INDIAN INSTITUTE OF TECHNOLOGY KANPUR

CHE-616
End-Term Project

Evolution of binary size granular mixture over a long chute for rectangular cross-section with bumpy base in the presence of side walls.

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INTRODUCTION

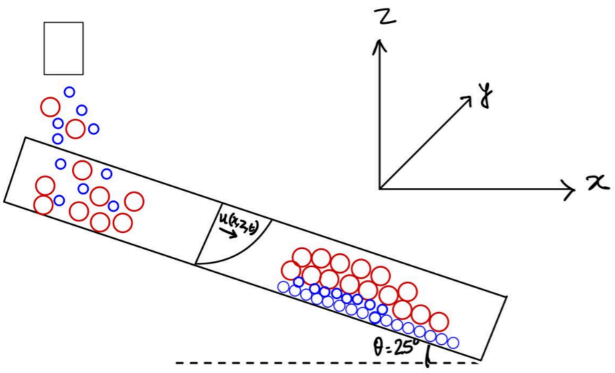
The dynamics of granular materials, such as coke particles, flowing over inclined surfaces is important in various industrial applications, including chemical reactors, furnaces, and material handling systems. Understanding the behaviour of granular flows—specifically the packing fraction and velocity profiles—under steady-state conditions is critical for optimising processes and ensuring operational efficiency. However, the complex nature of particle interactions and boundary conditions, especially in irregular geometries like bumpy bases, poses challenges for both experimental and theoretical studies.

This project employs a Discrete Element Method (DEM) simulation in the Musen framework to address these challenges. The simulation models the flow of approximately 400,000 coke particles of two distinct sizes over an inclined chute with a bumpy base. The study aims to analyse the variations in packing fraction and velocity profiles during steady-state flow and compare the simulation results with analytical predictions. This comparison not only validates the simulation model but also provides insights into the limitations and applicability of theoretical frameworks for granular flow dynamics.

SIMULATION PARAMETERS

-LONG CHUTE FLOW-:

Inclination Angle(ϴ)	**Base**	**Height**	**No of Particles**
25 deg	1000d	50d	4.1 Lakh



Schematic of chute position

-MATERIAL PROPERTIES:-

- COKE-

Density	kg/m^3	1100
Dynamic Viscosity	Pa.s	0.1
Youngs Modulus	Pa	5e+07
Poisson Ratio	-	0.2
Yield Strength	Pa	2e+10

- GLASS-

Density	kg/m^3	2500
Dynamic Viscosity	Pa.s	0.1
Youngs Modulus	Pa	1e+09

Poisson Ratio	-	0.2
Yield Strength	Pa	2e+10

- HEAVY COKE-

Density	kg/m^3	100000
Dynamic Viscosity	Pa.s	0.1
Youngs Modulus	Pa	1e+09
Poisson Ratio	-	0.2
Yield Strength	Pa	2e+10

MATERIAL-MATERIAL INTERACTION:

	Coke-Coke	Coke-Glass	H Coke-H Coke	H Coke-Glass	H Coke-Coke
Restitution Coefficient	0.5	0.6	0.001	0.001	0.6
Sliding Friction	0.3	0.3	0.2	0.2	0.3
Rolling Friction	0.01	0.01	0.1	0.1	0.01

BINARY SIZE GRANULAR MIXTURE:

Sno	Material	Diameter(mm)	Fraction
1	Coke	1	0.4
2	Coke	2	0.6

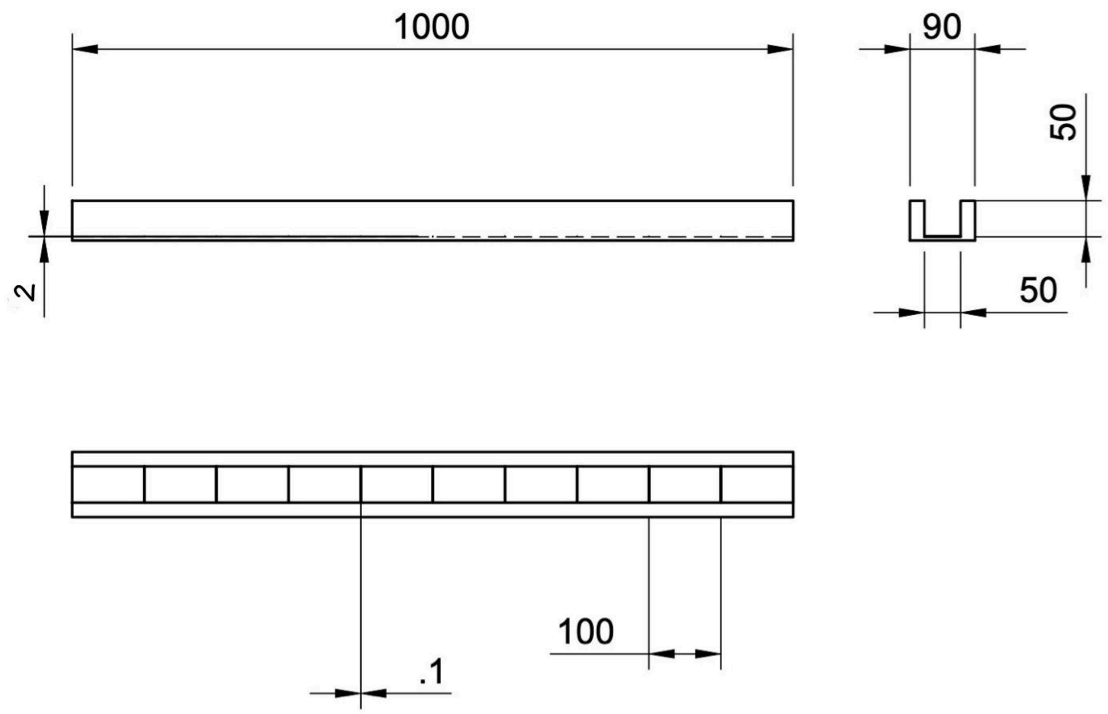
SIMULATION:

