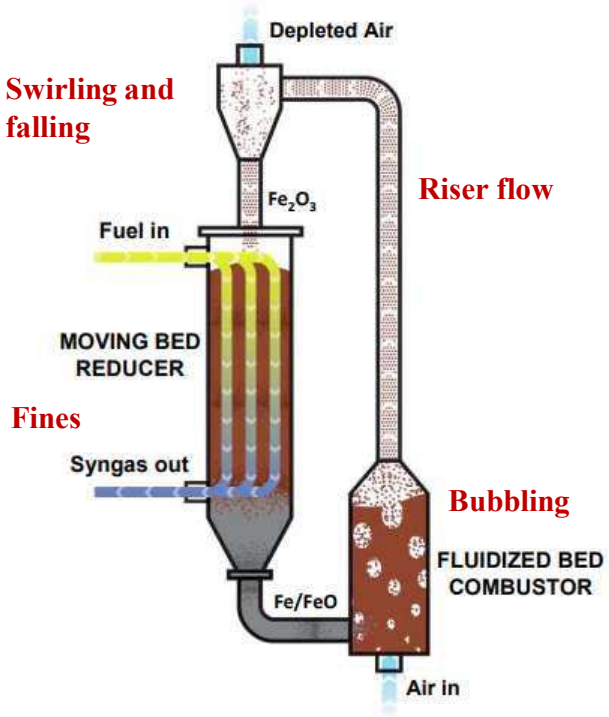
THE OHIO STATE UNIVERSITY

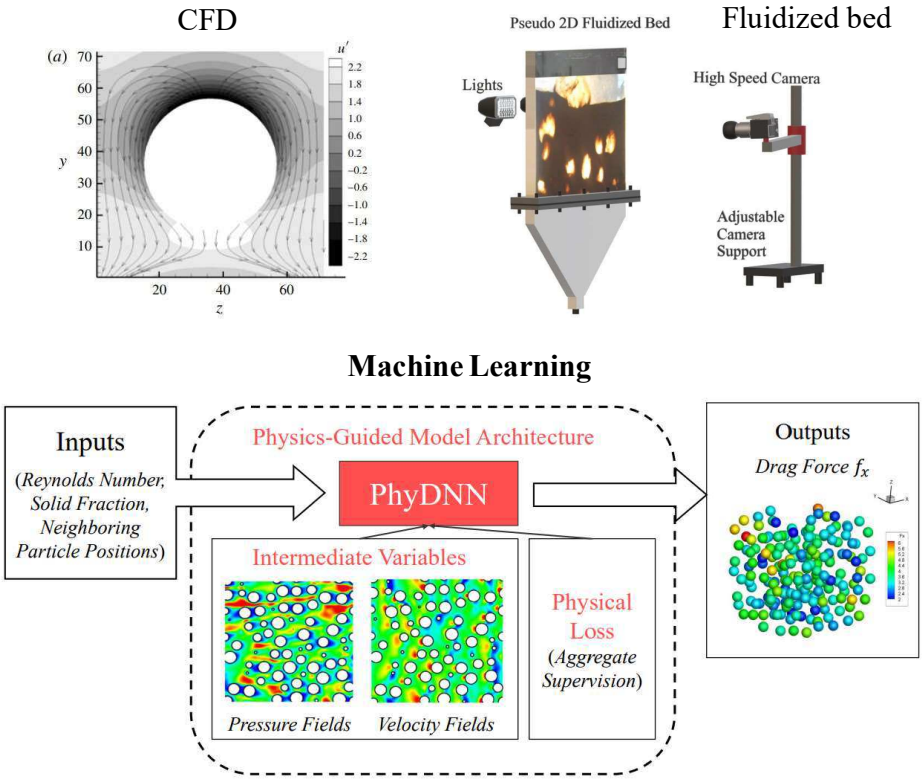
MACHINE LEARNING-BASED FORCE MODEL FOR IRREGULAR-SHAPED PARTICLES IN GAS-SOLID FLOWS

