B. Tech Project Progress Report

STUDY OF SEGREGATION OF NON-SPHERICAL PARTICLES USING DEM IN A VIBRATING PACKED BED

Nishant Singh Sikarwar
(16112051)

Department of Chemical Engineering
Indian Institute of Technology, Roorkee

Under the guidance of

Dr. ANSHU ANAND

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ABSTRACT

In this work, we have investigated segregation of granular particles inside a vertical vibrating packed bed using open source software package LIGGGHTS. In the first part of this thesis, we have described about LIGGGHTS and come computation techniques for simulating the vibrating bed filled with non-spherical particles and in later report will do a quantitative analysis of segregation of mixed particles. We will measure the degree of segregation and study how the segregation pattern evolves with time. In the later half, we will also investigate the effect of particle shape on the degree of segregation. Specifically taking all combinations of prolate and oblate spheroids, their size segregation will be analyzed. Vibratory packed beds are mainly used in several industries such as pharmaceutical, agricultural, catalyst, plastics, minerals, food processes.

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CHAPTER 1
INTRODUCTION

1.1 What is granular materials?

Granular materials are a collection of discrete particles of similar kind. Since these materials are macroscopic, Newton's laws can be applied on them to predict their motions accurately. Many researchers have found that their behavior is very much different from solids. This result is interesting because each granular particle itself is a solid. It is also known that the granular material also distinguishes itself from other state of matter such as liquid and gases. Therefore, many researchers and scientists consider granular material as a new form of matter. Hence it could be concluded that describing each solid particle is easy, but understanding the combined behavior of granular materials is complex allowing it to exhibit striking properties.

Several variations of granular materials appear in nature, like sand or snow, but they can also be found in the industry with the shape of powders, chemicals or groups of products that are processed together. The popularisation of the DEM as a solid method and the appearance of different codes and softwares ready to solve problems related with granular materials have increased the appearances of this kind of simulations in all the engineering fields and day after day they are becoming more and more part of the aspects taken into account for scientists and engineer

1.2 Segregation

Segregation is a property of particles in which granular materials when subjected to processes like shaking or vibration will exhibit circulation patterns similar to types of fluid convection. This effect occurs due to differences in their physical properties like difference in size, shape, orientation density etc. This affects the processes which involves two or more types of granular materials in the process. This has a huge impact on the final results or products. Studying these segregation mechanisms of granular material will help in improving different industrial processes and increase the product quality.

Generally, segregation can be performed in many ways like vibration of the container containing granular material, flow them on inclined surface, percolation or passing them through fluidised bed. It this, fluidised method is used. Non-spherical particles of different physical properties like shape, density are passed in fluidised bed in the flow of air and behaviour of both types of particles is tried to observed.

1.3 Motivation and Approach of study

The process of mixing different kinds of granular particles is a common unit-operation adopted in a chemical industry. Therefore, a large fraction of equipment in industries are columns like vibrating bed and fluidized beds. They spend millions of dollars on these equipment to produce desirable mixing.

A problem faced by these industries is that under certain conditions, particles are segregated instead of getting mixed. This result is counterintuitive but has been proved by various researches both theoretically and experimentally. This segregation of particles is a problem for the industries that needs to be tackled by proper design of the Mixing equipment. This can only be done by fully understanding the segregation phenomena.

CHAPTER 2
TOOLS OVERVIEW

1.1 TOOLS

LIGGGHTS - Create the boundary of vibrating bed and then generates and settles the granular particles in the bed. Also calculates the force fields for on each particle during simulation.

Paraview - Visualisation of dump (*.VTK) files created after the simulation.

Octave - Extracts values from the dump files and apply specified operations on data for plotting the graph.

1.2 Discrete Element Method model (DEM)

The discrete element method is a numerical method used to compute different characteristics of systems that can be represented by particles. The philosophy behind the DEM is to model the actions that happen at a microscopic level and study how these actions affect the evolution of the motion of a whole media in a macroscopic level. This method needs mainly a contact detection strategy, time-discretized equations of motion governing the particle displacements and interaction laws describing the inter-particle relations.
The DEM is especially useful for granular media as its main feature is that it is modelled by particles, so either each particle simulated is going to be a single element or in case it is required to apply it to a continuous media (not usual) the material would be discretized into particle shaped elements. While the behaviour of such small elements as particles may not be valuable enough to study in a microscopic way, the gathering of all these particles acting together involves a certain magnitude of facts more than valuable enough to study in a macroscopic Basis.

