Development and Evaluation of a General Drag Model for Gas-Solid Flows via Physics-Informed Deep Machine Learning

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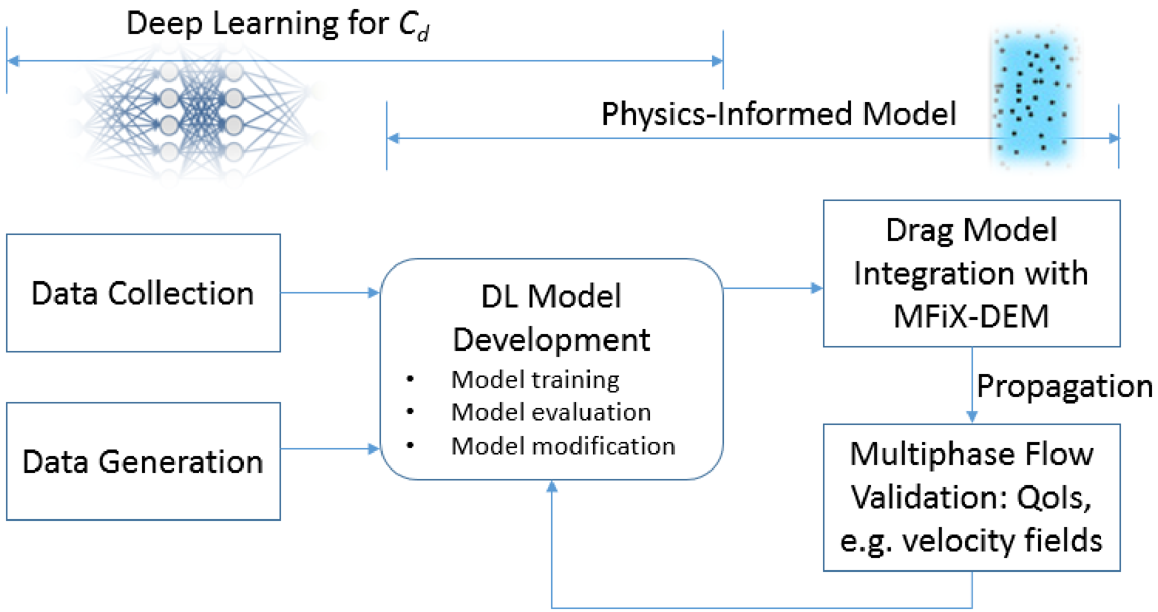
Agenda

- Project Objective
- Project Status
- Technical Progress
  - Background/Motivation for the Project
  - Data collection
  - Features considered
  - Gated DNN modeling
  - Integration with MFiX
  - CFD validation with single particle
  - Assemblies of particles
  - CFD validation with Fluidized bed
- Conclusions

Project Objective

The overall objective of this project is to develop, test, and validate a general drag model for multiphase flows in assemblies of non-spherical particles by a physics-informed deep machine learning (PIDML) approach using artificial neural network (ANN).

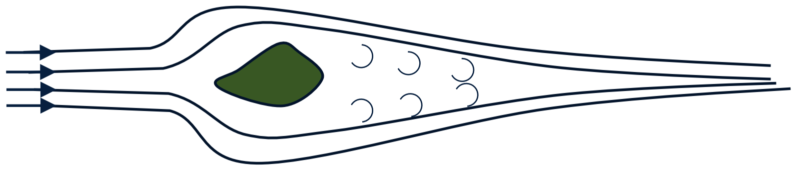


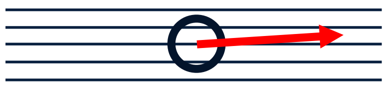
CFD Software

Project Status

Task Name	Assigned Resources	Year 1				Year 2				Year 3			
		Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4
Task 1.0 - Project Management and Planning	**PI**												
Task 2.0 - Data Collection and Generation	**Team**												
Subtask 2.1 Data Collection	Team												
Milestone A													
Subtask 2.2 Data Generation	Co-PI												
Milestone B													
Decision Point 1	Team												
Task 3.0 - ANN Model Development	**Co-PI**												
Subtask 3.1 ANN Model Training & Test	Co-PI												
Milestone C													
Subtask 3.2 ANN Algorithm Evaluation	Team												
Milestone D													
Decision Point 2	Team												
Task 4.0 - Drag Model Integration	**Team**												
Milestone E													
Decision Point 3	Team												
Task 5.0 - Multiphase Flow CFD Validation	**Team**												
Subtask 5.1 Multiphase Flow Validation	PI												
Milestone F													
Subtask 5.2 ANN Model Modification	Co-PI												
Milestone G													

Motivation

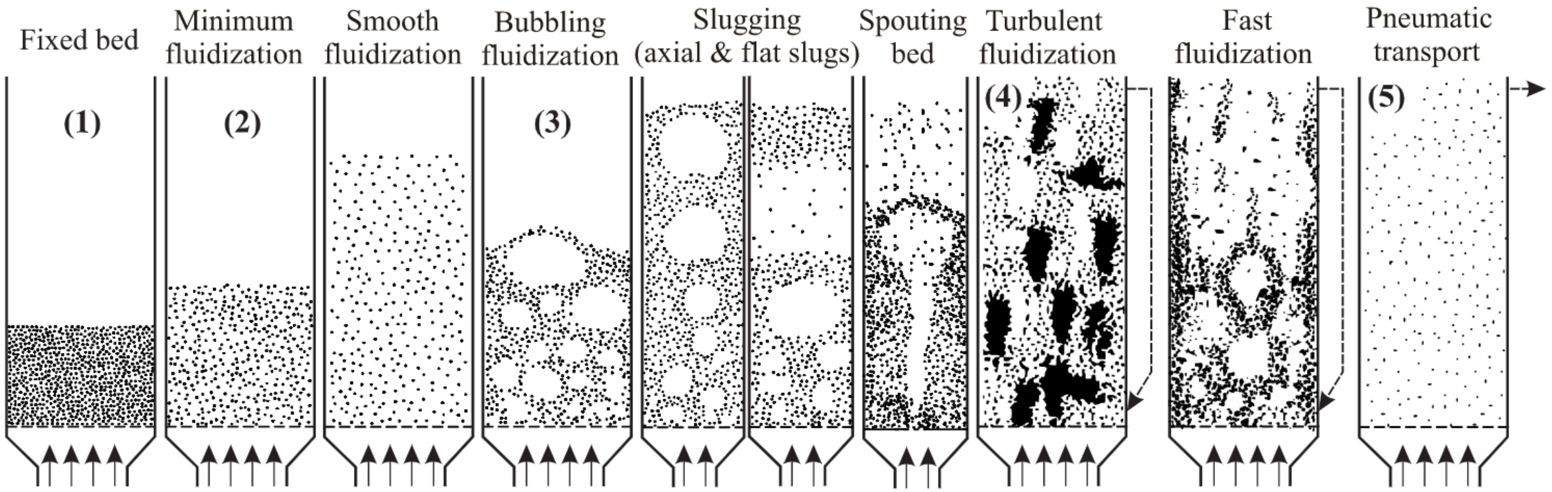




$$\rho_g \frac{DV}{Dt} = -\nabla p + \nabla \overleftrightarrow{\tau} + \overrightarrow{F_D}$$

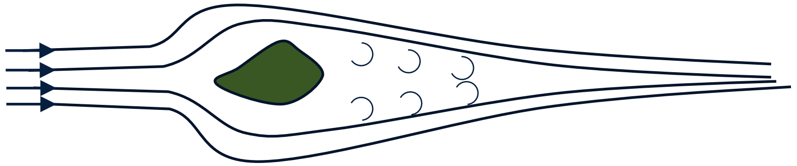
$$Drag\ force\ (F_D) = \frac{1}{2} \rho_g |V_r|^2\ A_p\ C_D$$

1. Energy industry
   - Gasifiers
   - Combustion
2. Food industry
3. Chemical process

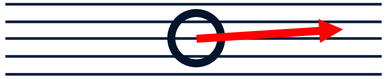


Alobaid, F., Almohammed, N., Farid, M.M., May, J., Rößger, P., Richter, A. and Epple, B., 2022. Progress in CFD simulations of fluidized beds for chemical and energy process engineering. *Progress in Energy and Combustion Science*, *91*, p.100930.

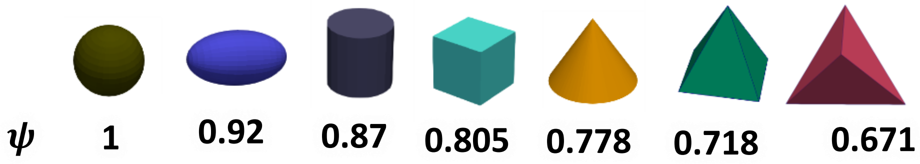
Motivation



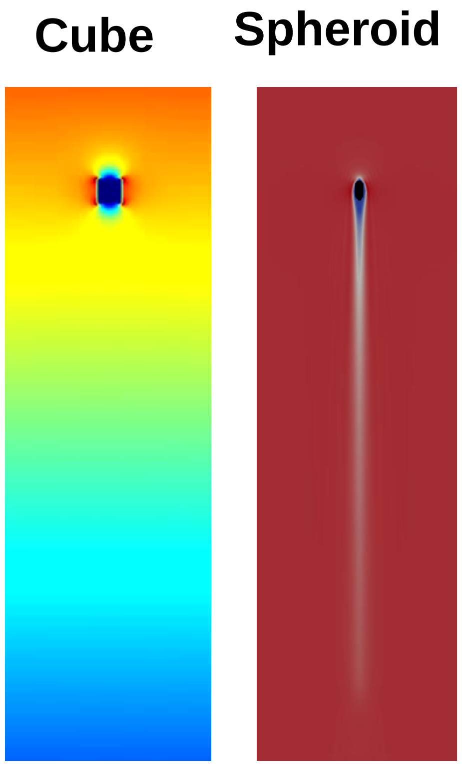
$$Drag\ force\ (F_D) = \frac{1}{2}\rho_g |V_r|^2\ A_p\ C_D$$