Soohwan Hwang, Liang-Shih Fan

Gas-Solid Flows



Interaction Forces



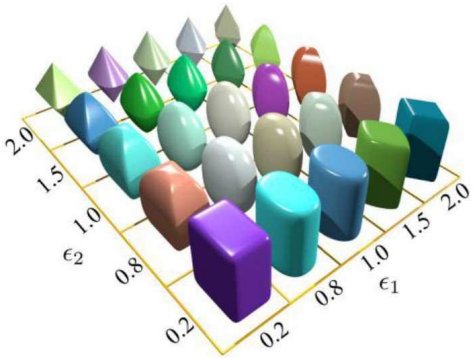
Qiang Zhou et al., *Journal of Fluid Mechanics*, 765 (2015)
Cesar Martin Venier et al. *International Journal of Numerical Methods for Heat and Fluid Flow* (2019)
Long He et al., *Powder Technology* 345 (2019)

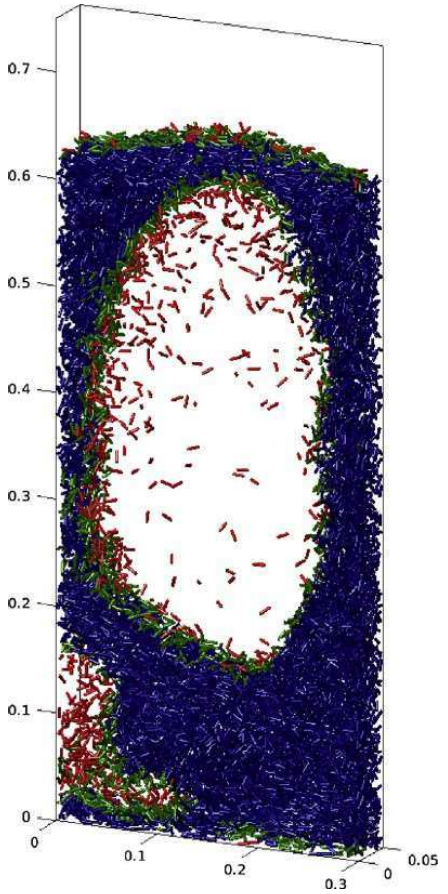
Non-spherical particle

- Difficult to define the geometrical factors sphericity, flatness, elongation and circularity, etc.
- Data for the interaction force between non-spherical particles and the fluids are limited.
- Correlation may be highly-nonlinear.

Objectives

- Developing a neural network-based force model for a diversity of non-spherical particles.





Shiwei Zhao et al., Int J Numer Anal Methods Geomech., 43 (2019)

Vinay V. Mahajan et al., Chemical Engineering Science, 192 (2018)

Spherical Harmonic (SH)

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\varphi^2} = 0.$$

$$f(r,\theta,\varphi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} f_\ell^m r^\ell Y_\ell^m(\theta,\varphi)$$

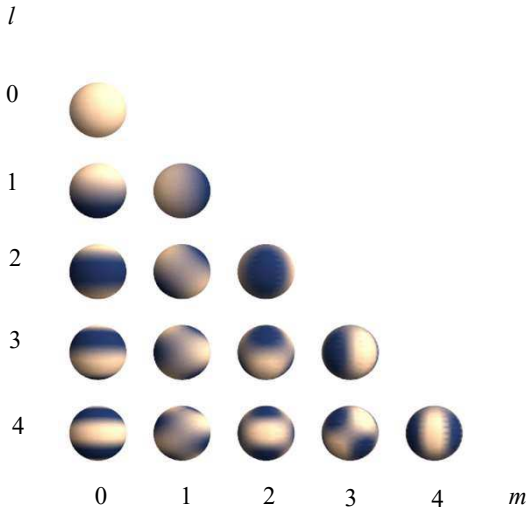
$$\boldsymbol{X} = (x,y,z) = \sum_{l=1}^{l=8}\sum_{m=-l}^{l} \boldsymbol{C}_l^m Y_l^m(\varphi_1,\varphi_2)$$

$$\boldsymbol{C}_l = \begin{pmatrix} C_{x,l}^{-l} & \cdots & C_{x,l}^{0} & \cdots C_{x,l}^{l} \\ C_{y,l}^{-l} & \cdots & C_{y,l}^{0} & \cdots C_{y,l}^{l} \\ C_{z,l}^{-l} & \cdots & C_{z,l}^{0} & \cdots C_{z,l}^{l} \end{pmatrix}$$

