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 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 spherical particles having different radius. Also, density based simulation is also going on parallel.

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INTRODUCTION

1.1 What are granular materials

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

If a granular material is placed on an inclined plane, the mass position of the system depends on the angle of the plane. For larger angles the granular material flows like a non-Newtonian liquid. For small angles the granular material will behave like a solid and remain stable. The value of the critical angle between these phases depends on the history of preparation, and the transition between phases is the manifestation of the glass transition. As the composition becomes more complex, the behavior becomes even more enriched.

1.2 Segregation

Separation is a property of particles in which granular materials when subjected to processes such as shaking or vibration will exhibit a circulation pattern similar to the type of liquid convection. This effect is caused by differences in their physical properties such as differences in shape, size, orientation density, etc. It affects processes in which two or more types of granular substances are involved in the process. This has a huge impact on the end results or products. The study of these separation mechanisms of granular materials will help improve various industrial processes and increase product quality.

In general, isolation can be performed in many ways such as the vibration of containers with granular materials, passing them through an inclined surface, orifice, or a fluid bed. This, the liquefied method, is used. Non-spherical particles of different physical properties, such as size, density, are passed into a fluidized bed in an air flow and try to observe the behavior of both types of particles.

1.3 Need For The Study

Granular particles are being used in various industries like medicine, cosmetics, agriculture, chemicals, cement etc. Blender is usually used to mix grains, but due to lack of knowledge about particle technology, they often break apart. Typically, industries have to waste large amounts of money for efficient mixing. Sometimes, particle operations cause accidents in which particles exit the drum which is so destructive.

In addition, fluidized bed is widely used in today's industries. Over time, liquefied bedding has become increasingly complex and diverse to meet industrial needs. Typically, concrete can constitute two or more types of materials, depending on the specific requirements of each application. Furthermore, as already discussed it is very difficult to guarantee a narrow particle size distribution in an actual industrial fluidized bed. A problem facing these industries is that under certain conditions, the particles are separated rather than mixed. This result is counterproductive but has been proved by various researches both theoretically and experimentally. This separation of particles is a problem for industries that need to deal with the proper design of mixers. This can only be done by fully understanding the events of isolation. In addition, it is important to understand the conditions at which separation of granular material will occur.

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 in each timestep during coupling.

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 coupling.

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 the synthesis of CFD and DEM to model coupled fluid-granular systems (Wikipedia article on CFDEM).

The motion of the particles is solved with a dem, and the CFD method is used to calculate the fluid flow. The granular phase residing in a certain volume in each computational cell is responsible for introducing the "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. AlfaL is the fluid (liquid) content of a compute-cell, the zero fraction. "RhoL" is the fluid (liquid) density, uL fluid (liquid) velocity, p pressure, Ksl underlying solid exchange period between solid and liquid phase, us solid velocity, tau liquid-stress-tusser, g. Gravity Vector and T Time. "F" is a generic explicit term that can be used to explicitly speed from solid to liquid phase.

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

1.3 LIGGGHTS

LIGGHTS means improvements in LAMMPS for general granular and granular heat transfer simulations. It is an Open Source Discrete Element Method Particle Simulation Software. It inherits all capabilities Standard offers for the simulation of standard granule distribution materials. It contains:

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

A typical LIGGGHTS script consists of:

- Initialization - This includes the inclusion of atomic style parameters, types of boundaries (moving, fixed or periodic), units, processors to be included during simulation, etc.
- Defining an area - This includes defining the area size (cylinder, cuboid, etc.) and its shape.
- Atomic Definition - This involves generating particles by defining the area in which the particles are inserted.
- Settings - This includes defining all properties of the 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 Models - This includes defining the thermal properties of a particle. Also, the model to be used or the variable we want to calculate and dump it.
- Running simulation - It only launches based on the simulation 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 many broad features to solve anything from complex fluid flow to chemical reactions, turbulence and heat transfer, etc. This includes more advantages over other CFD software:

- Utilities to convert mesh generated from other software to its own format.
- Tools for decomposing, reconstructing, and redistributing the computational case to perform parallel calculations.
- Data can be visualized using Paraway, exported to other software for visualization. In addition, Octave supports which gives the graph of the plot automatically picking up the data during simulation.
- The syntax suited for partial differential equations and includes incompressible fluid flow, bounce-driven flow solver.