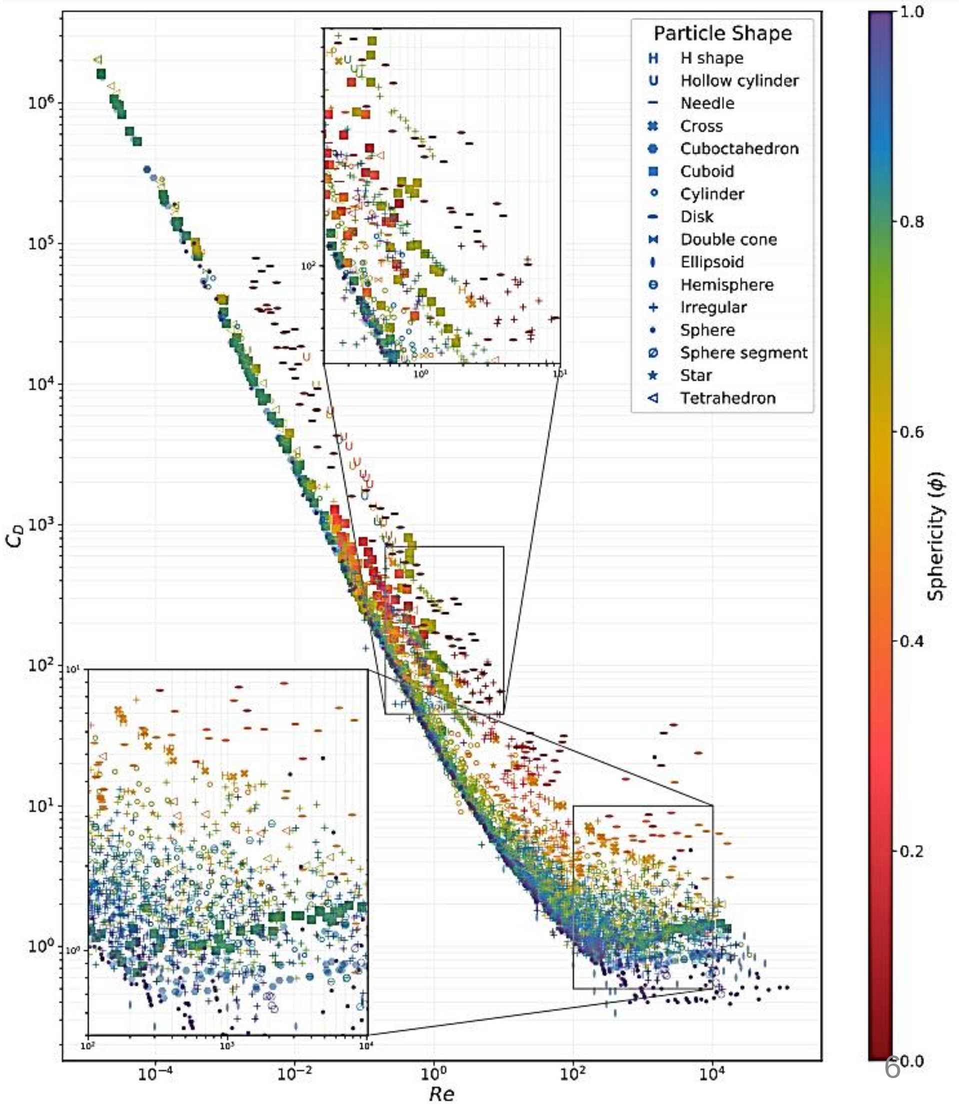


$$\rho_g \frac{DV}{Dt} = -\nabla p + \nabla \overleftrightarrow{\tau} + \overrightarrow{F_D}$$



- The drag coefficient primarily depends on
  - Shape
  - Reynold number
- The variations are highly non-linear
- Single correlation cannot cover all the particles
- Requires more sophisticated modelling such as Neural network





Current State-of-Art

$$C_D = \frac{24}{Re}(1 + 8.1716\exp(-4.0655\psi) * Re^{0.0964+0.5565\psi} + 73.69 * Re * \frac{\exp(-5.0748\,\psi)}{Re + 5.378\exp(6.2122\,\psi)} \qquad \boldsymbol{\psi > 0.67}$$

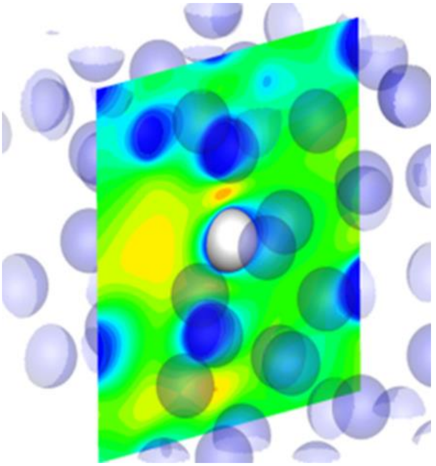
- Haider & Levenspiel (1989)
- Yow et al. (2005)
- Hölzer & Sommerfeld (2008)
- He & Tafti (2019)
- Yan et al. (2019)

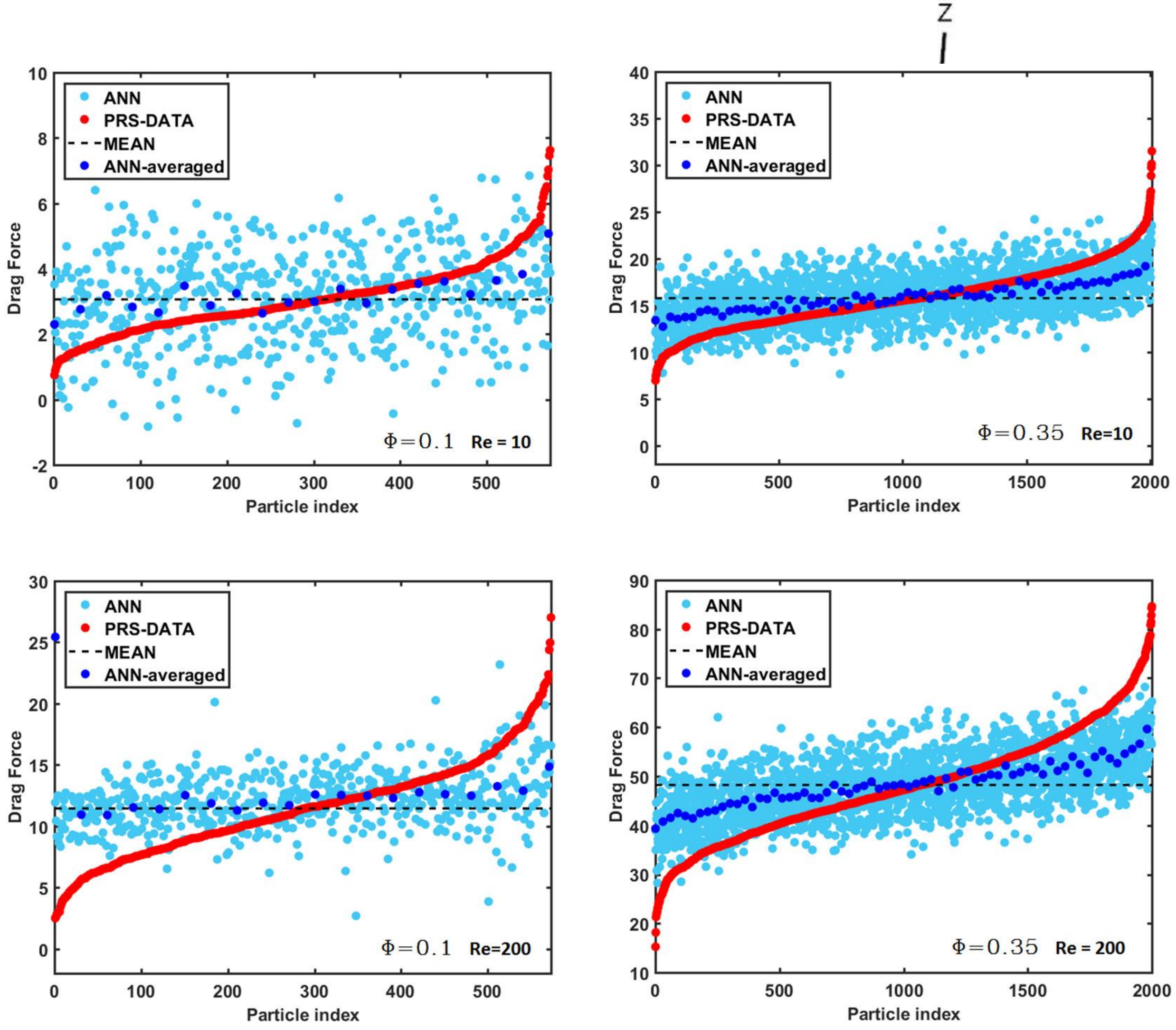
$$C_D = \frac{a_1}{Re} + \frac{b_1}{\sqrt{Re}} + c1$$

$$C_D = \frac{8}{Re}\frac{1}{\sqrt{\boldsymbol{\psi}_{||}}} + \frac{16}{Re}\frac{1}{\sqrt{\boldsymbol{\psi}}} + \frac{3}{\sqrt{Re}}\frac{1}{\boldsymbol{\psi}^{3/4}} + 0.421^{0.4(-\log\boldsymbol{\psi})^{0.2}}\frac{1}{\boldsymbol{\psi}_{\perp}}$$