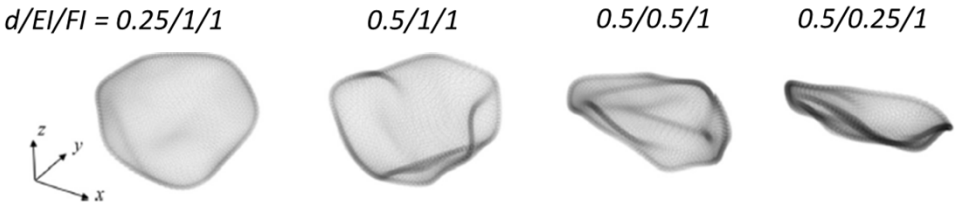
$$= \begin{pmatrix} k_{x,l}(\alpha_{x,2l} - \alpha_{x,2l+1}i) & \cdots & k_{x,l}\alpha_{x,1} & \cdots k_{x,l}(\alpha_{x,2l} + \alpha_{x,2l+1}i) \\ k_{y,l}(\alpha_{y,2l} - \alpha_{y,2l+1}i) & \cdots & k_{y,l}\alpha_{y,1} & \cdots k_{y,l}(\alpha_{y,2l} + \alpha_{y,2l+1}i) \\ k_{z,l}(\alpha_{z,2l} - \alpha_{z,2l+1}i) & \cdots & k_{z,l}\alpha_{z,1} & \cdots k_{z,l}(\alpha_{z,2l} + \alpha_{z,2l+1}i) \end{pmatrix}$$

$$k_{i,l} = \sqrt{\frac{d_{i,l}^2}{\alpha_{1,1}^2 + 2\sum_{j=2}^{2l+1}\alpha_{i,j}^2}}, \quad i \in (x,y,z)$$

$$d_{i,l} = \frac{d\sqrt{\frac{\pi}{3}(1+EI^2+EI^2FI^2)}}{\sum_{k=2}^{8}(\frac{2}{k})^{1.387}}(\frac{2}{l})^{1.387}$$

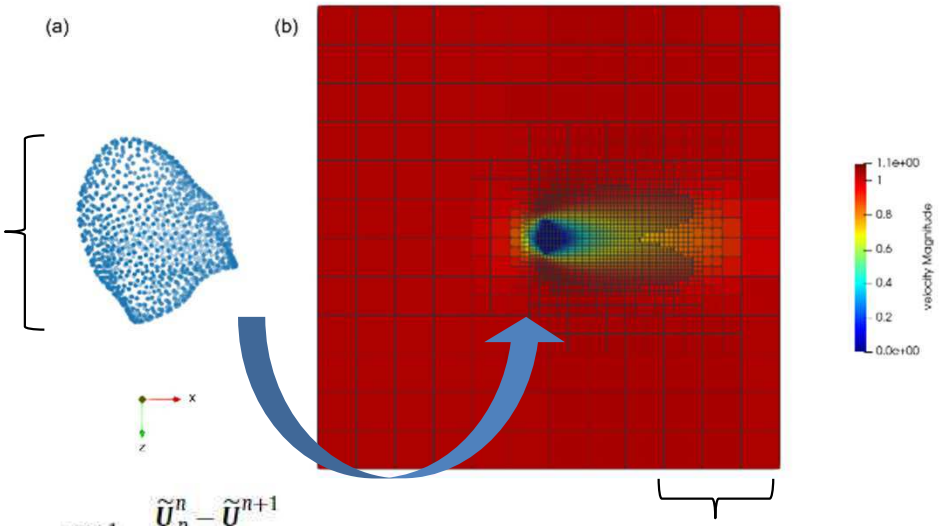


Combine linearly,
Higher weight on higher l → high ***d***
d ~ roughness



Wei, D., Wang, J., & Zhao, B. (2018). *Powder Technology*, *330*, 284-291.
https://en.wikipedia.org/wiki/Spherical_harmonics

Particle-Resolved Direct Numerical Simulation (PR-DNS)



