Revisiting Wen and Yu: An empirical drag model based on the foundational data sets in fluidization

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CPFD Software

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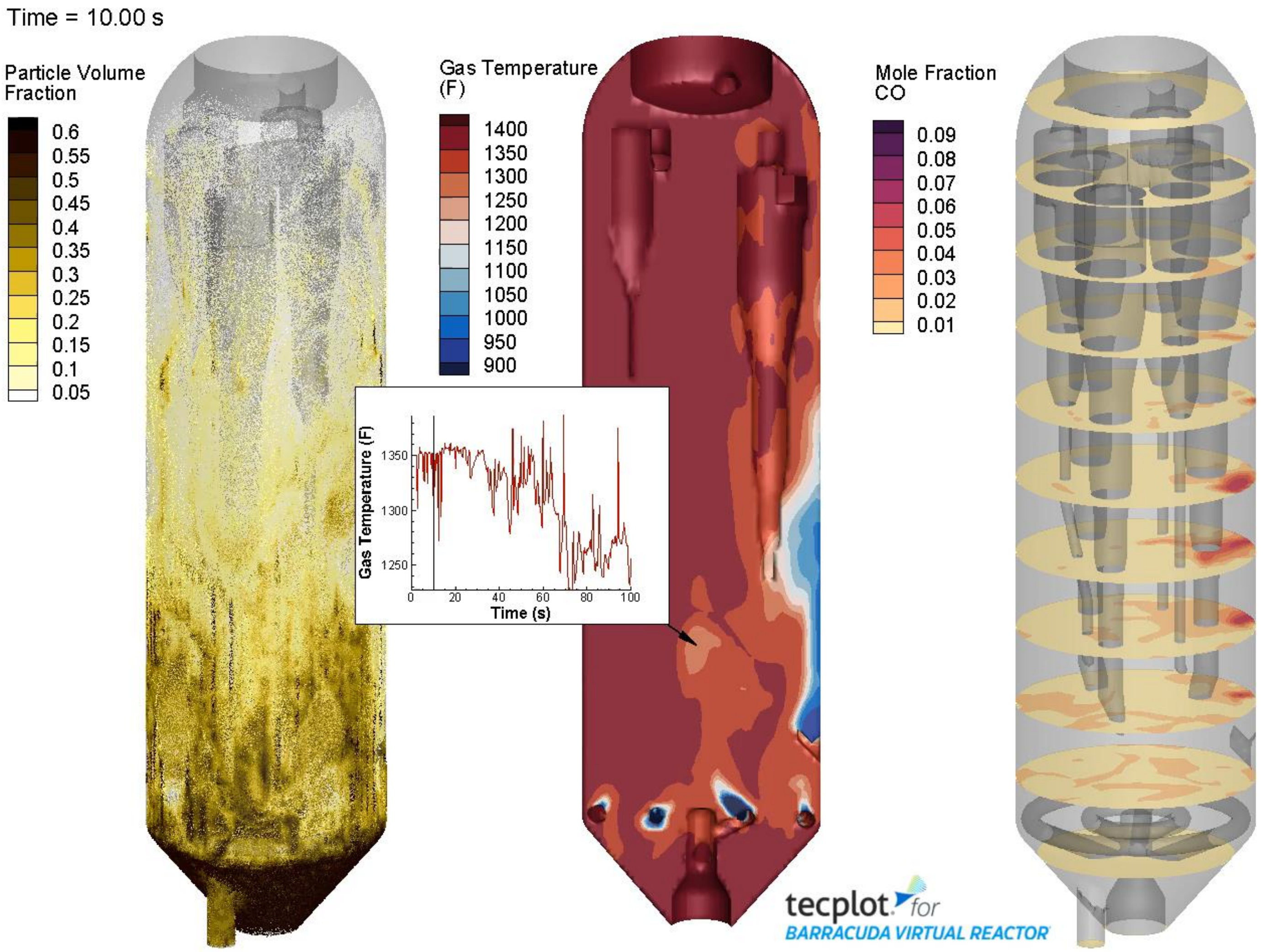
Background on CPFD Software

- Developer of Barracuda Virtual Reactor, a multiphase CFD software for the simulation of particle – fluid systems at the industrial-scale

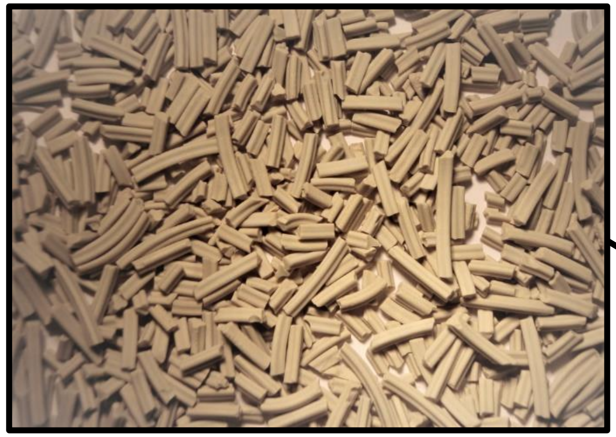
- Key capabilities of Barracuda Virtual Reactor for modeling of industrial reactors
  - Multiphase Particle-in-Cell (MP-PIC) approach
  - Parallelized for computation on multiple GPU cards
  - Heat transfer – convective and radiative
  - Gas-solid reaction chemistry – homogeneous and heterogeneous
  - Advanced boundary conditions
  - Data analysis with Tecplot for Barracuda



