B. Tech Project Progress Report

STUDY OF SEGREGATION OF NON-SPHERICAL PARTICLES IN A FLUIDISED BED USING LIGGGHTS AND OpenFOAM

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ABSTRACT

Granular particles of different radius, surfaces, sizes and shapes may get unexpected segregation when subjected to any process. As the shaking or shearing of two or more different material is subjected to any process particles of same type get segregate, unabling the circulation patterns similar to types of fluid convection. This creates a major concern to food, cosmetics, pharmaceutical industries where mixing type processes are key operation. It depends on different factors like physical properties of materials or the method used for that process or equipment used during the process.

My work contains the study of behaviour of two types of non-spherical particles when subjected to air flow in same fluidised bed using LIGGGHTS and CFDEM softwares which are open source and much more flexible to edit according to the need. Mainly, in this work only elliptical particles in taken into consideration. Till now, I have simulated two types of elliptical particles having different shapes. Also, density based simulation is also going on parallel.

TABLE OF CONTENT

CHAPTER 1
INTRODUCTION

1.1 What are granular materials

Generally, matter is classified into three solid, gas and liquid. But what about the sand or powder which take shape of the container in which they are stored. A particle of sand is obvious a solid but a pile of sand is considered as a granular particles. They are generally a collection of macroscopic particles such as wheat stored in the container. These particles are generally evaluated on the basis of Newton's equations, which have repulsive forces between them that are non-zero only when there is a contact between particles.

If a granular material is heaped on an inclined plane, then the large scale state of the system depends on the angle of the plane. For large angles the granular material flows like a non-Newtonian liquid. For small angles the granular material will behave like a solid and remain stationary. The value of the critical angle between these phases depends on the preparation history, and the transition between the phases is a manifestation of the glass transition. As the composition becomes more complicated, the behavior becomes even richer.

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 Need For The Study

Granular particles are being used in different industries like pharmaceutical, cosmetics, agriculture, chemical, cement, etc. Blenders are generally employed to mix the grains but due to lack of knowledge of particle technology, they often get segregated. Usually, industries waste a large amount of money in order to have efficient mixing. Sometimes, particle operations lead to accidents in which particles moves out of the drum which is so much destructive.

Also, the fluidized bed is widely used in today's industries. Over time, the fluidized bed has become increasingly complex and diverse to satisfy industrial needs. Generally, based on the specific requirements of each application, the solid may constitute two or more types of materials. Also, as it is already discussed it is very difficult to guarantee a narrow particle size distribution in a real industrial fluidized bed. 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 blenders. This can only be done by fully understanding the segregation phenomena.Therefore, it is crucial to understand the conditions at which the segregation of granular material would take place.

CHAPTER 2
SOFTWARE OVERVIEW

1.1 Methodology

CFDEM - Use to couple LIGGGHTS and OpenFoam and provides solver to combine both.

LIGGGHTS - Setting the different shape column of fluidised bed and generating and settling the granular particles in the bed. Also calculates the all types of forces exerted on each particle during simulation.

OpenFOAM - Fluidise the bed by passing air from the bottom of the bed as well as creating mesh of the bed. It also calculate the velocities and temperature variation during simulation.

Paraview - Visualisation of log files after the simulation.

Octave - Extracts values automatically during the simulations and represent them by plotting the graph.

1.2 Computational Fluid Dynamics / Discrete Element Method model (CFDEM)

The CFDEM method is a synthesis of CFD and DEM to model coupled fluid-granular systems(Wikipedia article on CFDEM).