Lagrangian points

$$F^{n+1} = \frac{\tilde{U}_p^n - \tilde{U}^{n+1}}{\Delta t}$$

Direct forcing scheme
$\tilde{U}_p^n = 0$ for fixed particles

Adaptive mesh refinement based on:

$$\Omega = \frac{b}{a+b}$$

$$a = \mathrm{trace}(A^T A) = \sum_{i=1}^{3}\sum_{j=1}^{3}(A_{ij})^2, \qquad b = \mathrm{trace}(B^T B) = \sum_{i=1}^{3}\sum_{j=1}^{3}(B_{ij})^2.$$

$$\nabla V = \frac{1}{2}(\nabla V + \nabla V^T) + \frac{1}{2}(\nabla V - \nabla V^T) = A + B,$$

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = \frac{g-f}{\tau}$$

$$f(0,t) \approx g(0,t) + \frac{\tau}{\delta t}(g(-v\delta t, t-\delta t) + g(0,t))$$

$$F = \int f(0,t) v_x \Xi dv\ ,\ \Xi = \begin{pmatrix} 1 \\ v \end{pmatrix}$$

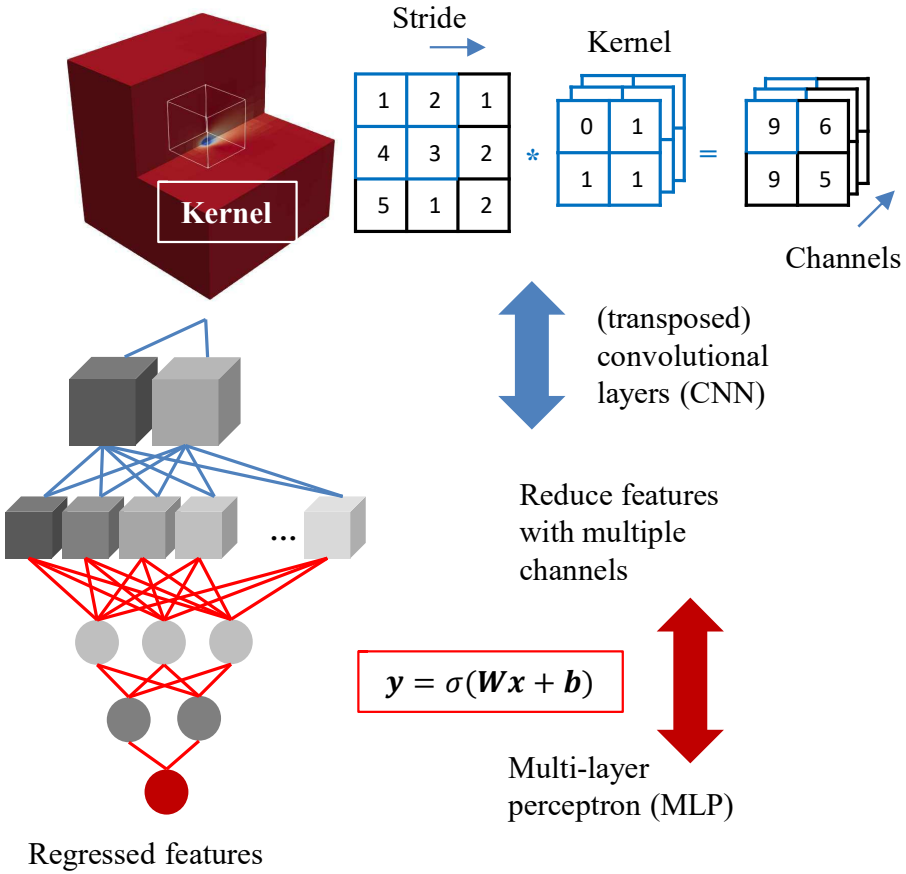
$$\frac{\partial W}{\partial t} + \nabla \cdot F = 0,\ W = \begin{pmatrix} \rho \\ \rho u \end{pmatrix}$$