Current State-of-Art

Nearest Particles' location





- Haider & Levenspiel (1989)
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- He & Tafti (2019)
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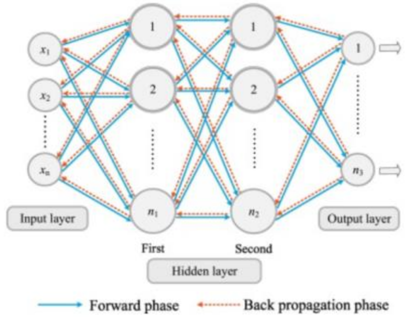
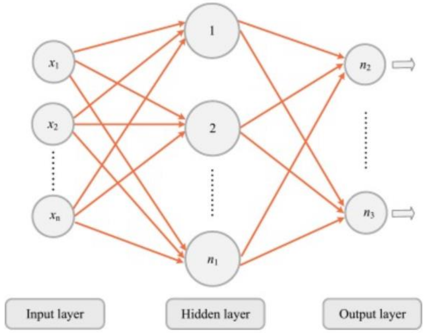
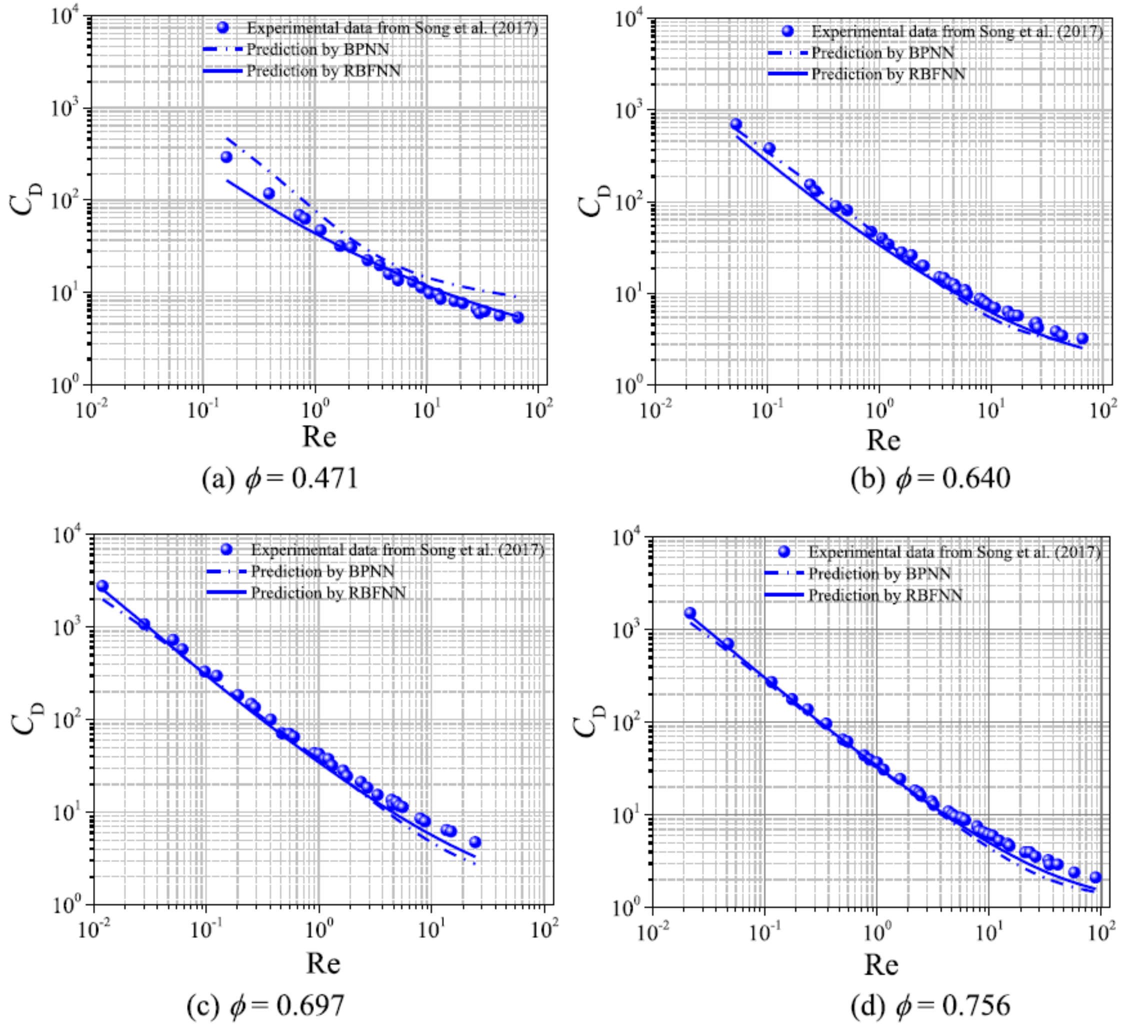
Current State-of-Art

BPNN



RBFNN





$$\lg C_D = A_0 + A_1 \lg \mathrm{Re} + A_2 (\lg \mathrm{Re})^2 + A_3 (\lg \mathrm{Re})^3 + A_4 (\lg \mathrm{Re})^4$$

- Haider & Levenspiel (1989)
- Yow et al. (2005)
- Hölzer & Sommerfeld (2008)
- He & Tafti (2019)
- Yan et al. (2019)

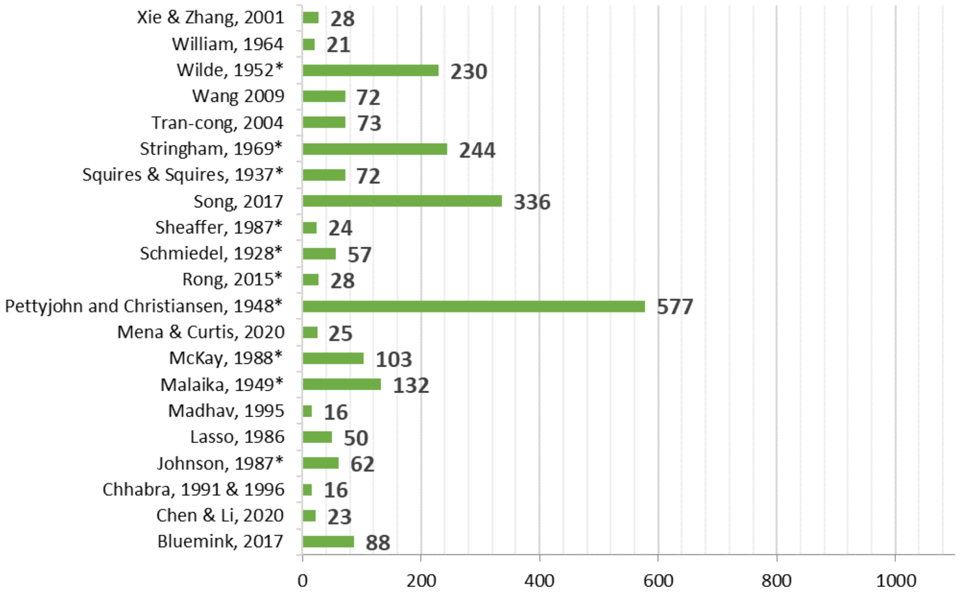
Knowledge gap: A drag model which can effectively discriminate shape of the particles and easy to apply in the current MFiX framework

Data Collected

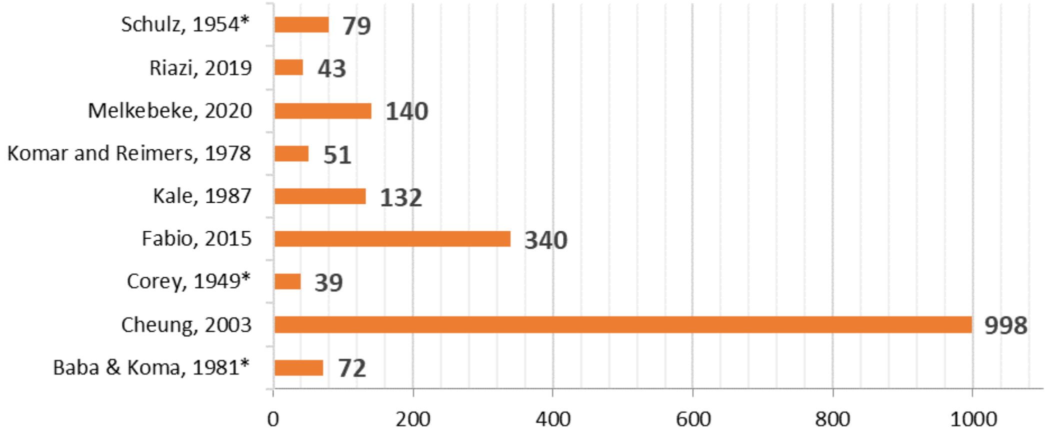
Digitalized several more papers/reports

(**> 4K data points**)

- Created a combined spreadsheet with data of drag coefficients at identified features
- Performed preliminary data analysis of feature importance and feature correlation
- Conducted a systematic experimental analysis on various data configurations



Regular-shaped Particles (Total: 2277)

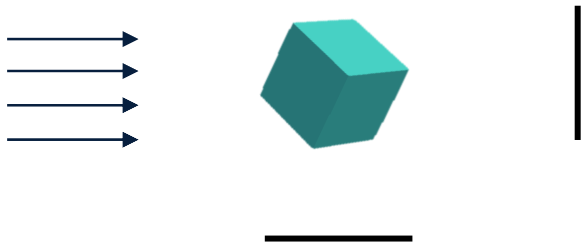


Irregular-shaped Particles (Total: 1894)

* Particle shape and settling velocity are retrieved from David, 2017. Other parameters including Re and Cd are calculated ourselves to be consistant with other data

