2022 DOE/FECM Spring R&D Project Review Meeting

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

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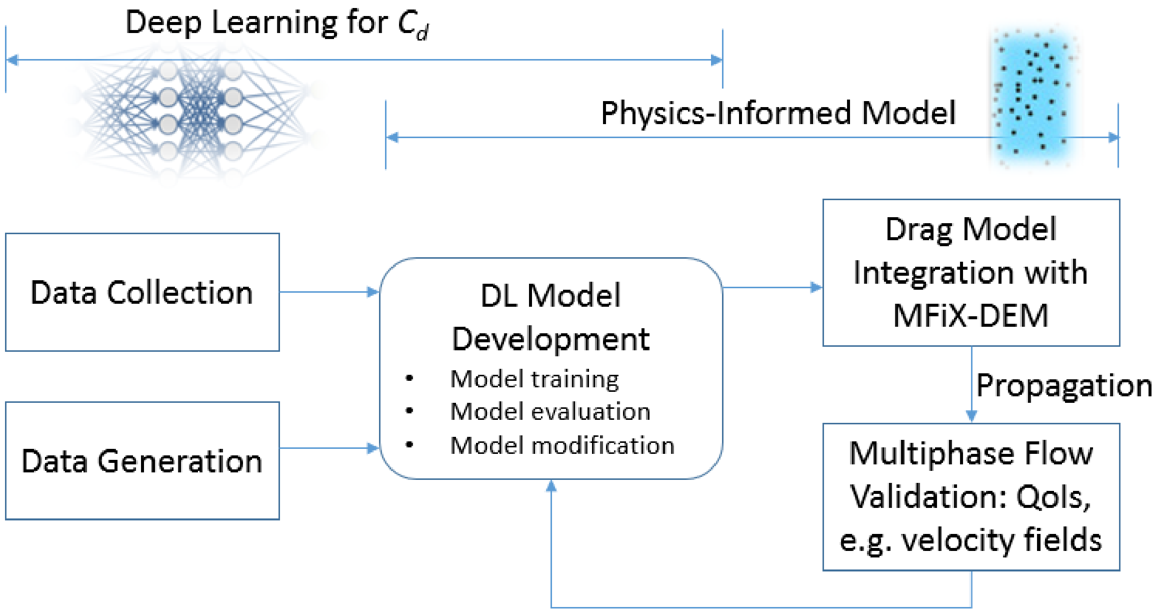
Agenda

- Project Objective
- Project Status
- Technical Progress
    - Introduction and Motivation
    - Data Collection
    - Data Analysis
    - DNN Model Development
    - Performance Results
- Conclusion
- Plan for the Next Few Months

Project Objective

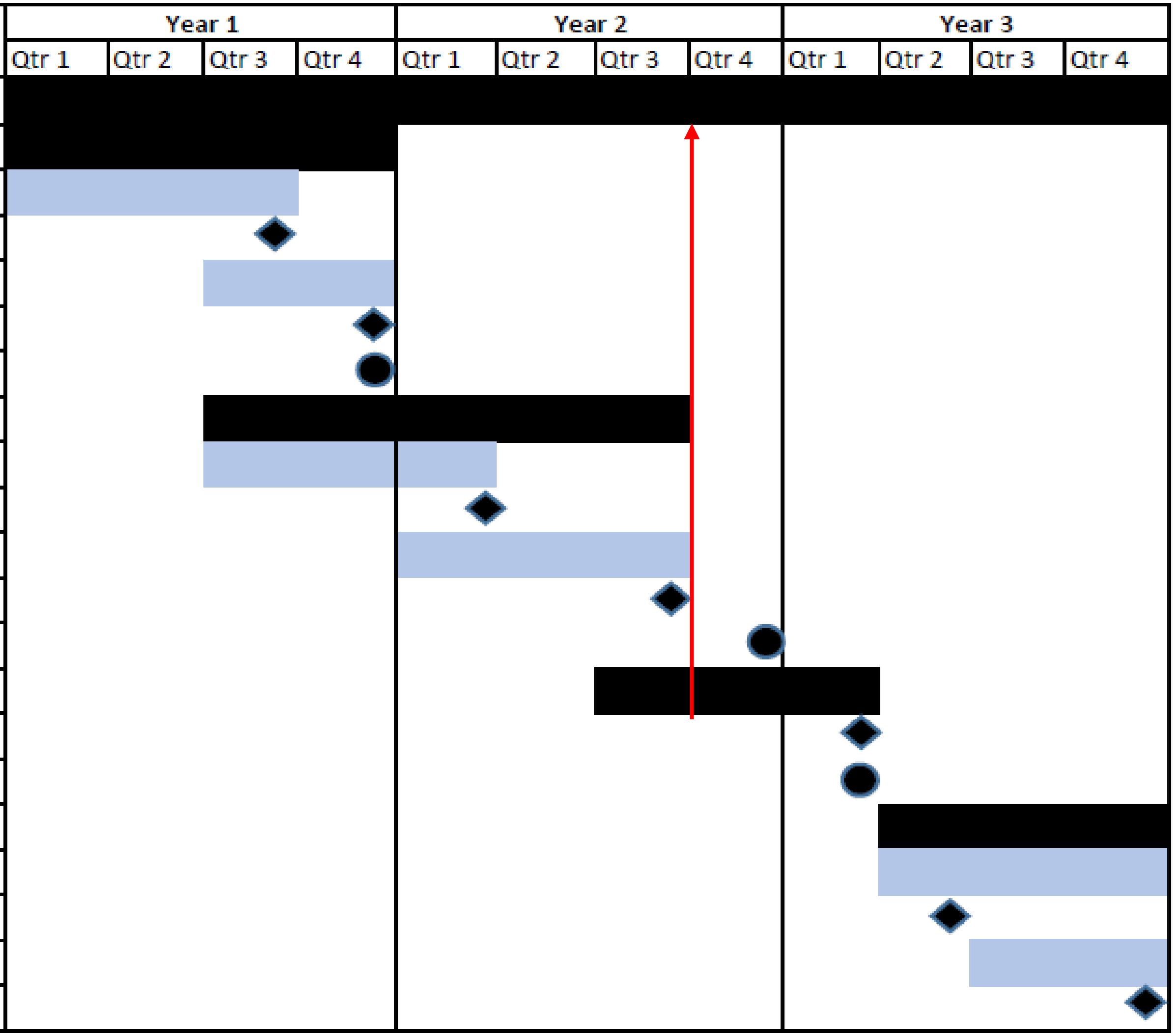
The overall objective of this project is to develop, test, and validate a general drag model for multiphase flows in assemblies of non-spherical particles by a physics-informed deep machine learning (PIDML) approach using artificial neural network (ANN).



Project Status

Project Timeline

Task Name	Assigned Resources
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	

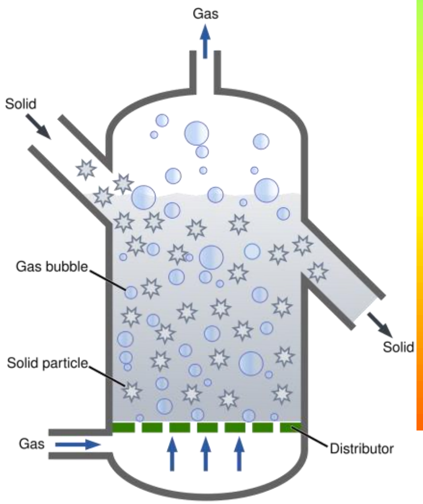


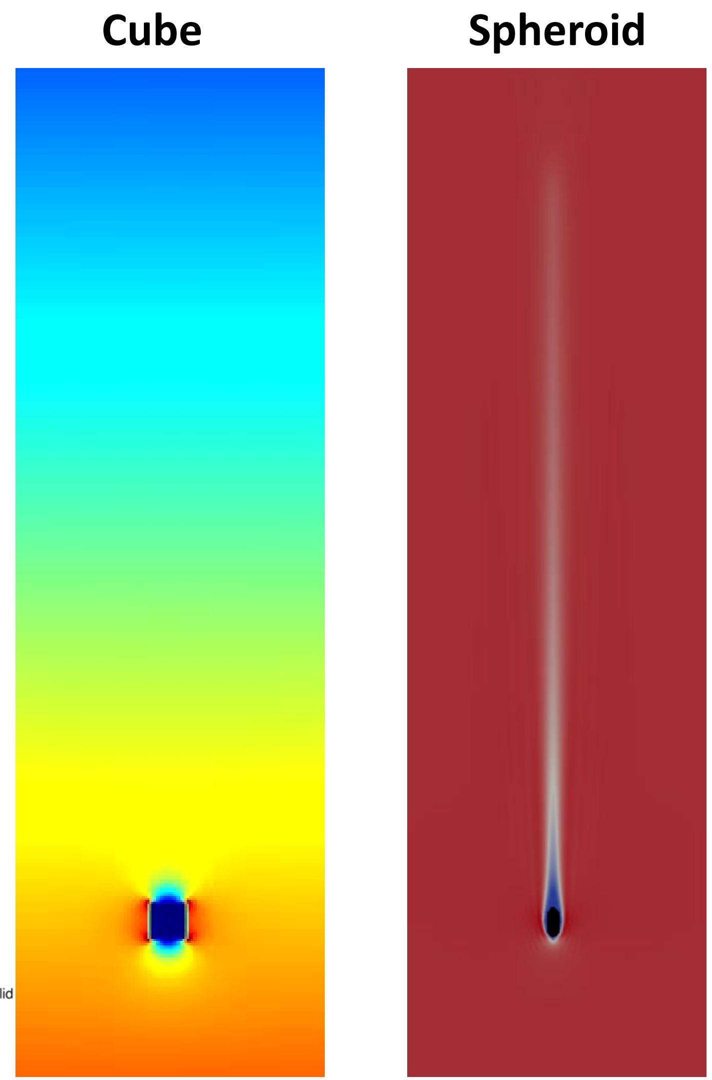
Introduction

- The particle laden flow is found in many industrial and natural processes
- The accuracy of simulation of multiphase flow system mainly governs by the fidelity of the **particle drag model** employed