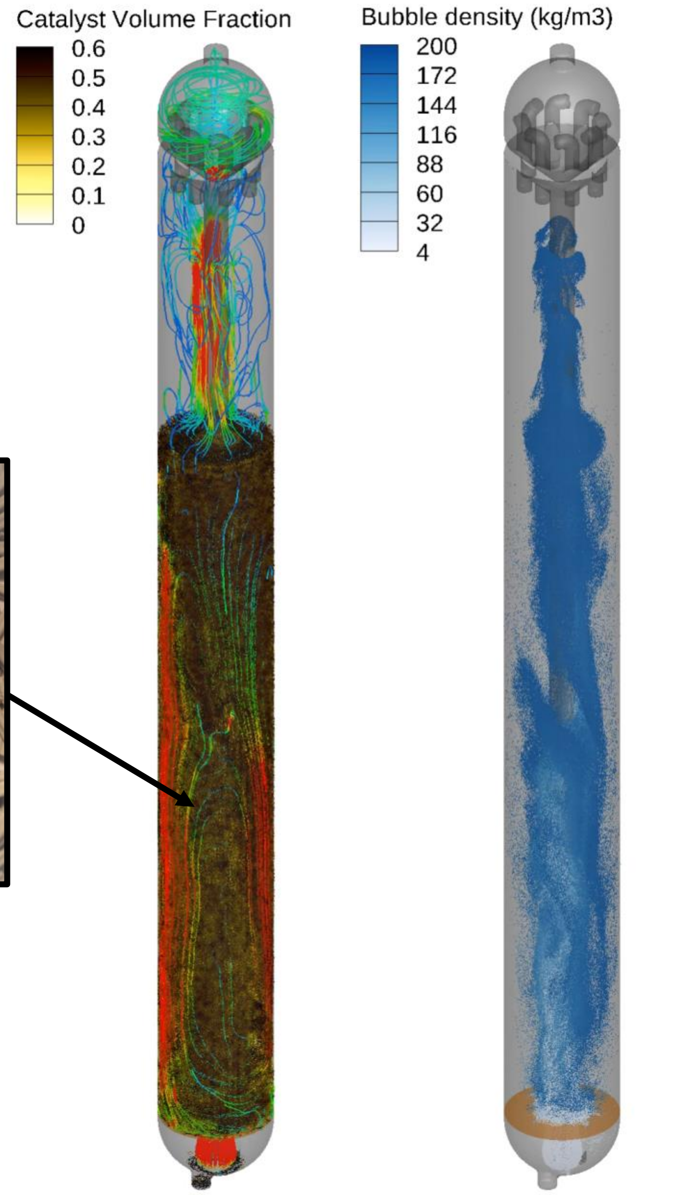
Motivation

Common questions from CFD users:

- What drag model to use for CFD?
- What experiments or particle characterization should be performed?
- How can a drag model be improved (tuned) from experimental data?



Hydrocracking Catalyst (Extrudate)



Industrial scale hydrocracker with extrudate catalyst

Parker & Blaser (2022), Application of MP-PIC method to Ebullated Bed Reactors. GLS-15 Conference

Motivation for drag model work

- Diverse particle shapes in gas-phase and liquid-phase systems are commonplace in CFD for wide range of established and emerging applications

Solid waste, fluffy or pelletized

Chipped wind turbine blades

Hydrocracking Catalyst (Extrudate)

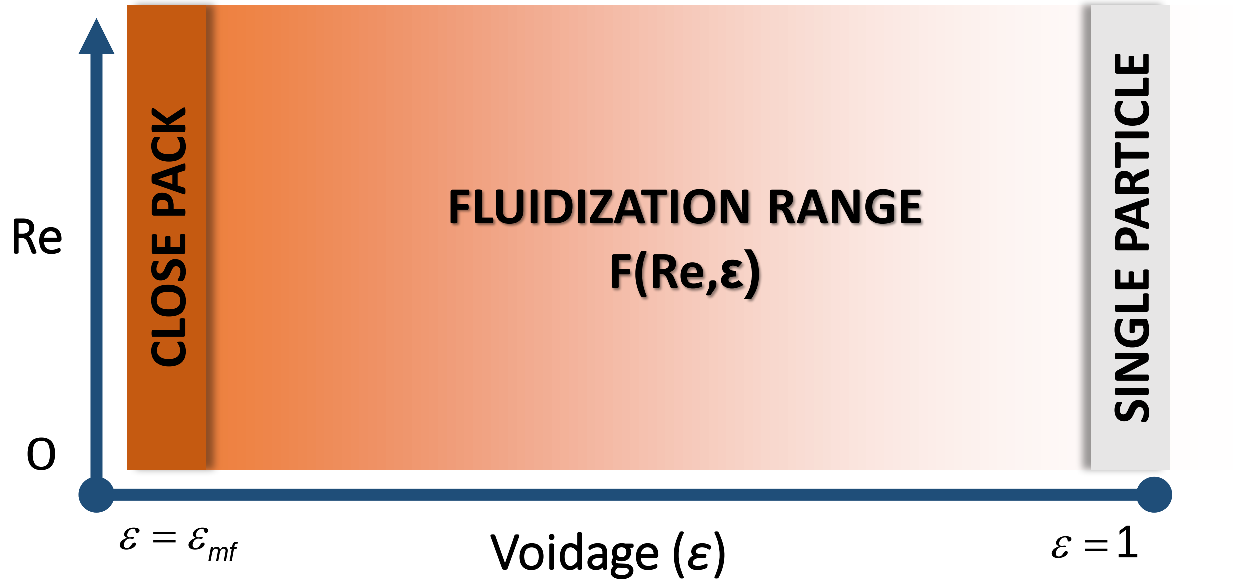
Plastics

Biomass

Shredded tires

Drag models

- Close-pack
  - Ergun (1949)
- Single particle drag
  - Schiller-Naumann (1933)
  - Variety of non-spherical drag models
- Full range models
  - Wen-Yu (1966)
  - Gidaspow (1986)
  - *Di Felice (1994)*
  - *Beetstra (2007)*
  - *Tenneti (2011)*
  - *Tang (2015)*
  - *EMMS models*
  - *Wen-Yu Ergun blend*