Gas Kinetic Scheme

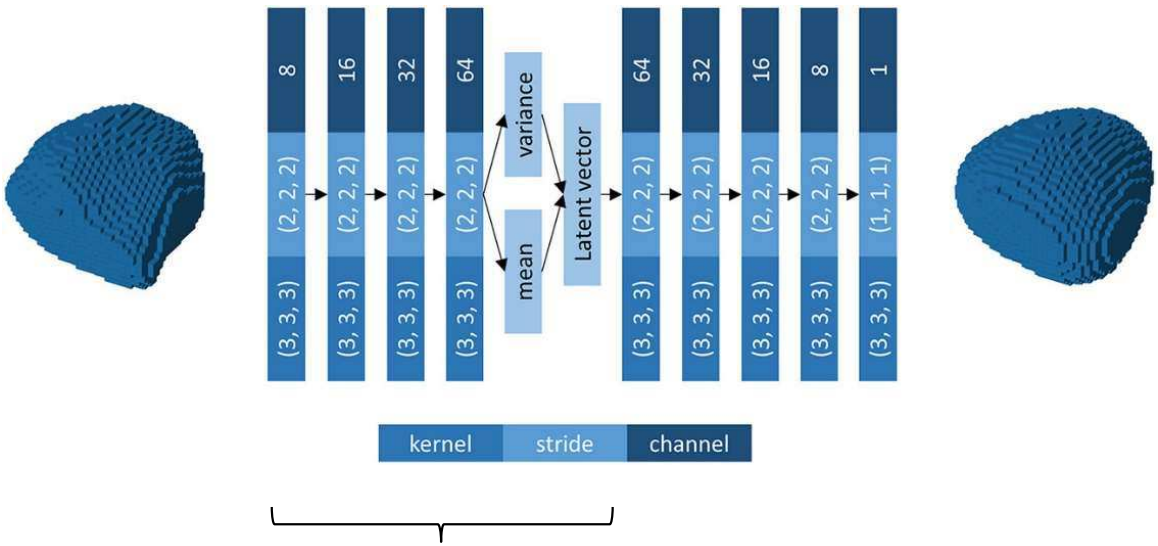
$$g = \begin{cases} \frac{\rho}{4\pi}, & if\ (u-v)^2 = c^2 \\ 0, & otherwise \end{cases}$$

Simplified Sphere function for incompressible flows

Neural Networks



Variational Auto-Encoder (VAE)



- Encoder

$48^3 \rightarrow 24^3 \times 8 \rightarrow 12^3 \times 16 \rightarrow 6^3 \times 32 \rightarrow 3^3 \times 64 \rightarrow 27$

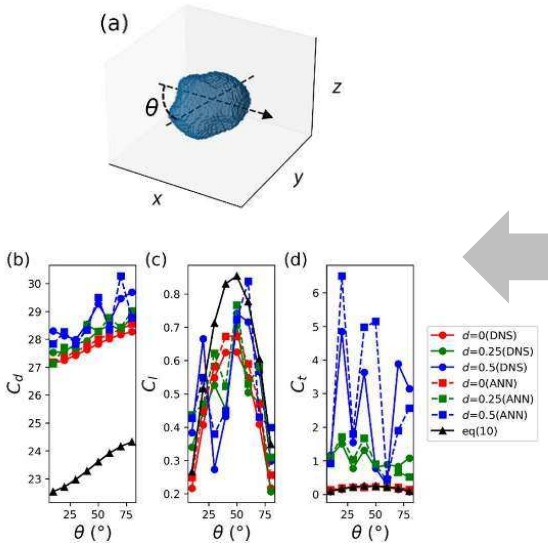
- MLP/Regularization

$27 \rightarrow 128 \times 2 \rightarrow$ **128 (latent)**

- Vertices (Decoder, TCNN)
- Force coefficients (MLP)
- Flow fields (PIEP, TCNN)

Re

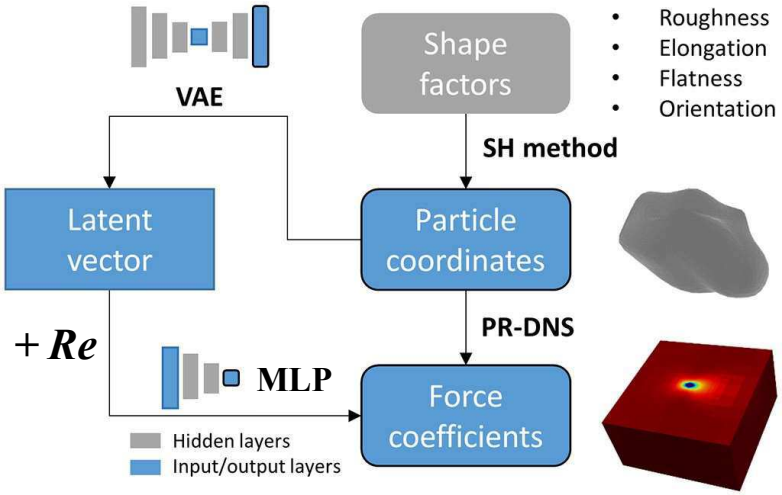
Interaction Force Model for Single Particles