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.

BACKGROUND THEORY

1.1 Pressure drop through packed bed

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

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

Where P is the pressure, U is the surface velocity, H is the height of the pack bed.

The pressure drop for the laminar fluid flow through a randomly filled bed of monosized areas with diameter X can be calculated using the Carman – Cozenian 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 filled bed can be calculated from the turbulent component of the Irgun equation:

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

The Ergon equation combines both the laminar and turbulent components of the pressure loss of a filled bed. The equation is represented as:

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

variations in the constants used due to differences in experimental data. . In the laminar region, the pressure drop through the packed bed is independent of the density of the fluid and has a linear relationship with surface velocity.

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

1.2 Packed bed friction factor

The Irgun equation can also be expressed through the use of a pack bed friction factor in a similar way to how the pressure drop for fluid flow in a pipe with the Darcy friction factor is calculated. The packed bed friction factor can be calculated using the packed bed Reynolds number:

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

The Ergon equation can be calculated using the packed bed friction factor as expressed below:

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

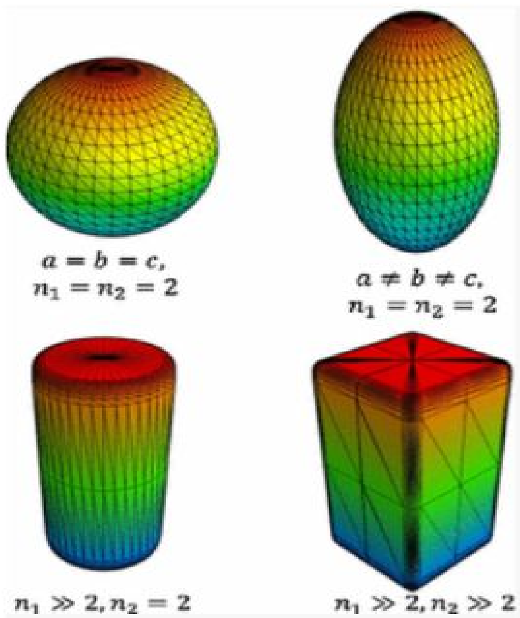
1.3 Implementation of non-spherical particles

A lot of studies have been done on spherical particles using DEM due to its simplicity in implementation. The simulation of non-spherical particles is challenging because the orientation of the particles also becomes important and hence it becomes difficult to detect the contact. Realistic representation of size in DEMs remains a challenge for researchers.

But even then, it is not possible to introduce typically shaped particles in DEMs. 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 of its principal axes. From fig. 2.7 It is clear that the superquadric equation is capable of describing four common shapes such as spheres, ellipses, cylinders, and cuboids by varying 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 more. Another disadvantage compared to similar simulations launched for spherical particles is the drastic increase in computation time. Computation time also increases greatly with interruption parameters n 1 and n 2.

Simulations

First of all, I have performed a coupling of two types of spherical particle having different radius in the cylindrical fluidised bed using open source software CFDEM on a system of particles having density 2000kg/m3. Here, initially the particles generated are already mixed. Then, I have changed this and settled the particles layer wise according to their radius. Then, I have changed the radius of both types of particles for next coupling setup just 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 1.3kg/m3 and simulations is run 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
Coupling time (sec.)	10
FLuidised bed diameter(cm)	1.5
Fluidised bed height (cm)	50

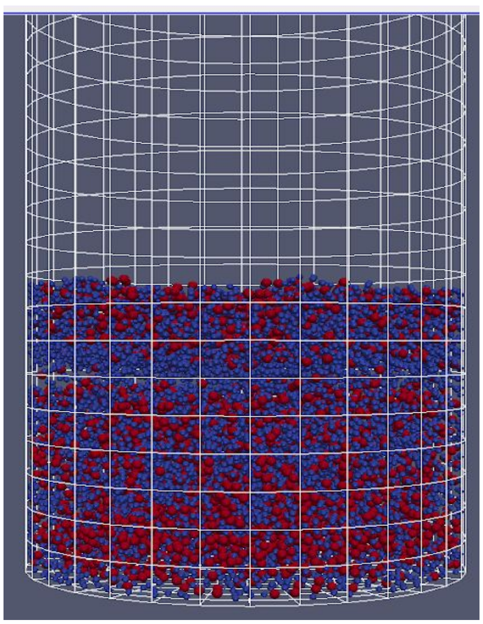
Velocity of the air (m/s)	0.1
Density of the air (kg/m3)	1.3
Gravity constant (m/s2)	9.81
Types of particles	Granular, Spherical and dense