The motion of the particles is resolved with DEM, and the CFD method is used to calculate the fluid flow. The granular phase which occupies a certain volume in each computational cell, is accounted for by introducing a "volume fraction" into the Navier-Stokes equations.

$$\frac{\partial \alpha_l \rho_l}{\partial t} + \nabla \cdot (\alpha_l \rho_l \mathbf{u_l}) = 0$$

$$\frac{\partial (\alpha_l \rho_l \mathbf{u_l})}{\partial t} + \nabla \cdot (\alpha_l \rho_l \mathbf{u_l} \mathbf{u_l}) = -\alpha_l \nabla p - \mathrm{K}_{sl} (\mathbf{u_l} - \mathbf{u_s}) + \nabla \cdot (\alpha_l \ \boldsymbol{\tau}) + \alpha_l \rho_l \mathbf{g} + \mathbf{f}$$

In general “l” denotes liquid and “s” solid properties. AlphaL is the fluid (liquid) content of a calculation-cell, the void fraction. “rhoL” is the fluid (liquid) density, uL the fluid (liquid) velocity, p the pressure, Ksl the implicit momentum exchange term between solid and liquid phase, us the solid velocity, tau the liquid-stress-tensor, g the gravity vector and t the time. “f” is a general explicit term which can be used to explicitly exchange momentum from the solid to the liquid phase.

The CFDEM method can, in principle, be used for any fluid-granular system. Some typical applications for the CFDEM method are fluidized bed, chemical and pharmaceutical reactors.

1.3 LIGGGHTS

LIGGGHTS stands for LAMMPS improved for general granular and granular heat transfer simulations. It is an Open Source Discrete Element Method Particle Simulation Software. It inherits all the abilities the standard LAMMPS distribution offers for the simulation of granular materials. It includes:

- Import and handling of complex wall geometries from CAD.
- A moving mesh feature to account for moving geometry
- Heat conduction between particles in contact
- A "template" mechanism to account for particle non-uniformity

A general LIGGGHTS script consists of these parts:

- Initialization - It involves setting the parameters of the atom style, types of bound - aries (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 OpenFOAM

Openfoam is a free and open source CFD toolbox. OpenFOAM stands for Open source Field Operation And Manipulation. It has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, etc. It includes more benefits over other CFD software:

- Utilities to convert mesh generated from other software to its own format.
- Tools to decompose, reconstruct and redistribute the computational case to perform parallel calculations.
- Data can be visualised using paraview, can be exported to other software for visualization. Also, supports octave which plots graph automatically picking the data during the simulation.
- Friendly syntanxing for partial differential equations and also includes flow of incompressible fluid, buoyancy driven flow solvers.

1.5 Visualisation Tools and Post Processing

Once the script in CFD and Dem is complete and the system is described fully with appropriate mesh files and variable values are set according to the problem simulations can be launched. During the simulation log 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 so generated position data was converted to a number of snapshots with the help of Paraview. The data containing particle coordinates as a function of time were used by paraview to show the dynamic and smooth movement of the particle during fluidisation. Also, the graph between pressure and velocity is generated in parallel by using octave script.

CHAPTER 3
BACKGROUND THEORY

1.1 Pressure drop through packed bed

As a fluid passes through a packed bed it experiences pressure loss due to factors such as friction. The relationships required to predict the pressure drop for a fluid flowing through a packed bed have been known that the laminar flow of water through a bed of sand was governed by the following relationship:

$$\frac{-\Delta P}{H} \propto U$$

Where P is the pressure, U is superficial velocity, H is the height of packed bed.

The pressure drop for laminar fluid flow through a randomly packed bed of monosized spheres with diameter x may be calculated using the Carman-Kozeny equation as follows:

$$\frac{-\Delta P}{H} = 180\frac{\mu U\left(1-\varepsilon\right)^2}{x^2\varepsilon^3}$$

Where x is the spherical equivalent particle diameter.

The pressure drop for turbulent flow through a packed bed may be calculated from the turbulent component of the Ergun equation:

$$\frac{-\Delta P}{H} = 1.75\frac{\rho_f U^2\left(1-\varepsilon\right)}{x\varepsilon^3}$$

The Ergun equation combines both the laminar and turbulent components of the pressure loss across a packed bed. The equation is represented as:

$$\frac{-\Delta P}{H} = 150\frac{\mu U\left(1-\varepsilon\right)^2}{x^2\varepsilon^3} + 1.75\frac{\rho_f U^2\left(1-\varepsilon\right)}{x\varepsilon^3}$$

In laminar flow conditions the first component of the equation dominates with the Ergun equation essentially reducing to the Carman-Kozeny equation, although with a slight variation in the constants used due to variations in the experimental data with which the correlations was developed. In the laminar region the pressure drop through the packed bed is independent of fluid density and has a linear relationship with superficial velocity.

