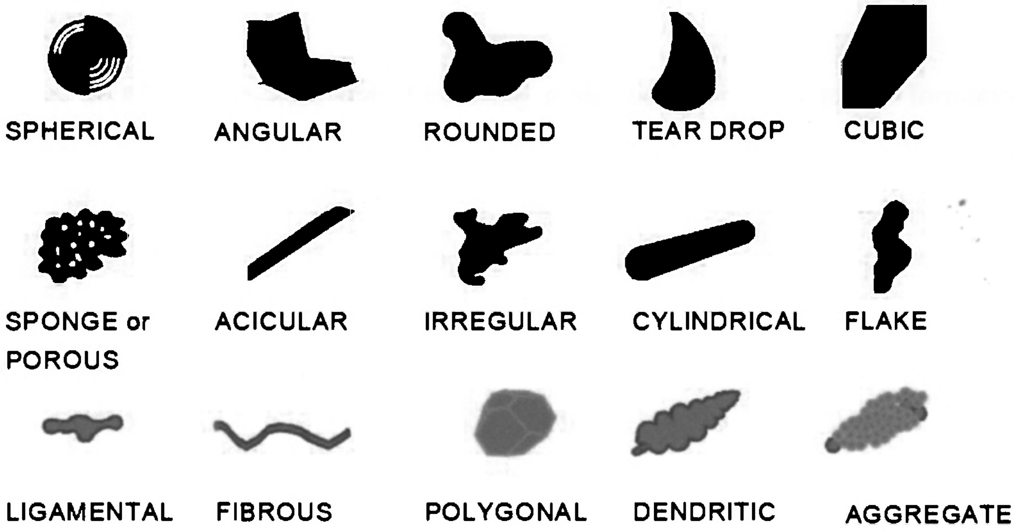

Figure 2.2 Possible particle shapes and qualitative descriptors [Verlinden, 2006].

Cleary [1999] investigated the effect of particle aspect ratio and blockiness on hopper discharge. He reported that the increase in blockiness in his simulations has reduced the flow rate by 28 percent. He found that the flow rate of elliptical particles with aspect ratio of 5:1 to be 29 percent lower compared to circular particles while angular and blocky shaped particles showed an increase in interlocking, and inhibit rolling which increases voids within the powder mass. Blocky particles with rough surfaces are found to be better at resisting flow.

Cleary [2001] reported that elongated particles produce flow rates up to 30 percent lower than those that are circular in shape. Abbaspour-Fard [2005] reported a fluid-like flow of spherical particles in a hopper simulation. Spherical particles were observed to move individually and rolled over each other during flow, resulting in a lower resistance to shear, whereas elongated particles exhibited a stronger shear due to interlocking between particles. Li et al. [2005] considered rolling friction to obtain good agreement between simulations and experiments on angle of repose for piles of spherical particles.

2.3.2 Particle Size

Kadau et al. [2003] reported that decreasing grain diameter leads to the formation of a porous media because the cohesive forces within fine particles increase. They also observed that for particle diameters in the nanometer range, the cohesive force becomes the dominant force, where particles stick together upon contact. The cohesiveness of powder was found to increase as the particle size decreases because of the increase in specific surface area. As particles decrease in size, they are more susceptible to attractive weak forces like van der Waals, electrostatic, chemical bonding, capillary liquid forces, and magnetic force which impede particle movement. Small particles are found to be the primary cause of agglomeration [German, 1994]. Since fine powders have very poor flowablity, they are turned into granules. Rodiger et al., [2000] reported that hardmetal powders of the size between 0.5 and 10 /j, m are usually converted into grains of sizes between 100 to 300 ju m to reduce cohesion.