- Generation Rate (1/s)- 50000
- Updating Time Step(s)- 0.01
- Simulation Step- 8e-6
- Saving Step-0.1
- Particle-Particle Contact Model = Hertz Mindlin
- Particle- Wall Contact Model= Hertz Mindlin

PROJECT METHODOLOGY

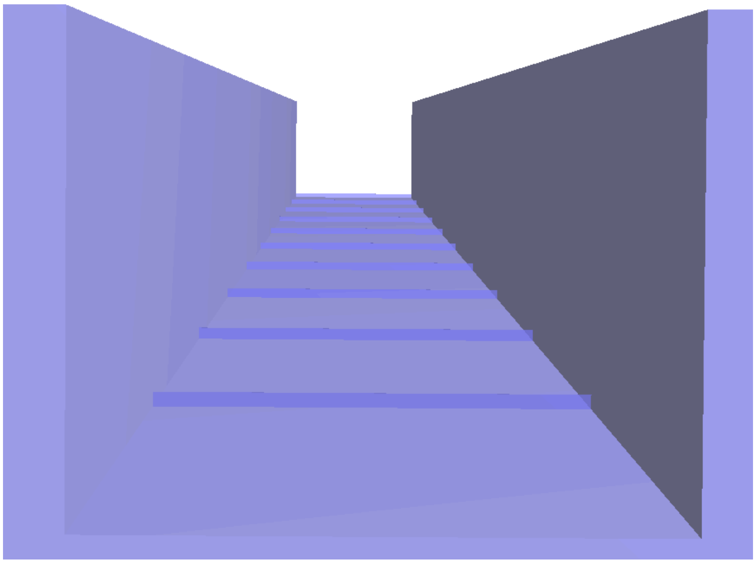
PHASE-1

BUMPY BASE:



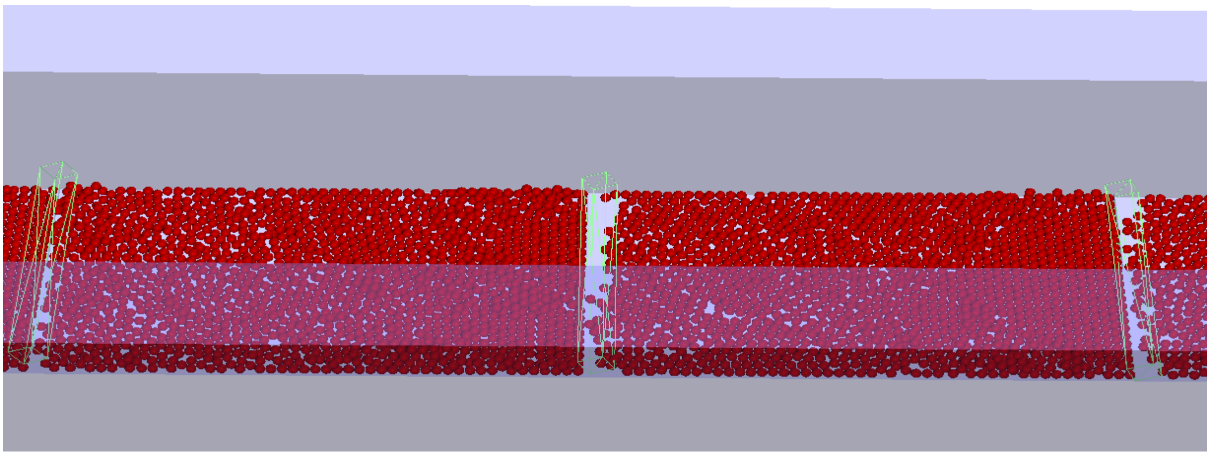
Schematic of Bumpy Base with Baffles (Measurements in mm)

Firstly, we made a long chute STL file, with baffles over a smooth surface (with the given dimensions).