1.3 LIGGGHTS

LIGGGHTS is an open source Discrete Element Method particle simulation software developed by Sandia National Labs. LIGGGHTS stands for LAMMPS Improved General Granular and Granular-heat transfer simulations, where LAMMPS is a molecular dynamics software simulator that preceded the creation of LIGGGHTS, an improved version that made the move from MD to DEM simulations by adding characteristic features from the method that cannot be found in the previous one such as the contact force formulation involving Hertz/Hooke pair styles, cohesional and rolling friction forces and heat conduction between particles.
Another LIGGGHTS's goal, besides approaching the DEM in a reliable and complete way, is to be used in industrial applications, that is the reason why it also includes the possibility of importing and handling complex CAD geometries, moving meshes to account for moving geometries and much more particle insertion options.
The LIGGGHTS code is written in C++ and can be run either in a single processor or in parallel. Its main script and the functions and libraries called by the main code are not going to be commented as there is not interaction with them in the development of the present work, but the input le is going to be explained in general basis, getting into more detail for each specific case simulated in this thesis.

A general LIGGGHTS script consists of these parts:

- Initialization - It involves setting the parameters of the atom style, types of boundaries (moving, fixed or periodic), units, processors to be involved during simulation etc.
- Region defining - It involves defining region shape (cylinder, cuboid etc), and its size.
- Atom definition - It consists of generating particles by defining the region in which the particles are inserted.
- Settings - It involves defining all the properties of atoms and the granular wall such as young's modulus, poisson's ratio, coefficient of restitution, coefficient of friction. This section also defines the size of a time-step.
- Thermal properties and model - It includes defining thermal properties of particle. Also the model to be used or variables we want to calculate and dump it.
- Running a simulation - It simply launches the simulation based on what is defined in the above three sections.

1.4 VISUAL TOOL KIT (VTK) and POST PROCESSING

Once the script in DEM is complete and the system is configured with appropriate mesh files and environment values are set according to the problem statement simulations can be launched. During the simulation dump files are generated which includes all the values of variables like velocity, position, temperature etc. of each particle at every time-step (as specified in the input file). The generated data will be converted to a certain number of snapshots according to the data and time step defined. The data containing particle

coordinates as a function of time will be used by paraview to show the dynamic and smooth movement of the particle during vibration.

CHAPTER 3
THEORY

1.1 CONTACT MODELS MOLECULAR DYNAMICS

One of the main characteristics of two body collision method is that all particles are assumed rigid. When two particles collide, there is a relation between the velocity before and after the impact. This relation is called coefficient of restitution. This coefficient can be either given or computed and it can take values from 0 to 1. The bigger the coecient is, the more the energy is conserved until one can obtain a total
energy conservation for a value of e = 1

1.2 HERTZ CONTACT MODEL

This law states the relation between the compression or overlap of the particles and the force created when they collide. Suppose two rigid and elastic spheres with specific young's modulus, radius and velocity. The contact force generated by the impact of these two particles will be a straight line passing through the point where they established contact and the centres of the particles. The value of the force will be given by this equation:

$$P = \frac{4E^*\sqrt{R^*}}{3}\delta^{\frac{3}{2}}$$

$$\delta = R_1 + R_2 - d$$

$$\frac{1}{R^*} = \frac{1}{R_1} + \frac{1}{R_2}$$

$$\frac{1}{E^*} = \frac{1 - v_1^2}{E_1} + \frac{1 - v_2^2}{E_2}$$

Where each R corresponds to each radius and the d stands for the distance between the centres of the two particles.
For the Hertz contact model, no tension force is allowed in the contact area, neither is friction and the overlap can never be bigger than the radius of the particles.
The Hertz contact law is not the only law possible in DEM problems: This model stands for the forces caused by the physical contact between two particles due to an impact, but there are other contact laws to be considered such as the liquid bridge, Van der Waals, electromagnetic forces and so on.