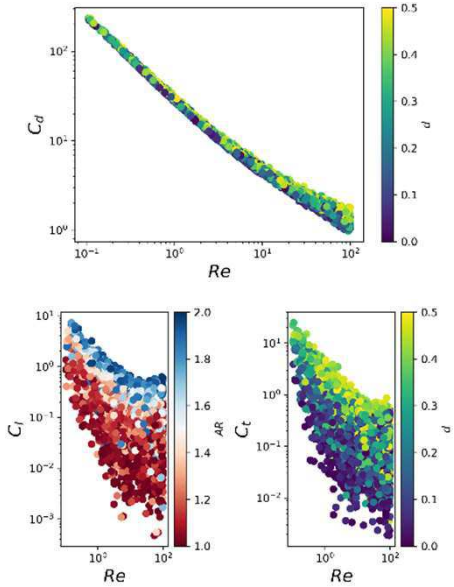


MLP results (MSE) C_d : 7.9 (3.3% MAPE)

C_l : 0.00546

C_t : 0.0647

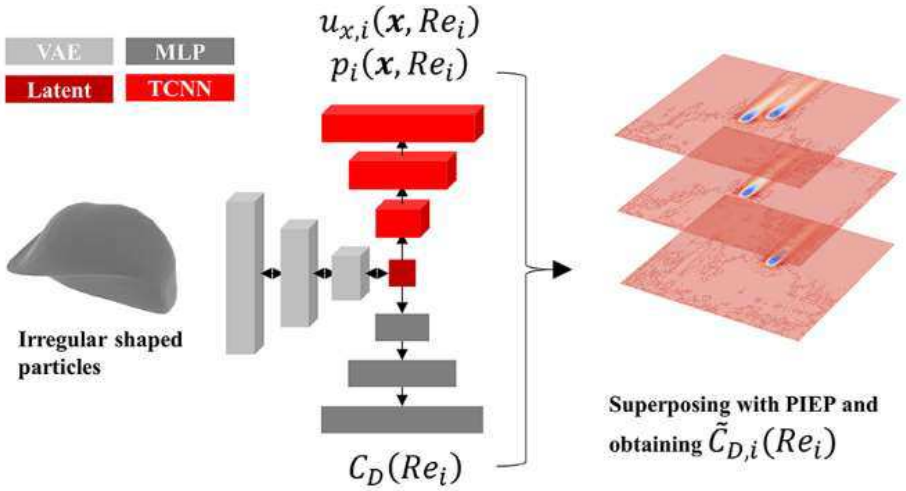




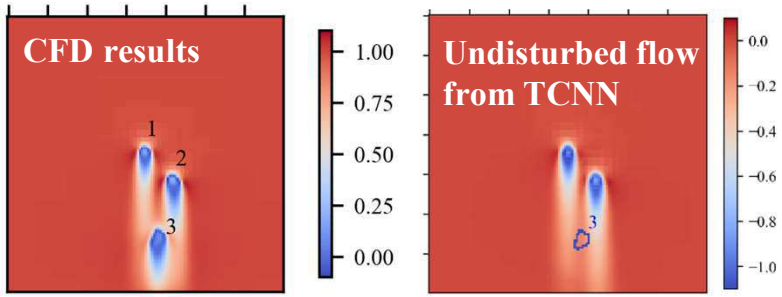
CFD results

Soohwan Hwang et al., *Powder Technology*, 392 (2021)