Example application: fluidized-beds

- ✓ Generate energy from a variety of solid fuels
- ✓ Reduce toxic emissions
- ✓ Promote environmental sustainability





Motivation

Existing work considers at most two features (i.e., Reynolds & sphericity)

Drag coefficient depends on multiple features such as aspect ratio, lengthwise sphericity, crosswise sphericity, density ratio, etc

Traditional correlation-based methods have drawbacks:

- Limited number of features
- Limited feature range
- Limited to specific experimental conditions

Neural network can efficiently consider the effects of all these features and predict drag coefficient with high accuracy

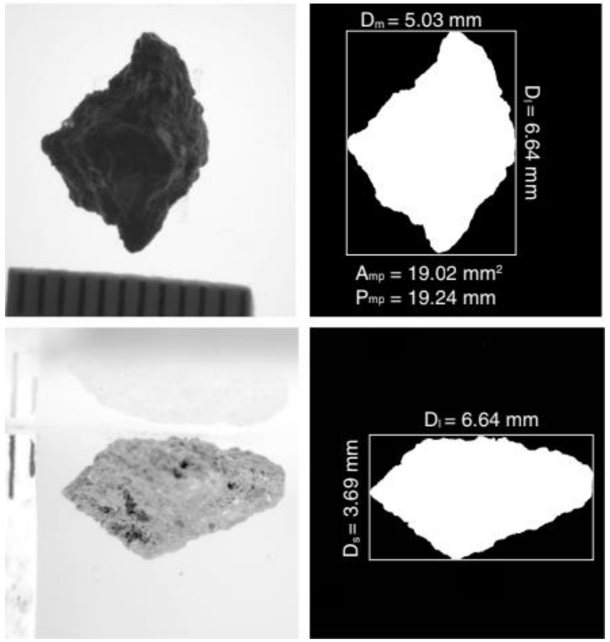
Regular vs. Irregular Shapes

Regular shaped particles:

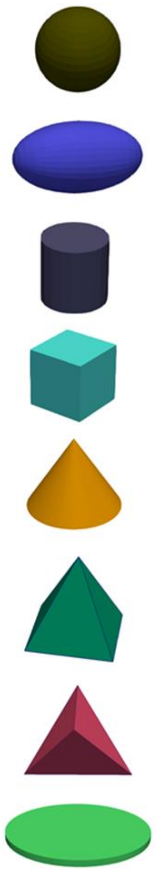
- Geometric parameters such as volume and surface area can be mathematically determined

Irregular shaped particles:

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



Irregular-shaped Particles[1]



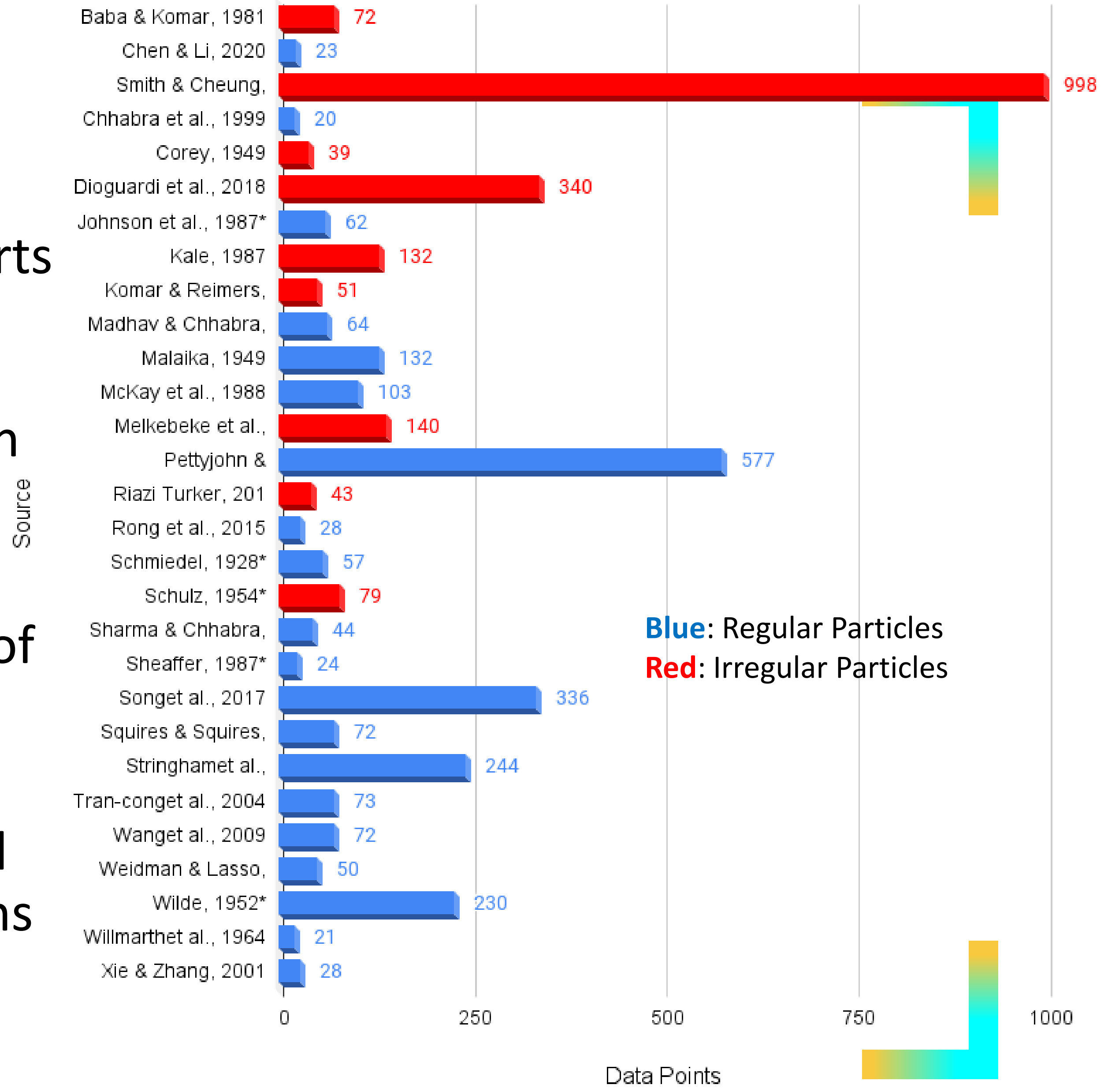
Particle Shape	Sphericity
Sphere	1
Spheroid	0.92
Cylinder	0.87
Cube	0.805
Cone	0.778
Pyramid	0.718
Tetrahedron	0.671
Disk	≈ 0.213

Regular-shaped Particles

[1]Dioguardi, F., D. Mele, and P. Dellino. "A new one-equation model of fluid drag for irregularly shaped particles valid over a wide range of Reynolds number." Journal of Geophysical Research: Solid Earth 123, no. 1 (2018): 144-156.

Data Collected So Far

- 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



* 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

Feature Generation

Drag Coefficient

$$C_D = f\left(Re, R_\rho, \Phi, AR, \varphi_\parallel, \varphi_\perp\right)$$

Flow property
- *Re*: Reynolds number
- R_ρ: Density ratio between fluid and particle

Particle geometry
- φ : Sphericity
- *AR* : Aspect ratio

Settling direction
- $\varphi_\parallel$: Lengthwise
- $\varphi_\perp$: Crosswise

$$Re = \frac{\rho_{fluid}\, u_{particle}\, d_{particle}}{\mu_{fluid}}$$

$$R_\rho = \frac{\rho_{fluid}}{\rho_{particle}}$$

$$\varphi = \frac{A_{volume\ equavlent\ sphere}}{A_{particle}}$$

$$AR = \frac{l_{max}}{l_{min}}$$

$$\varphi_\parallel = \frac{A'_{volume\ equavlent\ sphere}}{\frac{A_{particle}}{2} - A'_{lenthwise}}$$