1.3 INITIAL PACKING CONFIGURATION

The initial particle configuration is something determined by the problem that has to be represented as accurate as possible because in most of the problems it would play a crucial role. It can involve the initial position, velocity or distribution of the particles in the domain

1.4 CONTACT DETECTION

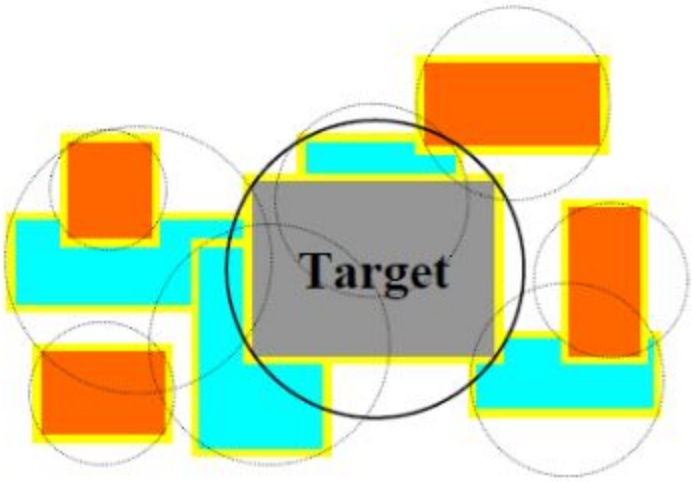


FIGURE 2.13: The idea of the contact detection

The idea of the contact detection Contacts are one of the most important aspects of the DEM and at the same time the most characteristic issue. Locating and solving them are aspects that need to be faced to obtain a realistic representation with less computational cost. This part will set the algorithm in charge of saying whether a particle is or is not in contact with another. Notice that the contact search can take up to 90 percent of the computation time as this action has to be done for every time step, following the evolution of the simulation taking into account the large number of particles involved and their specific shapes.
The contact detection is formed by three main steps:
1.The global contact search:
The first step, its mission is to locate all the possible contacts in the whole domain. In order to do that, each particle will be assigned a bounding box according to its shape. The global contact search will determine which bounding boxes overlap with a previously selected box called the target.
Bounding box:
The bounding boxes are volumes surrounding the particles that arbitrarily represent their shapes. Even if they are arbitrary geometries, each particle would have the bounding box with the closest geometry to its shape. The most common options are spheres, axis aligned and oriented bounding boxes

FIGURE 2.14: Circular bounding box

2.Locating possible contacts:
The following step is locating the possible contacts. There are several search methods:
Brutal search: Check the relation between all the bounding boxes. It requires a lot of memory, computationally expensive.
Cell/Grid based search: For that method the domain is going to be divided into a grid. The first step in this search method is finding the biggest particle in terms of size in order to give its measures to set the size of the cells. Afterwards, each particle has to be assigned into a cell in a step called the mapping stage