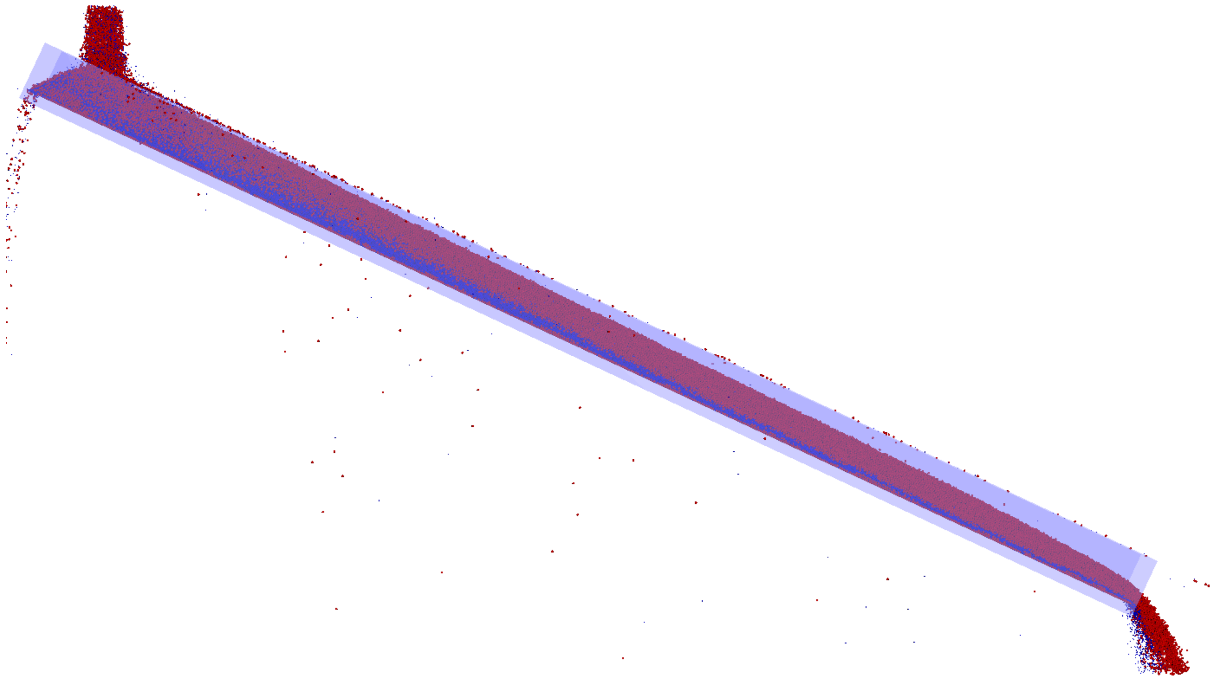
Then using multiple analysis volumes over each baffle , we generated particles of Heavy coke(2mm Dia) ,with appropriate parameters, so that they don't bounce over the glass surface along with negligible interaction with each other to act as a wall

(A single particle layer over the smooth surface)



Snapshot from Musen Scene

STEADY STATE

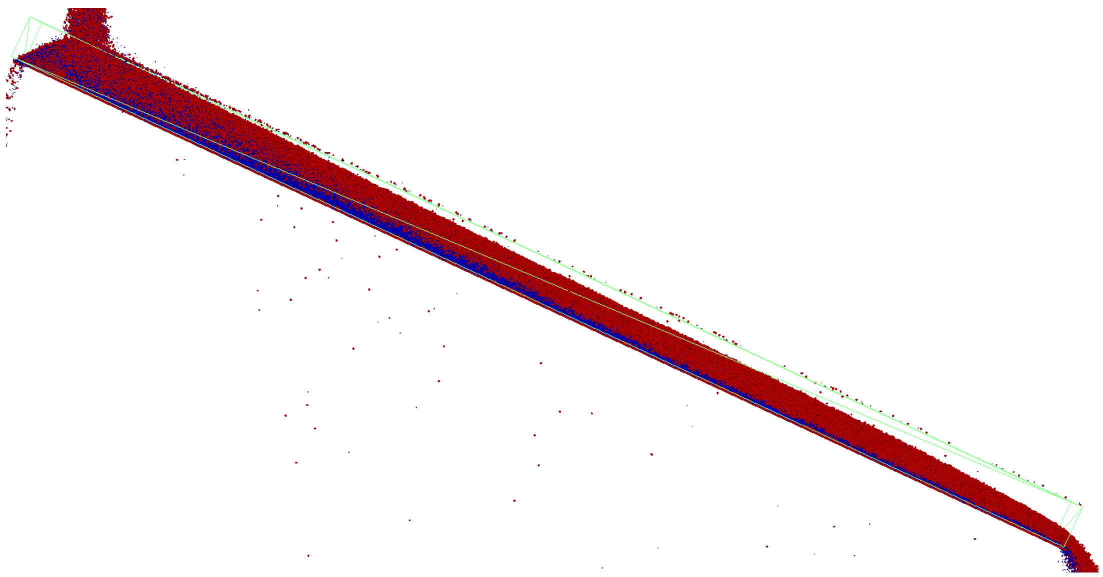


Snapshot From Musen Simulation- Last Time Step

Steady state was achieved ,with visible segregation of smaller (Blue) and Larger (Red) particles.

DATA RETRIEVAL:

Following image shows a Green Analysis Box over the region where particles are present in the steady state.



We exported a text file of the particle data and converted it into a dataframe. Following the extracted data (Un-clean) of the particles in the analysis box-