$$\varphi_\perp = \frac{A'_{volume\ equavlent\ sphere}}{A'_{Crosswise}}$$

A: Surface area
A’: Cross-sectional area

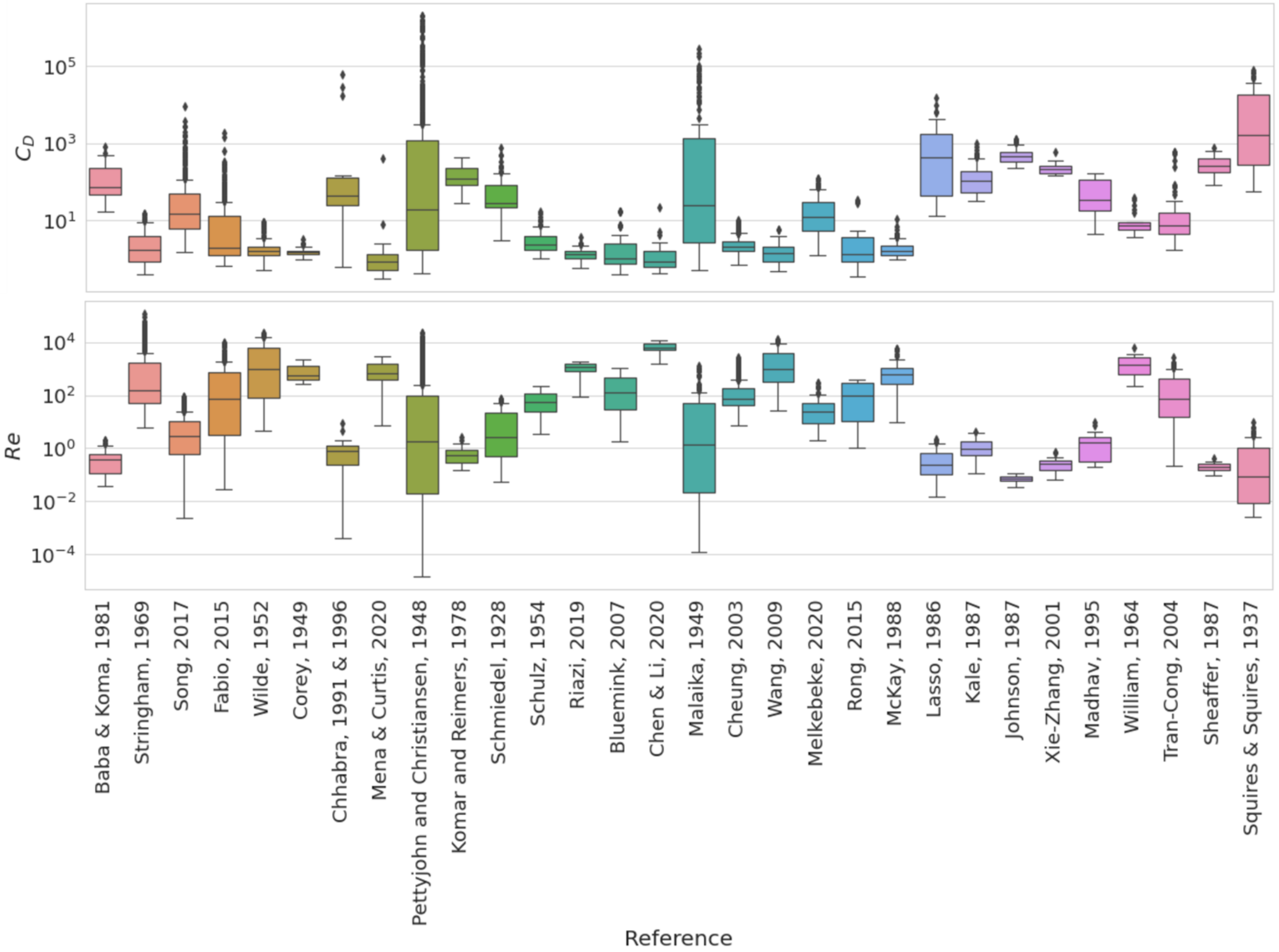
Data Challenges

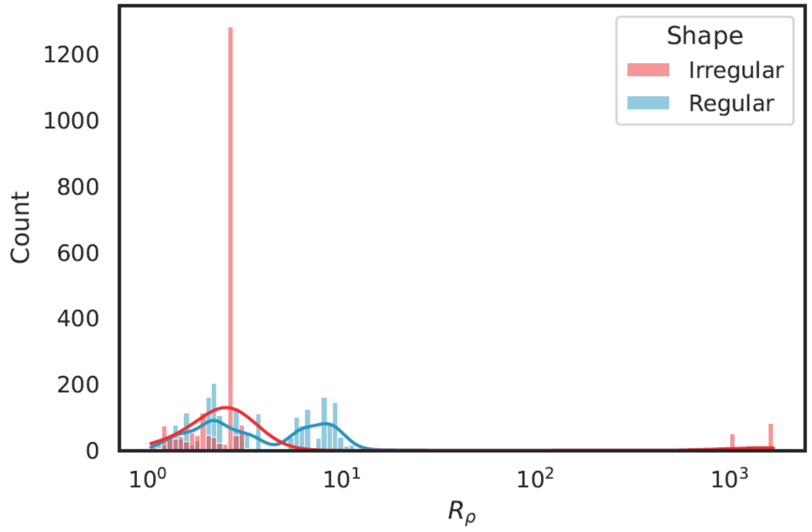
Learning from limited data sets

- Leads to overfitting

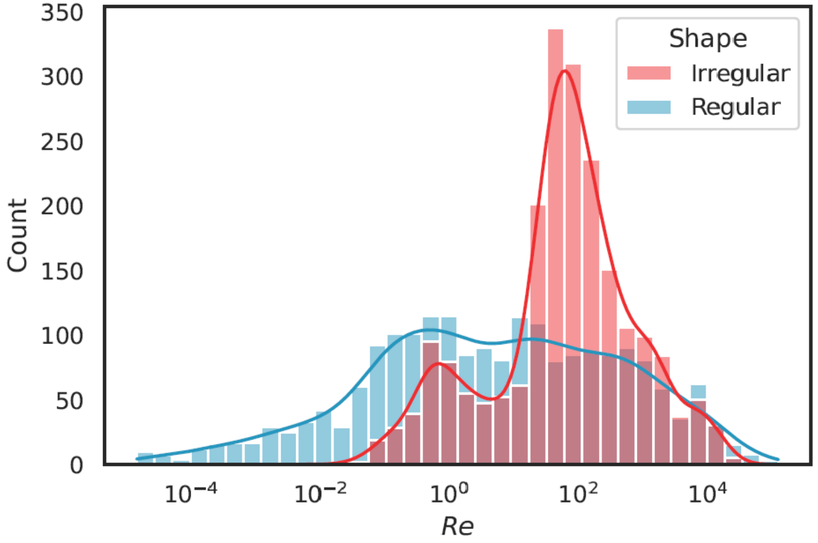
Extreme values

- Results in longer training times
- Less accurate models
- Can spoil and mislead the model training process