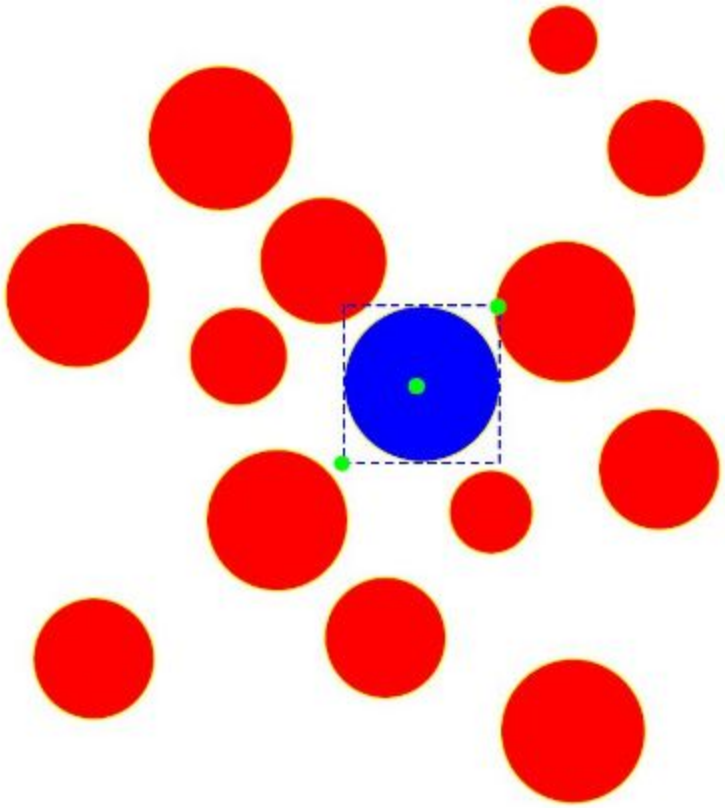


FIGURE 2.17: Brutal search: analysing the particles one by one

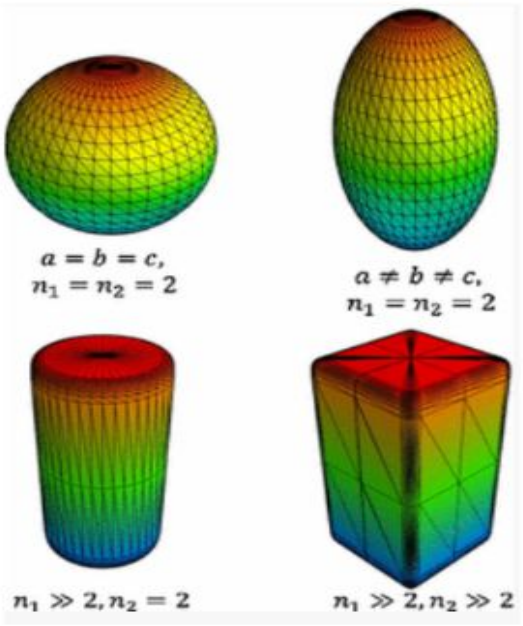
1.5 IMPLEMENTATION OF NON-SPHERICAL PARTICLES

A lot of studies using DEM are performed on spherical particles because of the simplicity in its implementation. Simulation of non-spherical particles is challenging as the orientation of particle also becomes important and therefore contact detection becomes difficult. Realistic representation of shape in DEM remains a challenge for the researchers.

But still, it has not been possible to introduce a general shaped particle in DEM. Nevertheless, the general equation of superquadrics can be written as:

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

Only recently it has been possible to introduce a class of 3-d shapes known as Superquadrics. This class of objects can represent some basic shapes like ellipsoid, cylinder and cuboids. Some of them are shown in the below figure:



The figure shows the different types of Superquadrics shapes obtained by just varying the parameters such as (a, b, c, n1 , n2) in the equation.

1.6 SUPERQUADRICS

a, b, c are the lengths along its principal axes. From fig. 2.4 it is clear that the superquadric equation is able to describe four common shapes such as sphere, ellipsoid, cylinder and cuboid by the variation in the five parameters ((a, b, c, n1 , n2)). The disadvantage of using superquadrics is that it is not able to describe shapes such as cones, pyramids and many others. Another disadvantage is the huge increase in the computation time as compared to a similar simulation launched for spherical particles. The computation times also drastically increases with the blockiness parameters n 1 and n 2 .

CHAPTER 4
SIMULATIONS

I have performed simulation using superquadric particle in the vibrating bed using LIGGGHTS on a system of 60000 particles having density 2600kg/m3.