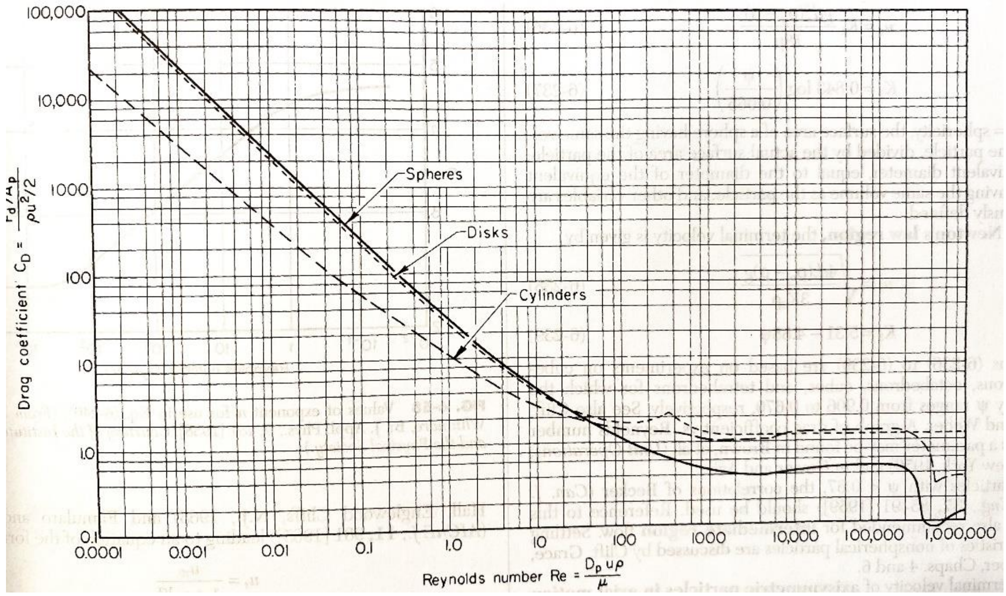


Foundational drag models

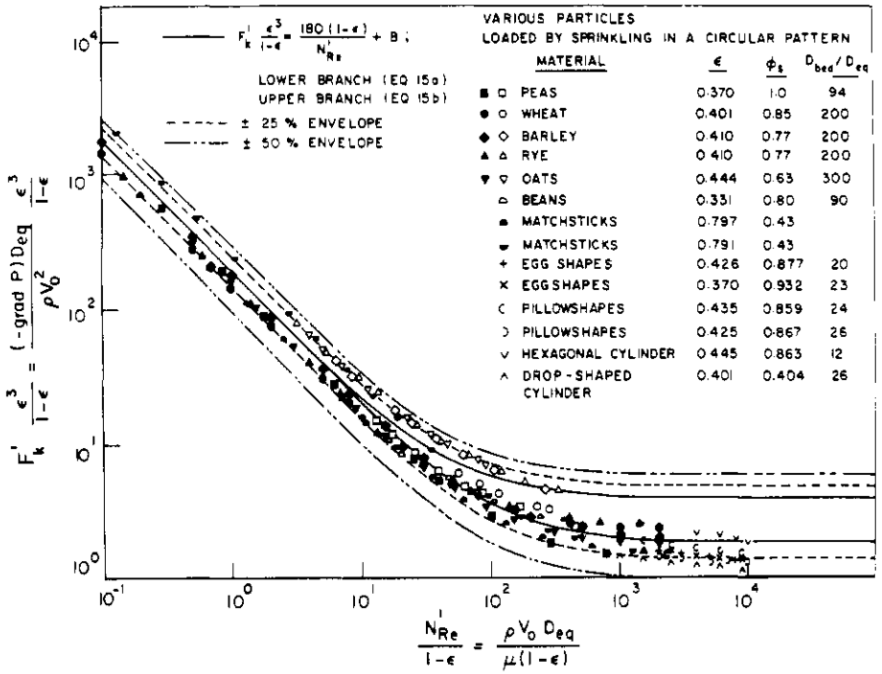
- Shape and sphericity has a significant effect on drag at extremes
- Sphericity is often estimated from pressure drop measurements and comparison with Ergun equation

Ergun equation (non-dimensional):

$$F_{Ergun}(\varepsilon, \mathrm{Re}) = \frac{A}{18}\frac{1-\varepsilon}{\phi^2\varepsilon^2} + \frac{B}{18}\frac{\mathrm{Re}}{\phi\varepsilon^2}$$



Drag coefficient for single particles by shape
Perry and Green (1997). Perry's Chemical Engineers Handbook



Test of modified Ergun Equation
Macdonald et al (1979). Flow through Porous Media – the Ergun Equation revisisted

Approach to improving drag

Goal

Build upon previous work to find a new drag model:

- Schiller-Naumann drag at $\varepsilon = 1$
- Ergun drag at close pack $\varepsilon = \varepsilon_{mf}$
- Continuous between $\varepsilon = \varepsilon_{mf}$ and $\varepsilon = 1$
- Can be improved by incorporating experimental data

Steps

1. Identify experimental data in literature where fixed bed pressure drops *and* bed expansion data exists
2. Determine Ergun parameters based on the pressure drop
3. Determine a best fit value drag model parameter
4. Compare with existing drag models in literature

Error = $\sqrt{\sum\left(F_{apparent} - F\right)^2}$

Dimensionless Drag

$$F(\varepsilon, \mathrm{Re}) = F_{drag}/F_{Stokes} \qquad F_{Stokes} = 3\pi\mu d_p U$$

Close pack or minimum fluidization (Ergun)

$$F_{mf}(\varepsilon, \mathrm{Re}) = \frac{A}{18}\frac{1-\varepsilon}{\phi^2\varepsilon^2} + \frac{B}{18}\frac{\mathrm{Re}}{\phi\varepsilon^2}$$

Single particle (Schiller-Naumann correlation)

$$F_{sp}(\varepsilon, \mathrm{Re}) = \begin{cases} 1 + 0.15\mathrm{Re}^{0.687} & \mathrm{Re} < 1000 \\ 0.44/24\mathrm{Re} & \mathrm{Re} \geq 1000 \end{cases}$$

Experimental data analysis

$$F_{apparent}(\varepsilon, \mathrm{Re}) = \mathrm{Ar}\frac{\varepsilon}{18\mathrm{Re}} \qquad \mathrm{Ar} = \frac{{d_p}^3\rho_f(\rho_s - \rho_f)g}{{\mu_f}^2}$$

Previous work

- In previous work, Wen-Yu form (power of voidage) was used as basis:

$$F = F_{sp}\varepsilon^{-\beta}$$

- The exponent is set as a function of Reynolds number such that Ergun's drag force is maintained for all Re at minimum fluidization:

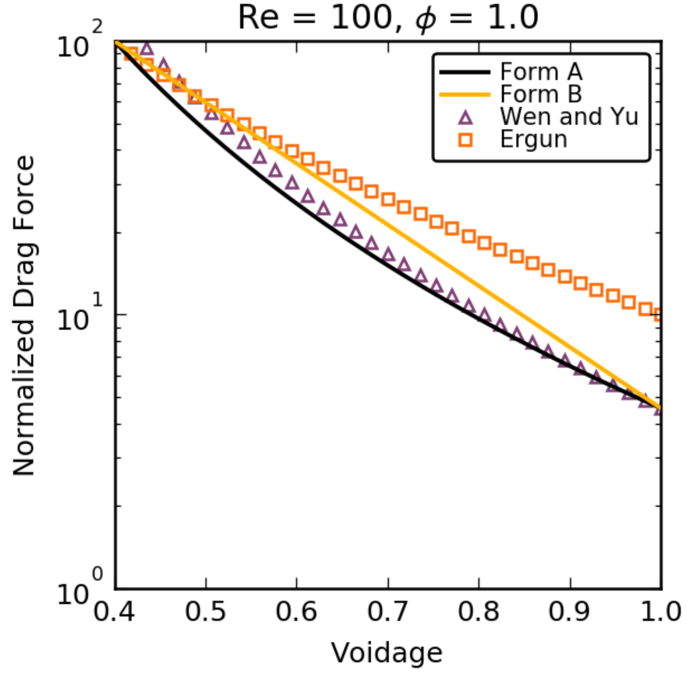
$$\beta = -\frac{\ln(F_{mf}/F_{sp})}{\ln(\varepsilon_{mf})}$$

$$F_{sp} = \begin{cases} 1 + 0.15\mathrm{Re}^{0.687} & \mathrm{Re} < 1000 \\ 0.44/24\mathrm{Re} & \mathrm{Re} \geq 1000 \end{cases} \qquad F_{mf} = \frac{A}{18}\frac{1-\varepsilon_{mf}}{\phi^2 {\varepsilon_{mf}}^2} + \frac{B}{18}\frac{\mathrm{Re}}{\phi {\varepsilon_{mf}}^2}$$