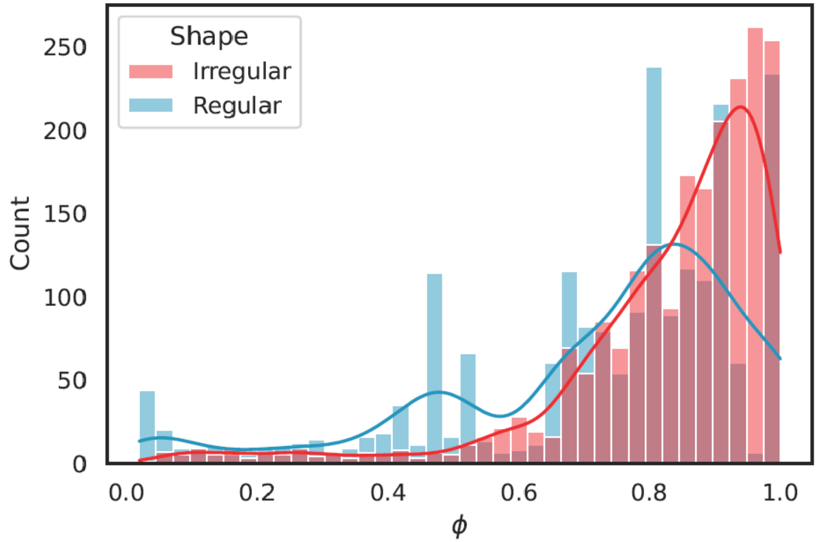




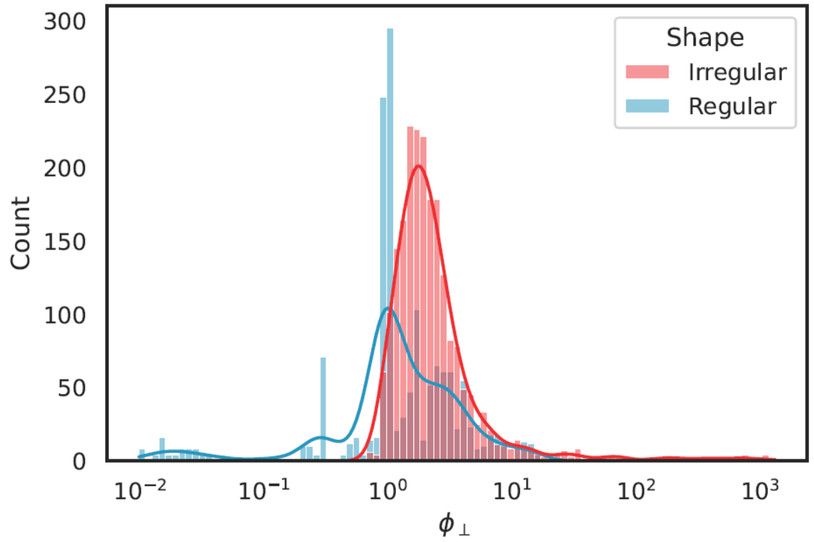
(a) Density ratio



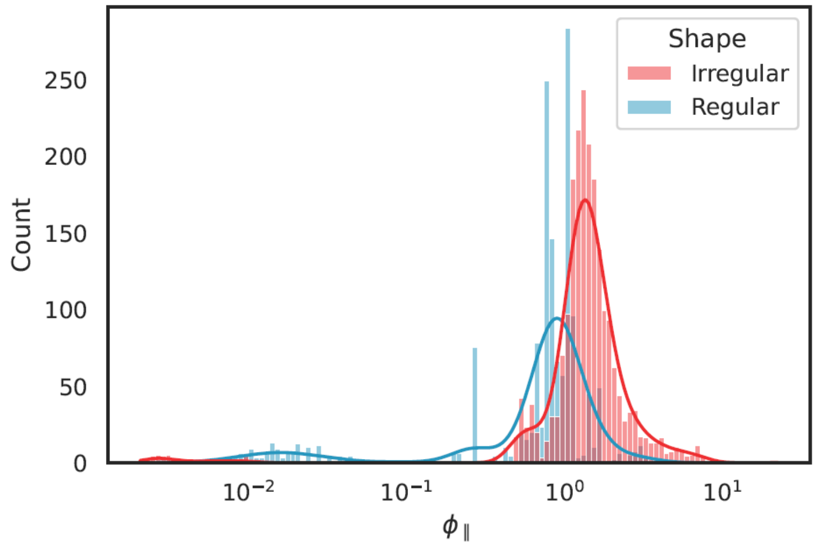
(b) Reynolds number



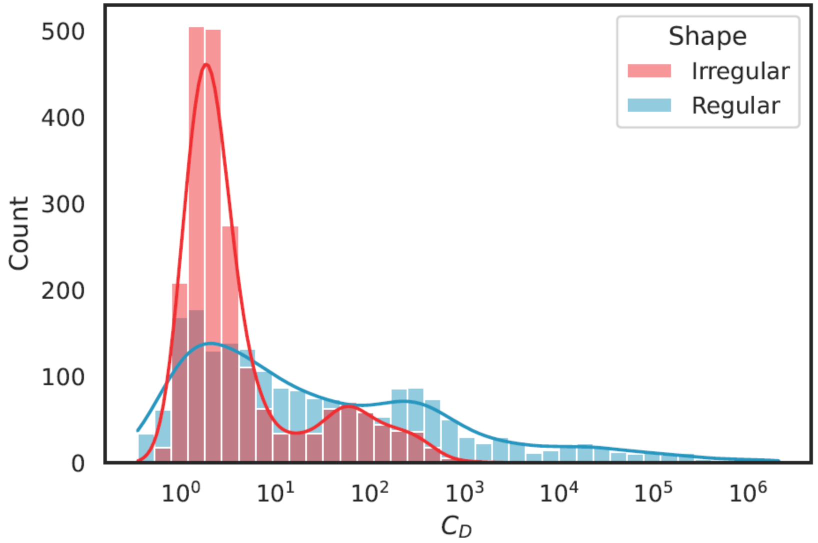
(c) Sphericity



(e) Crosswise sphericity

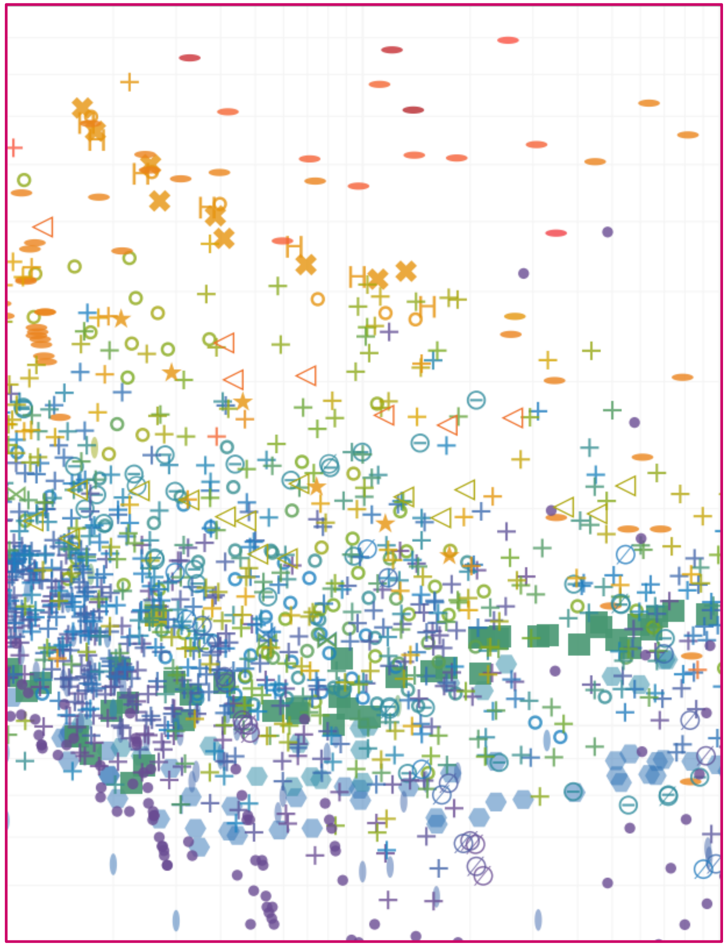


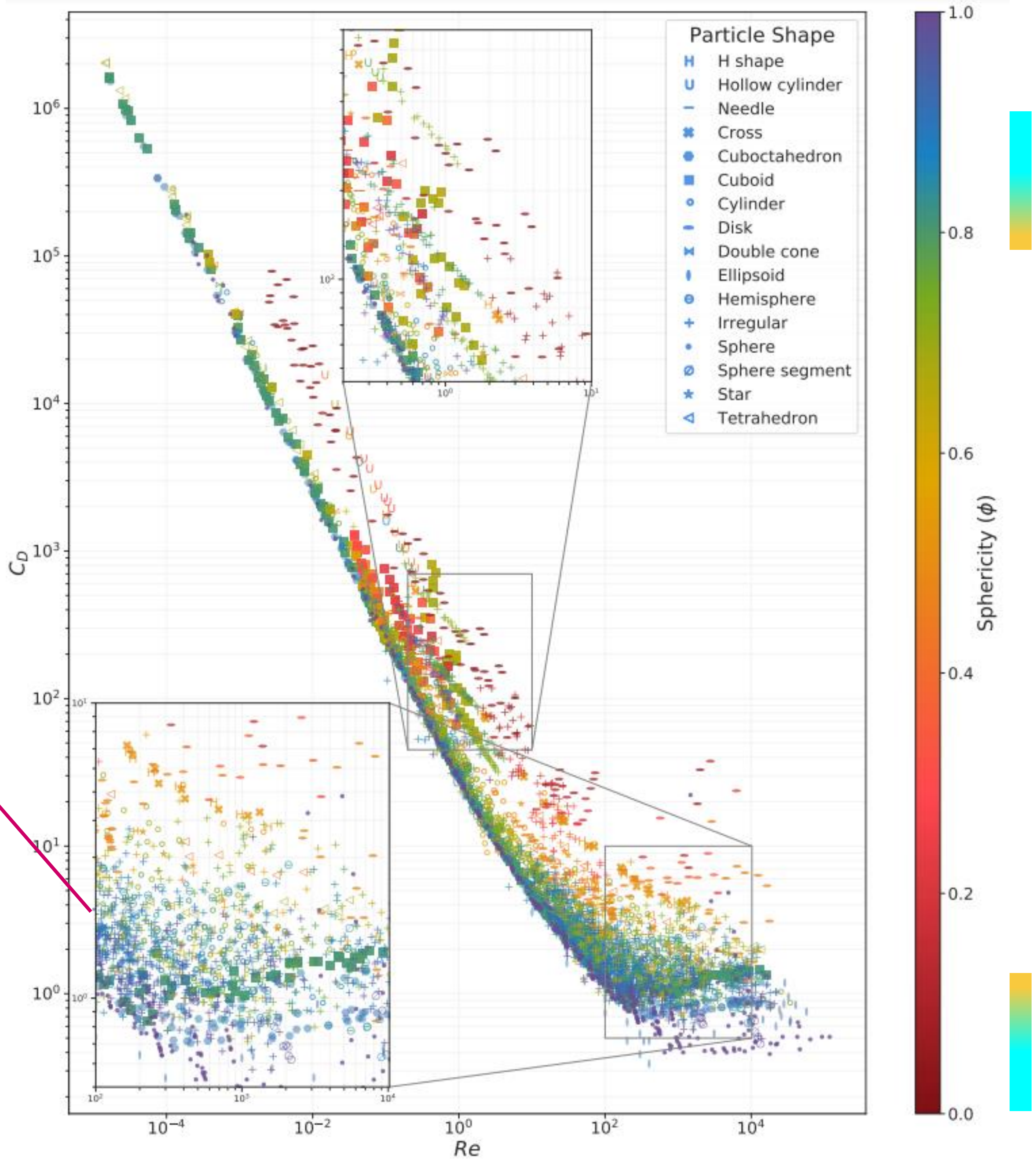
(f) Lengthwise sphericity



(g) Drag values

C_D vs. Re



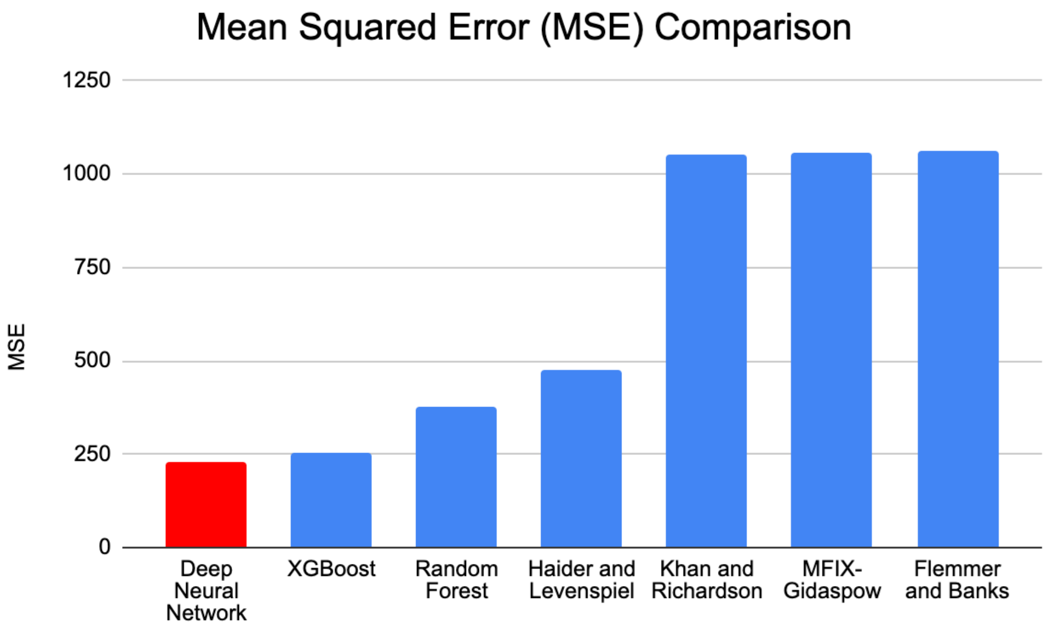


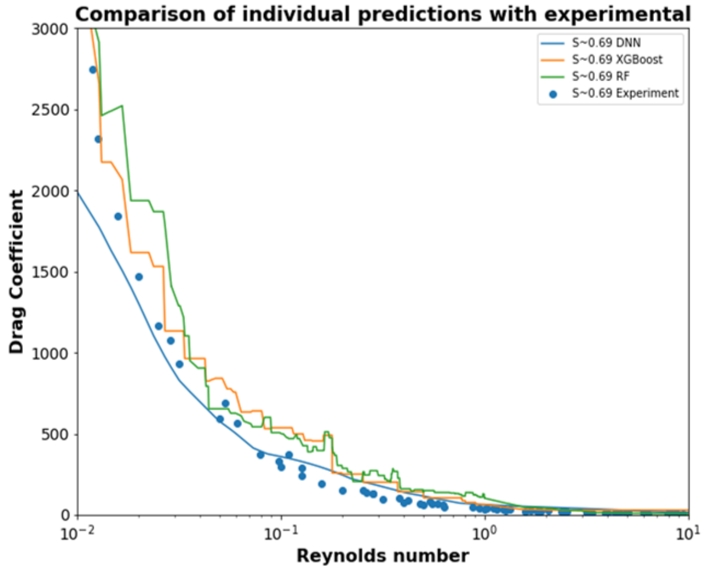
Particle Shape
H shape
Hollow cylinder
Needle
Cross
Cuboctahedron
Cuboid
Cylinder
Disk
Double cone
Ellipsoid
Hemisphere
Irregular
Sphere
Sphere segment
Star
Tetrahedron
C_D
Re
Sphericity (ϕ)