Features for Neural Network

- Reynold number (Re)
- Sphericity (ψ)
- Fixed Crosswise Sphericity ($\psi_{\perp}$)
- Fixed Lengthwise Sphericity ($\psi_{\parallel}$)
- Aspect ratio (AR)
- Density Ratio



$$Re = \frac{\rho_g V_r D}{\mu}$$

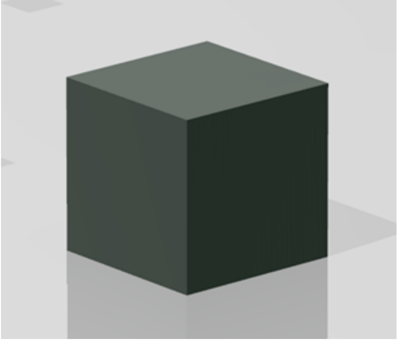
$$\psi = \frac{\pi D^2}{Surface\ area\ of\ the\ particle\ (A_s)}$$

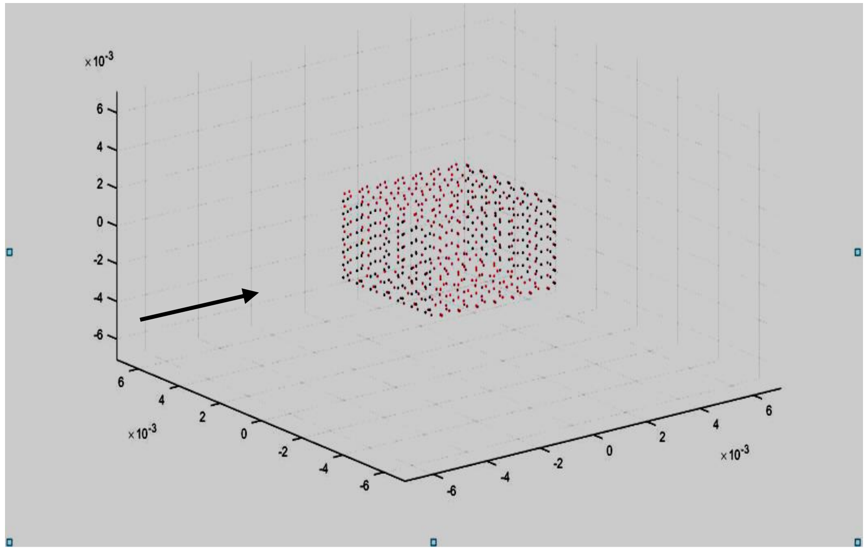
$$\psi_{\perp} = \frac{0.25\pi D^2}{Projected\ area\ of\ the\ particle\ perpendicul\ to\ the\ flow}$$

$$\psi_{\parallel} = \frac{0.25\pi D^2}{0.5A_s - Mean\ longitudinal\ projected\ area}$$

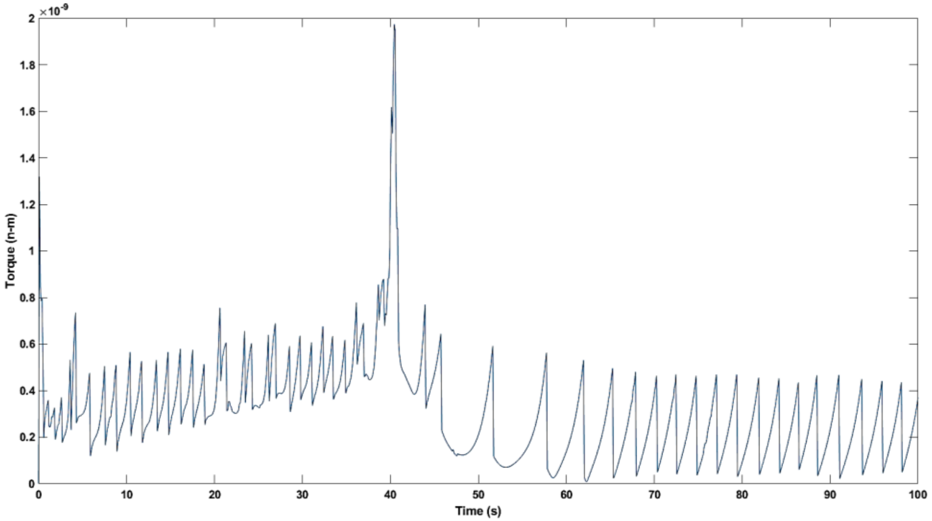
$$AR = \frac{Longest\ side}{Smallest\ side}$$

Particle Orientation Study





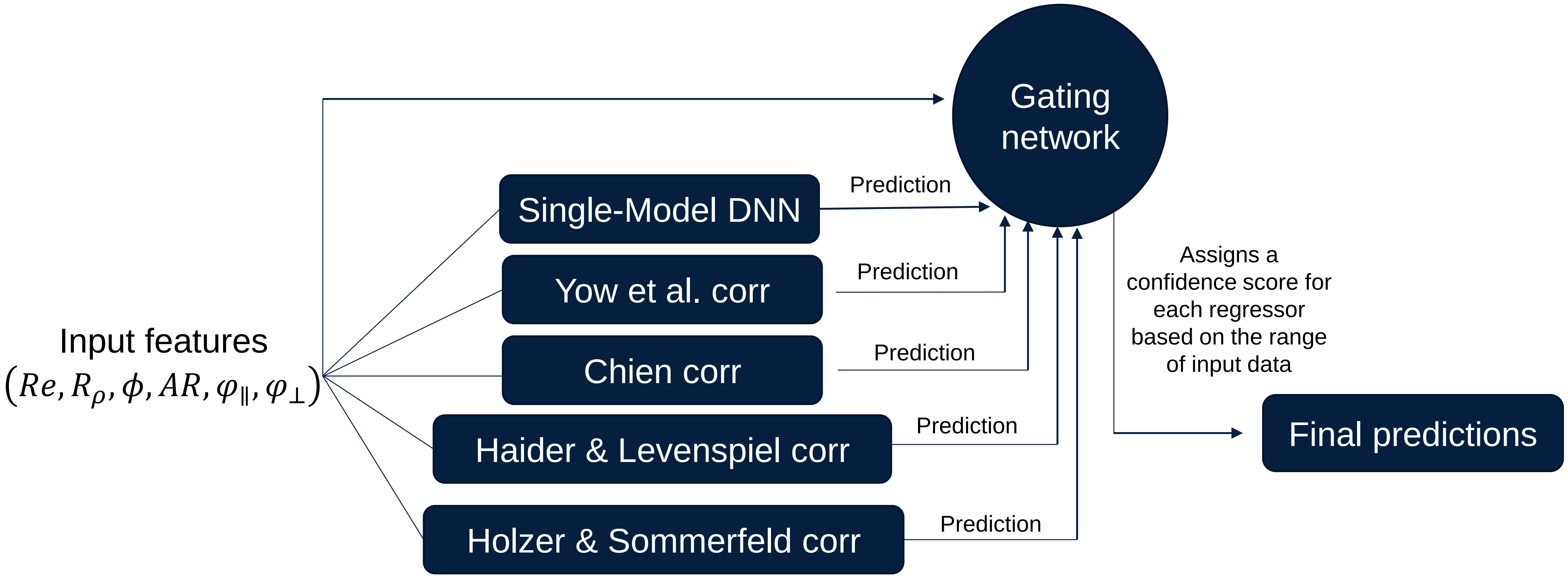
Methodology and Assumptions
1. Panel method to solve aerodynamics
2. Low Reynolds number
3. Flow leaves particle smoothly



Observations
1. Particle density impacts the orientations
2. Low sphericity particles fluctuates

Drag Coefficient Correlation-aided Deep Neural Network (DCC-DNN)

Mixture of Experts (MoE) Architecture



RMSE	MRAE	R^2
25.98	17.05	0.8569

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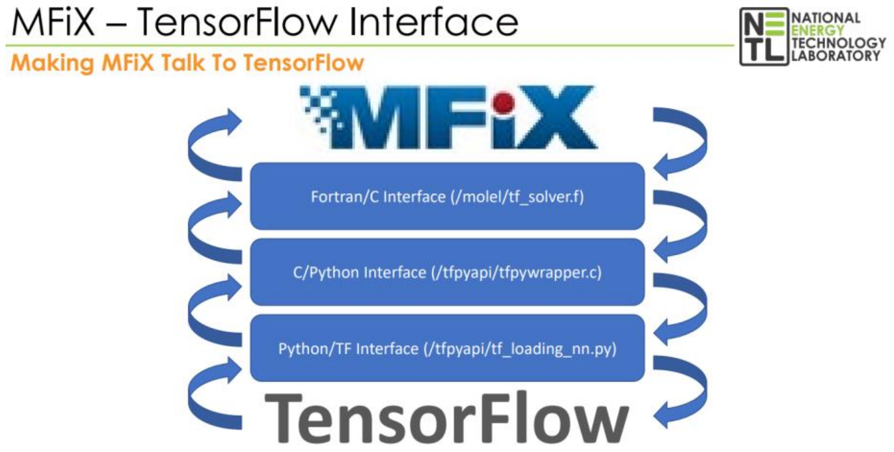
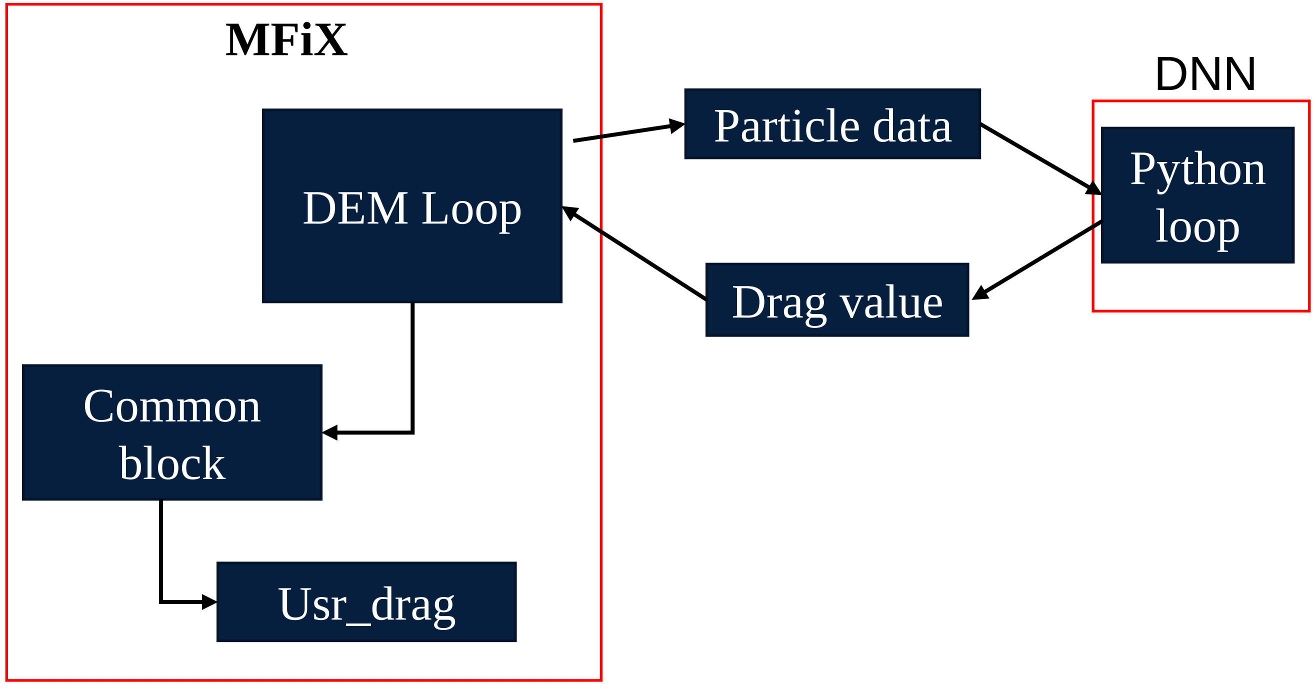
Integration with CFD (MFiX)