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

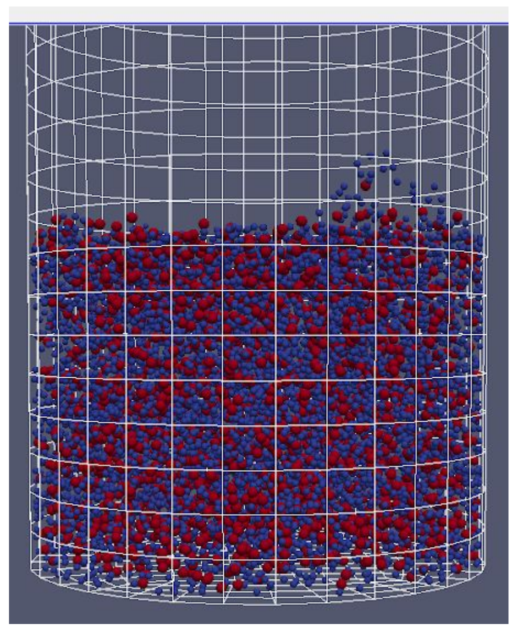
Radius of particle 1 (mm)	**Radius of particle 2 (mm)**
0.5	0.3 (without layering)
0.5	0.3
0.5	0.2
0.6	0.4
0.6	0.2

COUPLING PROTOTYPE

As, initially I have coupled simple fluidized bed containing two types of spherical particles of different radius (0.3 mm and 0.5 mm) having same mass ratio. Some screenshots of paraview visualisation is shown in below figure:



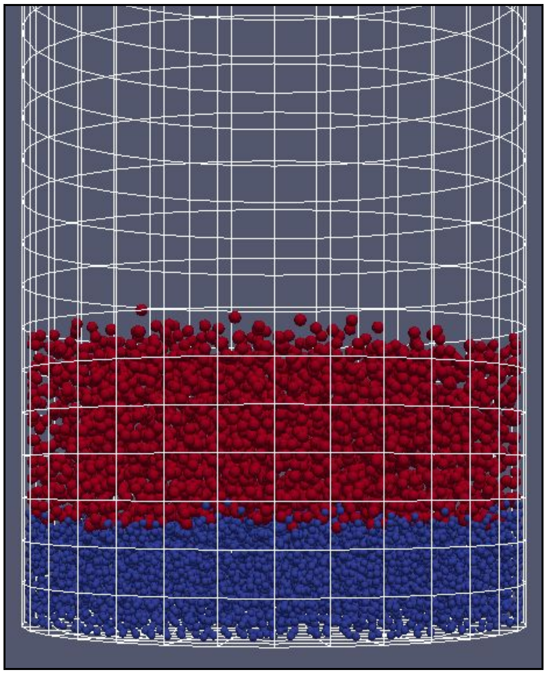
T = 0 (Initial dispersed mixture)



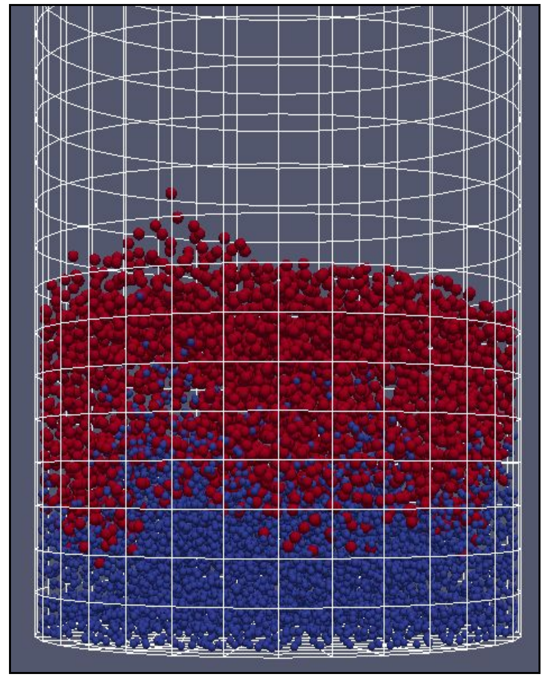
T = 10sec. (After coupling)

Here blue are smaller particles and res one large particles. Aloso, we can see in the figure that the height of the particle bed increases as fluidisation occur due to drag force on the particles due to the air passed from the bottom.