- With manipulation, the equation can be written in a simplified form:

$$F_p = \left(F_{sp}\right)^{\chi}\left(F_{mf}\right)^{1-\chi} \qquad \chi = 1 - \left(\frac{\ln \varepsilon}{\ln \varepsilon_{mf}}\right)^{n}$$

New

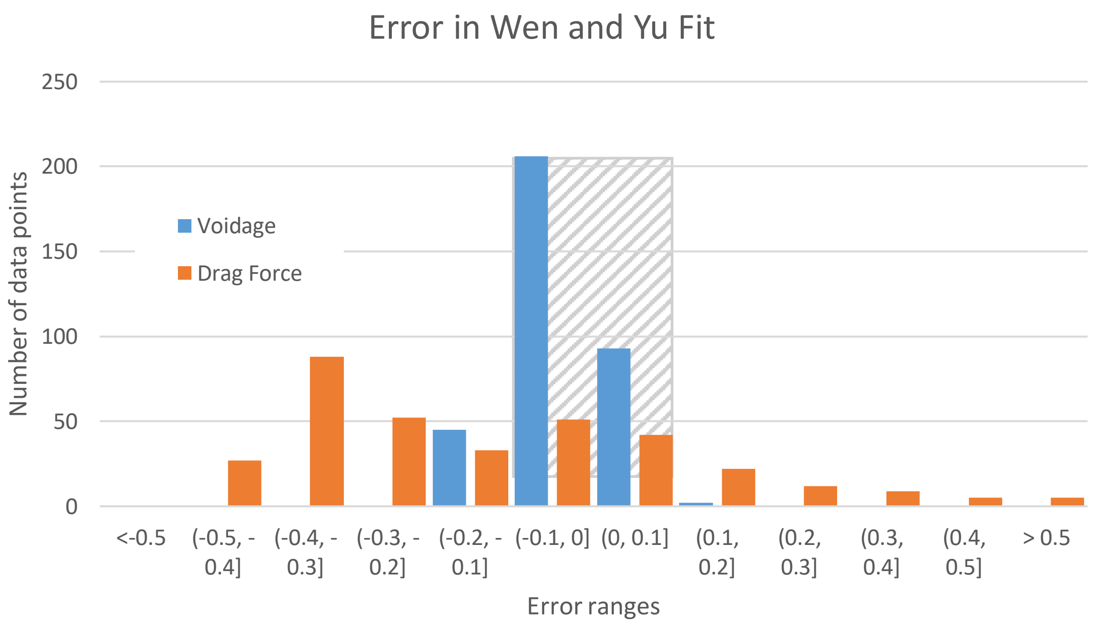


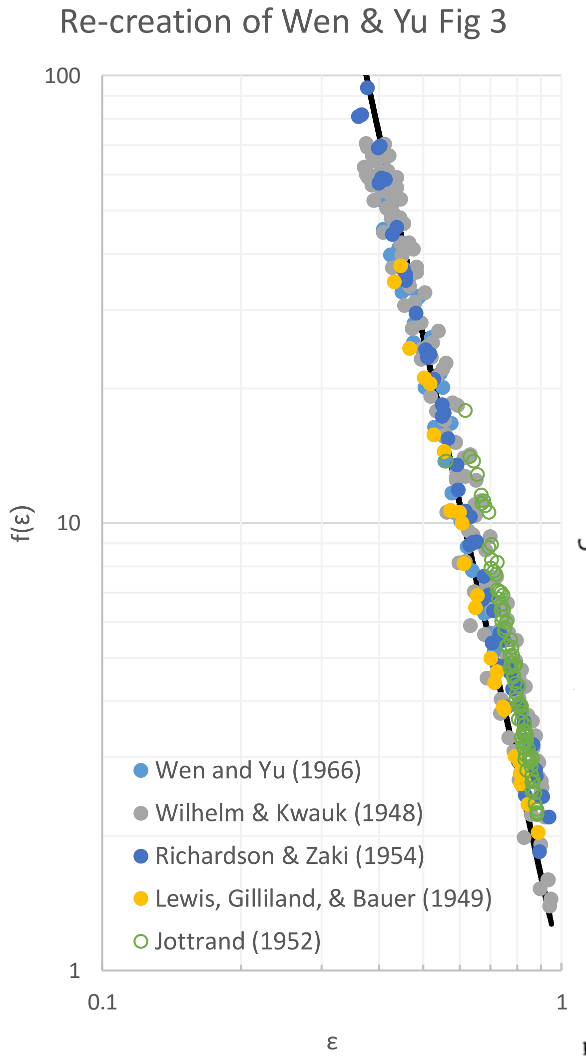
Demonstration of drag transitions

Parker (2016), NETL Workshop on Multiphase Flow Science, Morgantown WV

Foundational data sets

- Assembled the data sets used by Wen and Yu (1966) plus data of Jottrand (1952)
- Voidage error consistent with +/- 10% reported by Wen and Yu
- Drag force errors are significantly higher