DNN vs. Machine Learning

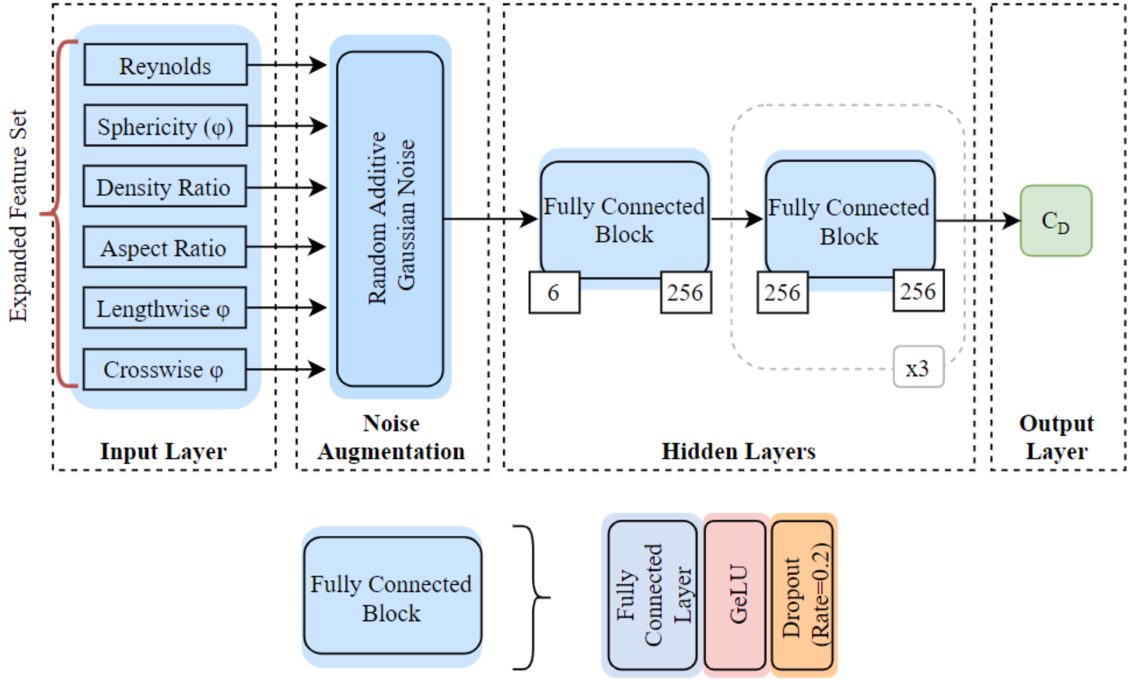
Preliminary study and results demonstrate DL/ML models can achieve better performance.

The more data we can feed the model to learn, the better result we obtain.



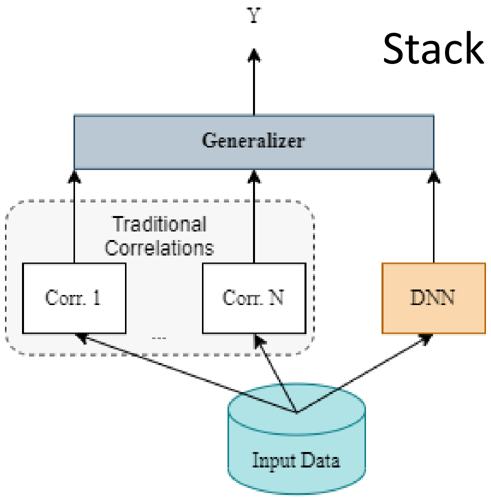


Proposed General Drag Model

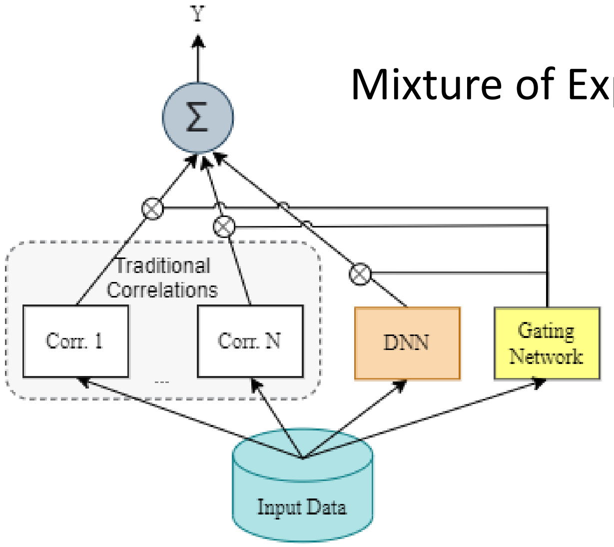


Proposed Deep Neural Network (DNN) Architecture

Stack Generalization (SG)



Mixture of Experts (MoE)

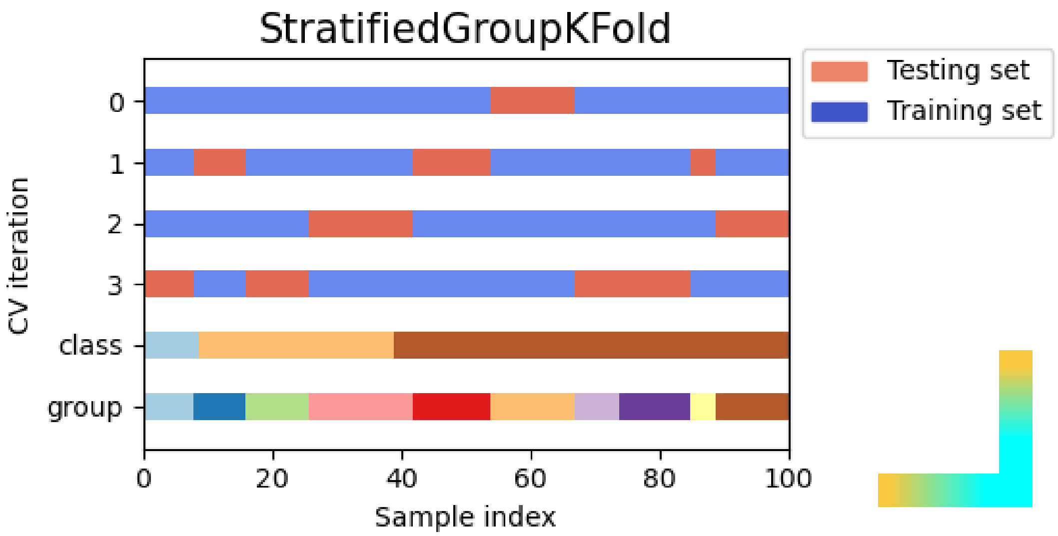


Analytic Setup

- Apply log transform to Re and C_D
- Apply a standard scaling to input features
- Huber Loss: using MAE for bigger loss values and reduces the weight given to outliers