1. MFiX is written on Fortran
2. Neural network model is written on Python
3. Available wrappers cannot work with advance libraries such as Pytorch.



https://www.netl.doe.gov/sites/default/files/2020-11/UCR_HBCU_OMI/Dirk%20VanEssendelft%20Presentation-2020UCRHBCU_Kickoff_MFIXAI_Overview.pdf

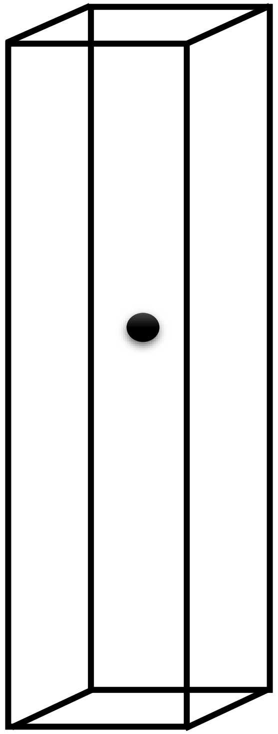


- **~11000 particles cost approximately 5 seconds to complete the DEM loop.**
- File writing takes place only once
- CFD of lab scale setup is practical
- Large scale can be time consuming

CFD Validation
Settling of Single Non-Spherical Particle

1. Non-spherical particle
2. Glycerin and water
3. Al, Ti and Steel
4. Terminal velocity measurement

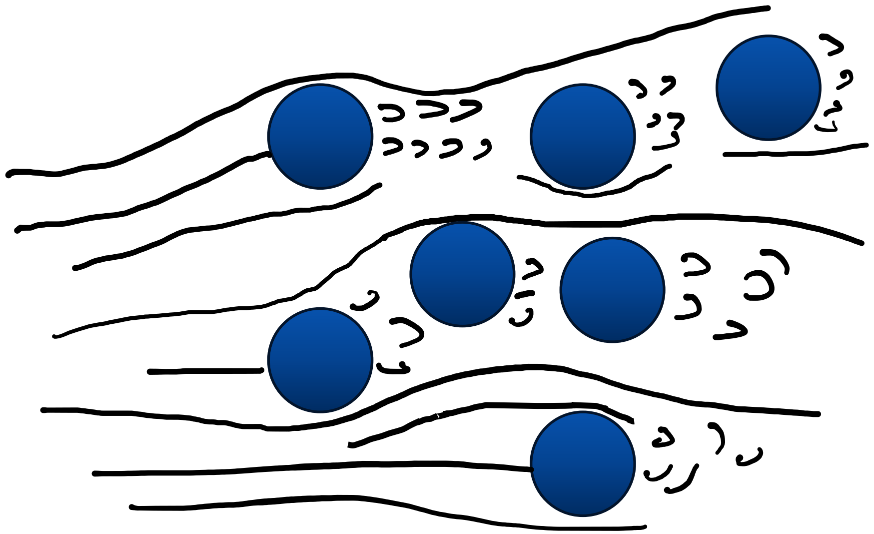
1. DEM simulation
2. Gravity
3. Particle velocity is monitored



Drag Predictions error < 30 %

Song, X., Xu, Z., Li, G., Pang, Z., & Zhu, Z. (2017). A new model for predicting drag coefficient and settling velocity of spherical and non-spherical particle in Newtonian fluid. *Powder Technology*, *321*, 242-250.

Assemblies of particles



Fluidized Bed

Vollmari, K., Jasevičius, R. and Kruggel-Emden, H., 2016. Experimental and numerical study of fluidization and pressure drop of spherical and non-spherical particles in a model scale fluidized bed. *Powder Technology*, *291*, pp.506-521.

