2021 DOE/FE 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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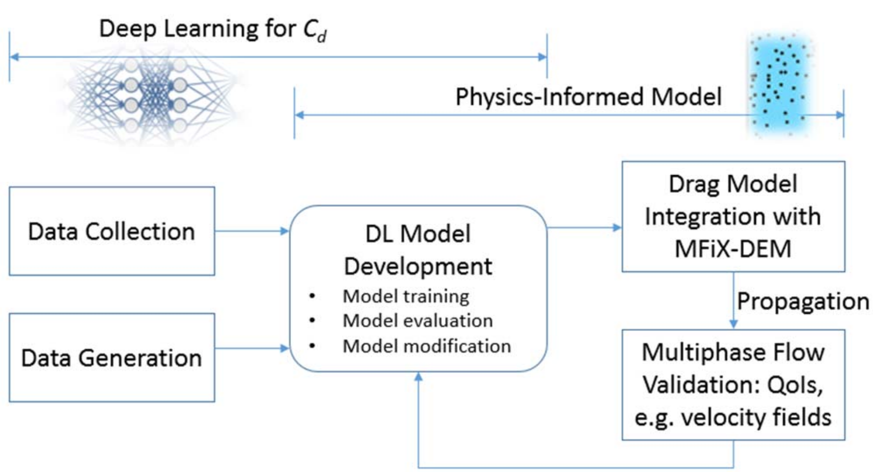
# Agenda

- Project Objective
- Project Status
- Technical Progress
  - Background/Motivation for the Project
  - Regular vs. Irregular Shapes
  - Data Collected So Far
  - Data Challenges
  - $C_D$ of Particles of Different Shapes
  - DNN Model Development
  - Performance Summary
- Conclusion
- Plan for the Next Few Months

# Project Objective

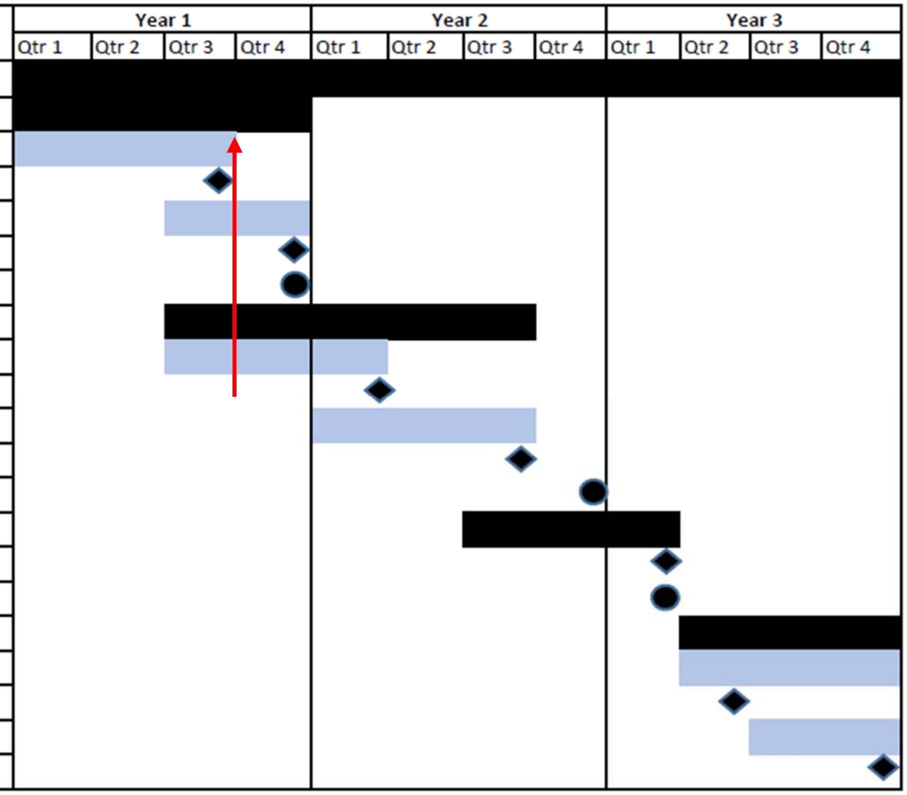
The overall objective of this project is to develop, test, and validate a general drag model for multiphase flows in assemblies of non-spherical particles by a physics-informed deep machine learning (PIDML) approach using artificial neural network (ANN).



# 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 | |



# Technical Background/Motivation for the Project

Most of existing work considers at most two features (i.e., Reynolds & sphericity)

Drag coefficient also depends on multiple other 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.