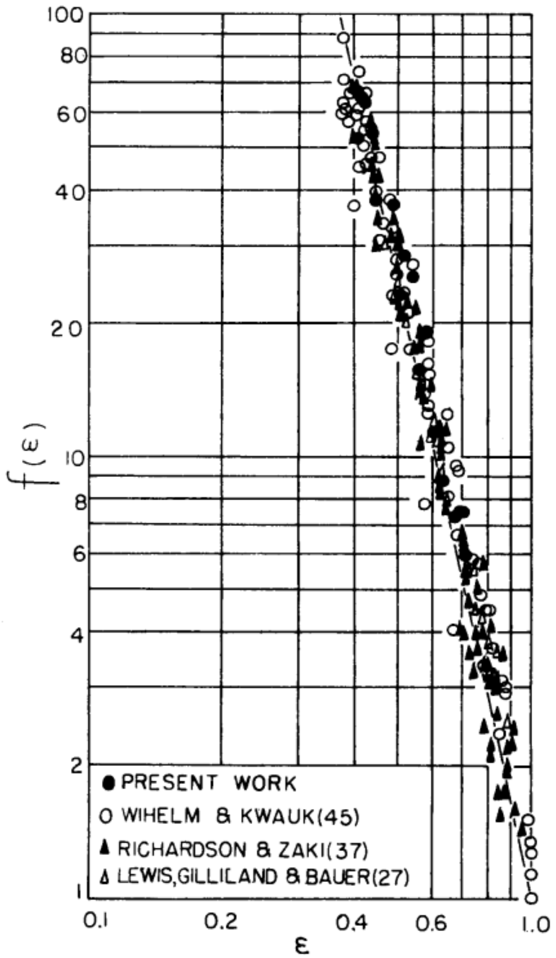


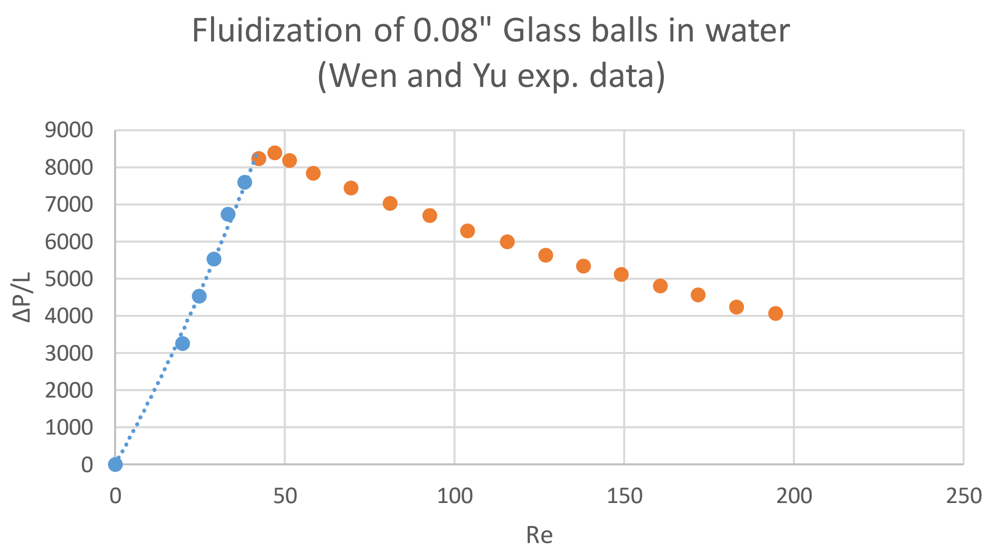
Fig. 3. Correlation of the voidage function of multiparticle system.

$$F_{WY}/F_{Stokes} = (1 + 0.15\,\mathrm{Re}^{0.687})\varepsilon^{-3.65}$$

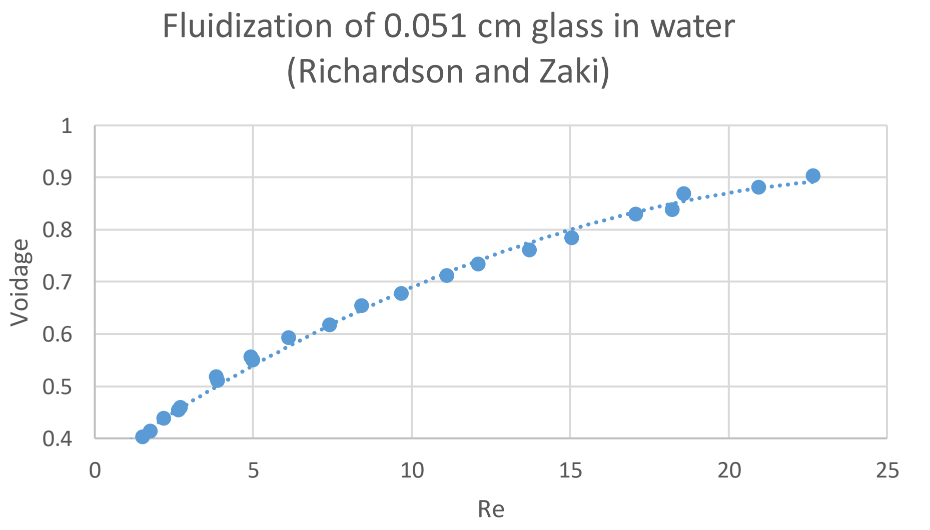
Foundational data sets

- Liquid – solid bed expansion and settling data formed the full data set
- A subset of the data that included fixed bed pressure drop data information was isolated as a Tuning dataset

Data Set Parameters	Full Data Set *Min*	*Max*	Tuning Set Min	*Max*
Reynolds	1.18E-03	2176.4	9.5	1620
Voidage	0.36	0.95	0.37	0.94
Particle size (mm)	0.02	6.35	1.00	6.35
Data points	346		154	
Sources	Wen & Yu, Wilhelm & Kwak, Lewis, Gilliland, and Bauer, Richardson & Zaki, Jottrand		Wen & Yu, Wilhelm & Kwauk	