Sedimentation

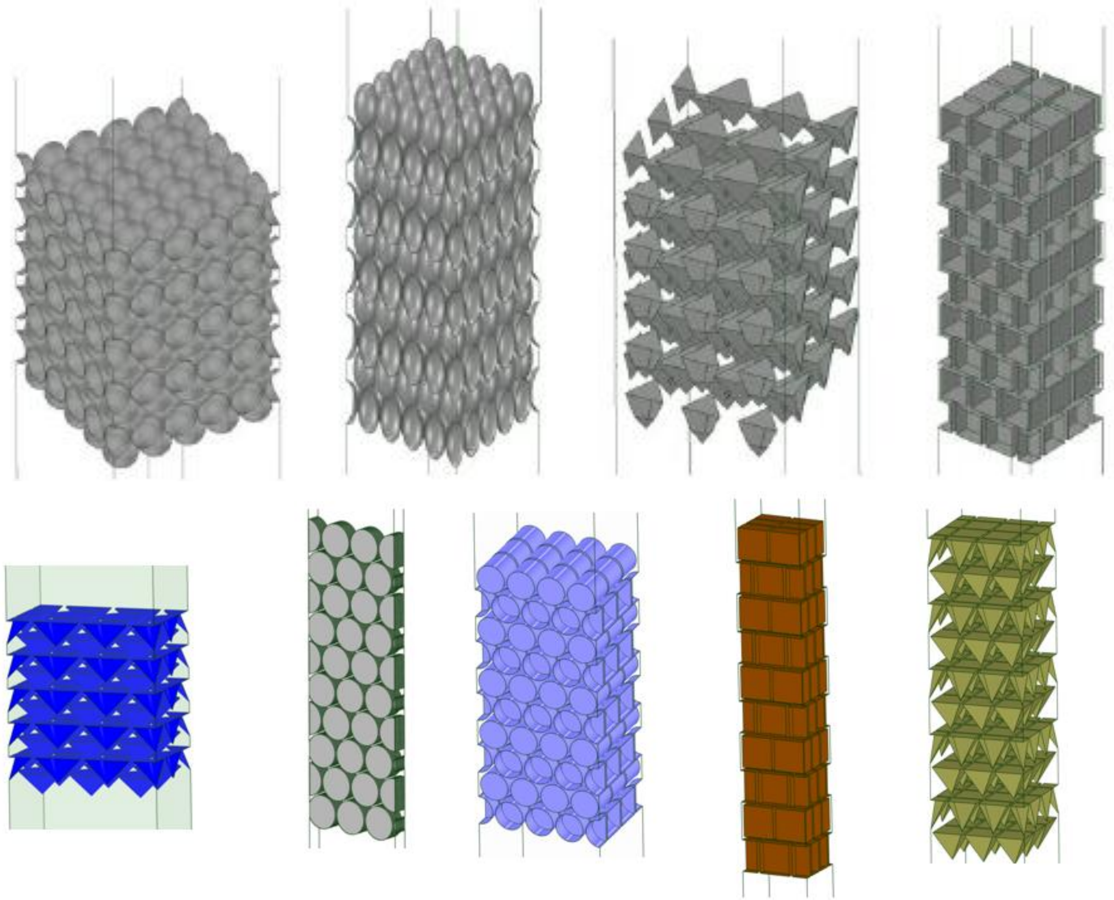
https://physics.aps.org/articles/v10/40

Volcanic debris

https://volcanoes.usgs.gov/volcanic_ash/ash_gas_vog.html

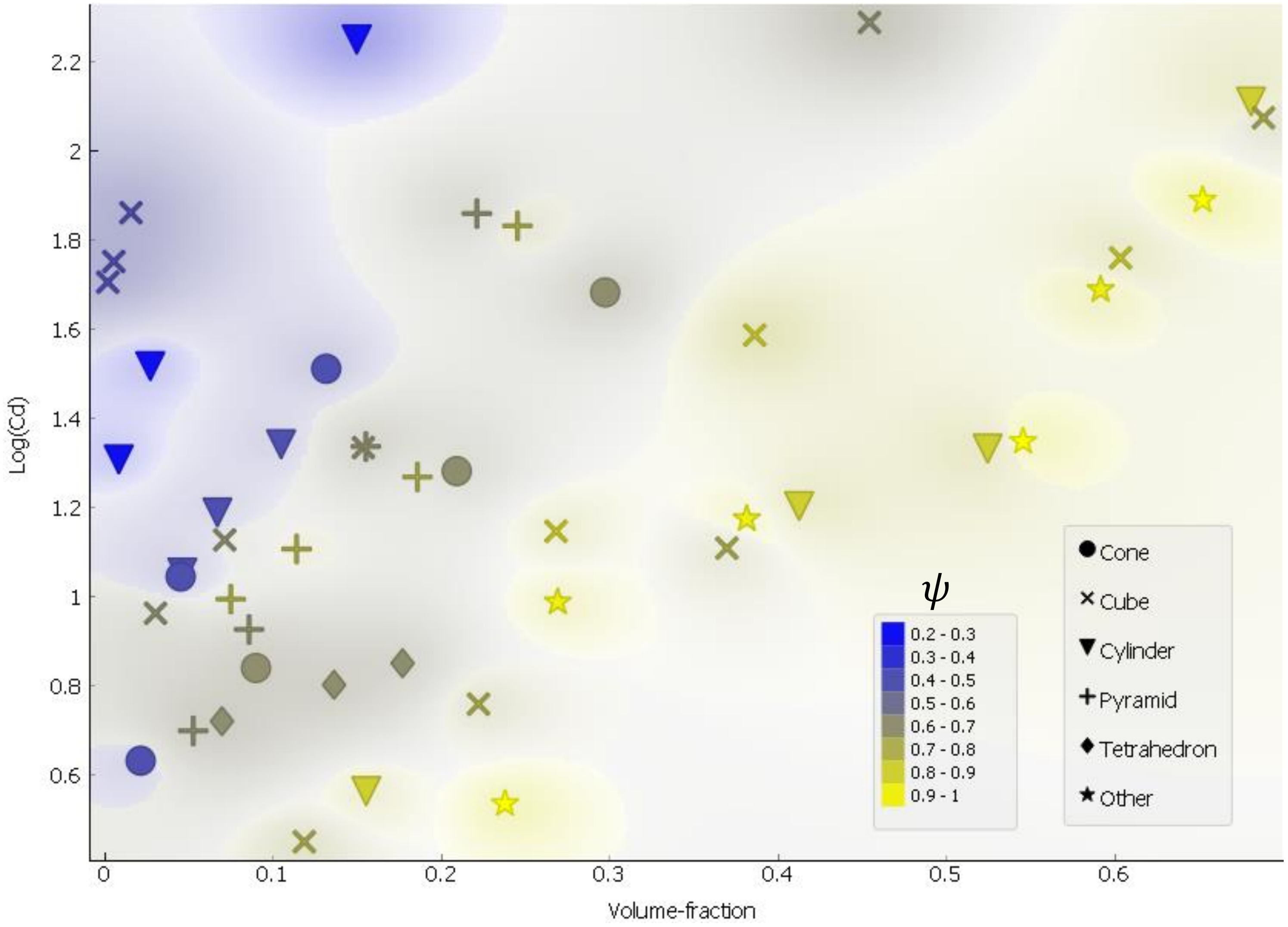
Effect of Volume Fractions on Drag

- Experimental studies typically do not report drag of a particle in a group.
- CFD simulations are carried out to generate drag data of particles found in beds.
- Re: 1~500



Mahyawansi, P. and Lin, C.X., 2021, August. An Investigation of the Effects of Volume Fraction on Drag Coefficient of Non-Spherical Particles Using PR-DNS. In *Fluids Engineering Division Summer Meeting* (Vol. 85284, p. V001T02A024). American Society of Mechanical Engineers.

Effect of Volume Fractions on Drag for Re = 500



Modelling Volume fraction

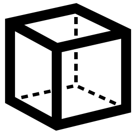
$$\boldsymbol{C_d = C_{d_0}(1-\epsilon_s)^n}$$

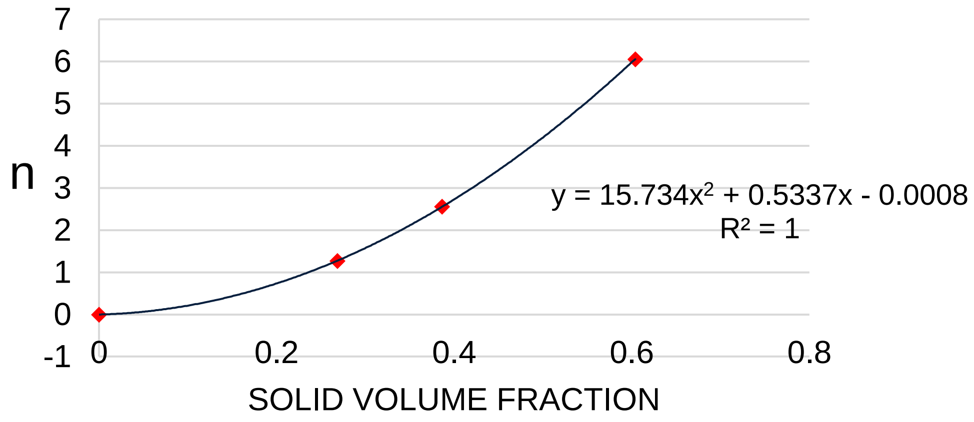
$$C_d = C_{d_0}\phi_v^n$$

$$n \approx f(\phi_v, Re, \psi)$$

For Re < 10, $n = -0.0008 + 0.532\phi_v + 15.73\phi_v^2$

	ϕ_v				n		
Re	**0.2683**	**0.3864**	**0.6038**	**Single Particle**	**0.2683**	**0.3864**	**0.6038**
10	40.57	83.791	365.266	28.0152	0.281444	1.15217	5.089824
100	13.9877	38.582	57.522	3.7008	1.010626	2.465328	5.43816
500	7.6399	12.317	28.357	1.3449	1.32031	2.329059	6.042577
1000	7.5487	12.86072	25.744	1.2051	1.394606	2.489914	6.068513





$For\ Re > 10,\ n \approx f(\phi_v)$

If $\phi_v \to 0$, then $n \to 0$

ϕ_v	0	**0.2683**	**0.3864**	**0.6038**
n	0	1.270517	2.559466	6.056596

$$n = 15.734\phi_v^2 + 0.5337\phi_v - 0.0008$$

Di Felice, R., 1994. The voidage function for fluid-particle interaction systems. *International journal of multiphase flow*, *20*(1), pp.153-159.

Experimental Data

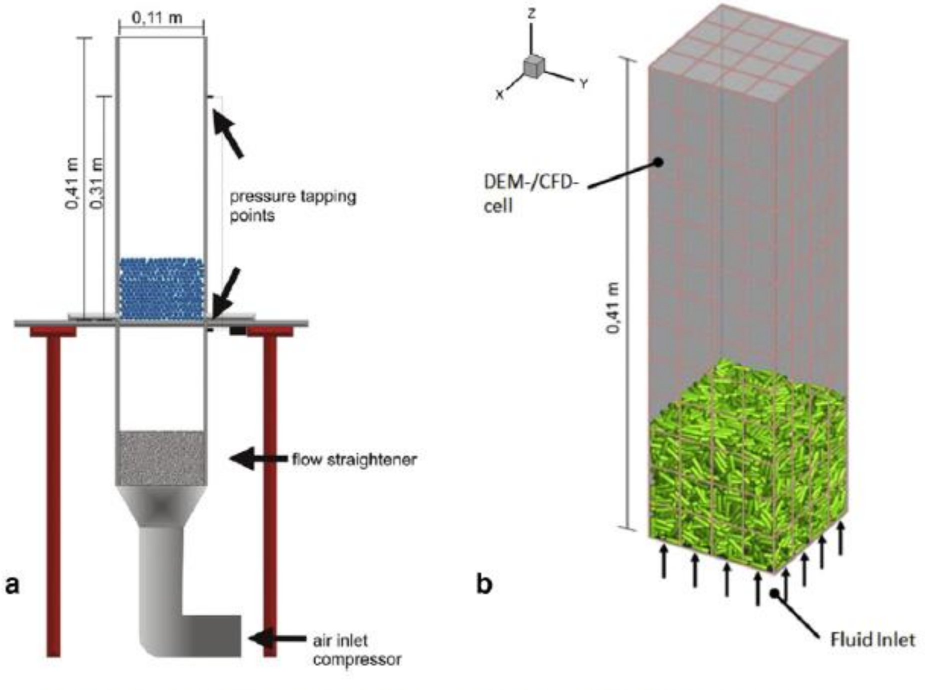
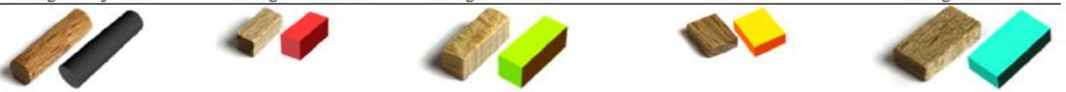
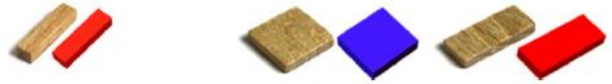


Fig. 2. Experimental (a) and numerical (b) setup and its division into a number of DEM–CFD cells larger than the particle size.

