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May 12, 2022
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

<table>
<thead>
<tr>
<th>Task Name</th>
<th>Assigned Resources</th>
<th>Year 1</th>
<th>Year 2</th>
<th>Year 3</th>
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<td><strong>Task 1.0 - Project Management and Planning</strong></td>
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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

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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 consistent with other data
Feature Generation

Drag Coefficient

\[ C_D = f(Re, R\rho, \Phi, AR, \varphi_{\parallel}, \varphi_{\perp}) \]

Flow property
- \( Re \): Reynolds number
- \( R\rho \): Density ratio between fluid and particle

Particle geometry
- \( \Phi \): Sphericity
- \( AR \): Aspect ratio

Settling direction
- \( \varphi_{\parallel} \): Lengthwise
- \( \varphi_{\perp} \): Crosswise

Reynolds number:
\[ Re = \frac{\rho_{\text{fluid}} u_{\text{particle}} d_{\text{particle}}}{\mu_{\text{fluid}}} \]

Density ratio:
\[ R\rho = \frac{\rho_{\text{fluid}}}{\rho_{\text{particle}}} \]

Sphericity:
\[ \Phi = \frac{A_{\text{volume equivalent sphere}}}{A_{\text{particle}}} \]

Aspect ratio:
\[ AR = \frac{l_{\text{max}}}{l_{\text{min}}} \]

Settling direction:
- \( \varphi_{\parallel} \): Lengthwise
- \( \varphi_{\perp} \): Crosswise

Cross-sectional area:
\[ A' = \frac{A'_{\text{volume equivalent sphere}}}{A'_{\text{Crosswise}}} \]

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
* Particle shape and settling velocity are retrieved from David, 2017. Other parameters including Re and Cd are calculated ourselves to be consistent with other data.
$C_D$ vs. $Re$
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)
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 $S$: $< Re, \phi, \phi_\perp, \phi_\parallel, AR, R_\rho >$

<table>
<thead>
<tr>
<th>Type</th>
<th>Method</th>
<th>Input Features</th>
<th>RMSE</th>
<th>MRAE</th>
<th>NRSS</th>
<th>SSLE</th>
<th>$R^2$</th>
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<tr>
<td></td>
<td></td>
<td>$&lt; Re, \phi &gt;$</td>
<td>37.93±12.13</td>
<td>30.08±11.08</td>
<td>56.06±54.48</td>
<td>19.52±21.10</td>
<td>0.7146±0.38</td>
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<td>TC</td>
<td>Haider &amp; Levenspiel, 1989</td>
<td>$&lt; Re, \phi &gt;$</td>
<td>49.46±12.29</td>
<td>38.59±9.06</td>
<td>92.21±90.81</td>
<td>26.14±29.03</td>
<td>0.6259±0.40</td>
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<td>Chien, 1994</td>
<td>$&lt; Re, \phi &gt;$</td>
<td>200.91±92.01</td>
<td>164.10±85.42</td>
<td>2001.56±2686.58</td>
<td>31.47±34.76</td>
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<td>Yow et al., 2005</td>
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<td>55.13±28.29</td>
<td>46.26±24.90</td>
<td>111.61±127.72</td>
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<td>ML</td>
<td>Random Forest</td>
<td>$S$</td>
<td>48.52±12.73</td>
<td>34.70±9.08</td>
<td>121.77±190.37</td>
<td>19.85±20.62</td>
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<td>Gradient Boosting</td>
<td>$S$</td>
<td>45.12±14.10</td>
<td>33.01±8.21</td>
<td>108.76±152.78</td>
<td>18.23±20.01</td>
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<td>DL</td>
<td>Baseline</td>
<td>$&lt; Re, \phi &gt;$</td>
<td>36.38±9.72</td>
<td>28.59±6.16</td>
<td>62.14±87.10</td>
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<td>$S$</td>
<td>37.09±8.92</td>
<td>27.65±5.18</td>
<td>72.66±116.09</td>
<td>72.66±116.09</td>
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<td>Single-Model DNN</td>
<td>$&lt; Re, \phi &gt;$</td>
<td>31.54±12.89</td>
<td>23.60±9.41</td>
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<td>$S$</td>
<td>26.63±10.63</td>
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<td>DCC-DNN (SG)</td>
<td>$S$</td>
<td>44.66±12.47</td>
<td>33.92±7.29</td>
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<td>DCC-DNN (MoE)</td>
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Results (cont.)

(a) $\phi = 0.1$

RF (Random Forest) and GB (Gradient Boosting)

(b) $\phi = 0.3$
Results: Ablation Study
Results: Feature Importance
CTGAN: Synthetic Data Generation
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.
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.
- Implementation of the best drag model the CFD code, MFIX.
- Verification and validation of the multiphase flow modeling results for selected cases.
Acknowledgement

This material is based upon work supported by the Office of Fossil Energy, U.S. Department of Energy under Grant DE-FE0031904.

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THANK YOU!

Questions?

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