Developing drag models for non-spherical particles through machine learning

Rui Ni, Gretar Tryggvason, Jiacai Lu, Xu Xu

Department of Mechanical Engineering
Johns Hopkins University

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Motivation: coal and biomass gasification

- Thermal conversion systems are very challenging to model:
  - Particles have complex shapes, a broad range of sizes, shapes and density.
  - Non-spherical particle interact with other particles.
  - Force closures are needed for non-spherical particles, i.e. drag and lift (maybe even other unsteady forces such as added mass and history force)

Objective: develop validated drag models for non-spherical particles
Drag Coefficient on Single Spherical and Non-Spherical Particle

Different drag correlations proposed by different groups based on the Reynolds number and sphericity ($\Phi$) projected to different directions.

Sphere (Stokes flow): $c_D = \frac{24}{Re}$


Non-spherical particle (Stokes flow):

$\frac{c_D}{K_2} = \frac{24}{ReK_1K_2} \left( 1 + 0.1118(ReK_1K_2)^{0.0567} \right)$

$+ \frac{0.4305}{1 + \frac{3305}{ReK_1K_2}}$

$K_2 = 10^{1.8148(- \log \phi)^{0.5743}}$ (Newton factor)

G. H. Ganser, Powder Technol. 77 (1993) 143

Non-spherical particle ($Re < 10^5$):

$c_D = \frac{8}{Re} \frac{1}{\sqrt{\Phi}} + \frac{16}{Re} \frac{1}{\sqrt{\Phi}} + \frac{3}{\sqrt{Re}} \frac{1}{\Phi^{\frac{3}{4}}} + 0.4210^{0.4(- \log \Phi)^{0.2}} \frac{1}{\Phi}$


Drag Coefficient on Packed Spherical Particle

\[ F(\phi, Re_m) = \frac{F_{isol}(Re_m)}{(1 - \phi)^3} + F_\phi(\phi) + F_{\phi,Re_m}(\phi, Re_m) \]

\[ F_\phi(\phi) = \frac{5.81\phi}{(1-\phi)^3} + 0.48\phi^{1/3}(1-\phi)^4 \]

\[ F_{\phi,Re_m}(\phi, Re_m) = \phi^3 Re_m \left(0.95 + \frac{0.61\phi^3}{(1-\phi)^2}\right) \]

Wen & Yu (1966) for dilute suspensions and Ergun’s equation (Ergun 1952) for denser systems are the earliest experimental efforts.

Tenneti et al. (2011); Hill et al. (2001); Beetstra et al. (2007); Gidaspow (1986); Syamlal and O’Brien (1987);
Drag Coefficient on Packed Non-spherical Particle

L. He et al. / Powder Technology 313 (2017) 332–343

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\[ c_D = \frac{8}{Re} \frac{1}{\sqrt{\Phi}} + \frac{16}{Re} \frac{1}{\sqrt{\Phi}} + \frac{3}{\sqrt{Re}} \frac{1}{\Phi_{\perp}^{3/4}} + 0.4210^{0.4(-\log\Phi)^{0.2}} \frac{1}{\Phi_{\perp}} \]

\( F_{\text{isol}}(Re_m) \) is the isolated drag model.
Human Learning versus Machine Learning

**Human Learning**

Sphere (Stokes flow): \( c_D = \frac{24}{Re} \)

Non-spherical particle (Stokes flow):
\[
  c_D = \frac{8}{Re} \frac{1}{\sqrt{\Phi}} + \frac{16}{Re} \frac{1}{\sqrt{\Phi}}
\]


**Machine Learning**

\[
  F_i = (F_i)(Re, \phi) + \Delta F_i(Re, \phi, \{r_{j=1}, \ldots, r_{j=M}\}),
\]

\[
  T_i = \Delta T_i(Re, \phi, \{r_{j=1}, \ldots, r_{j=M}\}),
\]

Seyed-Ahmadi and Wachs (2020)

**Neighbor configuration**

input features for ANN

\[
  \begin{bmatrix}
    Re, \phi, x_1, y_1, z_1, x_2, y_2, z_2 \ldots x_n, y_n, z_n
  \end{bmatrix}
\]

He and Tafti 2019

Still spherical particles
Problems

Curse of dimensionality:
As the number of features or dimensions grows, the amount of data we need to generate grows exponentially.

1 neighbor
Input: \( r_j = (x_j, y_j, z_j) \)
Output: \( F_d, c_d \)

15 neighbor
Input: \( 15 \times 3 = 45 \)
Output: \( F_d, c_d \)

\( D_1 = 3, \quad N_1 = 1000 \)
\( D_2 = 45, \quad N_2 = N_1^{D_2/D_1} = 1000^{15} \)

Each particle are collected, to yield 21,780 data points. All forces are further normalized using the Stokes-Einstein relation:

<table>
<thead>
<tr>
<th>Number of particles (N)</th>
<th>( \phi = 0.1 )</th>
<th>( \phi = 0.2 )</th>
<th>( \phi = 0.3 )</th>
<th>( \phi = 0.35 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>191</td>
<td>382</td>
<td>573</td>
<td>669</td>
<td></td>
</tr>
</tbody>
</table>

The input is a vector containing 47 features (1 Reynolds number, 1 solid fraction, relative distance in \((x,y,z)\) from the nearest 15 neighboring particles).

