CFD Models and Validation

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Particulate Solid Research, Inc. (PSRI)

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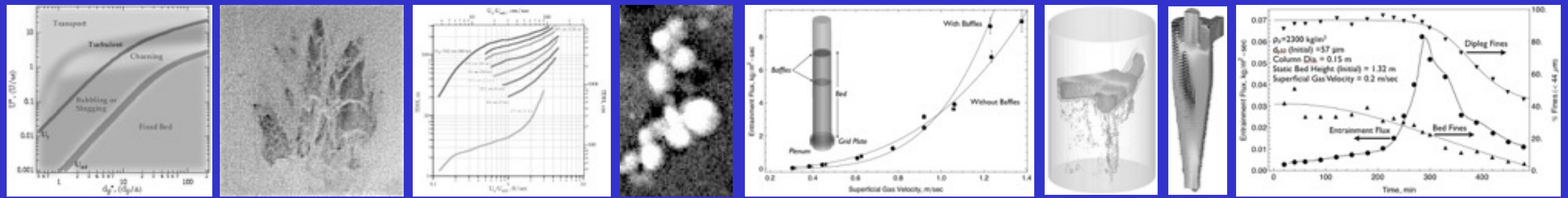
PSRI Particulate Solid Research, Inc.

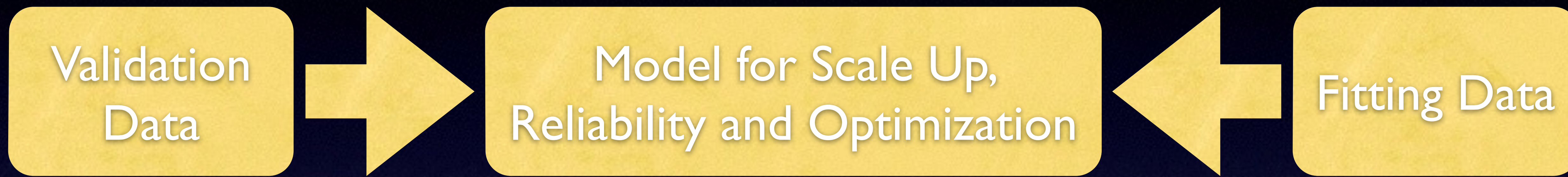
Applying the Fundamentals



Outline

- Validation challenges in fluidization
- PSRI's modeling methodology
- Gaps in PSRI's modeling methodology
- Summary

Challenges in Validating Fluidization Models



- Experiments have mostly been focused on providing validation for model development.
- Particle have a wide range of properties that may not be captured with a model
- Modeling with a commercial code of commercial systems requires a "fitting" of the drag model
- Experimental methods are limited for this "fitting"