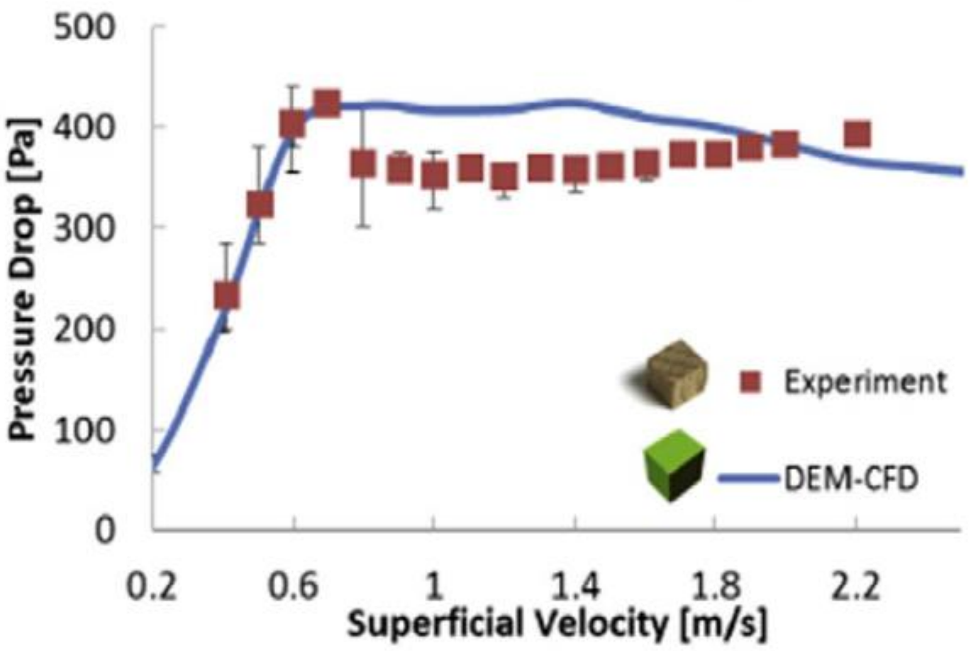
Table 1
Particle properties including the volume equivalent diameter d_e-*class*, the particle dimensions, the sphericity ϕ, the particle density ρ_p, the bed height L and the averaged porosity ε for the initial, unfluidized setup.

Shape	Sphere	Sphere	Ideal Cylinder	Cube	Cube
					
d_e–class [mm]	7	5	7	5	7
Size [mm]	7.2	5	6.1 6.2	4.2 4.3 4.5	5.2 6.3 6.3
ϕ [–]	1.00	1.00	0.87	0.81	0.80
ρ_p [kg/m³]	772.5	823.0	708.5	639.7	746.9
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	95 0.40	88 0.40	98 0.36	98 0.37	103 0.43
Shape	Elongated Cylinder	Elongated Cuboid	Elongated Cuboid	Plate	Elongated Plate
					
d_e–class [mm]	7	5	7	5	5
Size [mm]	3.9 14.0	3.0 3.0 7.1	4.2 4.2 11.4	2.0 4.9 6.0	2.0 4.0 8.0
ϕ [–]	0.75	0.75	0.73	0.71	0.69
ρ_p [kg/m³]	764.4	745.6	639.7	754.1	756.6
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	103 0.44	103 0.42	115 0.40	102 0.43	108 0.46
Shape	Elongated Cuboid	Plate	Elongated Plate		
					
d_e–class [mm]	5	7	7		
Size [mm]	2.0 3.0 11.0	2.2 9.0 9.8	2.0 6.0 14.9		
ϕ [–]	0.64	0.63	0.58		
ρ_p [kg/m³]	728.1	672.8	721.7		
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	117 0.48	121 0.46	124 0.51		

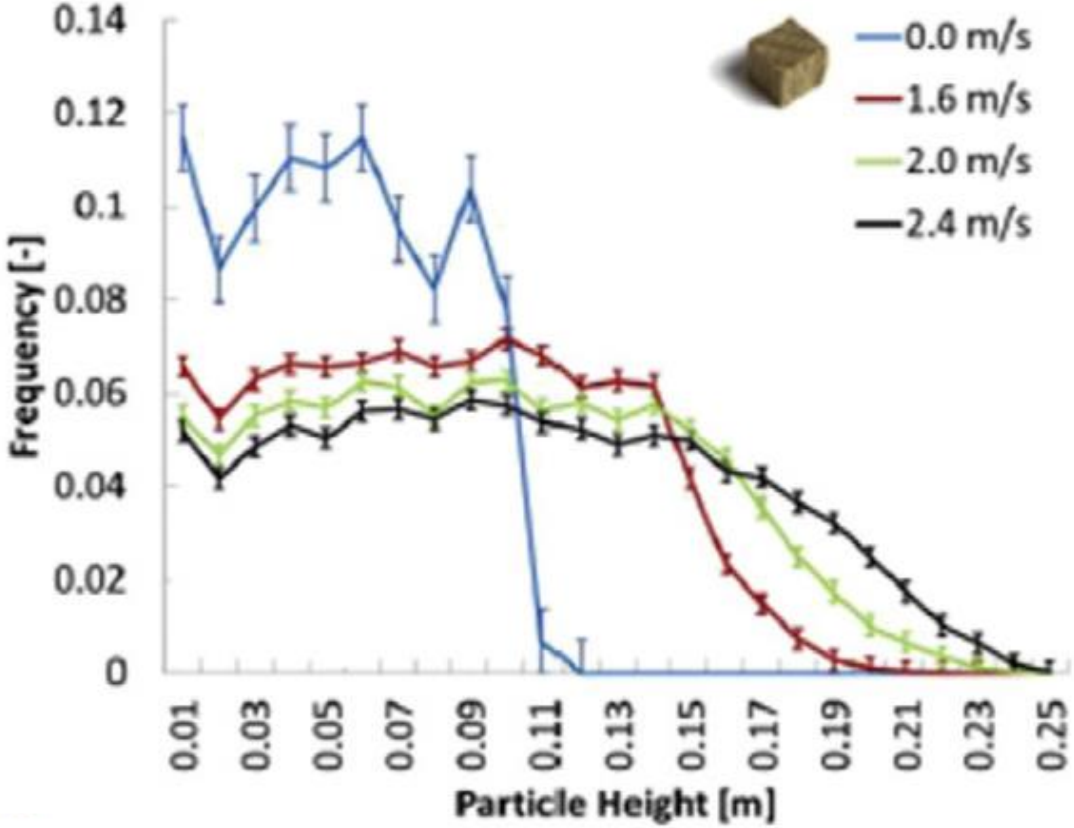
Vollmari, K., Jasevičius, R. and Kruggel-Emden, H., 2016. Experimental and numerical study of fluidization and pressure drop of spherical and non-spherical particles in a model scale fluidized bed. *Powder Technology*, *291*, pp.506-521.

Performance Metrics

Pressure drop



Frequency Distribution



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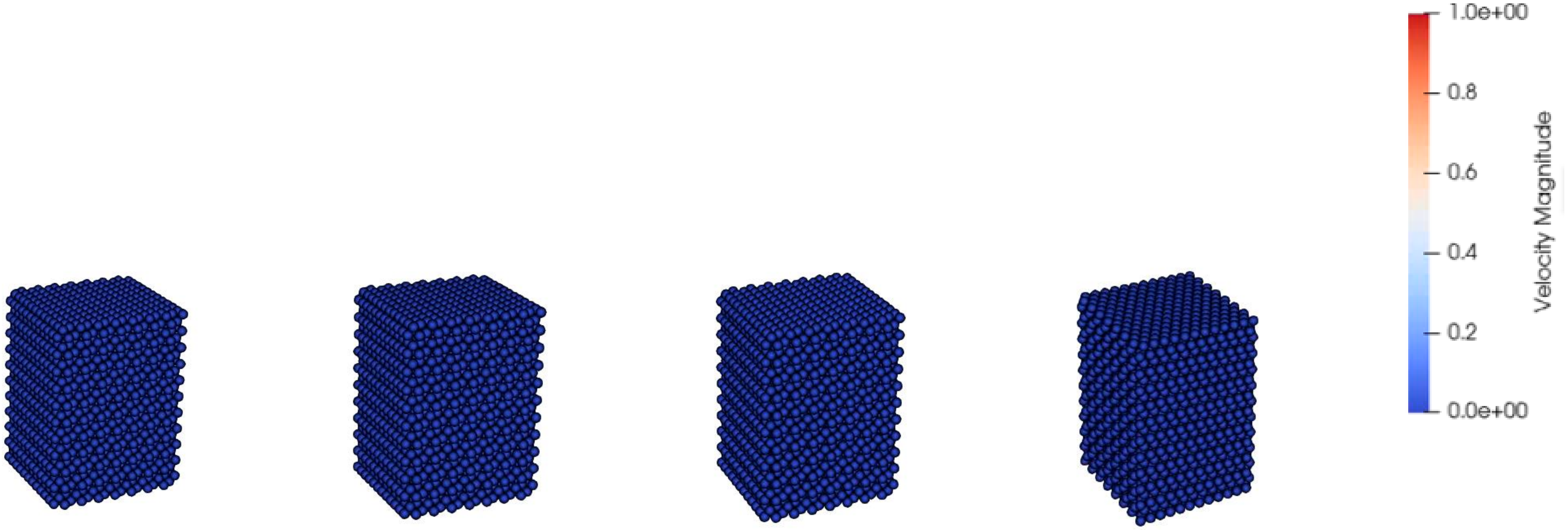
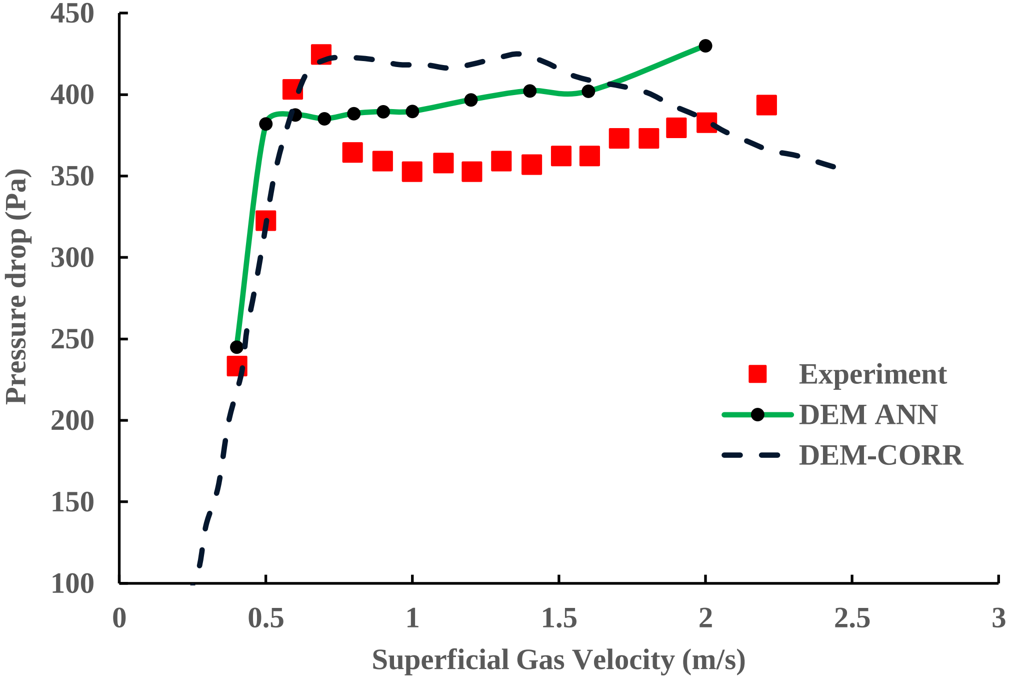
DEM Simulations of Cubic Particles