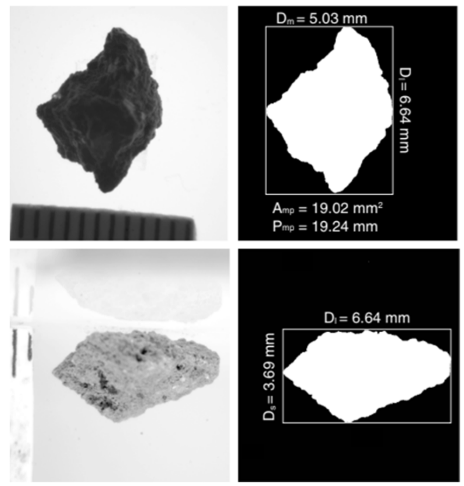
# Regular vs. Irregular Shaped Particles

Regular shaped particles:

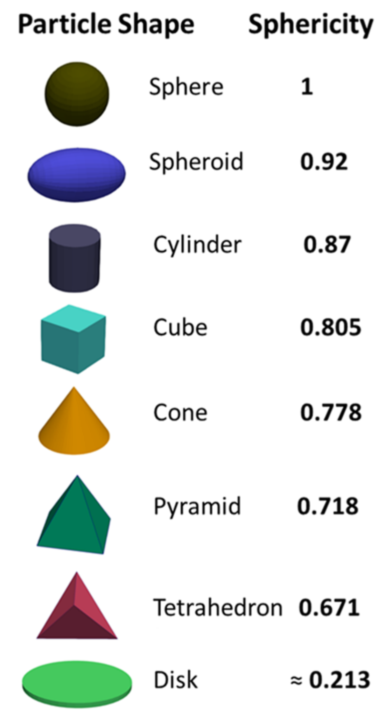
- A particle of geometric parameters such as volume and surface area that can be mathematically determined

Irregular shaped particles:

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




Irregular-shaped Particles[1]



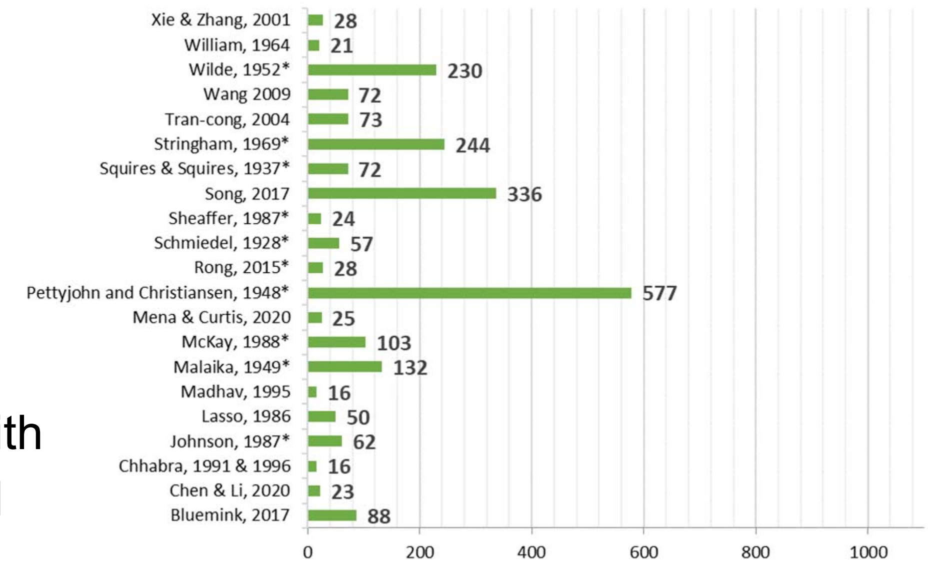

Regular-shaped Particles

[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.

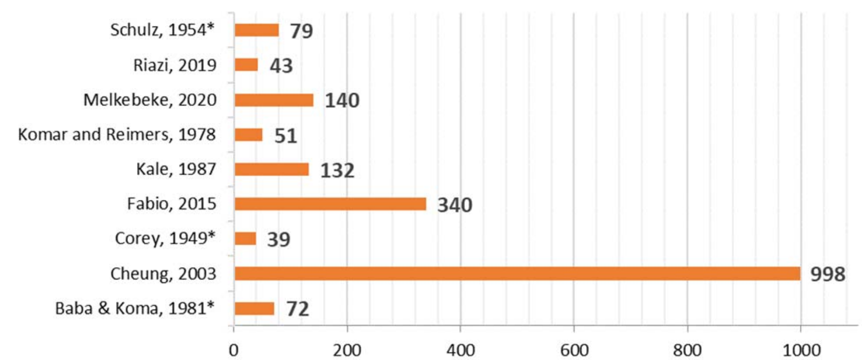
# Data Collected So Far

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




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

# Feature Generation

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

Flow property
- $Re$: Reynolds number
- $R_\rho$: Density ratio between fluid and particle

Particle geometry
- $\varphi$: 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

