

Advanced Training: Drag Calibration

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Outline

Empirical models in Virtual Reactor

Drag Models in Virtual Reactor

- Built-in drag models
- User-defined drag models
- Multipliers and multiplier tables

Calibration of Drag Models

- Using operational and experimental data
- Guidelines for applying calibrated drag models

Empirical Models in Virtual Reactor

All CFD tools are based on a mix of fundamentals and empirical models

Fundamentals

- Conservation of mass
- Conservation of momentum
- Conservation of energy

Empirical models

- Particle collision and bounce
- Fluid-particle drag models
- Turbulence models
- Chemical reactions and rates

Fluid-Particle Drag Models

Fluid-particle drag is an important empirical model in Virtual Reactor

Some aspects of drag are well-known

- Drag for a single particle (Schiller-Nauman Correlation)
- Drag for a group of particles at close-pack (Ergun)

Other aspects are not well-known

- Drag for volume fractions between single particle and close-pack (Wen-Yu, Wen-Yu/Ergun blend, EMMS)
- Drag for very small particles (< 44 microns diameter, i.e. fines)
 - Agglomeration
 - Hindrance effects

Audience Question

Which drag model do you usually use?

- How well does it work? How do you know?
- Do you ever perform calibration of the drag model?

Built-In Drag Models

Virtual Reactor includes several built-in drag models

- Wen-Yu/Ergun is a reasonable starting point for many Geldart Group A particles
- Nonspherical drag models are helpful when particles are very non-spherical in shape

The screenshot shows the Barracuda Virtual Reactor software interface. The main window title is "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/5_Wednesday_gasifier/demo/wednesday_gasifier.prj". The interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help) and a toolbar with various icons. The Project Tree on the left shows the following structure:

- Barracuda Virtual Reactor...
 - Setup Grid
 - Global Settings
 - Base Materials
 - Particles
 - Drag Models (selected)
 - Volatiles
 - Particle Species
 - Initial Conditions
 - Fluid ICs
 - Particle ICs
 - Boundary Conditions
 - Pressure BCs
 - Flow BCs
 - Injection BCs
 - Thermal Wall BCs
 - Passive Scalar BCs
 - BC Connections
 - Secondary Feeds
 - Secondary Exits
 - BC Connectors
 - Chemistry
 - Rate Coefficients
 - Reactions

The Drag Model Manager window is open, displaying a table of drag models:

	Name	Source	Description
1	Constant	System	Constant drag model
2	Stokes	System	Stokes drag model
3	Wen-Yu	System	Wen-Yu drag model
4	Ergun	System	Ergun drag model
5	WenYu-Ergun	System	WenYu-Ergun blended drag model
6	Turton-Levenspiel	System	Turton-Levenspiel drag model
7	Richardson-Davidson-Harrison	System	Richardson-Davidson-Harrison drag model
8	Haider-Levenspiel	System	Haider-Levenspiel drag model
9	EMMS-Yang-2004	System	EMMS-Yang-2004 drag model
10	Nonspherical-Ganser	System	Nonspherical-Ganser drag model
11	Nonspherical-Haider-Levenspiel	System	Nonspherical-Haider-Levenspiel drag model

Below the table, there is a text field with the prompt "Specify user-defined drag models here." and an information icon. At the bottom of the window, there are buttons for "Add", "Edit", "Copy", and "Delete". The status bar at the bottom shows the project name "wednesday_gasifier.prj" and the file path "C:/training/5_Wednesday_gasifier/demo".

User-Defined Drag Models

Can be based on built-in drag models

- Copy an existing model
- Modify as desired

Can be completely new

- Use the Drag Model Editor
- Define any constants
- Define $F_{custom}()$

The screenshot shows the 'Drag Model Editor' window. The 'Name' field is 'WenYu-Ergun_3' and the 'Comment' is 'Multiply Wen-Yu portion by M = 0.7, and Parker terms'. The 'Constants' table is as follows:

Name	Value
c2	0.44
c3	2
c4	250
n0	-2.65
n1	0.687
M	0.7

An orange box highlights the 'M' constant with the value 0.7, and an arrow points to it with the text 'Local Wen-Yu multiplier'. The 'Drag Model Definition' section contains the following code for $F_{custom}()$:

```
IF(volfracP<0.75*thetaCP, IF(Re<=1000, (c0+c1*Re^n1), c2*Re/24*M^volfracF^n0,
IF(volfracP>0.85*thetaCP, (c3*Re^4*(volfracP/volfracF))/18,
IF(Re<=1000, ((c0+c1*Re^n1)*M^volfracF^n0 + ((c3*Re+c4*(volfracP/volfracF))/18) - ((c0+c1*Re^n1)*M^volfracF^n0) * (volfracP-0.75*thetaCP) / (0.1*thetaCP))
((c2*Re^M*volfracF^n0)/24) + (((c3*Re+c4*(volfracP/volfracF))/18) - (c2*Re^M*volfracF^n0)/24))) * (diamP/diamSauterP)^2
```

