CHAPTER 1
INTRODUCTION

1.1 Granular materials: A fascinating field

Granular materials are large conglomerations of discrete microscopic particles of varying size, shape and material properties, which displace from one another and interact only at the contact points. Granular materials are ubiquitous; a few examples include food products such as rice, corn and breakfast cereal flakes, building materials (sand, gravel and soil) and chemicals (coal, plastics and pharmaceuticals). They play an important role in several of our industries such as mining, agriculture, civil engineering and pharmaceutical engineering. They are also important in geological processes where landslides and erosion occur on a larger scale.

The behaviour of granular materials is determined by the material and geometric properties of the particles at the contact points. Depending on these conditions the granular materials exhibit properties reminiscent of the various states of matter; they may be deformed as solids, may have flowability similar to liquids or compressibility like that of gases. For example, a sand pile at rest with a slope lower than the angle of repose, behaves like a solid: the material remains at rest even though gravitational forces create macroscopic stresses on its surface. If the pile is tilted several degrees above the angle of repose, grains start to flow. However, this flow is clearly not that of an ordinary fluid because it only exists in a boundary layer at the pile’s surface with no movement in the bulk.

A distinguishing feature of granular flows over other flows of solid-fluid mixtures is that in granular flows, the direct interaction of particles plays an important
role in the flow mechanics. The dynamics of granular materials are highly dissipative and a significant fraction of the energy dissipation and momentum transfer in granular flows occur when particles are in contact with each other or with a boundary. Unlike the flows of solid-liquid mixtures, the temperature has no effect on grain motion since external forces such as gravity dominate the behaviour. Further the frictional interactions between the individual grains are highly nonlinear and, for static friction, even discontinuous. Also the particle size in a granular system is comparable to the length scale of flow variation; for example, the patterns such as waves resulting from the flow of granular materials occur on scales only 10-100 times that of the individual grain. Due to these unique properties exhibited by granular systems they are usually considered as an additional state of matter in its own right.

The unusual and unique character exhibited by granular material systems have led to a resurgence of interest within several scientific and engineering disciplines ranging from physics, soil mechanics and chemical engineering (Jaeger and Nagel [1992]; Behringer [1993, 1995]; Bideau and Hansen [1993]; Jaeger et al. [1994, 1996a, 1996b]; Mehta [1994]; Hayakawa et al. [1995]).

The science of granular media has a long history. Much of the engineering literature has been devoted to understanding how to deal with these materials. Notable contributions in the literature include Coulomb [1773], who proposed the ideas of static friction; Faraday [1831], who discovered the convective instability in a vibrated container filled with powder, and Reynolds [1885], who introduced the notion of dilatancy, which implies that a compacted granular material must expand in order for it to undergo shear.

Finally, there is another vitally important reason for the recent activity in this field. As mentioned above, many of our industries rely on transporting and storing granular materials. These include the pharmaceutical industry which relies on the processing of powders and pills, agriculture and the food processing industry where
seeds, grains and foodstuffs are transported and manipulated, as well as all construction based industries. Similarly, manufacturing processes in the automotive industry rely on casting large metal parts in carefully packed beds of sand. Thus it is important to develop appropriate technology for handling and controlling granular materials effectively, and this still remains as an area not yet fully explored.

1.2 Why study granular materials?

A good understanding of the physics of granular materials is desirable in designing efficient processing and handling systems. The significance of this is apparent when one considers the following statistics:

- In chemical industry approximately one-half of the products and at least three-quarters of the raw materials are in granular form (Neddermann [1992]).
- Ennis et al. [1994] estimate that $61 billion in the chemical industry is linked to particle technology.
- Approximately 1.3% of the U.S. electrical power production goes toward grinding particles or ores (Ennis et al. [1994]).
- Landslides cause a minimum of $1.5 billion dollars of property damage and at least 25 fatalities in the United States annually.
- Each year over 1,000 silos, bins, and hoppers fail in North America (Knowlton et al. [1994]).
- In Mexico, 5 million tons of corn is handled each year, 30% of which is lost due to poor handling systems.

In the chemical industry alone, it is estimated that half the products and three-quarters of the raw materials are in the form of particulates (Neddermann [1992]) and also enormous costs are associated with handling these materials. For example, a
straightforward process such as crushing ores uses approximately 1.3% of the U.S. annual energy consumption. Estimates show that around 60% of the capacity of many of the industrial plants is wasted due to problems related to the transport of these materials from part of the factory floor to another (Ennis et al. [1994]). A recent study of 40 solids processing plants in U.S. and Canada showed that 80% of the plants experienced solids handling problems and most of the plants were slow coming on-line. Furthermore, once operational, handling problems continued resulting in achieving only 40% to 50% that of its desired performance (Knowlton et al. [1994]).

In order to avoid such problems and to properly design systems involving particulates, there needs to be a better understanding of the mechanics and dynamics of granular materials. Hence, even a small improvement in our understanding of how granular media behave should have a profound impact on industry. Unfortunately there remains a poor understanding of how to model and simulate flow of granular materials. Most of the particulate handling knowledge is empirical and a scientific approach to analyzing these flows does not yet exist fully.