He and Tafti 2019

1. Reduce the number of dimensions
2. Increase the sample size

Overfitting
Introduce our team and methodology

Subteam 1: Experiment
- Rui Ni
- Xu Xu

Subteam 2: Simulation
- Gretar Tryggvason
- Jiacai Lu

Diagnostic methods
- Drop tower \((Re, \Phi)\)

Dimension reduction
- Particle-resolved DNS

Training
- TensorFlow

Validation
Using Machine Learning for closure terms in multiphase flow modeling

For turbulent flow, the fluxes depend both on resolved variables like void fraction and vertical velocity and on variables describing the average state of the unresolved state.

\[ F_g \]: The correlation coefficient with various variables

\[ F_{gx}, F_{gy} \]: Horizontal gas fluxes
Using Machine Learning for closure terms in multiphase flow modeling

Fg: The importance of various features as measured by the Gini coefficient
Flow around a falling solid sphere

Solid motion is computed by solving the fluid equations for the whole domain, with the correct density in the solid and the fluid.

A solid body motion is imposed in the solid by correcting the velocity in an iterative manner.

Collision is accounted for by adding repulsion forces. Proximity is determined using index functions on the grid used for the solving the fluid equations.
Falling solid spheres

The unsteady motion of 8 spheres in a periodic domain, viewed from above.

The trajectories of the centroids of spheres in a periodic domain viewed from above. The circles denote the initial conditions. Trajectories leave and enter the domain.
Falling solid spheres

The Reynolds number of 8 solid spheres falling in a periodic domain versus time

The instantaneous drag coefficient of each sphere versus time, computed from the slip velocity and the acceleration of each sphere
Falling solid spheres

Domain Size: 2.0 x 2.0 x 2.0;  
Resolution: 180 x 180 x 180;  
Gravity: 0.6081;  
Fluid/solid density: 1.0 / 10.0  
Fluid viscosity: 0.005  
Number of Solid Spheres: 50  
Diameter of Spheres: 0.30  
Volume Fraction of Solids: 8.84%

The volume fraction is high, so the spheres collide frequently
Falling solid spheres

The spheres and the fluid velocity in one plane

The vorticity around the spheres, visualized by the $\lambda_2 = -4.0$ contour
Falling solid ellipsoids

Domain Size: 2.0 x 2.0 x 2.0;
Resolution: 200 x 200 x 200;
Gravity: 0.6081;
Fluid/solid density: 1.0 / 10.0
Fluid viscosity: 0.005
Number of Solid Spheres: 50
Size of Ellipsoids: 0.32 x 0.16 x 0.16
Volume Fraction of Solids: 2.68%

Notice that the volume fraction is lower than for the spheres. Although many fall broadside on, not all do
Falling solid ellipsoids

The ellipsoids and the fluid velocity in one plane

The vorticity around the ellipsoids, visualized by the $\lambda_2 = -4.0$ contour
Non-spherical particles

Formlabs Form2 3D printer
- Stereolithography technology
- $145 \times 145 \times 175$ mm build volume
- $25 \mu m$ minimum layer thickness

Non-spherical particles also exist in nature

The aspect ratios from left to right are roughly 5, 3.5 and 1.5.

This is a 3D printed particle with supporting material. It has a 2.5 mm major diameter and 0.5 mm minor diameter.
Preliminary drop tower

The goals of preliminary setup:

- Automated experiment procedure
- Data acquisition system
- Post-processing algorithm

Control Parameters:

- Particle shape
- Particle size
- Particle material density
- Particle number density

<table>
<thead>
<tr>
<th>Test section dimension</th>
<th>Funnel volume</th>
<th>Total number of cameras rack</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25×0.25×3 m</td>
<td>350 ml</td>
<td>4</td>
</tr>
</tbody>
</table>
The goals of this setup:

- Use tracer and LED backlighting to obtain fluid phase data.
- Experimentally investigate pair particle interaction with controlled initial conditions.
- Experimentally investigate fluid flow within a free-falling anisotropic particle swarm.
  - Fluid phase is quiescent water
  - Anisotropic particle is rice
Preliminary experimental tests

**Water channel:**
Left panel: 4 mm rice  
Right panel: 7.5 mm rice

Images taken at ~5cm below particle release location

**Preliminary drop tower:**
Left panel: 4 mm rice  
Right panel: 7.5 mm rice

Images taken at ~1m below particle release location
2D particle tracking velocimetry
Plan

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MFIX

Training

Validation
Acknowledgment

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