The code is annotated with orange boxes around several terms: M^{volfracF^n0} , $(c3*Re+c4*(volfracP/volfracF))/18$, $(c0+c1*Re^n1)*M^{\text{volfracF}^n0}$, and $(diamP/diamSauterP)^2$. A blue box highlights the $(diamP/diamSauterP)^2$ term, with an arrow pointing to it from the text 'Sauter Mean Diameter' below the window. The 'Drag Model Definition' section also shows the equation $F_{drag} = 3\pi\mu d_p(u_f - u_s)F_{custom}()$. The 'Model Tools' section includes 'Functions: ABS(val 1)', 'Variables: densityF', and 'Operators: +'. At the bottom, there are 'Check Model', 'OK', and 'Cancel' buttons.

Sauter Mean Diameter

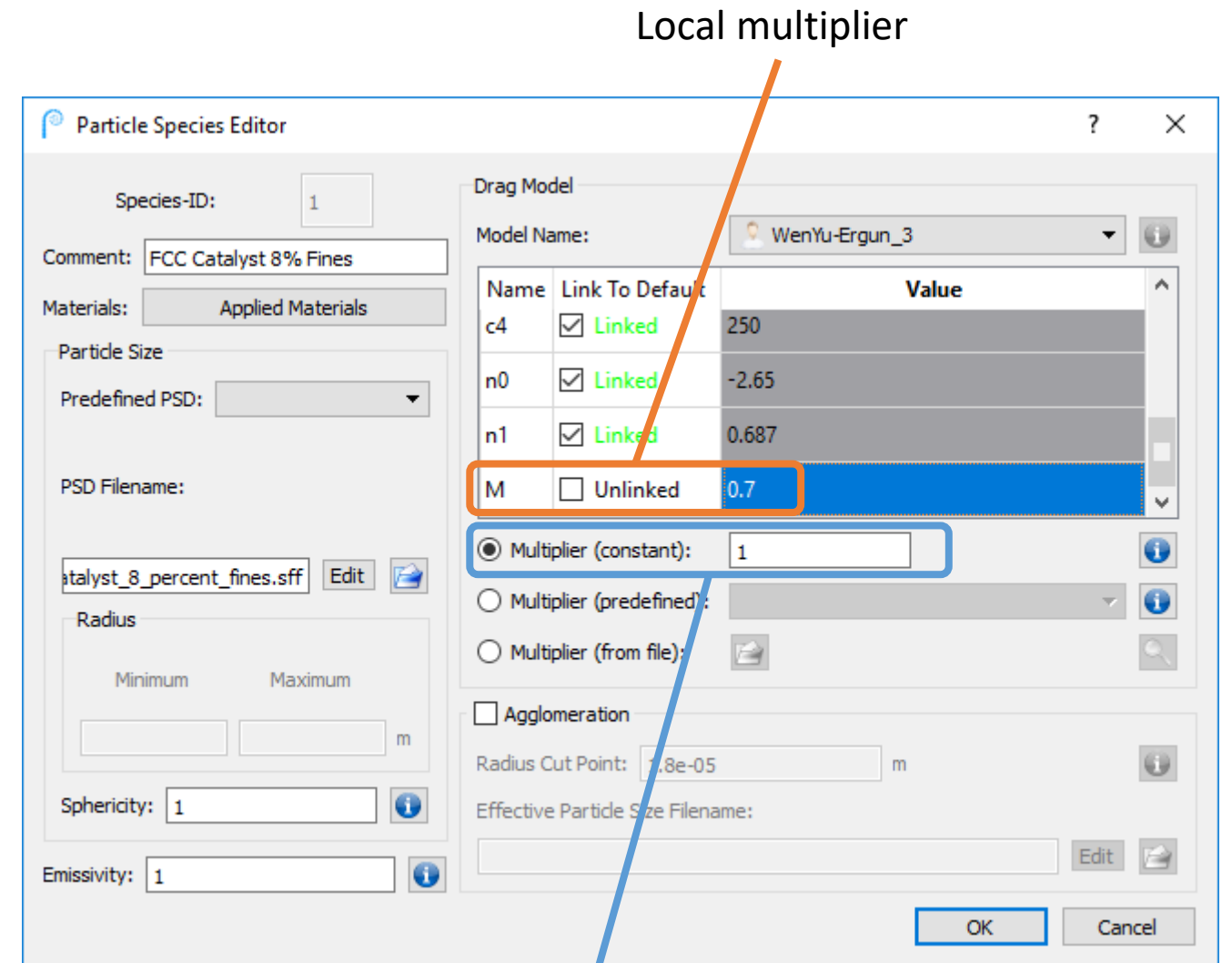
Multipliers: Global and Local