Under turbulent flow conditions the second component of the Ergun equation dominates. Here the pressure drop increases with the square of the superficial velocity and has a linear dependence on the density of the fluid passing through the bed.

1.2 Packed bed friction factor

The Ergun equation may also be expressed through the use of a packed bed friction factor in a similar manner to how pressure drop is calculated for fluid flow in a pipe with the Darcy friction factor. The packed bed friction factor may be calculated using the packed bed Reynolds number as follows:

$$f^* = \frac{150}{Re^*} + 1.75$$

The Ergun equation may then be calculated using the packed bed friction factor as expressed below:

$$\frac{-\Delta P}{H} = f^* \frac{\rho_f U^2 (1-\varepsilon)}{x\varepsilon^3}$$

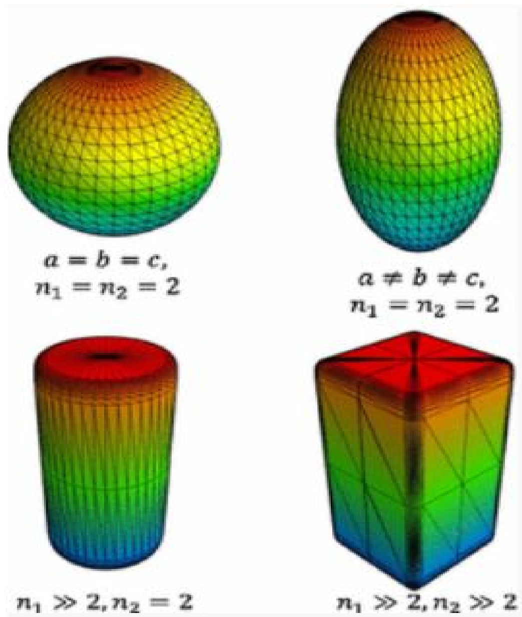
1.3 Implementation of non-spherical particles

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.

1.4 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 a coupling of two types spherical particle having different radius in the fluidised bed using open source software CFDEM on a system of 15000 particles (7500 of each type) having density 2000kg/m3. I have changed the radius of both types of particles for another simulations to detect the change in pressure drop vs velocity graph plot for all these couplings. The mass fractions of both types of particle is kept approx. 0.5.

So, initially granular particles were generated using LIGGGHTS script and settled down layer wise in the cylindrical packed bed generated using mesh files using OpenFOAM. After settling of particles, air is passed from the bottom of the bed at the velocity of 0.1 m/s having density constant of 20kg/m3 and simulations is run for 10s with logging the data of it at every 1000 time steps. Also it ensures that there will be no overlapping between particles throughout the fluidization.

So here are all the properties I have used for the fluidisation of two types of spherical particles:

Properties	Values
Density of the particles (kg/m3)	2000
Young's Modulus (Pa)	2.5*10^5
Poisson ratio	0.25
Coefficient of restitution	0.5
Friction between particles and wall	0.2
Number of particles (each)	7500
Timestep	0.0001
Friction between particles	0.25
Friction between particles and end plates	0.2
Coupling time (sec.)	10

Velocity of the air (m/s)	0.1
Density of the air (kg/m3)	20
Gravity constant (m/s2)	9.81
Types of particles	Granular, Spherical and dense

I have done coupling on these pairs of radii of the particles:

Radius of particle 1 (mm)	**Radius of particle 2 (mm)**
0.5	0.4
0.5	0.3
0.5	0.2
0.6	0.4
0.6	0.2

CHAPTER 5
RESULT AND DISCUSSION

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