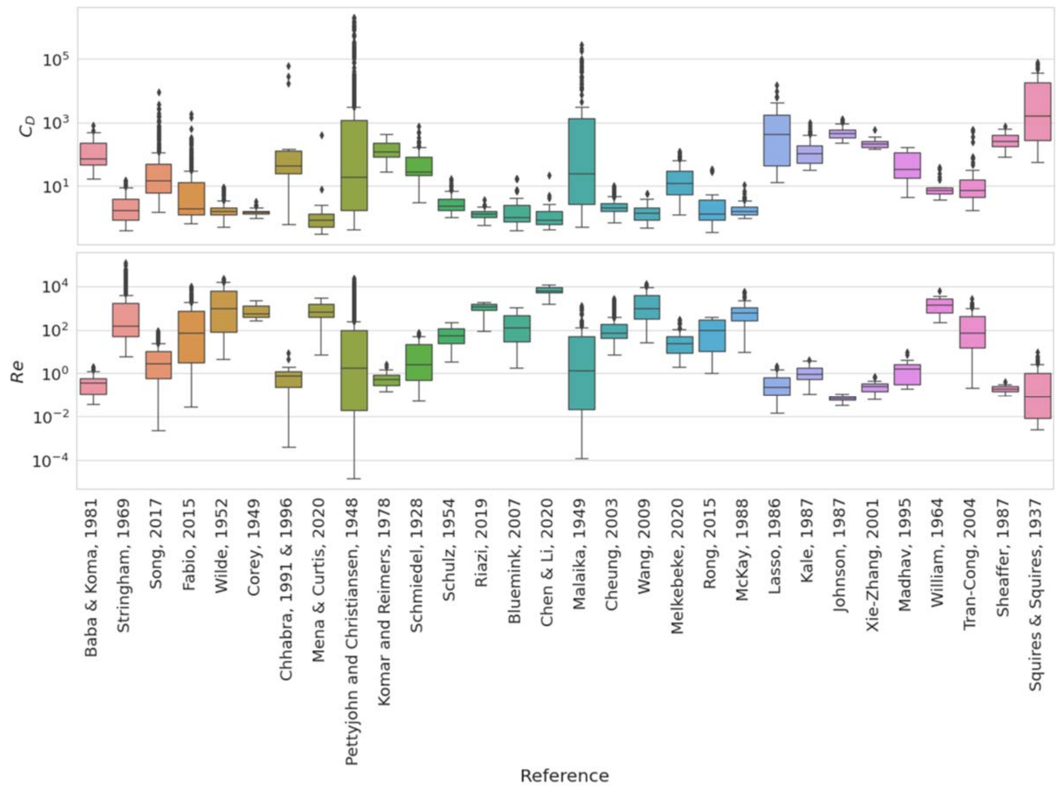
• The model doesn't generalize well from our training set to unseen set, resulting in overfitting