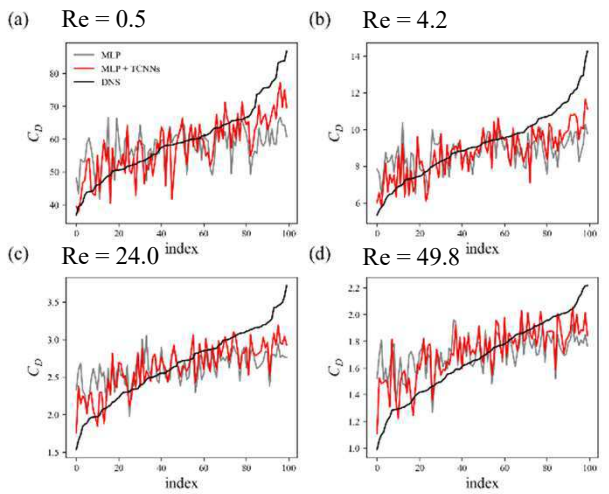
PIEP with MLP and TCNN



$$\tilde{F}_{qs,i} = \bar{F}_{drag}(Re_i, \varphi) + \frac{\rho {u_{mac}}^2 A}{2} C_{D,i} \left\{ \frac{1}{u_{mac}} \sum_{\substack{j=1 \\ j \neq i}}^{N} \overline{u_{j \to i}}^S \right\}$$

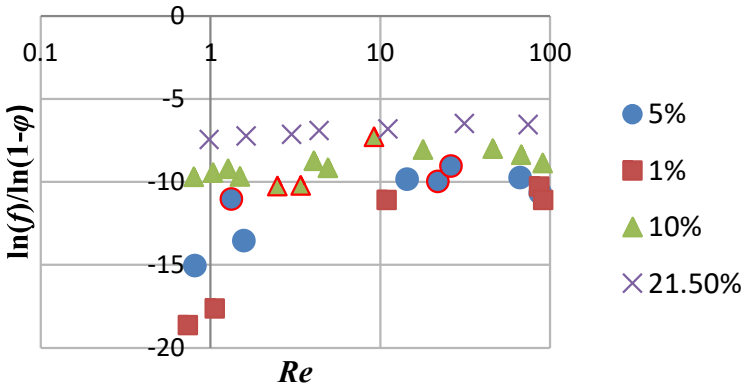


100 different particles with 0.5% ($1 < AR < 2$, $0 < d < 0.5$)



PIEP: Pairwise Interaction Extended Point-particle model
Soohwan Hwang et al., *Chemical Engineering Science* 266, 118299 (2023)

PIEP for dense systems



$$\bar{C}_D(Re_i, \varphi, d) = C_{D,i} \cdot f(Re_i, \varphi, d)$$

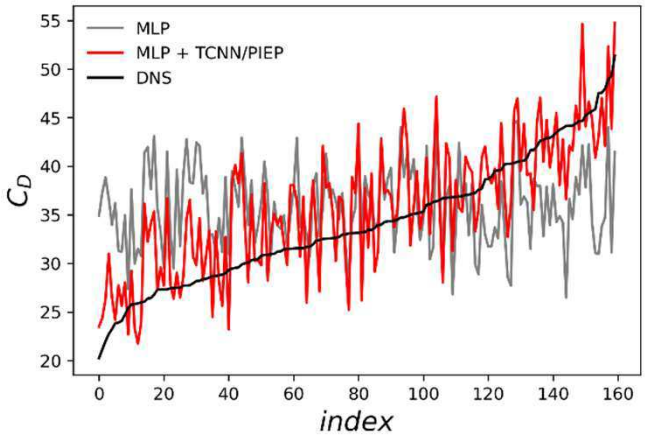
$$x = (\ln(Re) - 3.5)^2$$

$$\frac{\log(f)}{\log(1-\varphi)} = a(\varphi)x + b(\varphi)$$

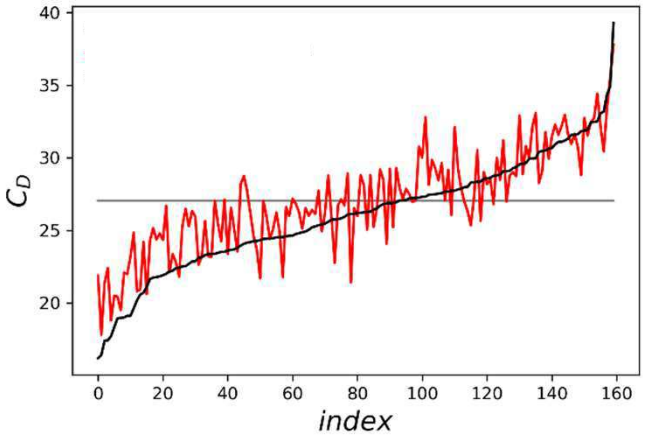
$$a(\varphi) = 0.18\ln(\varphi) + 0.23$$