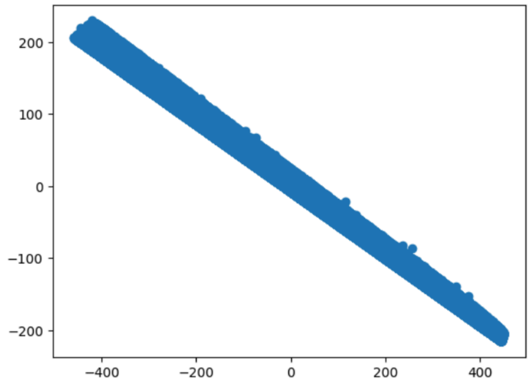
	0	1	2	3	4	5	6	7	8	9	...	30	31	32	33	34	35	36	37	38	39
0	0	192	1	1	5	0.0010	0.0010	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	0.057745	0.006391	-0.026560
1	0	195	1	1	5	0.0010	0.0010	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	0.173451	0.006024	-0.067080
2	0	243	1	1	5	0.0010	0.0010	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	0.000082	-0.000046	-0.000003
3	0	245	1	1	5	0.0010	0.0010	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	-0.000314	0.000073	-0.000171
4	0	292	1	1	5	0.0010	0.0010	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	-0.000054	-0.000105	0.000062
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
411371	0	956376	1	1	5	0.0005	0.0005	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	0.000000	0.000000	-0.117249
411372	0	956424	1	1	5	0.0010	0.0010	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	-0.006353	-0.142296	-0.370995
411373	0	956448	1	1	5	0.0005	0.0005	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	-0.199074	-0.083866	-0.719992
411374	0	956471	1	1	5	0.0005	0.0005	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	0.115690	0.057176	-0.166836
411375	0	956656	1	1	5	0.0005	0.0005	23	FTBX5F2QZF	24	...	0	0	0	0	0	0	15	-0.206153	0.053614	-0.150035

411376 rows × 40 columns

The data was very hard to interpret and so we used the documentation - (file:///C:/Program%20Files/MUSEN/Documentation/Text%20file%20format.pdf) To interpret the text file as meaningful data.

DATA PREPROCESSING:

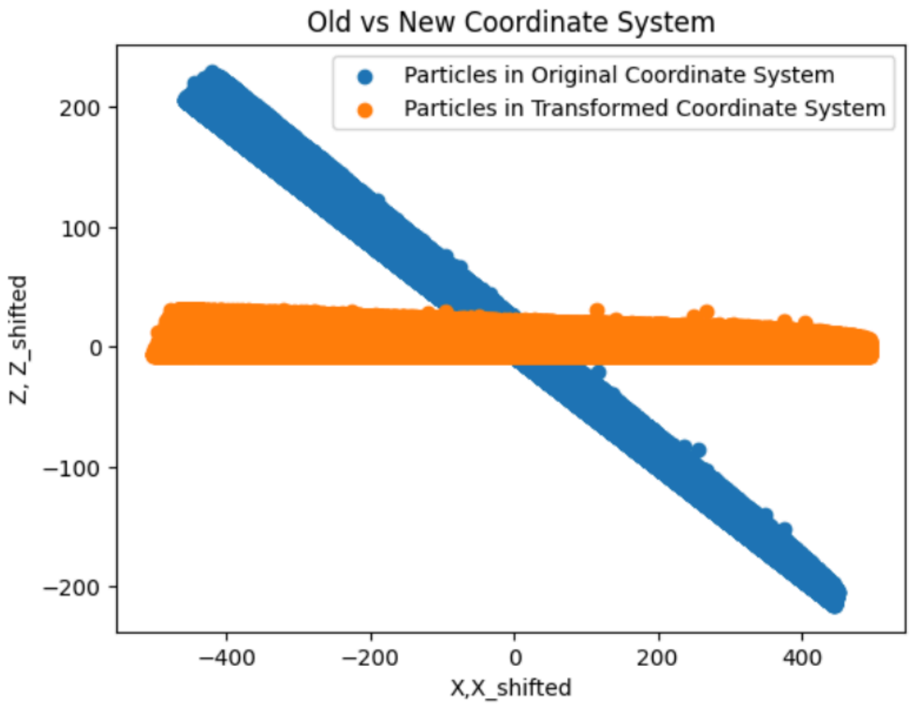
Object id	Dia (m)	x	y	z	Vx	Vy	Vz
192	2.0	61.4529	10.288400	-32.5134	0.057745	0.006391	-0.026560
195	2.0	335.1410	2.770710	-153.9060	0.173451	0.006024	-0.067080
243	2.0	-415.8060	-0.821557	187.8180	0.000082	-0.000046	-0.000003
245	2.0	-407.0930	12.307500	182.2080	-0.000314	0.000073	-0.000171
292	2.0	-408.6980	15.631600	184.4040	-0.000054	-0.000105	0.000062
...	...	...	...	...	...	...	...
956376	1.0	-411.9450	1.926480	225.4310	0.000000	0.000000	-0.117249
956424	2.0	-409.5200	-16.842000	222.9930	-0.006353	-0.142296	-0.370995
956448	1.0	-402.2590	-4.662650	221.0030	-0.199074	-0.083866	-0.719992
956471	1.0	-405.3730	-12.422100	220.8350	0.115690	0.057176	-0.166836
956656	1.0	-411.7920	6.572520	225.6590	-0.206153	0.053614	-0.150035



(X-Z scatter plot of all the particles)

To simplify the analysis in terms of x,y,z we transformed the coordinates and velocity using the coordinate transformation matrix, essentially changing the x an z coordinates

```python
def rotate_xz_clockwise(x, y, z, angle_degrees=25):

    # Convert the angle to radians
    angle_radians = np.radians(angle_degrees)

    # Define the rotation matrix for clockwise rotation in XZ plane
    rotation_matrix = np.array([
        [ np.cos(angle_radians), 0, np.sin(angle_radians)],
        [ 0,                     1, 0                    ],
        [-np.sin(angle_radians), 0, np.cos(angle_radians)]
    ])

    # Combine the coordinates into a single array for matrix multiplication
    coords = np.vstack((x, y, z))

    # Perform the rotation
    rotated_coords = rotation_matrix @ coords

    # Extract the new coordinates
    x_new, y_new, z_new = rotated_coords
    return x_new, y_new, z_new
```