Extreme values

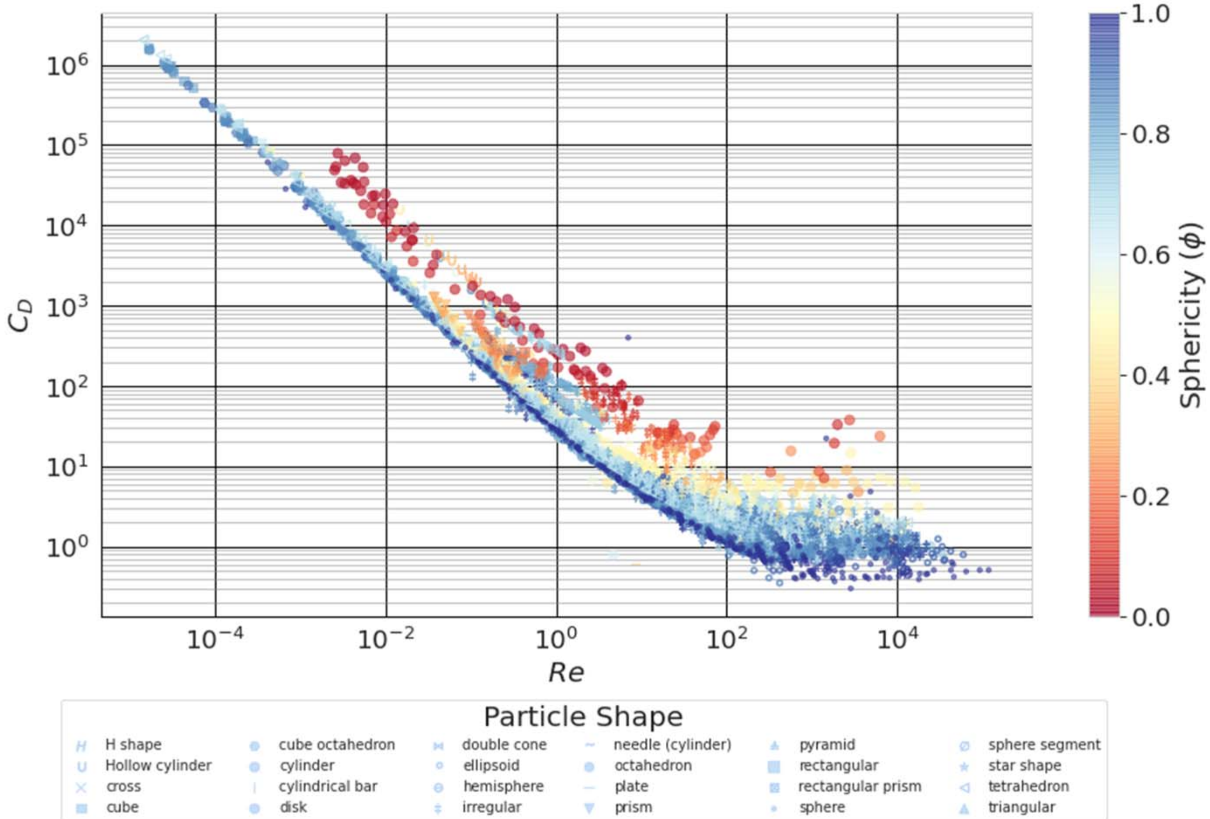
• Results in longer training times

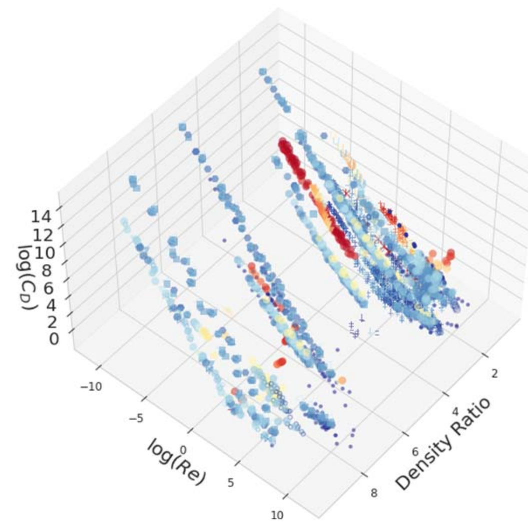
• Less accurate models

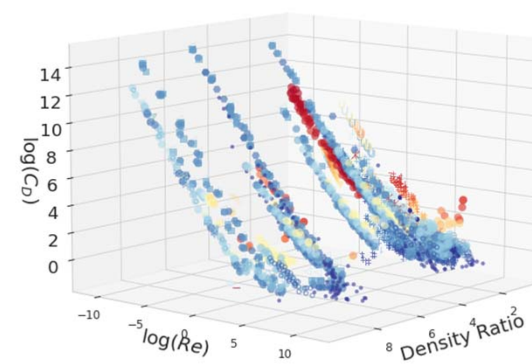
• Can spoil and mislead the model training process



# $C_D$ of Particles with Different Shapes



# Correlations-Based Drag Model

**Yow et al., 2005**

$$C_D = \frac{a_1}{Re} + \frac{b_1}{\sqrt{Re}} + c_1$$

where:

$$a_1 = 15.21 + \frac{10.82}{\varphi} - \frac{0.14}{\varphi^2}$$

$$b_1 = 13.41 - \frac{10.64}{\varphi} - \frac{0.06}{\varphi^2}$$

$$c_1 = -8.82 + \frac{5.70}{\varphi} + \frac{0.23}{\varphi^2}$$

**Chien, 1994**

$$C_D = \frac{30}{Re} + \frac{67.289}{e^{5.030\varphi}}$$

**Hölzer & Sommerfeld, 2008**

$$C_D = \frac{8}{Re}\frac{1}{\sqrt{\varphi_{\parallel}}} + \frac{16}{Re}\frac{1}{\sqrt{\varphi}} + \frac{3}{\sqrt{Re}}\frac{1}{\varphi^{3/4}} + 0.42 \times 10^{0.4(-\log(\varphi))^{0.2}}\frac{1}{\varphi_{\perp}}$$