2.3.3 Frictional Force

Friction is one of the major factors affecting particle flow. It is known to cause density variations in the final powder compact [Mesarovic, 1998]. Friction resists flow which in turn affects packing density. Interparticle friction arises from surface roughness and irregularities. The flow of powder becomes slow when interparticle friction is high. Nazer [2001] observed that an increase in friction and damping forces are responsible for significant loss in kinetic energy in gravity ore flow. In die filling, higher friction induces arching and interlocking, and voids are more likely to form which consequently lowers the packing density. On the contrary, lower interparticle friction results in a higher and a more homogeneous packing density. Coube et al. [2005] reported that the results of energy dissipation study are most sensitive to particle-particle and particle-wall frictions. The angle of repose is a simple indication for friction. The angle of repose increases significantly with the increase of sliding friction and rolling friction [Zhou et al., 2001]. A higher angle of repose relates to higher friction and lower density. Moon et al. [2003] reported that friction must be included in every simulation because it dissipates energy, reduces grain mobility, and increases overall collision rate. They observed that even though some phenomena in experiments such as pattern formation can be reproduced in simulations without the inclusion of friction, the overall effect of friction cannot be replaced by any other parameters.

2.3.4 Particle Packing

The initial packing condition of granular materials which consist of grains in contact and surrounding voids [Oda and Iwashita, 1999] has a big impact on powder flow. Singh [2007] reported that the packing state of powder has a significant influence on its flow behaviour. Modelling of particulates normally begins with settled particles. Preece [1999] adopted this technique to remove void space from the particles assemblages through gravity settling. The face centre cubic packing of spherical particles has the highest density. Initially known as the Kepler conjecture which was stated in 1611 by Johannes Kepler, this density is finally proven by Hales (2006). Theoretically, the maximum density for packs comprising identical spheres arranged in a face-centred cubic is found to be 0.7405. Munjiza [2004] showed that the theoretical density above is only achievable as spheres get smaller and smaller in size because larger particles leave a lot of pores between them during packing. For monosized spherical particles fractional densities in the range of 0.560 to 0.625 have been reported [Bocchini, 1987]. The actual packing density for PM powders ranges from 0.30 to 0.65 of the theoretical value but a mix of two monosized spherical powders can increase the maximum density from 0.637 to 0.734 [German, 1994]. The maximum density for spheres of bimodal mixture can be achieved when the large particles are in contact with one another while the interstitial voids are filled with small particles. Figure 2.3 shows that maximum density can be reached when small particles fill all the available spaces between the large particles.

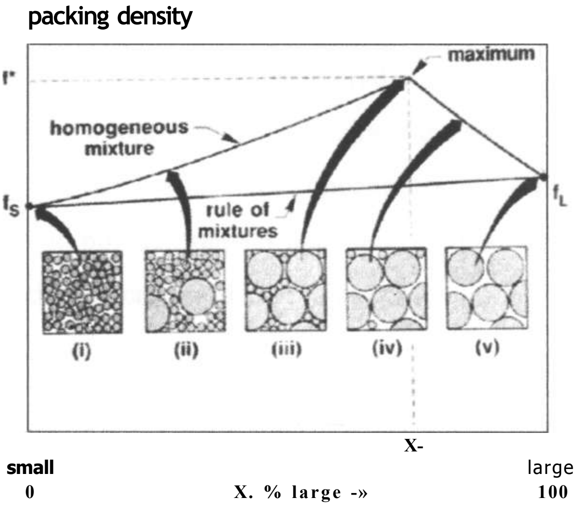

Figure 2.3 A plot of fractional packing density versus composition for bimodal mixtures of large and small spheres [German, 1994].

Packing density can also be increased by tapping and vibration [Takahashi and Suzuki, 1986]. Vibration improves the density by temporarily increasing the space around the grains, thus allowing them to rearrange. "Moving from one locally stable configuration to another, it improves the global density" [Ferrez, 2001]. Fluidization may also enhance flow. It loosens the particles by lubricating them. It reduces inter-particle friction and improves powder flow rates. Interaction of particles at rest is dominated by friction but in a fluidised state particles are readily separated from each other overcoming friction. Zahrah and Rowland [1999] reported a 31 percent to 55 percent increase in flow rate of 50 g of various powders flowing through a Hall flowmeter with the use of fluidization. They also showed that fluidization of the powder in a fill shoe can improve dimensional control and the quality of the final parts.