RESULTS AND ANALYSIS

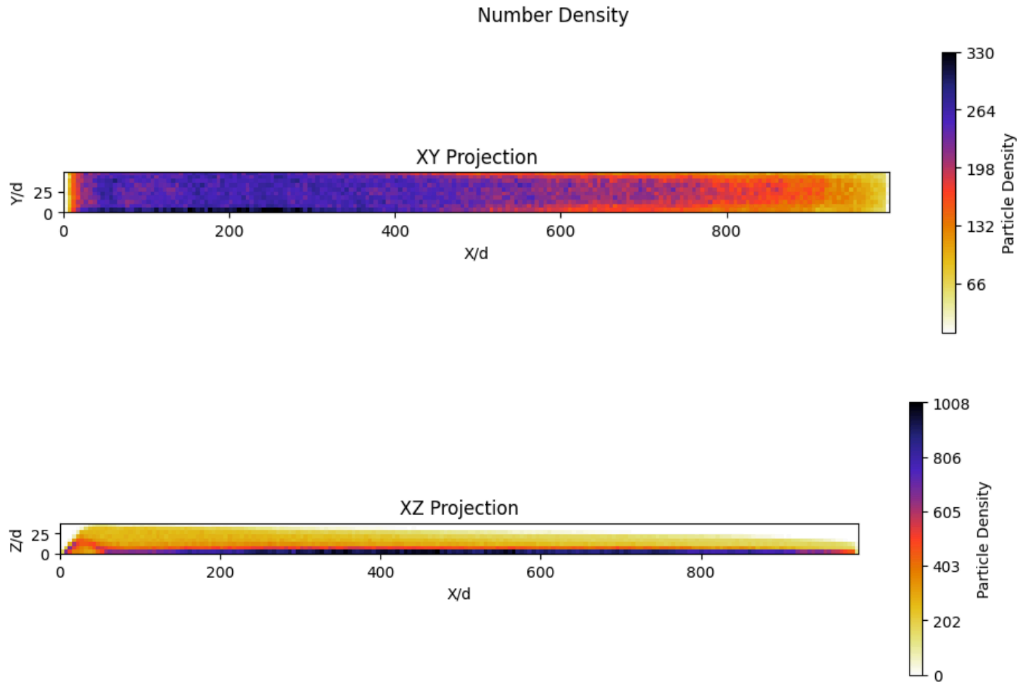
To analyse the spatial distribution of particle number density, packing fraction, and velocity profiles in the simulation, a 3D grid-based approach was employed. The simulation domain was divided into cubic cells of size 5 mm, and the following calculations were performed:

1. **Grid Setup**:
    - The simulation domain boundaries were determined (xmin, xmax, ymin, ymax, zmin, zmax), and the number of bins along each axis (x, y, z) was calculated based on the grid size.
2. **Density, Packing Fraction, and Velocity Calculations**:

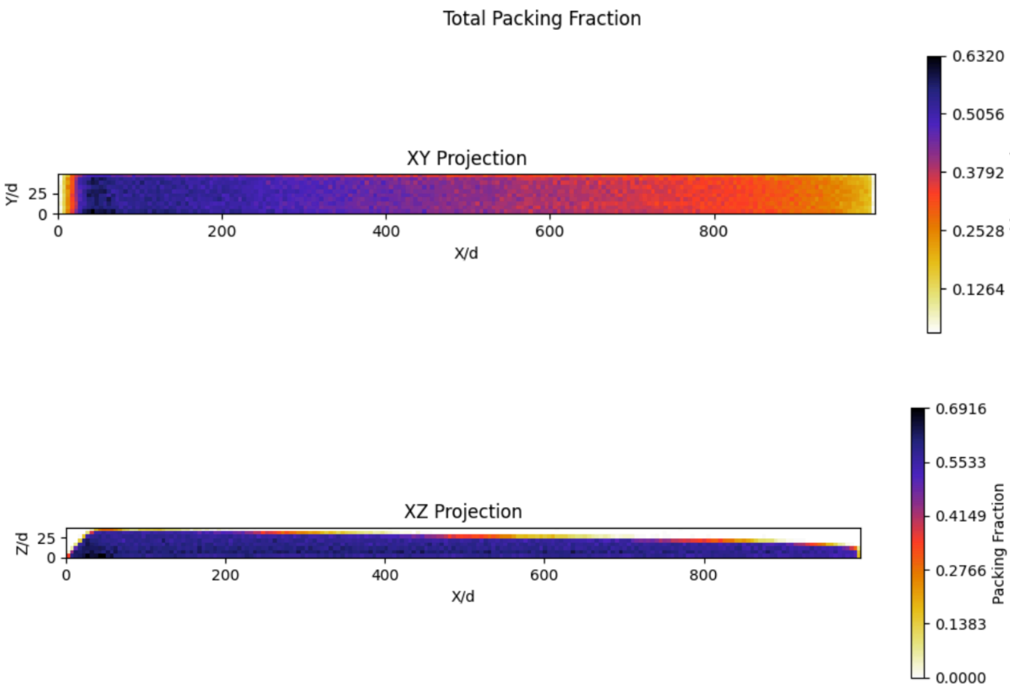
- A **density grid** was initialised to track the number of particles in each grid cell.
- A **packing fraction grid** was initialised to calculate the volume fraction occupied by particles in each cell.
- A **velocity grid** was introduced to compute the velocity profiles for the particles within each cell.