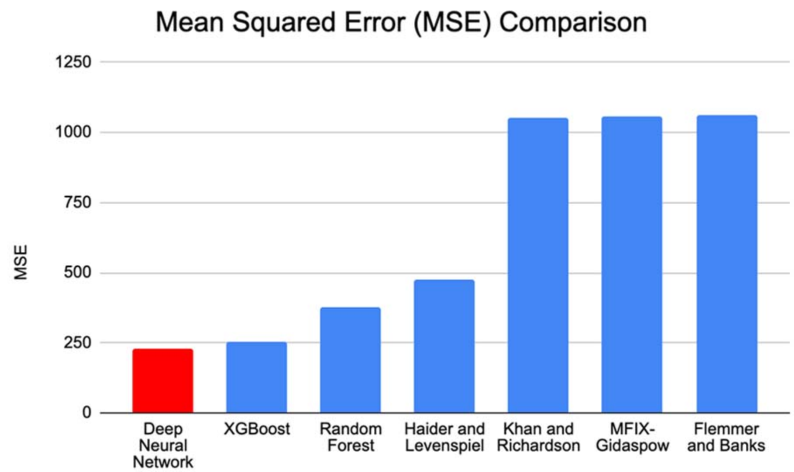
**Haider & Levenspiel, 1989**

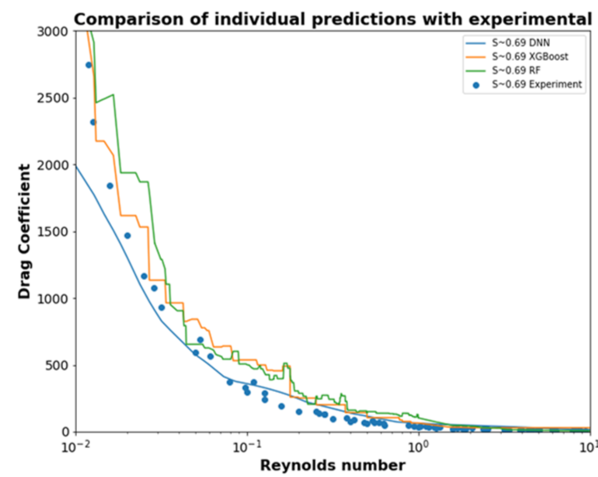
$$C_D = \frac{24}{Re}\left[1 + e^{2.3288 - 6.4581\varphi + 2.4486\varphi^2} Re^{0.0964 + 0.5565\varphi}\right] + \frac{Re \times e^{4.905 - 13.8944\varphi + 18.4222\varphi^2 - 10.2599\varphi^3}}{Re + e^{1.4681 + 12.2584\varphi - 20.7322\varphi^2 + 15.8855\varphi^3}}$$

# 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

**Data**: Tran-Cong, 2004; Song, 2017; Kale, 1987; Yow et al, 2005

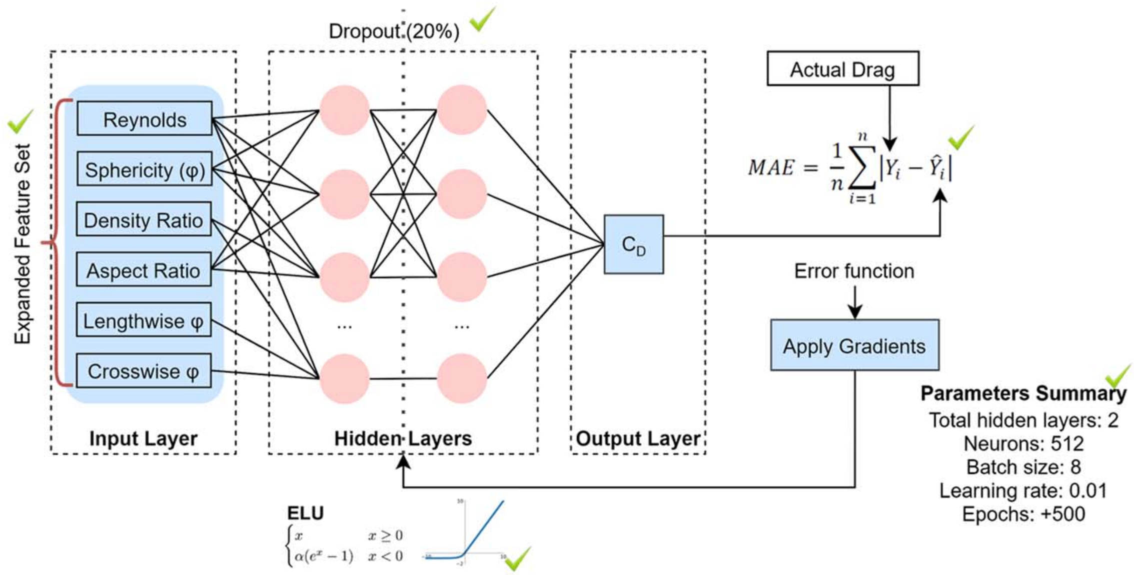


# DNN plus Additional Regularization Methods

Refining/Adjusting the DNN algorithm through model regularization and generalization

- Noise Augmentation
- Dropout Layer
- Mean Absolute Error (MAE) Loss Function
- Exponential Linear Unit (ELU) Activation