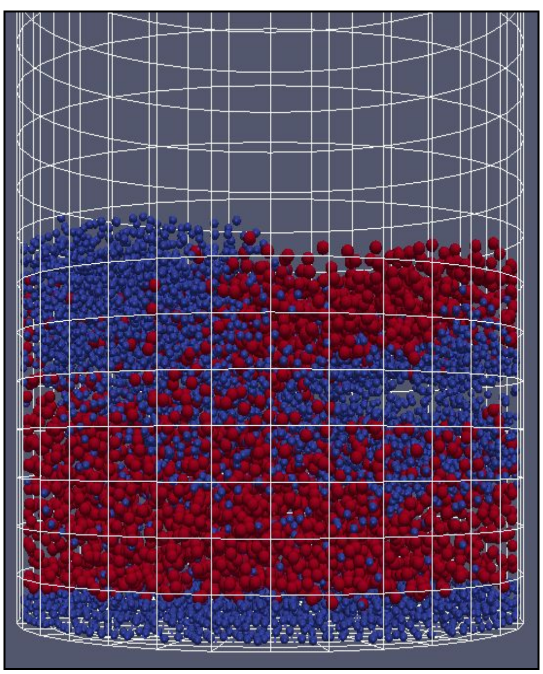
Then, I changed the script to settle the particles of different size according to their size. Such that, smaller particles settle first then bigger one. Now, I coupled some combination of layered binary mixtures having different radius spherical particles as described in the above table having same mass ratio. Some of the screenshots are added below.



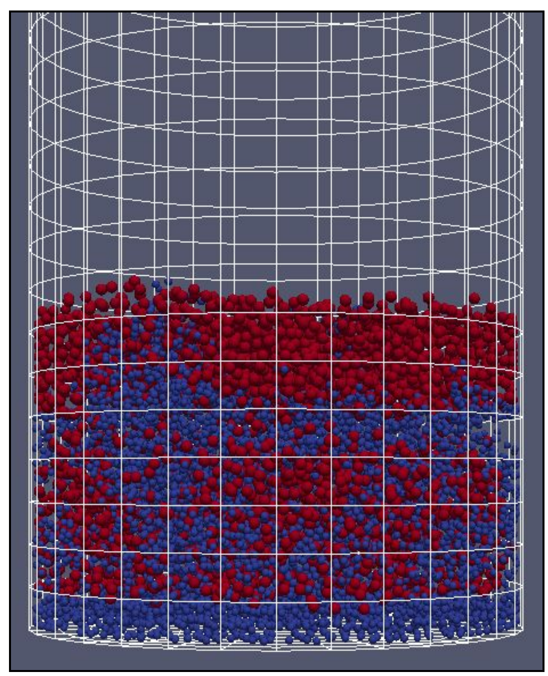
t = 0 (Initial layered set up)



t = 10s



t = 30s



t = 1min.

Here, blue one are the smaller particles whereas bigger one red. Also this is the set of particles of radius 0.6mm and 0.4mm containing 10,000 blue particles and 33,750 res particles as calculated manually to equalise the mass fraction.

- I have seen the pressure increases as the particles becomes smaller. This is also true because void fraction decreases as the particle size decreases and bed becomes dense due to which passes of air get restricted by these particles and drag force is exerted by the air leads to an increase in the size of particle bed.

- Also there is an increase in minimum fluidization velocity as the particle size becomes smaller. The reason behind this is that as the size decreases particle bed becomes more dense due to which more inertial force is required to neglect the downward gravitational force to fluidised it.

FUTURE GOALS

- Scale up the prototype to the lab fluidised bed and couple the bed containing same radius of particles used in the experiment.

- Evaluate and plot the graph of the mass fraction in each section of the bed divided into parts of the same length and compare these results with the experimental results.

- Study the coupling behaviour by changing the shape of the particles to oblate and prolate shape.

- Also, perform the coupling by changing the shape of the fluidised bed to rectangular and piramidal.

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