A global multiplier affects the entire drag model

- Use *Multiplier (constant)* in Particle Species Editor

A local multiplier can be defined to affect just a portion of the drag model

- Define a custom drag model
- Define a constant that affects just the desired portion



Global multiplier

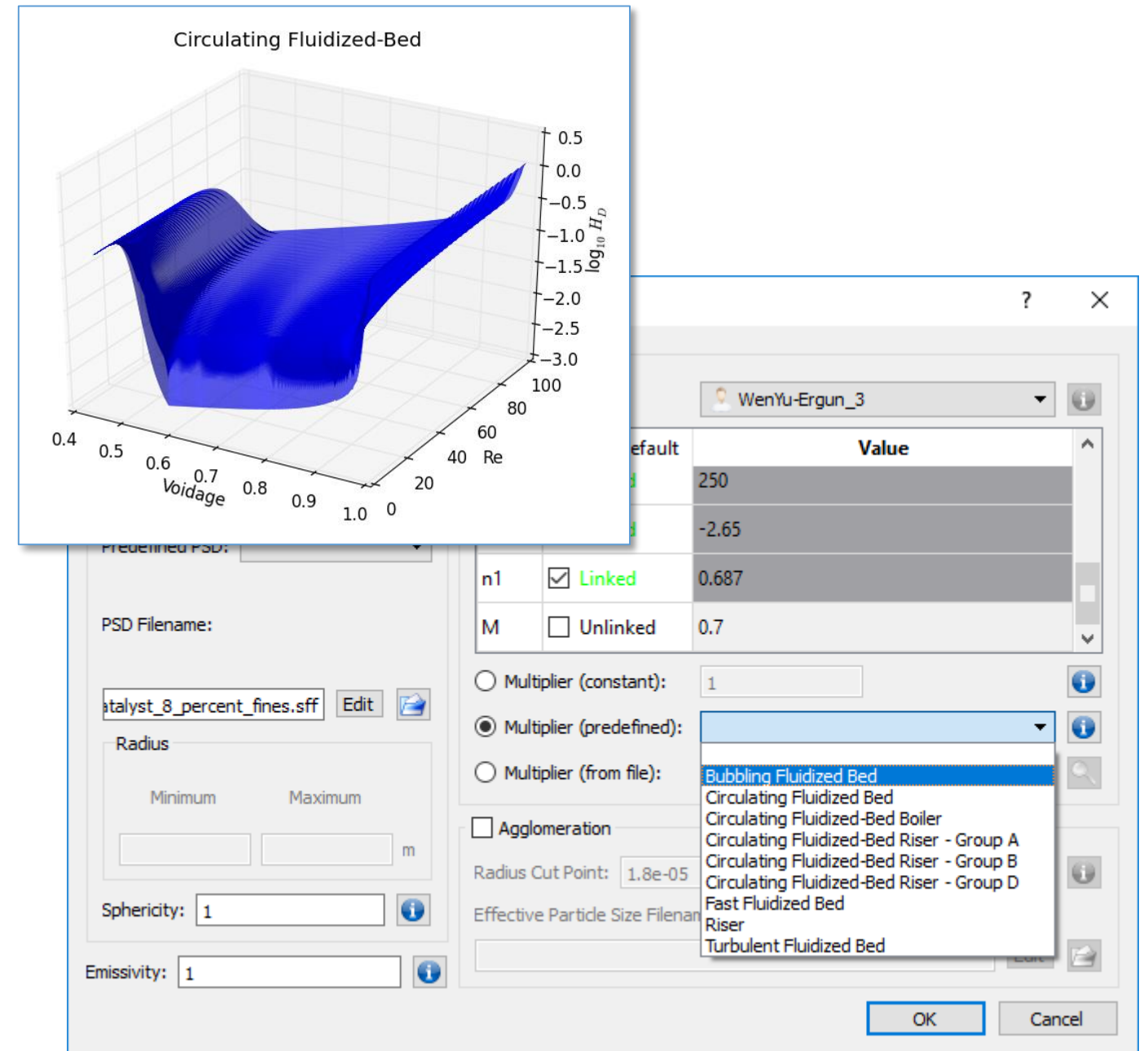
Multiplier Tables: EMMS

2-dimensional tables to adjust drag based on voidage and Re

Virtual Reactor has several predefined tables to choose from

CPFD has the ability to generate custom EMMS tables

- Highly recommend to use a custom-generated EMMS table
- Very dependent on particle properties and flow conditions



Drag Model Calibration

What adjustable parameters are available?