**Data**: Tran-Cong, 2004; Song, 2017; Kale, 1987; Chen & Li, 2020

# Experimental Setup

Performance metrics

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}_i - y_i)^2}{n}}$$

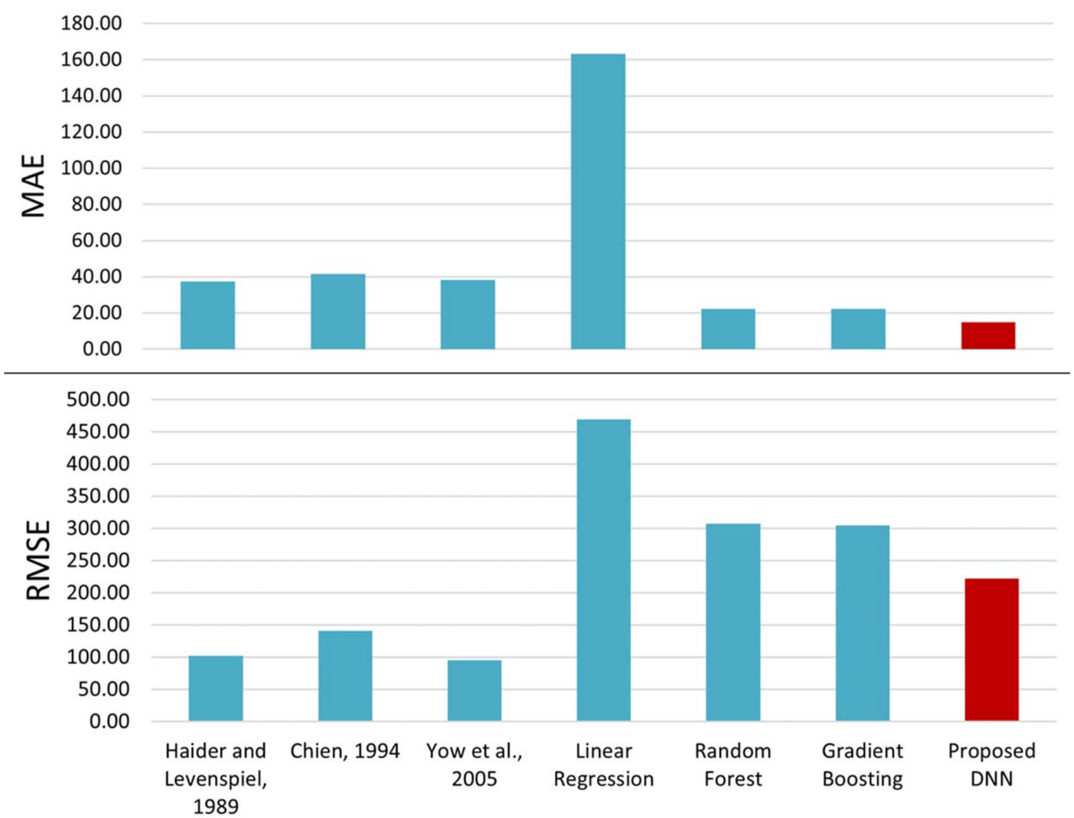
$$MAE = \frac{1}{n} \sum_{j=1}^{n} |y_j - \hat{y}_j|$$

Three-Fold Cross Validation

- Assessing how well the ML model will generalize to an independent data set

# Performance Summary

- Conventional methods may have lower RMSE values, and they are better at accounting for extreme cases
- However, higher MAE values demonstrates the it doesn’t generalize well to unseen data
- Our proposed DNN model can predict more robust results compared to traditional methods using MAE metric