Stratified Group KFold:

- Each experiment is a group
- Constraints:
  - Maintain proportion of target values
  - Non-overlapping experimental sources
- Test capability to generalize



Results

Full Feature Set S: $< Re, \phi, \phi_\perp, \phi_\parallel, AR, R_\rho >$

Type	Method	Input Features	RMSE	MRAE	NRSS	SSLE	R^2
TC	Haider & Levenspiel, 1989	$< Re, \phi >$	37.93±12.13	30.08±11.08	56.06±54.48	19.52±21.10	0.7146±0.38
	Chien, 1994	$< Re, \phi >$	49.46±12.29	38.59±9.06	92.21±90.81	26.14±29.03	0.6259±0.40
	Yow *et al.*, 2005	$< Re, \phi >$	200.91±92.01	164.10±85.42	2001.56±2686.58	31.47±34.76	-1.5375±7.44
	Holzer & Sommerfield, 2008	$< Re, \phi, \phi_\perp, \phi_\parallel >$	55.13±28.29	46.26±24.90	111.61±127.72	46.39±51.91	0.1171±1.71
ML	Random Forest	S	48.52±12.73	34.70±9.08	121.77±190.37	19.85±20.62	0.5426±0.33
	Gradient Boosting	S	45.12±14.10	33.01±8.21	108.76±152.78	18.23±20.01	0.5891±0.31
DL	Baseline	$< Re, \phi >$	36.38±9.72	28.59±6.16	62.14±87.10	11.84±13.33	0.7971±0.22
		S	37.09±8.92	27.05±5.18	72.66±116.09	72.66±116.09	0.7822±0.20
	Single-Model DNN	$< Re, \phi >$	31.54±12.89	23.60±9.41	42.62±49.90	8.31±9.76	0.7508±0.30
		S	26.63±10.63	17.43±6.29	40.83±62.95	6.96±10.50	0.8118±0.25
	DCC-DNN (SG)	S	44.66±12.47	33.92±7.29	76.41±81.48	13.22±12.52	0.8150±0.19
	DCC-DNN (MoE)	S	**25.98±10.18**	**17.05±6.03**	**38.00±58.17**	**6.76±10.02**	**0.8569±0.20**

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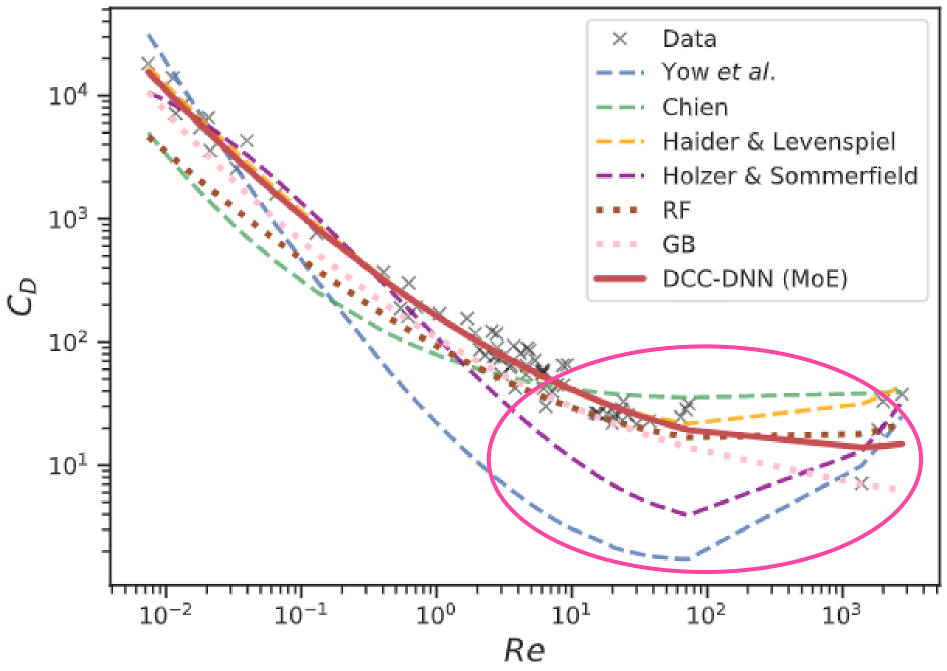
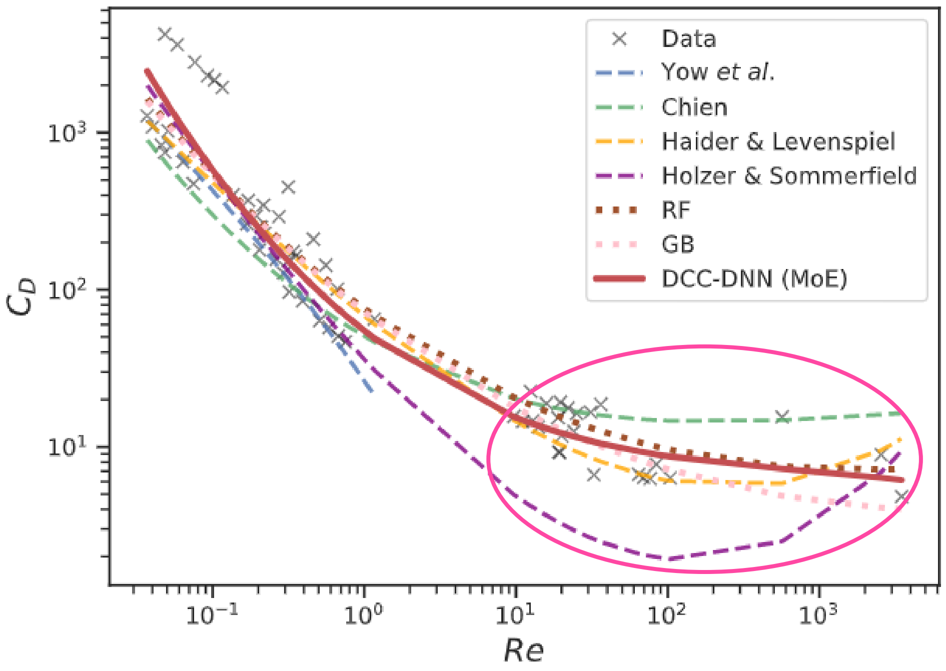
Results (cont.)