$$b(\varphi) = 18.1\varphi - 10.4$$

Re = 1.8, polydisperse (φ = 0.06, d = 0 ~ 0.5)
MAPE: 12%
R2 : 0.46

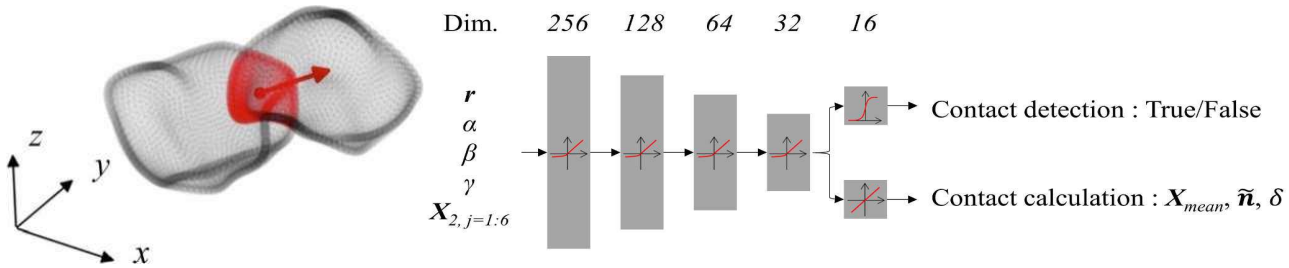


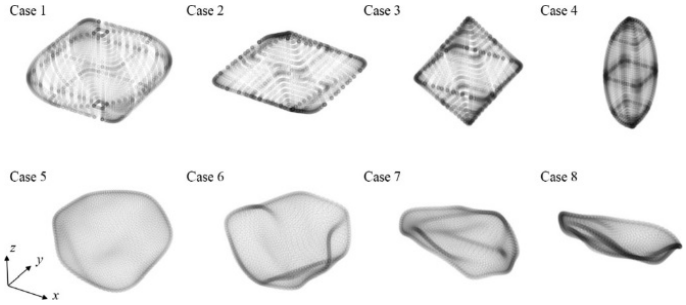
Re = 2.2, monodisperse (φ = 0.05, d = 0.49)
MAPE: 7%
R2: 0.70

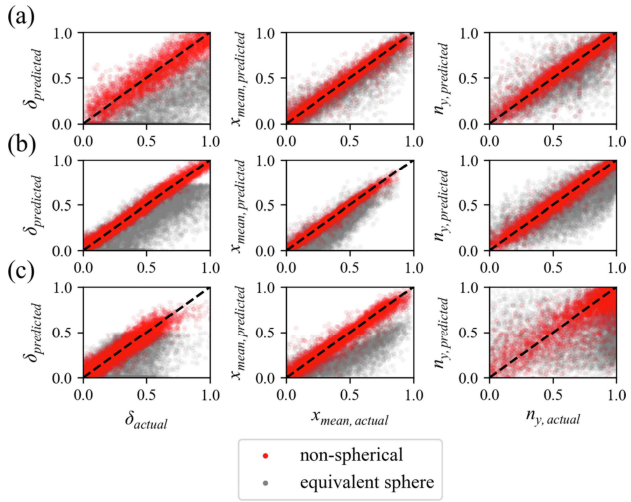


Contact model

- Develop a ML-based contact model outside of DEM loop to predict contact properties
- Regular, irregular-shaped particles
- Significant improvement of computational efficiency







Soohwan Hwang et al., *Chemical Engineering Science* 251, 117439 (2022)

CONCOLUSION

- This study provides ML-based force models for the irregular particle flows, which is practical in industry.
- The PIEP-based approach is efficient in that it mainly requires data for single particles.
- This study also provides computationally efficient collision force model, which can be applied to CFD-DEM.