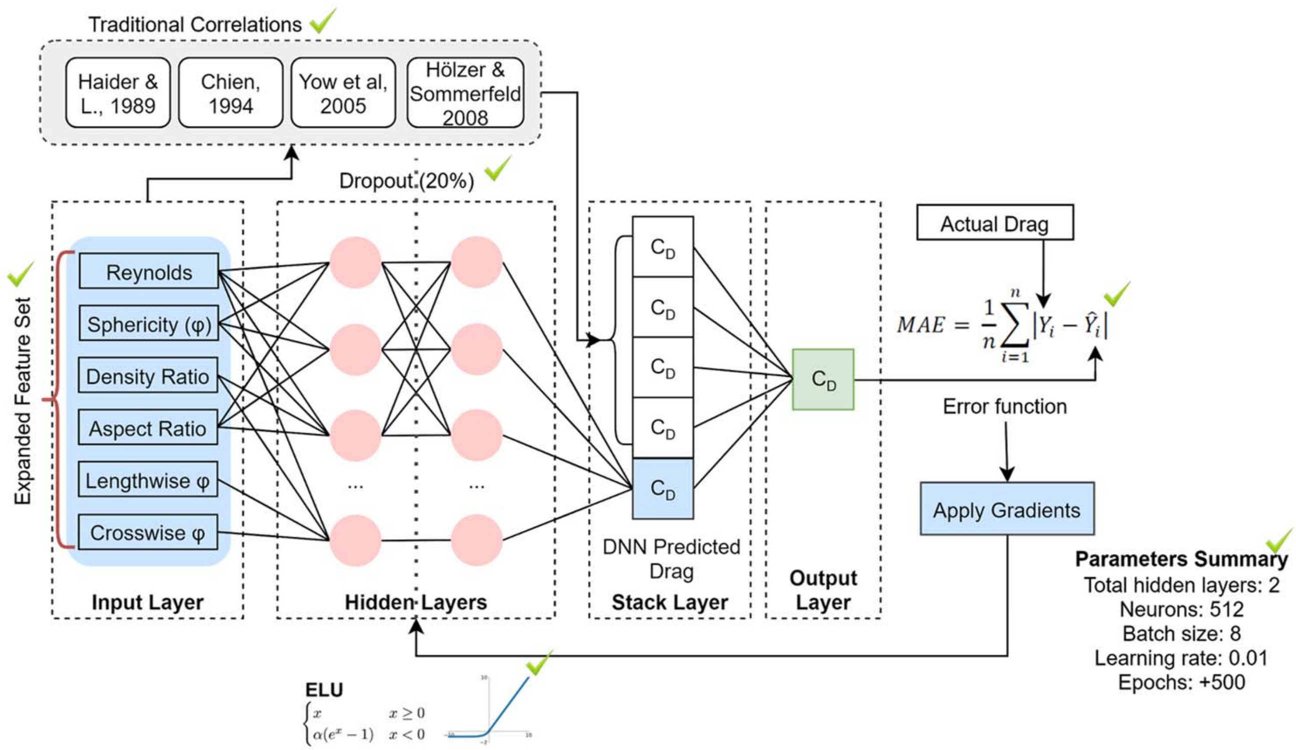


# Proposed DNN + Correlation-Based Methods

**Stacked Generalization** -

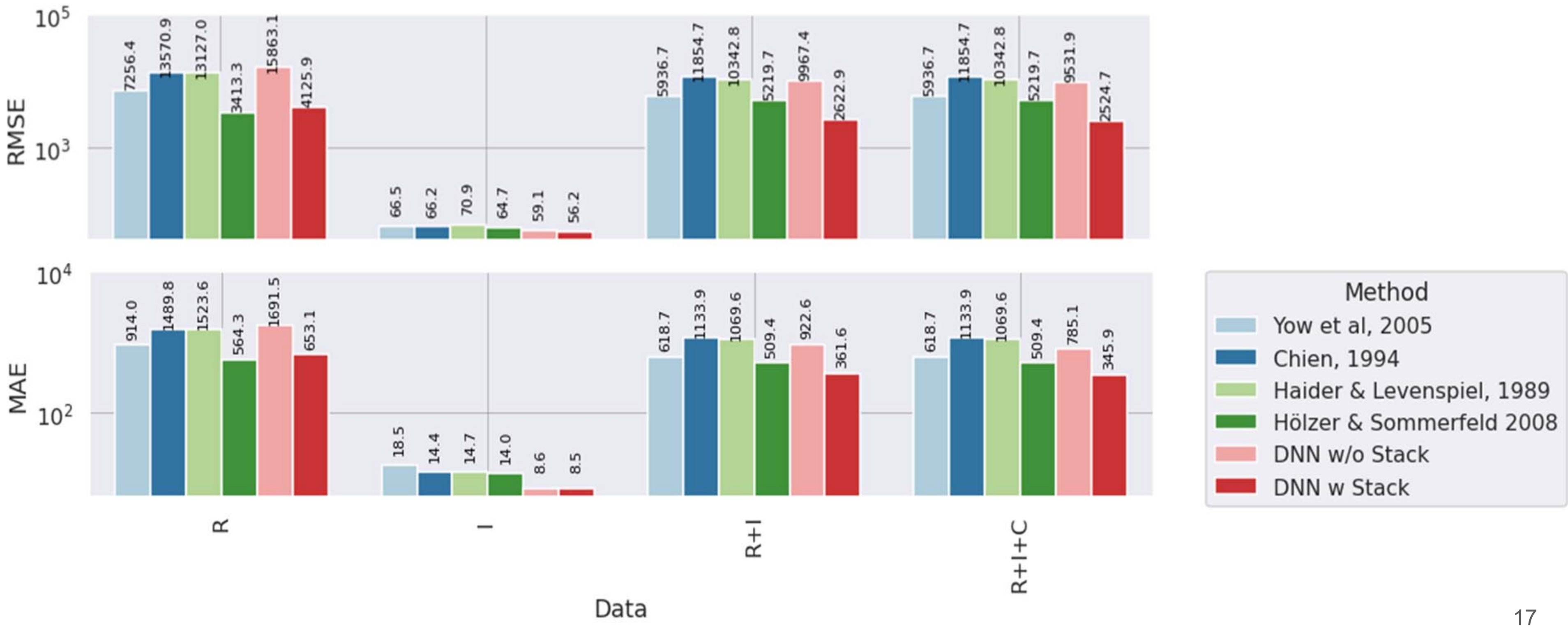
Learn how to combine the predictions from traditional correlation with proposed DNN