2.4 Density Gradient in Powder Compact

There are over forty definitions for density in the American Society's for Testing and Materials' book of standards. Even though determining the mass of granular material is fairly straightforward, the density varies depending on the way the volume of particles is determined. Figure 2.4 illustrates a few examples. Experimental method for density measurement can be found in Webb [2001], Density plays an important role in the quality of sintered products. Table 2.2 lists the density and the corresponding strength for sintered stainless steel. The density and strength increase with the decrease in porosity. Pores degrade the tensile properties and the hardness [German, 1999]. The stress on a product concentrates at pores. Density gradients which result from die filling and powder transfer may contribute to inconsistencies in dimensional changes, density, and properties of the final product which would affect product performance [Wu et al.(a), 2003].

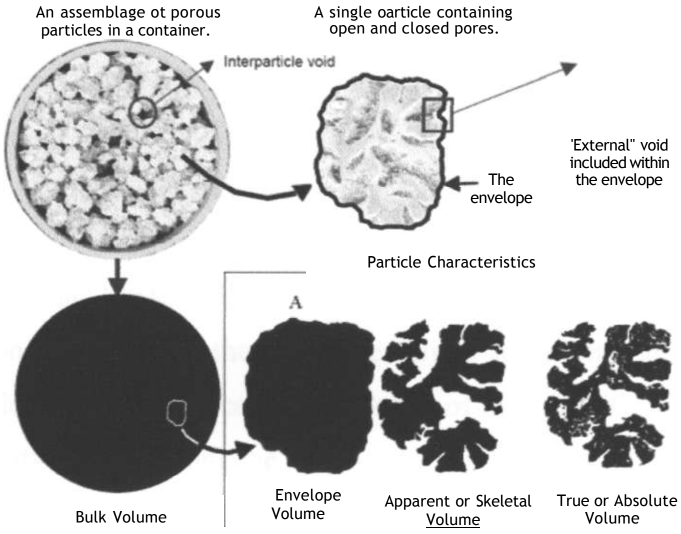

Figure 2.4 Granular density depends on the various definitions of volume [Webb, 2001].

Variations in density throughout compacts lead to variations in mechanical properties, distortion during sintering and inconsistent quality. Therefore, one of the major priorities of powder compaction is to minimise the density gradient.

Table 2.2 Density effects on Tensile Properties of Sintered 316L Stainless Steel [German, 1999].

Density, (g/cm^3)	6.31	6.66	6.82	6.94
Porosity, (%)	20.6	16.2	14.2	12.7
Yield strength, MPa	176	271	280	289
Tensile strength, MPa	308	417	444	468

Filling density in a die is often assumed to be uniform because the density gradient after initial die filling is very hard to determine experimentally. This assumption has recently been challenged. Hjortsberg [2000] reported a presence of 3% density variations specifically attributed to the filling operation. Shortened filling cycle time to increase the throughput was found to be the reason behind incomplete filling and inhomogeneous densities. He suggested controlling and eliminating this variation by the modification of the filling procedure. Ma [2004] found that two major contributors to density gradients within a compact are non-uniformity in the initial die filling, and friction between powder and the die walls. Friction was found to cause a reduction of the applied pressure with depth which results in a density gradient along the thickness of the compact. The study also reported that the density gradient increases with the increase of friction coefficient but decreases with the increase in compaction pressure.

Hjortsberg and Bergquist [2002] suspected that mechanical handling of powder from the feed shoe into the die as being a source of density variation. Wu et al. (c), [2003] reported a formation of depressions at the top of die cavity during powder transfer which would consequently affect density variation in powder compacts. Cante et al. [2005] reported that inhomogeneity of density distributions during powder filling and particle transfer can affect the subsequent compaction process.

2.5 Modelling of Powder Flow

The flow of particles is categorised as either rapid or slow. Loose rapid flows are characterized by instantaneous binary contacts with short collisions where the principle transport mechanisms are particle collisional transport and particle fluctuations, and the dense slow flows are characterized by enduring frictional contacts where the principle transport mechanisms occur through contact-force network created by continuous and simultaneous contact among particles [Chou, 2002], Both of these states of flow and a transition state in between exist together changing from one state to the other in powder delivery systems. Studies of particle flows have followed three parallel paths: (1) experiment, (2) analysis based on the assumption of a continuum, and (3) direct particle simulation. The performance of real particles can only be studied in physical experiments and DEM studies will always be based on idealised particles.