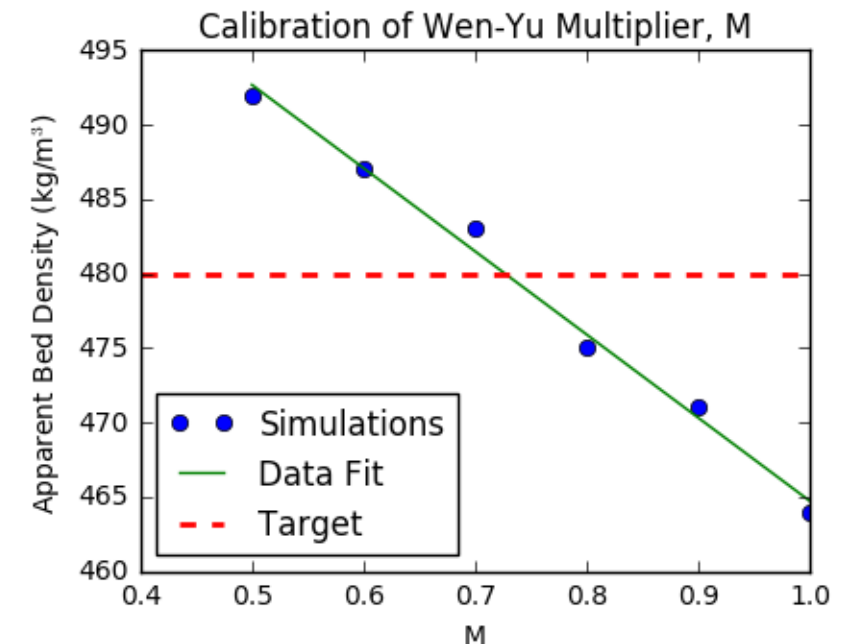
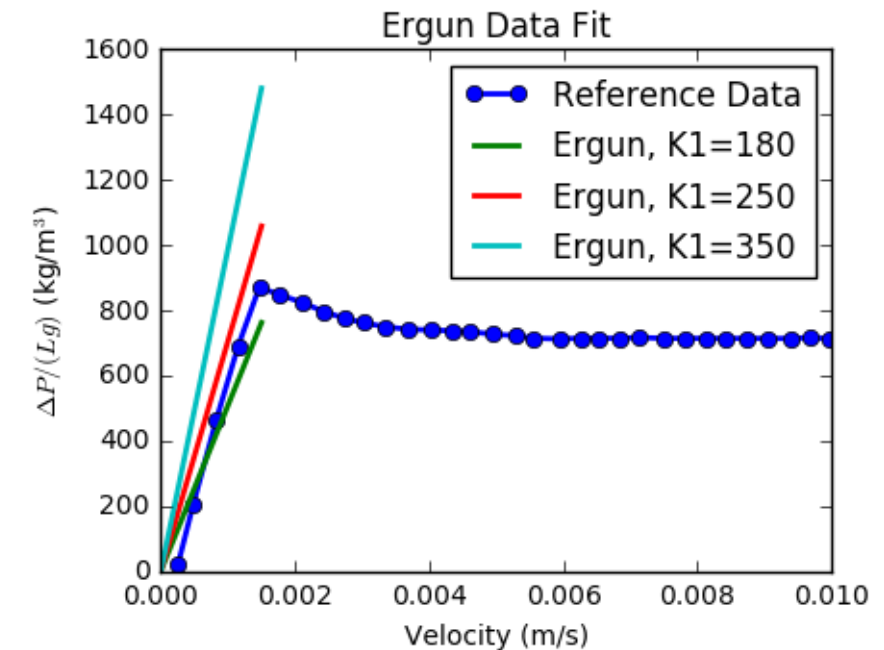
- Depends on which drag model you are using