**Data**: Latest database compiled from 30+ publications



# Performance Summary

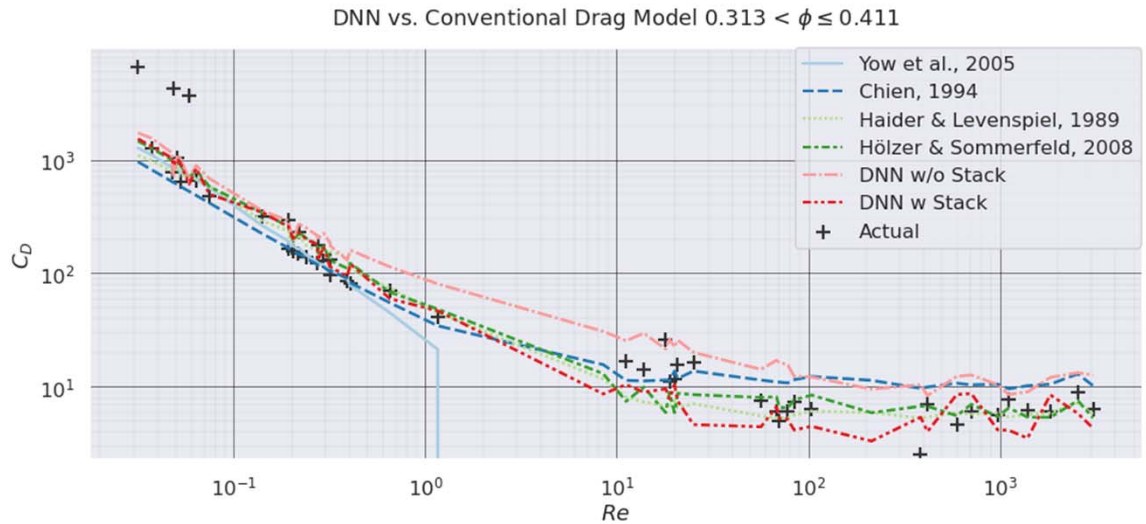
Data Configuration Key:
- (**R**) Regular Particles Experimental Drag Data
- (**I**) Irregular Particles Experimental Drag Data
- (**C**) Regular Particles Correlation-based Drag Data

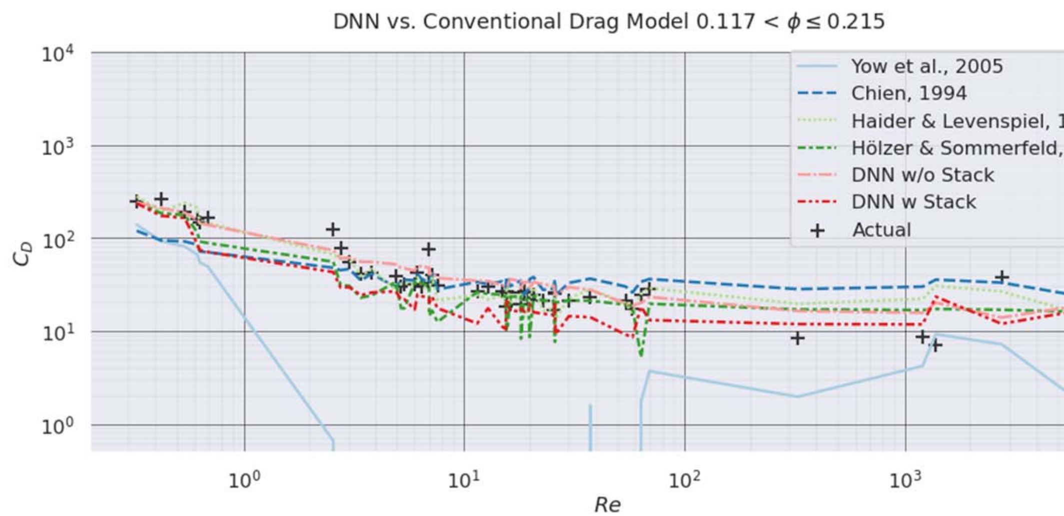


# Current Project Status

Proposed DNN vs. Conventional Drag Model

Performance comparison for particles of low sphericities demonstrate the capability of the proposed DNN



# Conclusion

In this work, we have used datasets available in the literature, 4171 samples from 30+ papers, to develop a general drag coefficient model.

Within the investigated parameter range, 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 with Stack Generalization ensemble can predict better results compared to traditional methods using RMSE and MAE metric.
- The proposed Stack Generalization technique is proven to achieve better performance, especially when irregular-shaped and low-sphericity particles are included in the dataset.

# Plan for the Next Few Months

- Continue to search for more data in the literature and expand the database.
- Perform synthetic data generation to further address the issue of missing values.
- Conduct further experiments to explore the combination of traditional correlation-based methods with DNN model in an ensemble approach.
- Apply more physics-informed methods to the DNN model to improve the performance.

# Acknowledgement

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U.S. DEPARTMENT OF ENERGY | Fossil Energy

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