3. For each particle:
   - The corresponding grid cell was identified based on its coordinates.
   - The density grid was updated by incrementing the particle count.
   - The packing fraction grid was updated using the particle's volume, calculated as πd^3/6, where d is the particle diameter.
   - The velocity data (e.g., magnitude or components) were added to the velocity grid for later contour visualisation.
4. **Projection and Averaging**:
   - **Number density** was computed as the sum of particle counts along specific axes to generate 2D projections (e.g., XY and XZ).
   - **Packing fraction** was averaged along specific axes to create corresponding 2D projections.
   - **Velocity profiles** were visualised through contour plots for 2D projections along with line diagrams, highlighting the flow dynamics.
5. **Visualisation**:
   - The 2D projections of number density, packing fraction, and velocity profiles were visualised using heatmaps and contour plots with appropriate colour scales.
   - Separate XY and XZ projections were plotted, with grid boundaries scaled to the simulation domain for intuitive interpretation.

NUMBER DENSITY- The number of particles(1mm and 2mm) in a given volume of grid. We see in the XZ projection that the number density is higher at the bottom as compared to top and the max height of particles decreases along the x axis. In the XY projection we can see that the number density (averaged out) is decreasing along the x axis , which again shows the decrease in particle layer thickness down the chute.

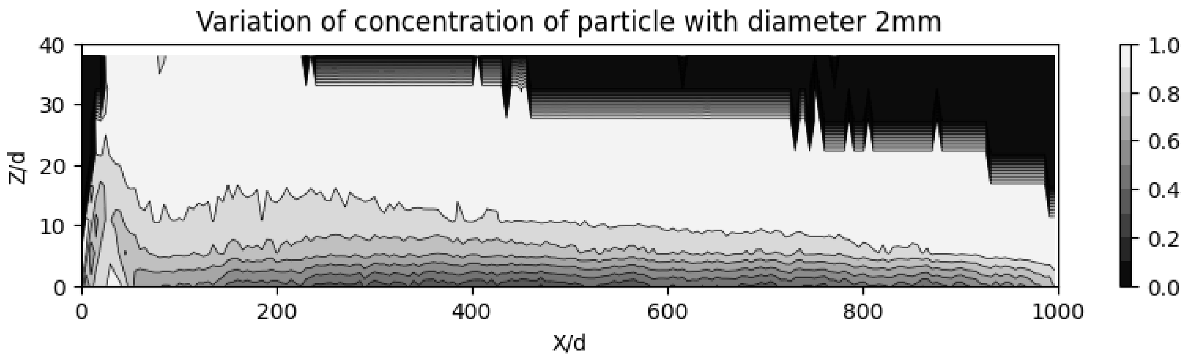


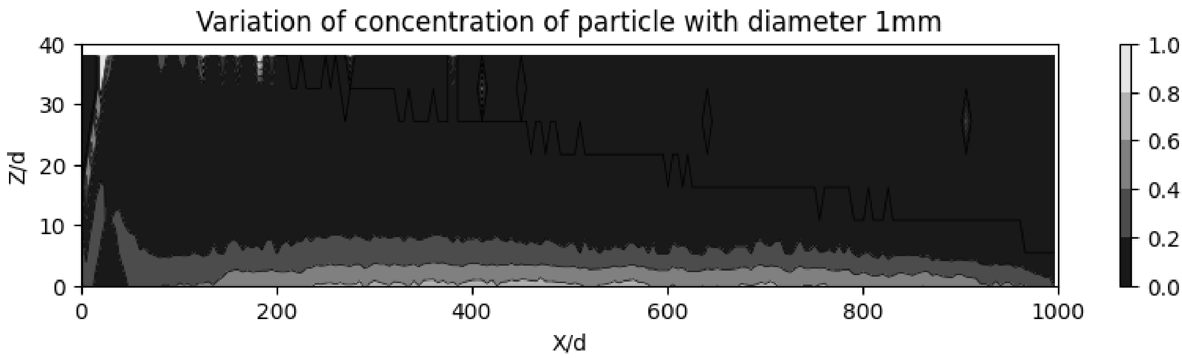
PACKING FRACTION- Similar inferences from the total packing fraction of both the particle sizes combined.PF is basically the fraction volume occupied by the particles in a grid. We have assumed that the particle is fully inside the grid containing its centre.



CONCENTRATION - It is basically the fraction of the PF of a particle type and the total PF of all particle types. Here we have 2 sizes of coke.

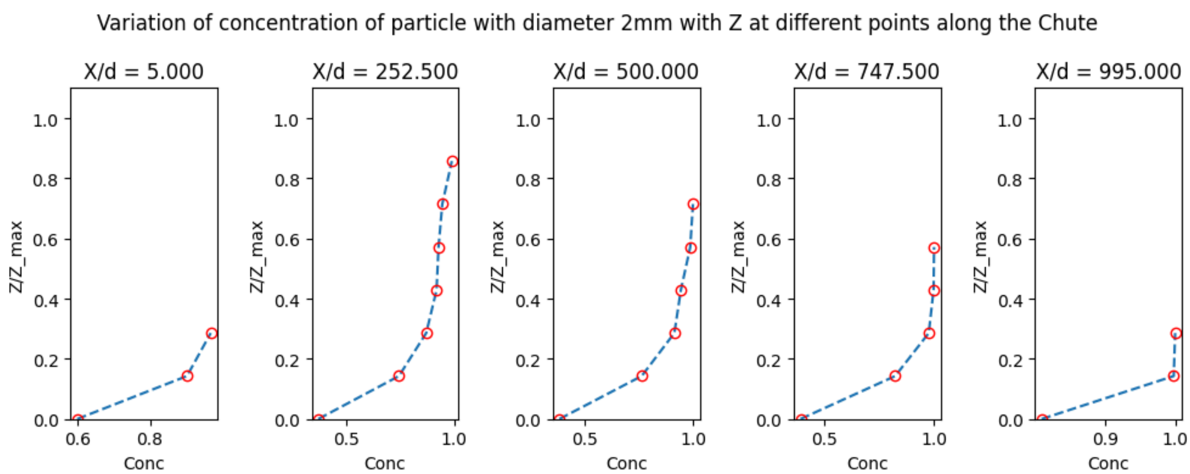
We will look particle wise concentration profile and try to compare it with the results of a similar published paper -