Ergun

- Linear coefficient can be calibrated using minimum fluidization (U_{mf}) data

User-defined Wen-Yu with local multiplier

- Multiplier “M” can be calibrated using operational pressure drop data

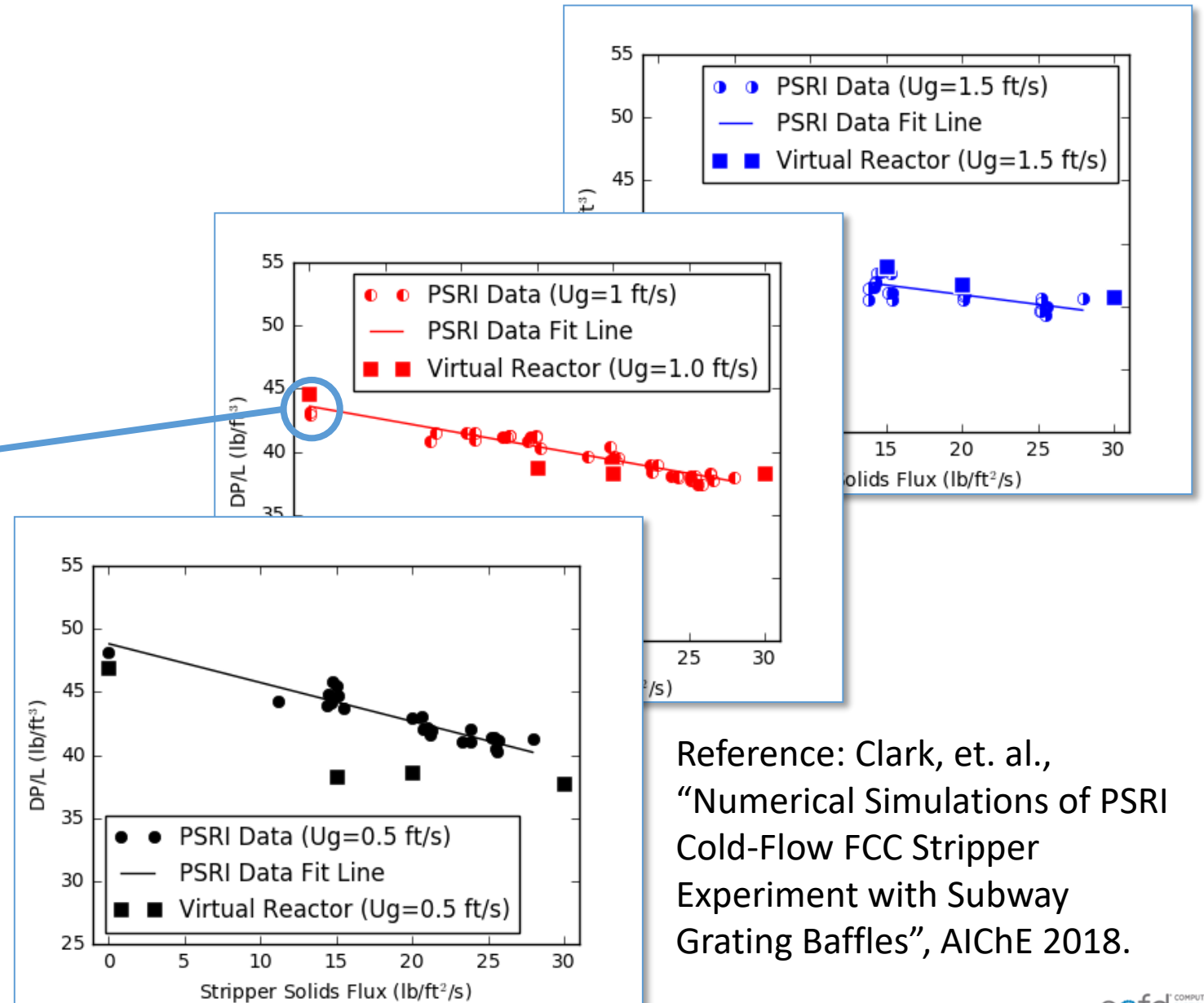


Guidelines for Applying Calibrated Drag Models

Goal: use Virtual Reactor as a reliable predictive tool

Do not “tune” every case

- Determine the calibrated parameters for a baseline case
- Use those parameters in all subsequent simulations of the system



Reference: Clark, et. al.,
“Numerical Simulations of PSRI
Cold-Flow FCC Stripper
Experiment with Subway
Grating Baffles”, AIChE 2018.

Conclusions

Drag is an important empirical model in Virtual Reactor

- Since it is not “fundamental”, calibration is necessary

Virtual Reactor provides several ways to handle drag

- Built-in drag models
- User-defined drag models
- Multipliers and multiplier tables

Guidelines for calibration of drag models

- Use operational and experimental data whenever possible
- Do not tune every case! Tune a base case, and use calibrated parameters.