The experimental and modelling techniques complement one another to enhance the understanding of powder flow. A conventional experimental technique mainly focuses on the phenomenon at macroscopic level but cannot obtain information at a microscopic or particle level. However, the experimental results provide evidence for the validation of simulation codes and the simulations can guide the evaluation of experimental observations. Simulations allow the factors that dominate overall flow response to be identified [Wu et al (a), 2003]. This may provide more understanding of the cause and effect relationships which govern powder flow [Baxter et al., 2000]. Prescott et al. [2000] reported that there is still no universal mathematical model that exists to predict the complex powder flow behaviour in every situation. Since there are so many parameters that may influence flow, approximations are necessary to save computation time. Models are often limited to idealized systems. Energy dissipation attributed to many factors are summarised by a single coefficient of restitution, and particles are often approximated by smooth circular shapes. Even so, models do offer many advantages.

The use of simulations allows researchers to obtain values for parameters that are difficult to measure experimentally and models can simulate physically unrealistic situations where the effect of individual mechanisms can be isolated, controlled, and studied. The results can then be compared to the results of a base simulation in order to determine the effect of the isolated mechanism. Mathematical modelling of particulate flow can be classified as a continuum approach (Eulerian) at a macroscopic level and a discrete-particle approach (Lagrangian) at the microscopic level [Weber, 2004].

2.5.1 Macro-mechanical Modelling

A continuum model or macro-mechanical model considers the particle working volume as a continuum which does not allow the separation of the mass, large scale deformation or large scale displacement. This modelling method generally provides predictions on the macroscopic behaviour of the powder, such as density and stress distribution, powder displacement, the pressures acting on container walls, and compact shape during and after each forming process. The macro-mechanical method is well established in simulating forming processes and widely applied to powder compaction. It provides macroscopic behaviour of powder assembly such as density distribution, stress distributions and powder movement during and after the process [Ariffin et al., 1998]. However, continuum models are unable to capture micro-structural effects like particle interactions, particle rotation, displacement, separation, and large deformations, and it does not take proper account of real material parameters measured at the single particle level, such as friction, elasticity, cohesion, and adhesion. A macroscopic constitutive equation which is able to predict the various complicated effects exerted by granular materials, is hardly found [Wellmann et al., 2007]. It has difficulty in modelling of highly localised phenomena like the formation of shear bands and the flow of material through an orifice.

2.5.2 Micro-mechanical Modelling

The micro-mechanical approach to particle modelling assumes that the bulk behaviour of a particle system is governed by particle scale effects. The most important micro-structural considerations in granular materials are the interparticle contacts because forces are transmitted through contacts between the particles [Sharma et al., 1999]. The most computationally demanding parts of DEM are contact detection and the resolution of the contact forces which determines whether particles intersect each other [Williams, 1996]. Every grain is identified separately, with its own mass, moment of inertia, and contact properties. Particles are described by their physical properties such as shape, size distribution, inter-particle friction, particle-wall friction, cohesion, damping, adhesion, density, and their material properties such as Poisson's ratio and Young's modulus.

The DEM is a computationally expensive numerical analysis method applied for cases where the model is composed of particulate matters instead of a continuum. Particles are treated as an assemblage of distinct bodies. Individual bodies in this case may undergo motion with large displacements and rotations as well as collisions. The DEM tracks the movement of individual particles which results from the interactions between individual particles with other particles and with their surroundings, taking into account the complex mechanics of particle contacts, particle shape, material inhomogeneity, the shear and bulk deformations, and the changes of material state through failure and deformation. Equations of motions are solved for all interactions to obtain the total force acting on each particle. Newton's equation of motion is then integrated to yield the new velocity, the rotations, the orientation and the position of all particles. The trajectories of particles are updated after each time step.

Micromechanical modelling enables researchers to investigate the micromechanics of granular materials in a way that cannot be achieved in continuum approaches. The global behaviour of a large assembly of particles is computed from the motions of individual particles, inter-particle behaviour, and particle-wall interactions. Jonsen [2001] compared the Computational Fluid Dynamics method and the Discrete Elements Method in

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