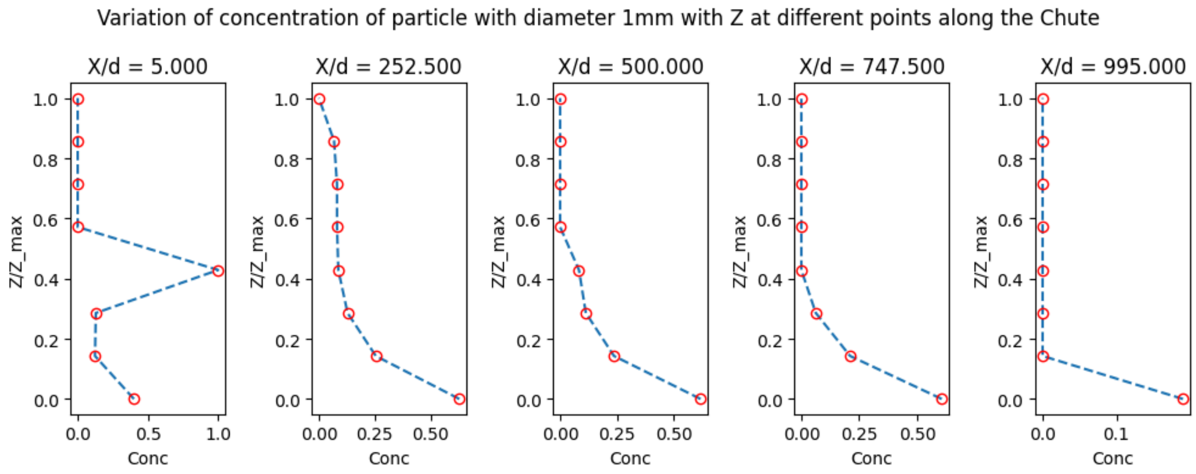




This is a contour plot of the concentration in the x-z plane. We have done gaussian smoothing in order to negate the effect of any particle which is not a part of the heap.

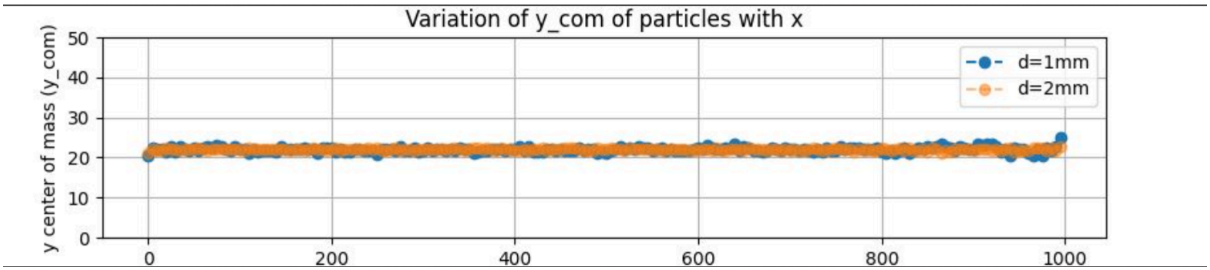
We can clearly see that the concentration of 2mm particles increases with increasing z/d whereas for 1mm particles it decreases.

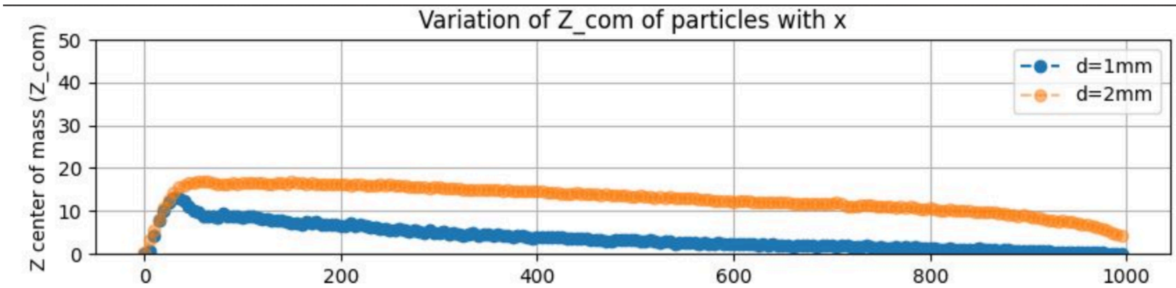




We see the effect of segregation of the particles in the above plots. And comparing it with the fig 7.c of the paper, we will focus mainly in the fully developed region (200-700 x/d)