Vg = 0.7 m/s   Vg = 1.2 m/s   Vg = 1.6 m/s   Vg = 2.4 m/s

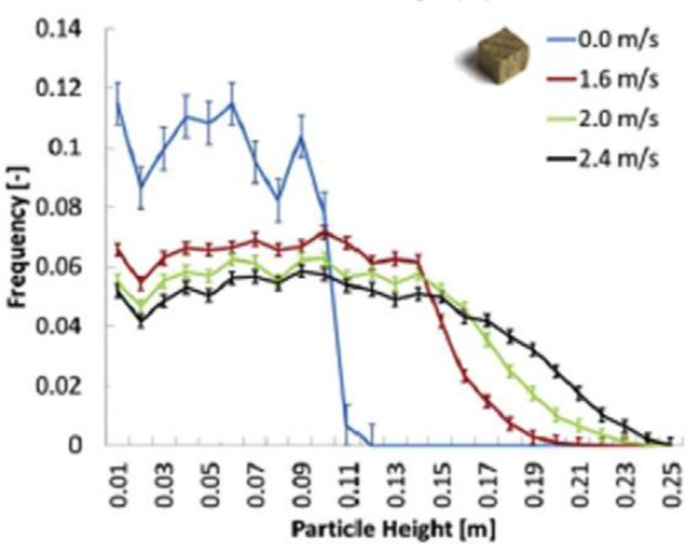
Results

Pressure drop across the bed

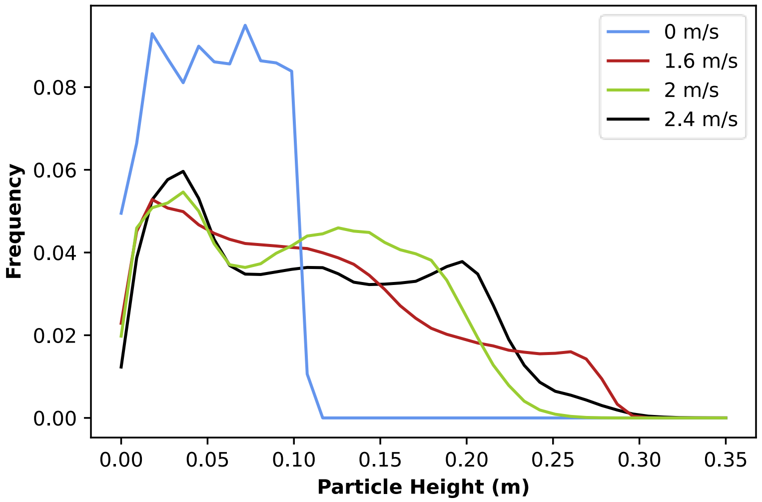


Frequency distribution

Experiments



DEM Simulations



Future Task
Modelling Volume Fraction Using Neural Network

$Re, AR, \psi, R_{\rho}, \psi_{\perp}, \psi_{||}$

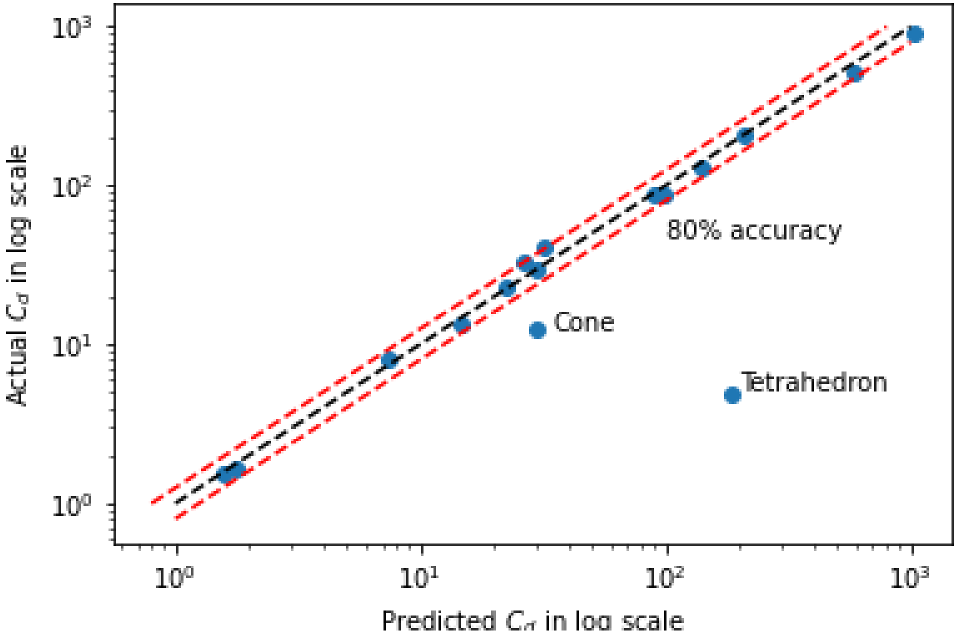
Deep Neural Network 1 (Mixture-of-Experts)

C_{d0} of a single particle

$C_{d0}, \phi_v, Re\ and\ \psi$

Deep Neural Network 2

C_d for group of particles



Predicted vs. Actual scatter plot

Conclusions

- Drag force on non-spherical particles depends on shape factor, inertia and Reynold number.
- Fixed crosswise and lengthwise sphericity is effective in discriminating the particles.
- Gated DNN model is integrated with MFiX to model particle drag.
- Single particle simulations with new drag model shows excellent predications.
- Solid volume fraction effect can be accounted using Di Felice's equation.
- DEM simulation using new drag model predicted fluidization of cubic particles.
- The pressure drop predictions across the bed are reasonably accurate.
- The pressure drop at the beginning of fluidization is under-estimated.
- The solid volume fraction effect are now accounted in the second level of DNN model.

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Appendix

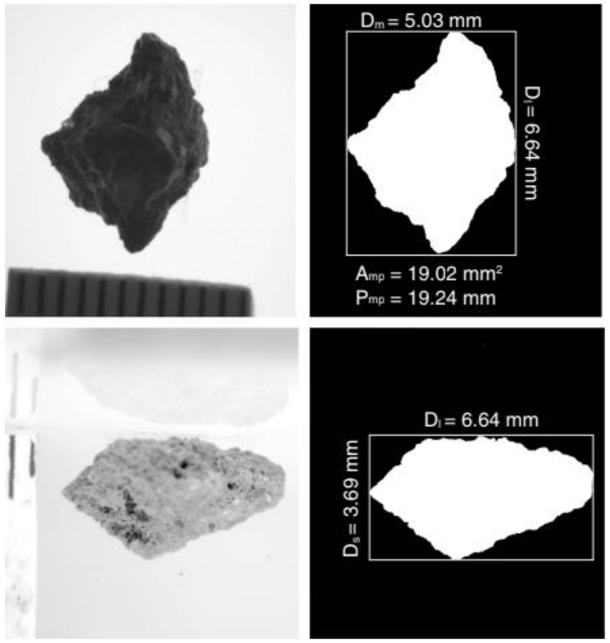
Regular vs. Irregular Shaped Particles

Regular shaped particles:

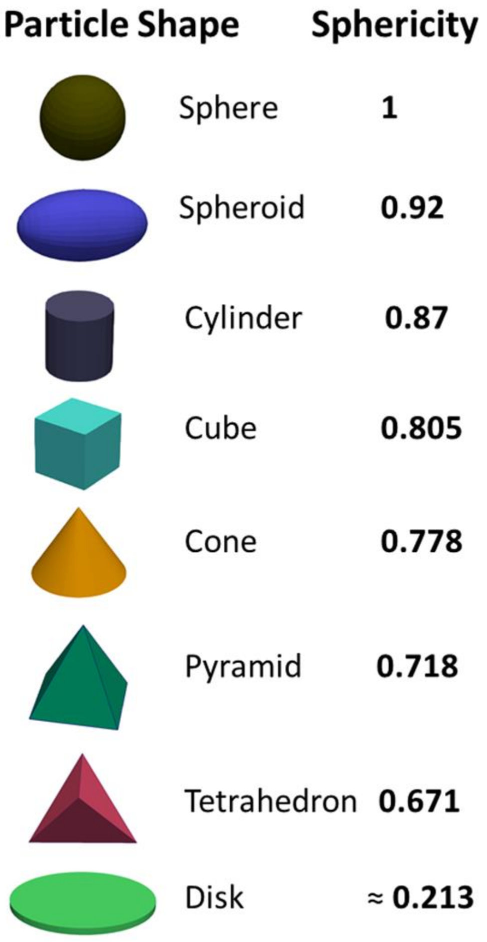
- A particle of geometric parameters such as volume and surface area that can be mathematically determined

Irregular shaped particles:

- An arbitrary random particle whose geometric parameters cannot be precisely calculated



Irregular-shaped Particles[1]



Regular-shaped Particles

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