Sample data with fixed bed pressure drop

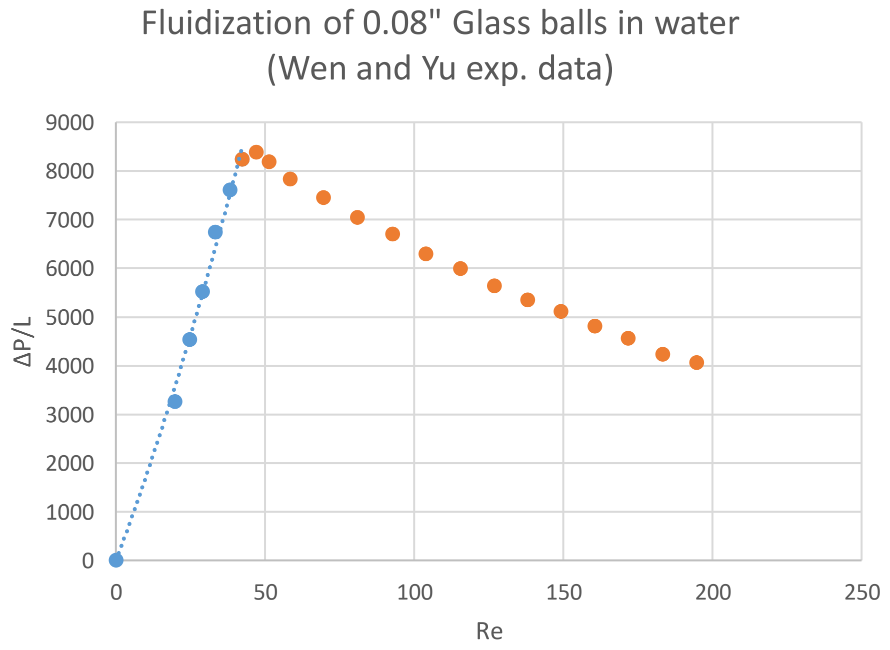


Expansion data only

Analysis – Tuning of Ergun Parameters

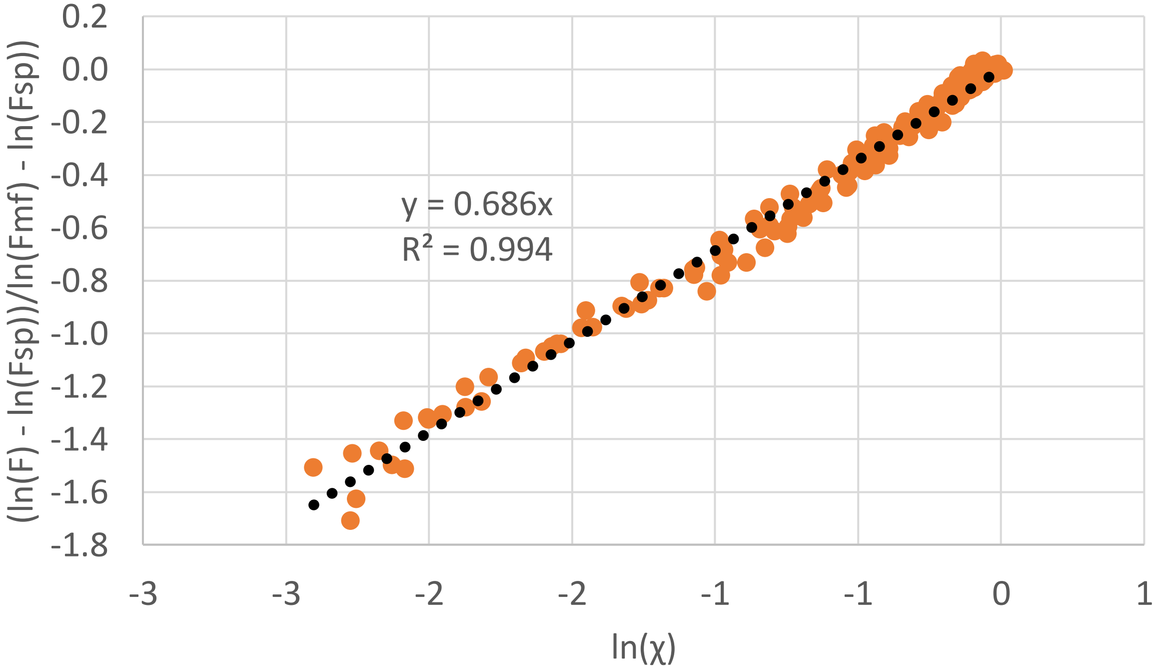
- Coefficient values in Ergun equation were fit from fixed bed data, from available voidage at close pack or bulk density information. Sphericity is assumed to be 1 (factored into values of A and B)
- Parameters are close to default Ergun coefficients (A=150, B=1.75) and coefficients of Macdonald et al (1979) (A = 180, B = 1.8 to 4.0)

Data set	A	B	ε_{mf}
Wen and Yu, Table 3, 0.08" glass balls	190.4	1.3	0.39
Wen and Yu, Table 3, 0.197" glass balls	302.6	1.3	0.394
Wen and Yu, Table 3, 0.25" glass balls	297.2	1.3	0.399
Wen and Yu, Table 3, 0.0937" steel balls	225.7	1.6	0.403
Wilhelm and Kwauk, Table 10, 0.0393" sea sand	171.7	2.4	0.4067
Wilhelm and Kwauk, Table 4, 0.129" saucony beads	134.7	1.7	0.3684
Wilhelm and Kwauk, Table 5, 0.174" saucony beads	160.0	2.0	0.3681
Wilhelm and Kwauk, Table 6, 0.205" glass beads	262.2	1.7	0.3839
Wilhelm and Kwauk, Table 7, 0.205" glass beads	178.3	1.9	0.385
Wilhelm and Kwauk, Table 9, 0.0505" lead shot	162.8	1.7	0.375



Determining the model exponent

- Exponent value was determined from a least-squares fit of the Tuning data set using some algebraic manipulation
- $(\ln F - \ln F_{sp})/(\ln F_{mf} - \ln F_{sp})$ vs $\ln \chi$ was plotted, where $F = Ar\frac{\varepsilon}{18\mathrm{Re}}$
- An exponent of $\boldsymbol{n \approx 0.7}$ was found to fit the data very well and the new drag model fully determined.



New drag model equation:

$$F_{sp} = \begin{cases} 1 + 0.15\mathrm{Re}^{0.687} & \mathrm{Re} < 1000 \\ 0.44/24\mathrm{Re} & \mathrm{Re} \geq 1000 \end{cases}$$

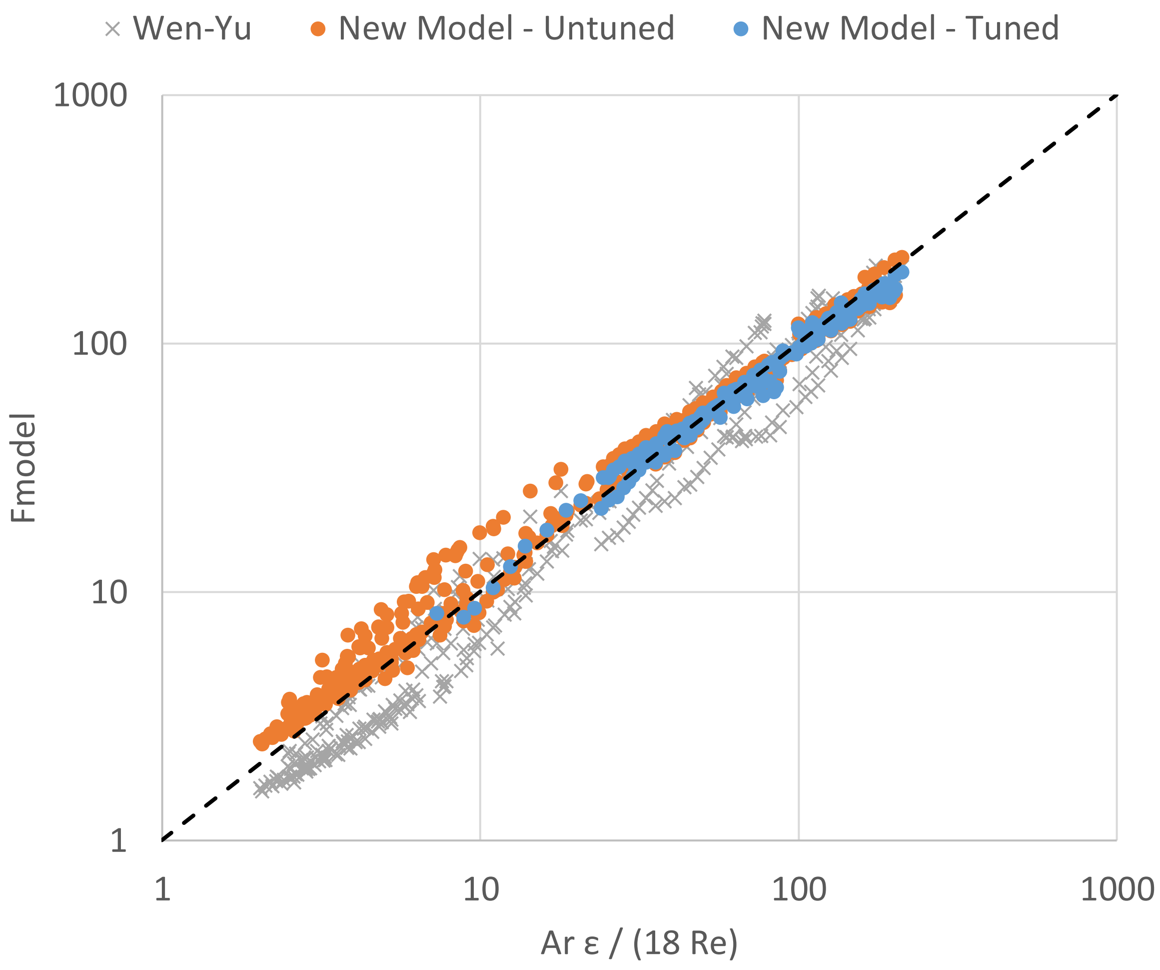
$$F_{mf} = \frac{A}{18}\frac{1-\varepsilon_{mf}}{\phi^2 {\varepsilon_{mf}}^2} + \frac{B}{18}\frac{\mathrm{Re}}{\phi {\varepsilon_{mf}}^2}$$