1.3 Granular Mixing and Segregation

Three mechanisms have been recognized as important in solids mixing (Lacey [1954]) namely, (i) convection, (ii) diffusion and (iii) shear. In any particular process one or more of these three basic mechanisms may be responsible for the course of the operation. In convective mixing, masses or group of particles transfer from one location to another while in diffusion mixing individual particles are distributed over a surface developed within the mixture. In shear mixing, groups of particles are mixed through the formation of slipping planes developed within the mass of the mixture, but this is often considered as part of a convective mechanism. A combination of the mechanisms described above promotes mixing in diverse types of mixers.
Solids mixing, also known as blending, is a common processing operation used in the manufacture of products such as ceramics, plastics, fertilizers, detergents, pharmaceuticals, food products, building materials, and cosmetics. The intent of mixing operations is to produce products of uniform quality and content and also to control the rates of heat and mass transfer and chemical reactions. Industrial devices designed to mix solids include tumblers, convective mixers, gravity flow mixers, and fluidized mixers.

However, the movement of particles during a mixing operation can also result in another manifestation known as segregation, which may retard, or even reverse, the mixing process (Henein et al. [1983a, 1983b], Nityanand [1986]). When particles differing in physical properties, particularly size and/or density, are mixed, mixing is accompanied by a tendency to segregate. Thus, in any mixing operation mixing and de-mixing may occur concurrently and the intimacy of the resulting mix depends on the predominance of the former over the latter. Apart from the properties already mentioned, surface properties, flow characteristics, friability, moisture content, and tendency to cluster or agglomerate, may also influence the tendency to segregate. The similar the ingredients are in size, shape and density, the easier the mixing operation is and the more intimate the final mix. Once the mixing and de-mixing mechanism reach a state of equilibrium, the condition of the final mix is determined and further mixing will not induce improved result.

The importance of segregation on the degree of homogeneity achieved in solids mixing cannot be over-emphasized. Any tendency for segregation to occur must be recognized when selecting solids mixing equipment. Segregation in a mixture of dry solids is readily detected by use of a heap test. A well-mixed sample of the solids is poured through a funnel so as to form a conical heap. Samples taken from the central core and from the outside edge of the cone should have essentially the same compositions if segregation is not to be a problem. When the two samples have
significantly different sizes or densities, it can be assumed that segregation would occur unless a very careful choice of equipment is made. It is generally accepted that the efficiency of a mixing process must be related to both the flow properties of the components, and to the selection or design of the mixer.

In some cases the phenomenon of segregation is exploited in order to separate or remove particles with different properties. Devices utilizing this phenomenon include vibratory sieves and Humphreys spirals and Reichert cones. In most instances, however, segregation is undesirable since it counteracts the intent of mixing operations. Even if a collection of particulates is well-mixed, subsequent transport and handling along conveyor belts or in railroad cars, for example, often results in segregation of the constituents. This is of particular concern for the pharmaceutical and ceramics industries where homogeneous blends of solids are critical.

A common approach to solids blending is to use the tumbling blender, which is essentially a hollow vessel attached to a horizontal rotating shaft. Tumblers are perhaps the most common among solid processing and mixing devices. In addition to mixing, this type of apparatus impacts such applications as drying kilns, ball mills, and coating processes. In any tumbler, the bulk of the granular material moves as a solid body, while the surface layer forms the down-surface flow. It is within this region of downward flow that mixing and segregation occurs.

Considerable efforts have been made to design mixing processes that maximize homogeneity and minimize mixing times. However, progress in understanding flow and mixing of granular materials has been hindered by the lack of understanding of their constitutive behaviour. In recent years, many constitutive relations have been proposed to model granular flows. Most of these theories are limited to a situation of either a rapid flow or a quasi-static flow. However, the flow
pattern within tumbling mixers generally consists of a rapid flowing region and a non-deforming region that usually contains a large part of the material to be mixed and therefore a scientific approach to investigate granular mixing in tumbling blenders is not yet possible.

1.4 Need for the present study

Granular flow in rotating cylinders is encountered in practical applications such as drying, mixing, and separation of particulate materials. Hence a fundamental understanding of mixing and blending of granular materials in horizontal rotating cylinders can be beneficial to a wide range of industries, namely; pharmaceuticals, metallurgy, ceramics, composites, polymers, food processing and agriculture, to name a few. Yet, in relation to its industrial relevance, the understanding of mixing of granular materials lags considerably behind that of liquid mixing (Ottino [1989]). Even though fundamental solids mixing mechanisms have been widely studied by investigators over the years (Lacey [1954]; Hogg et al. [1966]; Bridgwater et al., [1985], Bridgwater [1995]), a synthesis of these fundamentals into a coherent mixing description has been elusive. In fact, despite a substantial amount of work during the past few years aimed at understanding granular mechanics (Henein. et al. [1983a, 1983b]; Nityanand et al., [1986]; Jaeger and Nagel [1992]; Jaeger et al. [1996a, 1996b]) and powder mixing (Fan et al. [1990]; Poux. et al. [1991]) we do not yet have a full understanding of even the simplest case, namely; the mixing mechanism of two identical powders in a slowly rotated container.