POSITION OF COM-

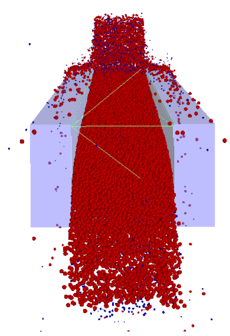




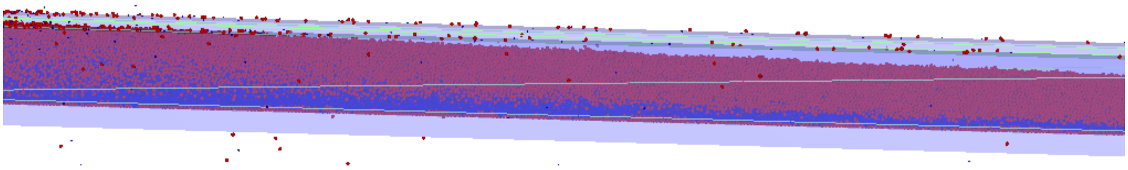
Position of the centre of mass shows the overall general distribution of particles.

We see the Ycom is similar for both the particle types
Showing overall central flow (within Y), since no external
Force in this direction and also the side walls which keep
All the particles motion restricted to the flow direction.

←Y→



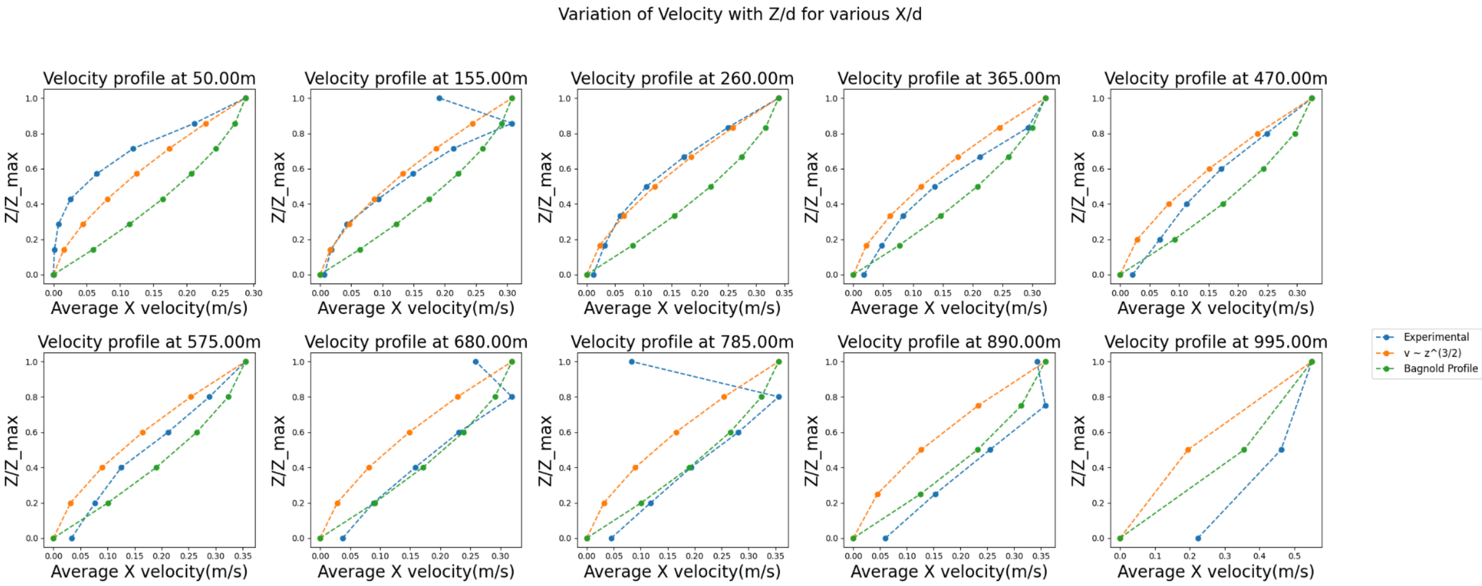
I
Z
I



We see that the Zcom of 1 mm particles is below that of 2 mm particles due to segregation of the two, down the chute.

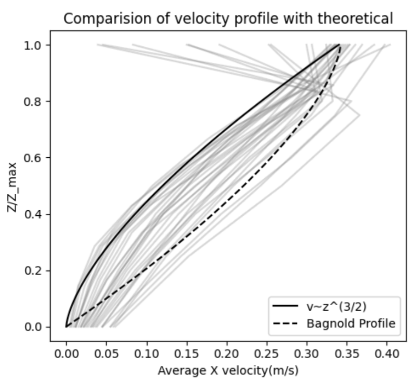
VARIATION OF VELOCITY-

We plot the variation of velocity along X with respect of Z at different equally spaced points along the chute.



For the fully developed region we can see that velocity mostly varies as a function of z^(3/2).

According to theoretical derivations of steady fully developed flow down an inclined surface, we know that V_x depends on z^(3/2).



Hence our experimental results match with theoretical findings. We also compare our results with Fig 5 of Wiederseiner et al.

The grey line indicate actual velocity profiles down at points down the chute.

CONCLUSION

We perform analysis of fully developed flow down an inclined surface for a mixture of particles with diameters 1mm and 2mm.
We find that segregation of particles occurs, and the particles with a diameter of 1mm settle below the particles with a diameter of 2mm.
We also perform an analysis of how mixture velocity varies with with height of heap down the chute. We find that in the fully developed region, simulation results are close with theoretically derived equations for velocity.