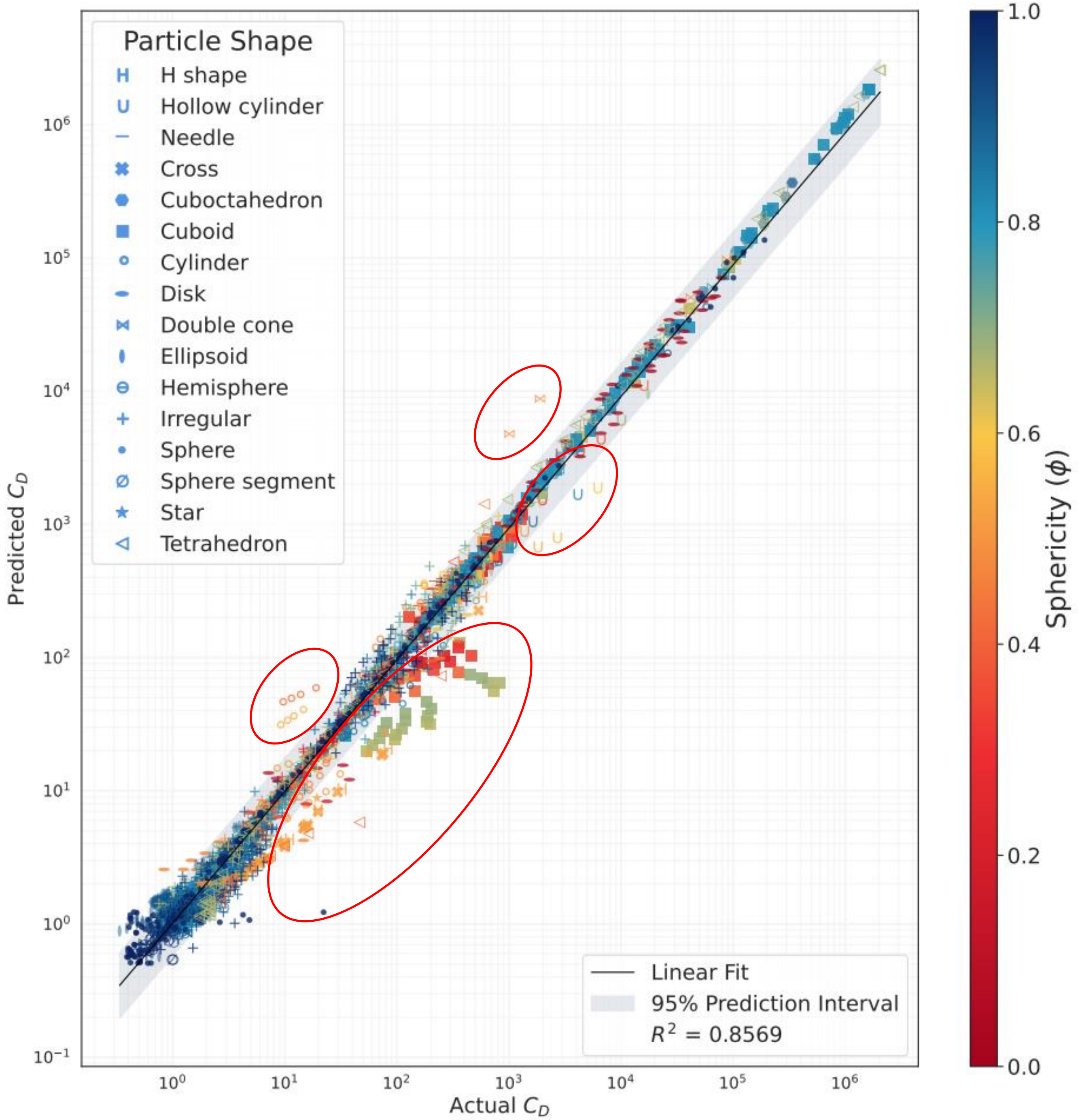


(a) $\phi = 0.1$



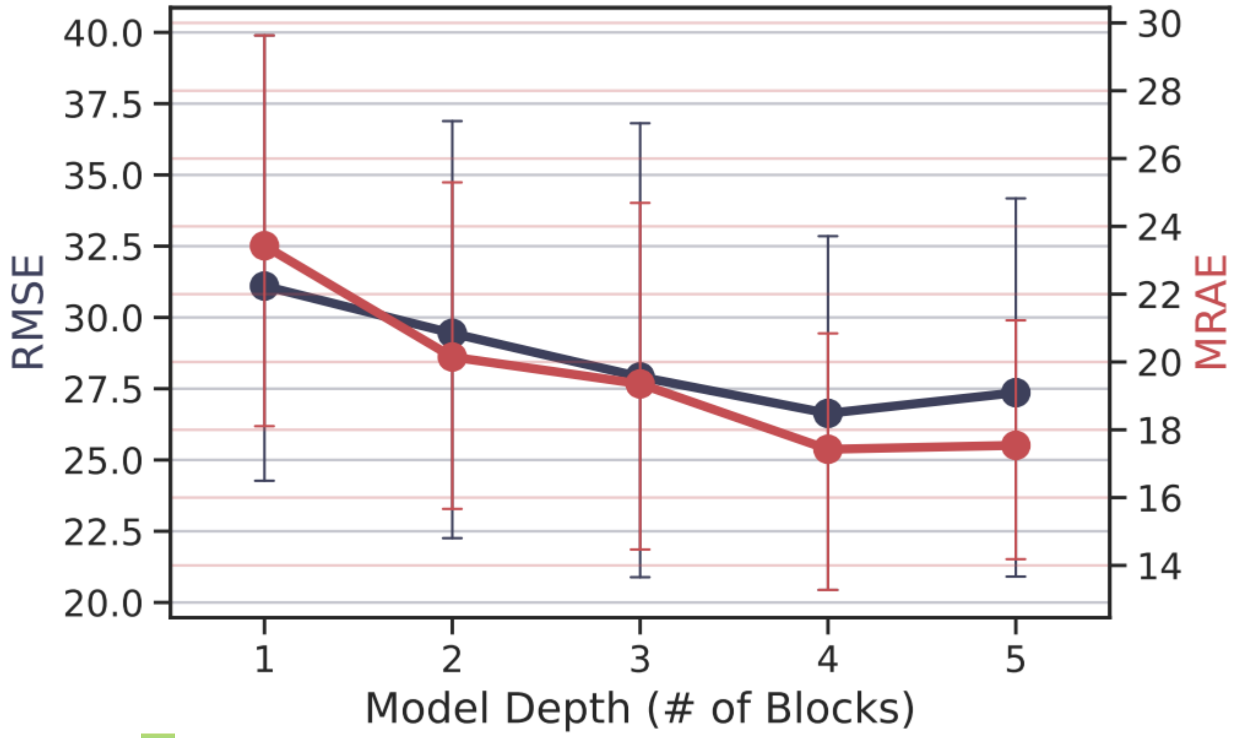
(b) $\phi = 0.3$

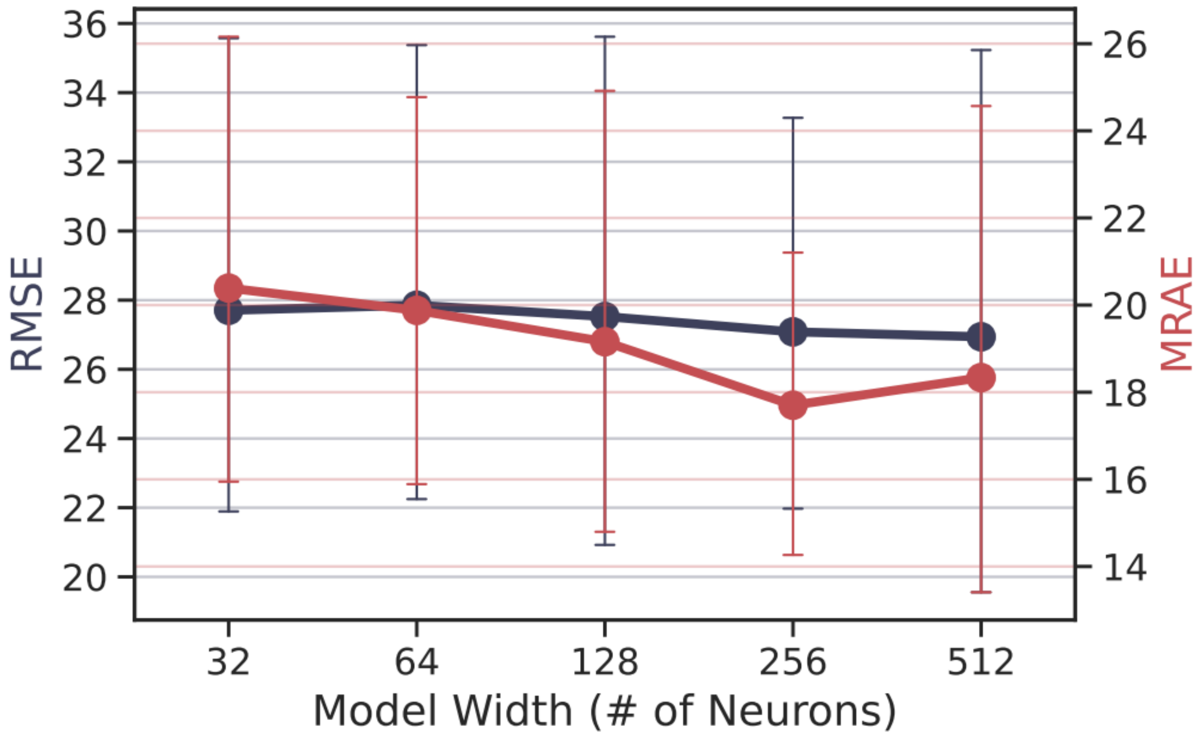
RF (Random Forest) and GB (Gradient Boosting)



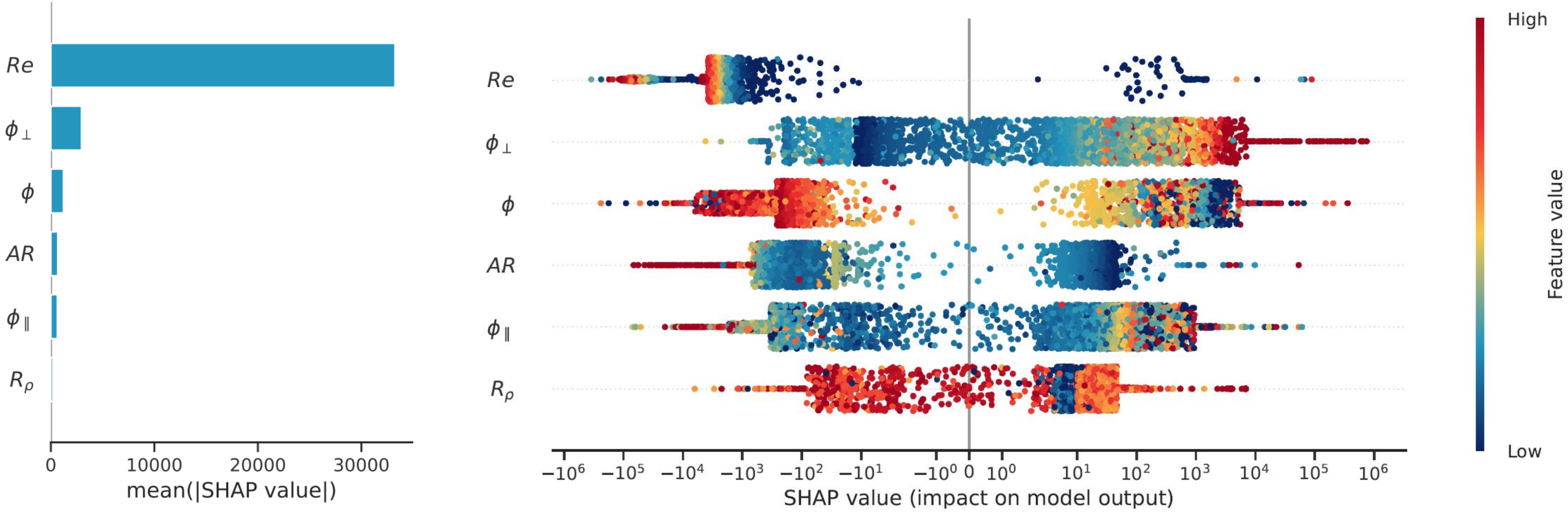
Particle Shape
H shape
Hollow cylinder
Needle
Cross
Cuboctahedron
Cuboid
Cylinder
Disk
Double cone
Ellipsoid
Hemisphere
Irregular
Sphere
Sphere segment
Star
Tetrahedron
Predicted C_D
Actual C_D
Linear Fit
95% Prediction Interval
R^2 = 0.8569
Sphericity (ϕ)