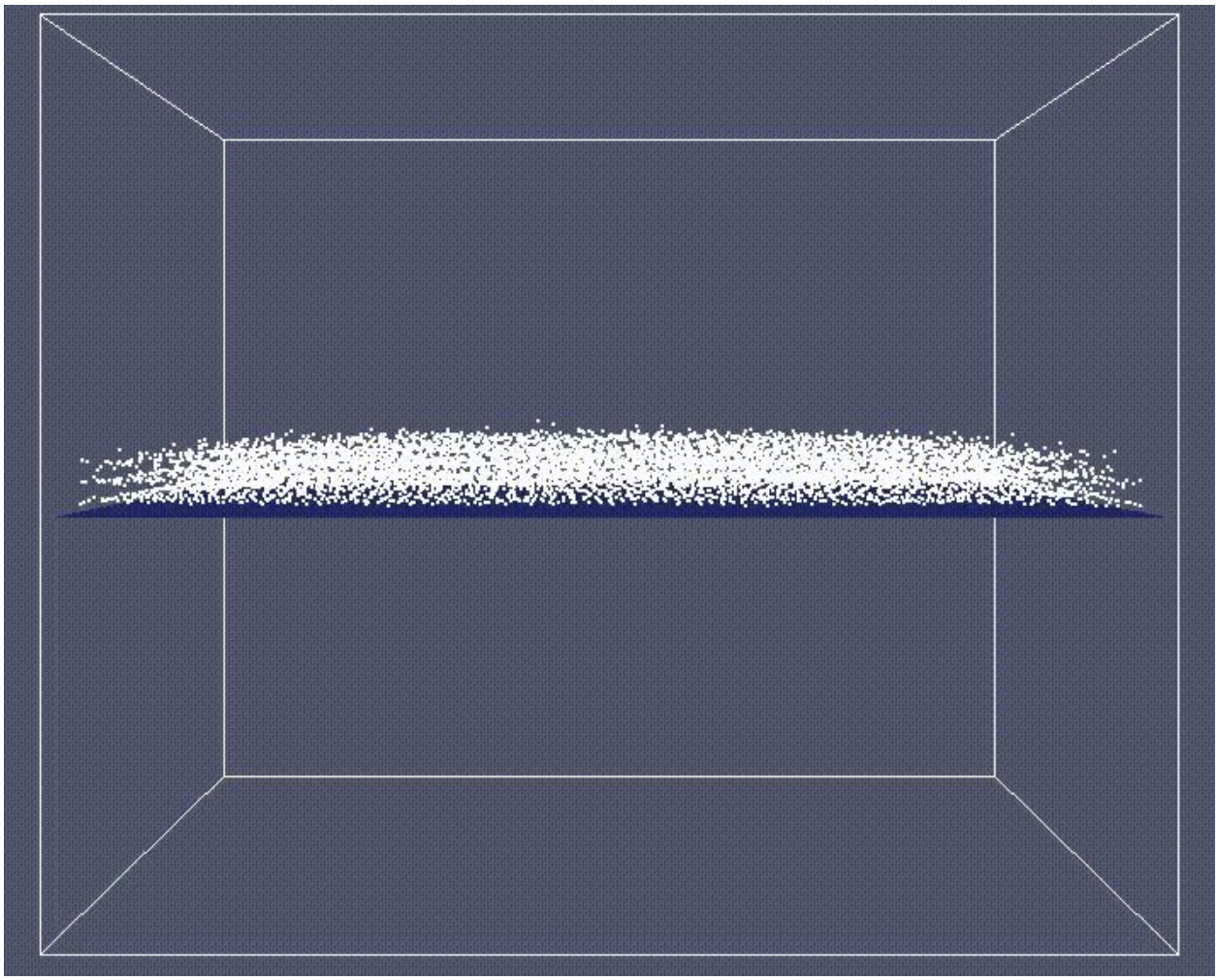
Granular particles are generated using LIGGGHTS script and settled down in packed bed generated using mesh files. After settling of particles, the bed is vibrated at two different frequencies 15Hz and 30 Hz and data is dumped at every time-step specified

So here are all the properties of system or its default configuration:

Properties	Values
Density of the particles (kg/m3)	2600
Young's Modulus (Pa)	2.3e7
Poisson ratio	0.3
Coefficient of restitution	0.1
Friction between particles and wall	0.1
Number of particles	60000
Timestep	1/512
Friction between particles	0.5
Friction between particles and end plates	0.1
Gravity constant (m/s2)	9.81
Types of particles	Granular, Superquadric

CHAPTER 5
SIMULATION PROTOTYPE

Using default configuration of system defined above here are some sample screenshots of vibrating bed using paraview:



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