Hence our research is focused on granular mixing in tumbling mixers, the simplest prototype being a horizontal cylinder, partially filled with granular material and rotated about its axis. Tumbling mixers are widely used in industry and current design practices are primarily based on empirical data. The goal of this work is to build a numerical simulation tool, which will help to evolve better designs for
equipment as well as improved industrial practice. One of the objectives of the work is to arrive at a mathematical model for the dynamics of mixing and use it to simulate real-world systems, which in turn can be used for a rational approach to design.

Engineers and physicists interested in complex non-Newtonian behaviour of granular flows have developed several continuum theories (Ottino [1989], Khakhar et al. [1997a, 1997b]). However, it is difficult to measure bulk properties such as stress, strain, and void fraction, which are necessary to develop a continuum theory, and hence continuum approach has achieved only limited success in mixing problems. Similarly, the other approaches to modelling granular flow, such as those based on statistical mechanics and cellular automata (Baxter and Behringer [1990, 1991]), while useful in certain regimes, are not general enough for all types of granular flow, and have not been successfully used as a predictive tool in granular mixing.

The success of molecular dynamic simulations for gas and liquid systems has motivated the use of the Discrete Element Methods (DEM) (Cundall and Strack [1979]; Walton and Braun [1993]; Tsuji [1993]; Mishra and Rajamani [1992]; Ristow [1994]) in modelling granular flows. These methods consider the granular material as a collection of a large number of discrete solid particles, which move independently from each other according to the deterministic laws of Newtonian mechanics. The advantage of these methods over the continuum models is their ability to simulate a wide range of granular flows with different particle sizes, shapes, and physical properties. The major drawback of the discrete models is the excessive run time for relatively small number of particles even with state of the art computers. When the number of particles is of the same order as in real flows of fine materials, the computation time becomes extremely long. Therefore, it is expensive or impossible to apply the discrete particle simulation to the case of fine powder.
Hence this work is directed towards a theoretical investigation based on Discrete Element Method (DEM) of the motion of granular solids in the radial direction of the horizontal cylinder to elucidate the relationship between the operating parameters of the rotating cylinder geometry and physical properties of the granular solid.

The operating parameters of the rotating cylinder include the various rotational velocities of the cylinder and volumetric fill. The physical properties of the granular solids proposed to investigate include particle sizes, densities, stiffness coefficients, and coefficient of friction. Finally the thesis will also investigate the following three factors of the system namely;

- **The different modes of solids motion observed in a transverse cross-section of the rotating cylinder for various rotational speeds**,  
- **The radial mixing of the granular solid as well as the transition behaviour in terms of the bed turnover time and rotational speed**  
- **Segregation mechanisms resulting from differences in the size and density of particles**.

### 1.5 Layout of the thesis

Chapter 2 contains a state of art of literature review of the transverse solids bed motion in a rotating cylinder. A comprehensive overview of all experimental and theoretical studies related to the granular solids motion in rotating cylinders is presented. The advantages and disadvantages of the various theoretical and computer aided simulation methods are also discussed.
Introduction

A detailed description of the mathematical model based on Discrete Element Method is provided in Chapter 3. The different types of contact forces available in the literature are discussed. Then formulation suitable for the dynamics of granular material motion in radial direction of the horizontal rotating cylinder is presented along with appropriate contact forces. The flow chart of the algorithm along with initial configuration generation is presented. This chapter concludes with a discussion on the validation of the software code DEMCYL developed for the present study.

Chapter 4 discusses the numerical results obtained by the simulation tool developed in Chapter 3 for a rotating cylinder of inner radius 1.5 m. The results obtained are presented both at the micro-level and macro-level. The micro dynamic analysis of the granular flow behaviour is presented in terms of the kinetic energy of the system and the radial position of the granular particles and as velocity vector plots. At the macro level, the effect of the rotational speed, fill fraction and coefficient of friction on the dynamic angle of repose are presented and discussed. Also the different types of the transverse solids motion with respect to changes in the rotational speed of the cylinder is presented in terms of the bed turnover time. The Active layer depth with respect to fill fraction and rotational speed are presented. The results obtained through simulation are compared with the experimental results of Van Puyvelde et al. [2000] and Ding et al. [2002].

An analysis of mixing and segregation in the transverse direction for different particle sizes and their size ratios is carried out in Chapter 5. The effect of fill fraction and rotational speed on the transverse mixing behaviour is presented in the form of a mixing index and mixing kinetics curve. The segregation pattern obtained by the simulation of the granular solid bed with respect to the rotational speed of the cylinder is presented. The segregation behaviour of the granular solid bed with respect to particle size, density and volume fraction of particle size has been investigated. From the results of the numerical experiments through computer
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