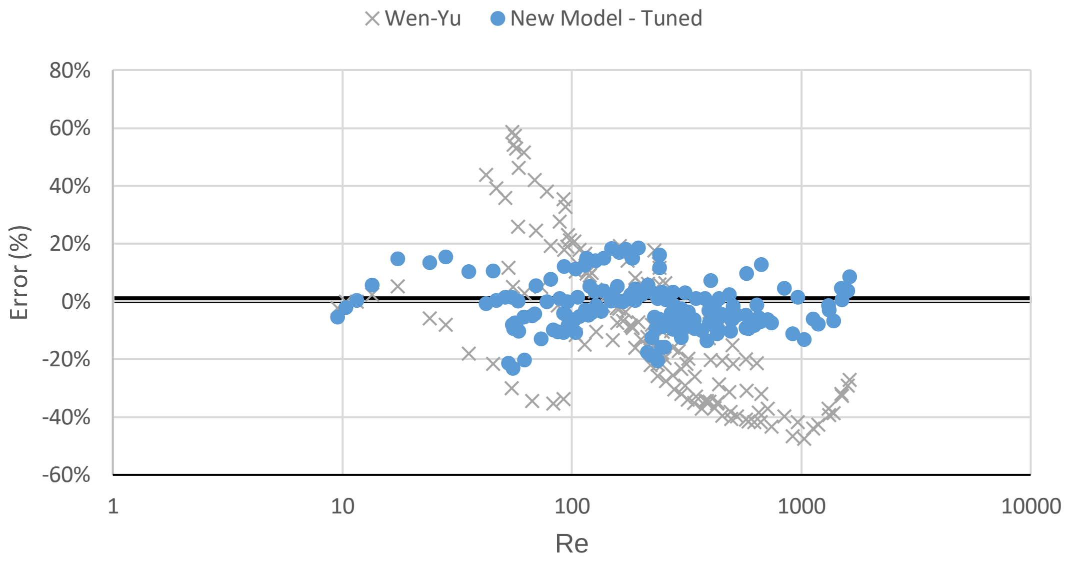
$$F_p = (F_{sp})^{\chi}(F_{mf})^{1-\chi} \qquad \chi = 1 - \left(\frac{\ln \varepsilon}{\ln \varepsilon_{mf}}\right)^{0.7}$$