Results: Ablation Study

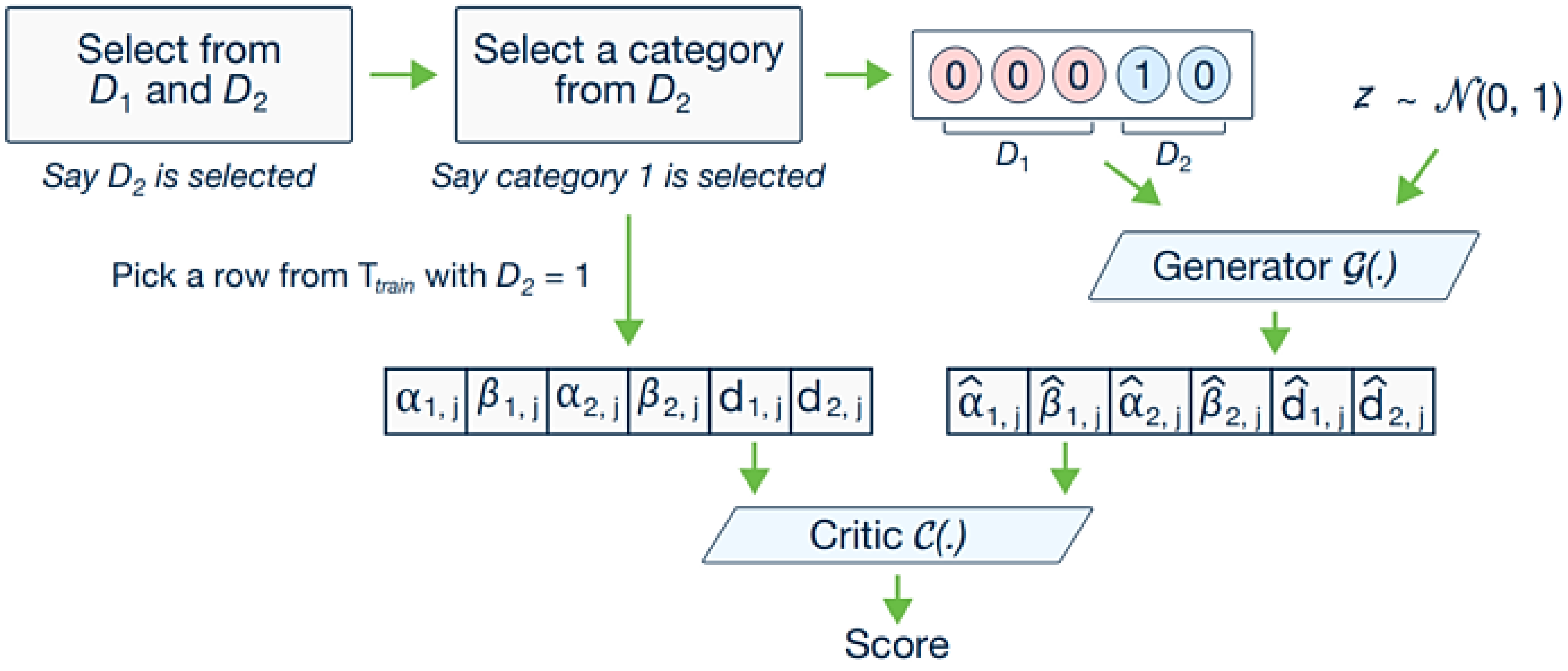




Results: Feature Importance



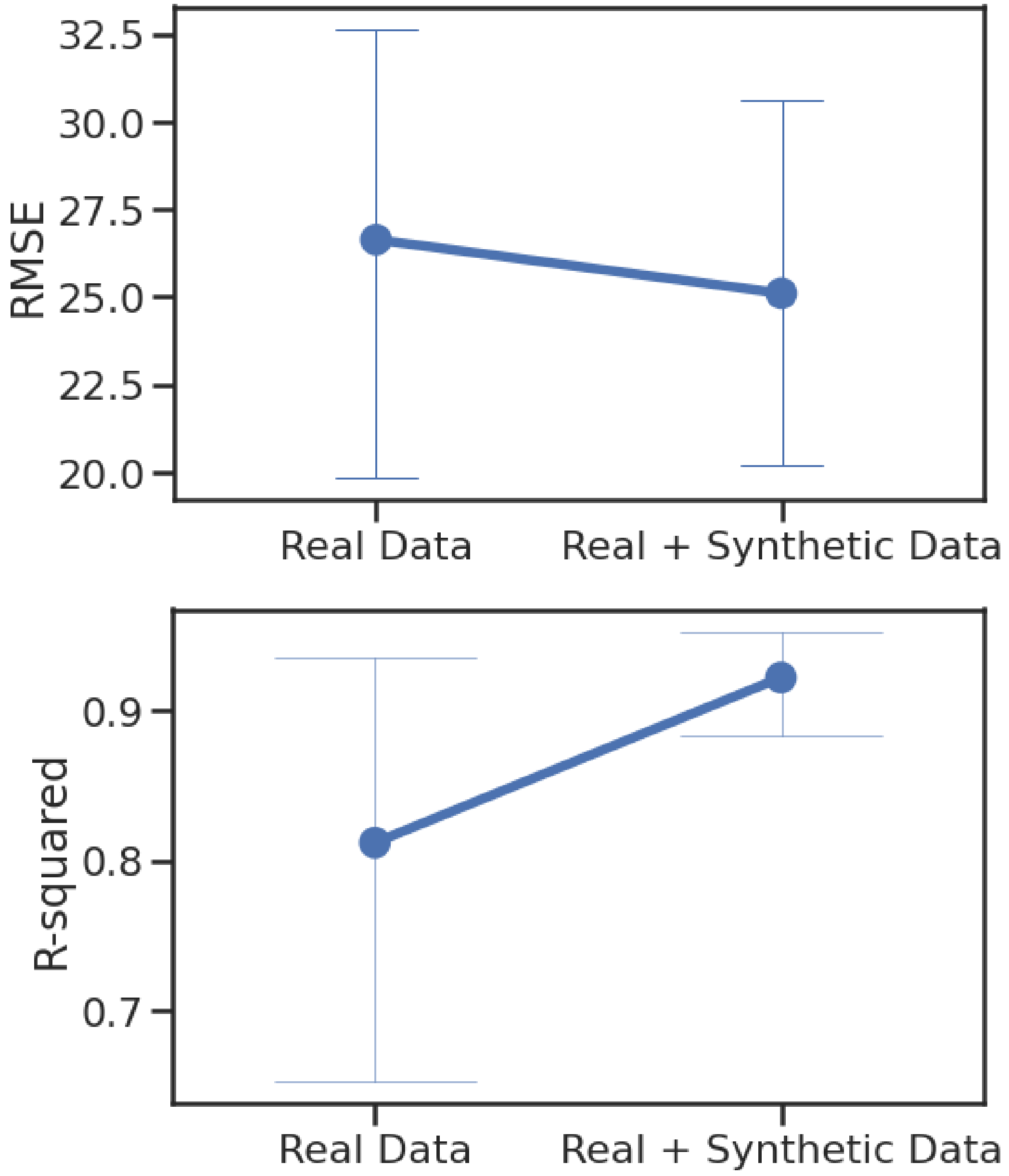
CTGAN: Synthetic Data Generation



CTGAN (cont.)

Preliminary results show:

- Model trained on the real data along with synthetic data generated by GAN achieves better performance
- Mean R-squared is 0.9215
- On average, when including Synthetic data, our model can explain about 92.15 % of the variations in the test data



Conclusion

Within the investigated parameter ranges, it is found:

- An improved drag coefficient model was developed by considering more features such as, aspect ratio, lengthwise sphericity, crosswise sphericity, and density ratio
- DNN model can predict better results compared to traditional methods using various regression metrics
- The proposed model addresses data challenges such as limited data and extreme data points through expanded feature-set, model regularization, and synthetic GAN data generation

Plan for the Next Few Months

- Continued effort to improve the DNN-based drag model in an ensemble approach.
- Implemenation of the best drag model the CFD code, MFIX.
- Verification and validation of the multiphase flow modeling results for selected cases.

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Fossil Energy and Carbon Management

THANK YOU!

Questions?

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