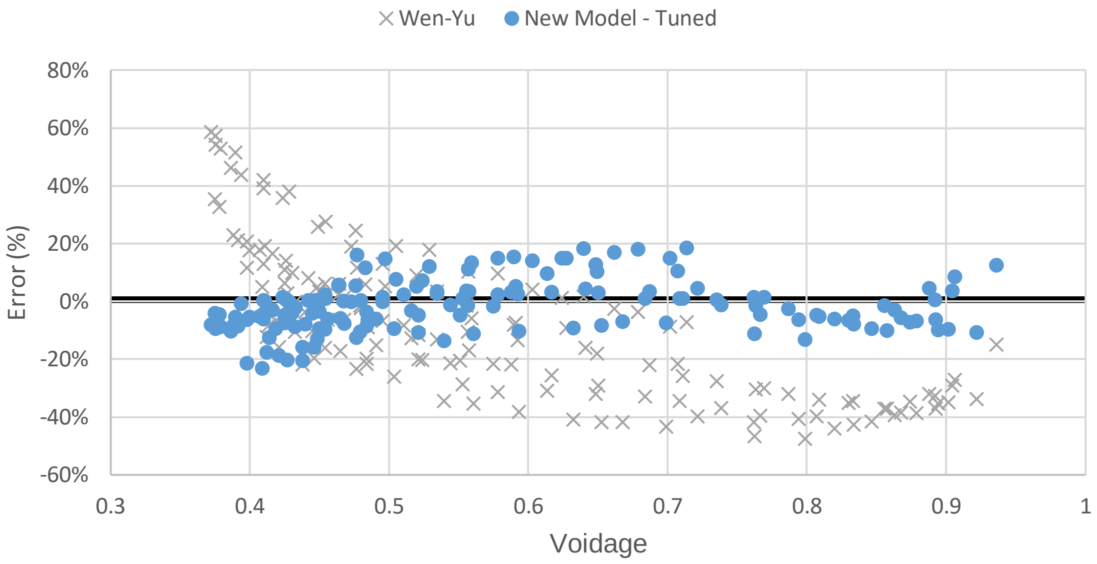
Model Results

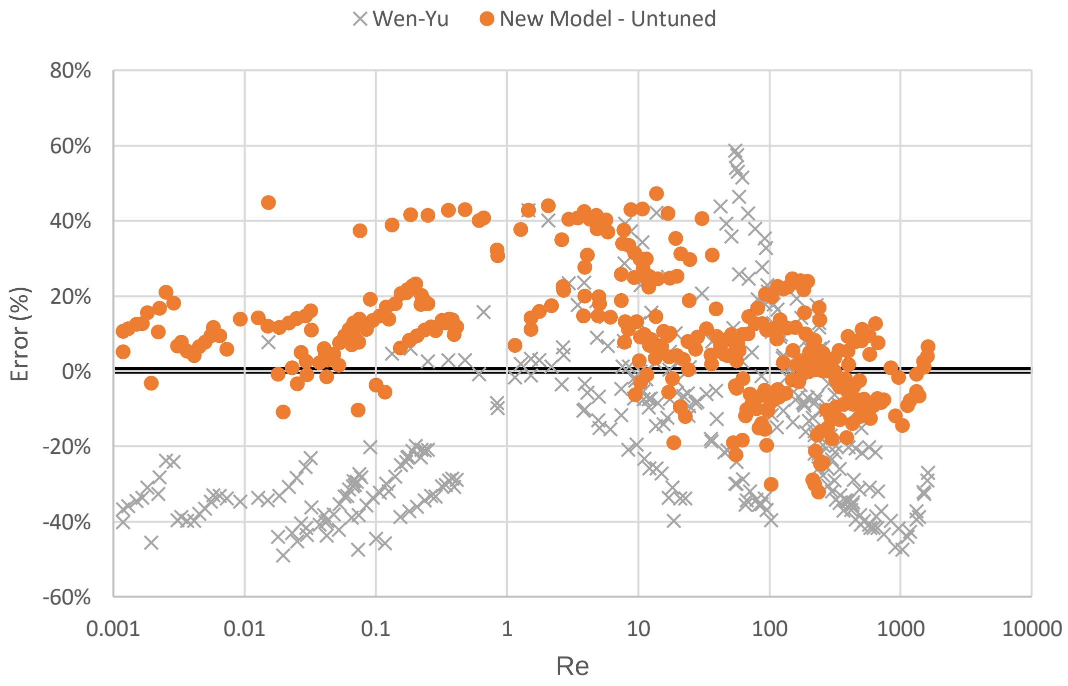
- Tuned model is compared with Untuned version (A = 180, B = 1.8) and other drag models from literature
- Tuned model outperforms all models when fitted data is available
- Untuned model outperforms the existing models on the full data set

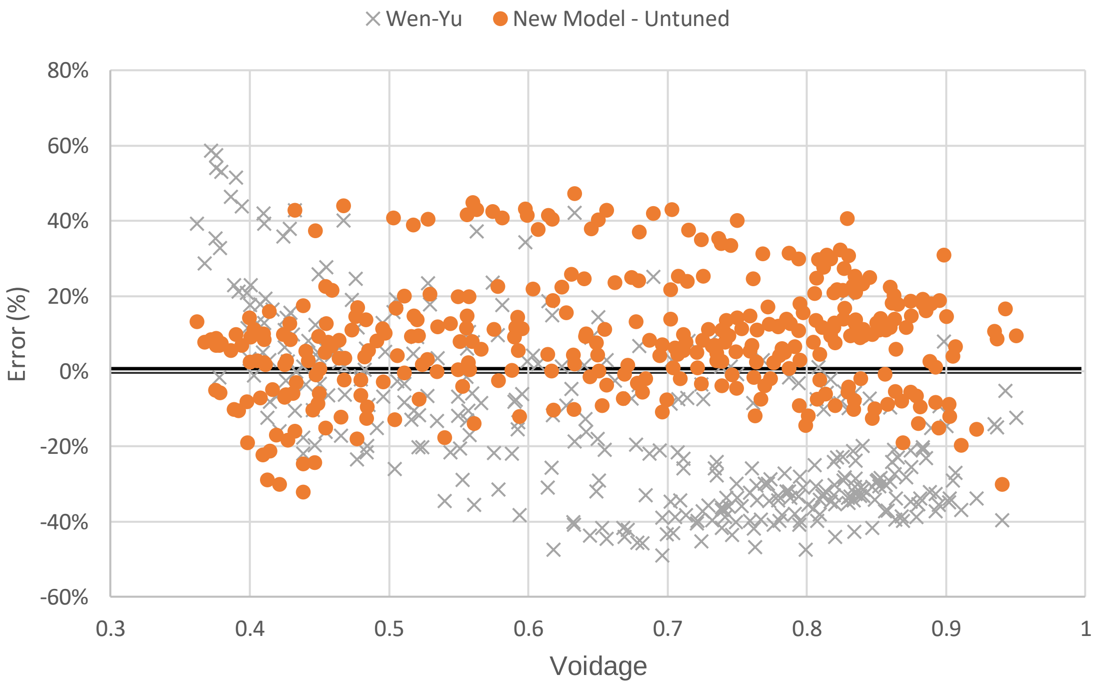
Drag model	Tuning Dataset		Full Dataset	
	Avg. Err.	*Max. Err.*	*Avg. Err.*	*Max. Err.*
New model - Tuned	**8.9%**	**23.3%**	**-**	**-**
New Model - Untuned (A=180, B=1.8)	**11.6%**	**32.3%**	**17.6%**	**47.2%**
Beetstra et al (2007)	15.5%	37.6%	25.2%	88.6%
Di Felice (1994)	20.9%	33.9%	24.5%	49.0%
Wen-Yu / Ergun Blend (A=180, B=1.8)	22.6%	47.6%	26.3%	77.1%
Wen and Yu (1966)	26.6%	58.6%	26.9%	58.6%
Gidaspow (1986)	31.2%	98.9%	27.5%	98.9%
Tang (2015)	32.1%	53.9%	34.5%	89.6%
Tenneti (2011)	36.3%	54.3%	31.7%	73.1%
Ergun (1949)	57.7%	230.3%	42.7%	230.3%




Wen-Yu
New Model - Tuned
80%
60%
40%
20%
0%
-20%
-40%
-60%
Error (%)
1
10
100
1000
10000
Re


Wen-Yu
New Model - Tuned
80%
60%
40%
20%
0%
-20%
-40%
-60%
Error (%)
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Voidage


Wen-Yu
New Model - Untuned
80%
60%
40%
20%
0%
-20%
-40%
-60%
Error (%)
0.001
0.01
0.1
1
10
100
1000
10000
Re


Wen-Yu
New Model - Untuned
80%
60%
40%
20%
0%
-20%
-40%
-60%
Error (%)
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Voidage

Conclusions

- A new drag model has been fit to foundational data sets.
- The model has a simple form and matches the Ergun drag model at close-pack volume fractions and the Schiller-Naumann correlation for a single particle
- The model has increased accuracy over commonly used drag models in the range of data tested using default Ergun coefficients of A=180 and B=1.8.
- Ergun coefficients of A and B can be fit to experimental data to further improve the accuracy

New drag model equation:

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$$F_{mf} = \frac{A}{18}\frac{1-\varepsilon_{mf}}{\phi^2 {\varepsilon_{mf}}^2} + \frac{B}{18}\frac{\mathrm{Re}}{\phi {\varepsilon_{mf}}^2}$$

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Thank you

- Questions?