The Multi-scale Validation Paradox

Micro-scale	*Meso-scale*	*Macro-scale*
1 to 100's Particles	Millions to Billions of Particles	Trillions of Particles
10^{-6} to 10^{-4} m	10^{-2} to 10^{-1} m	10^{-1} to 10^{2} m
Experiments are cheap	Experiments are inexpensive	Experiments are expensive
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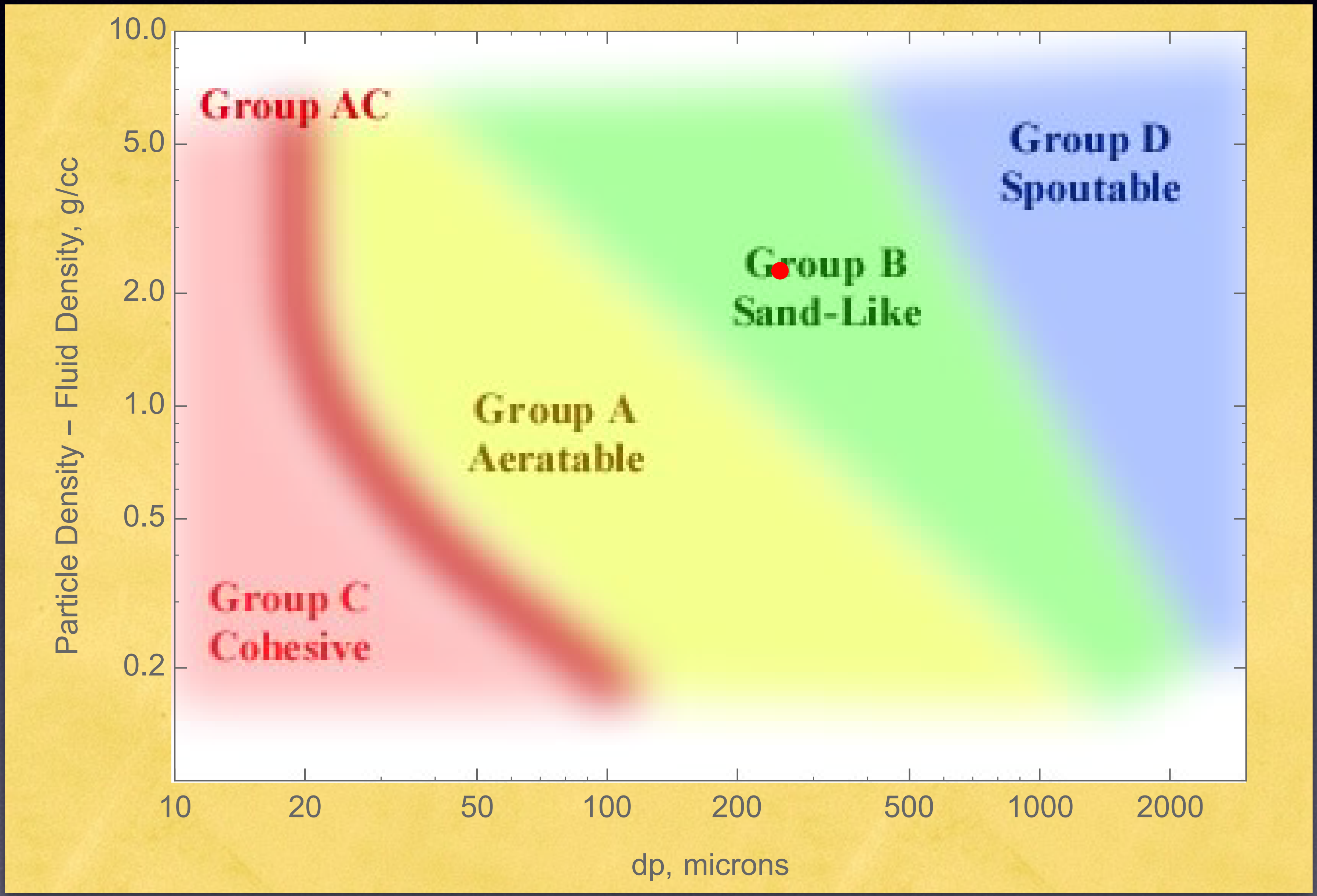
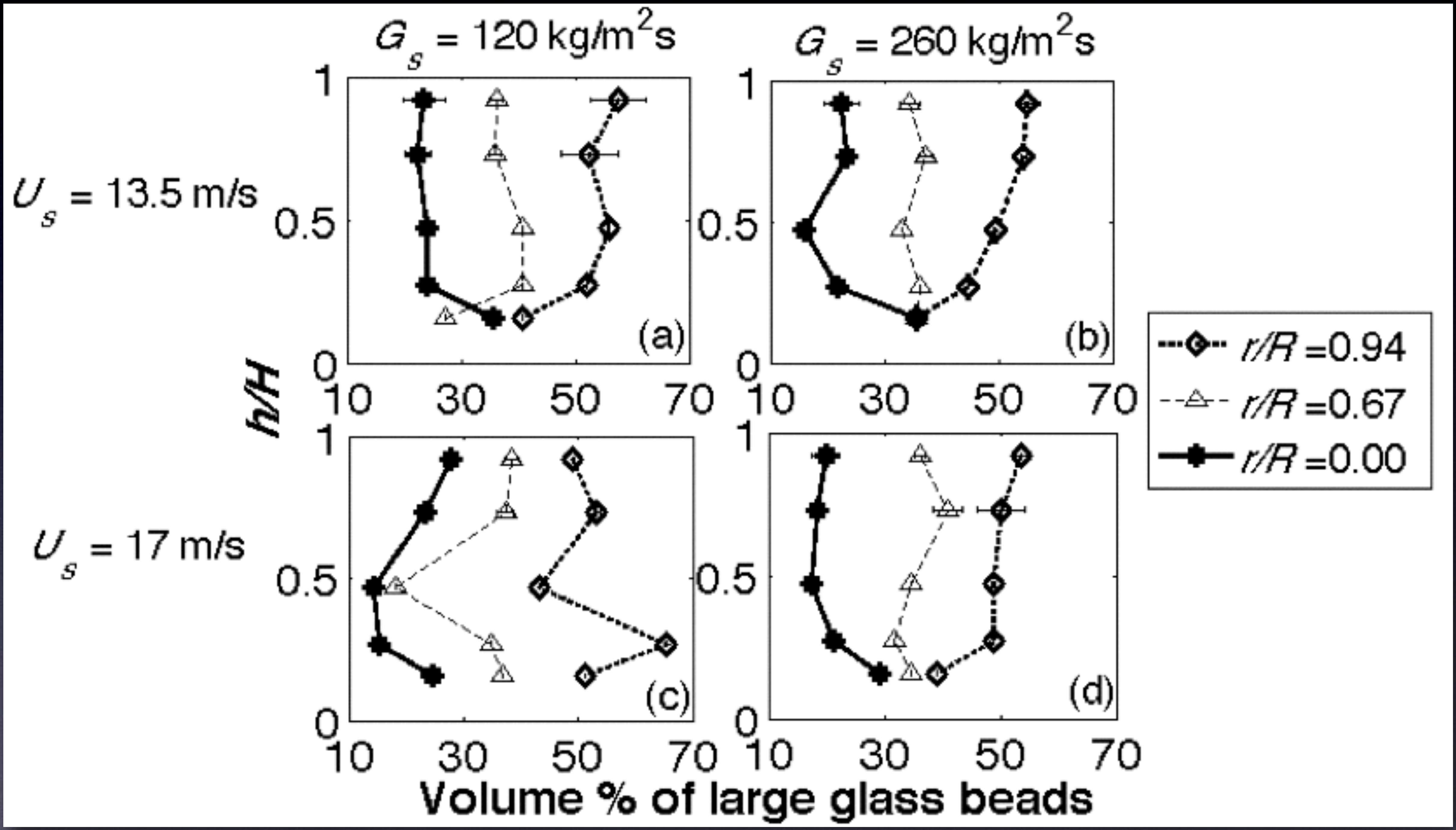
Factors Effecting the Fundamentals

- Particle diameter
- Particle density
- Particle size distribution
- Particle shape
- Particle morphology
- Particle adsorbates

Particle Size and Density

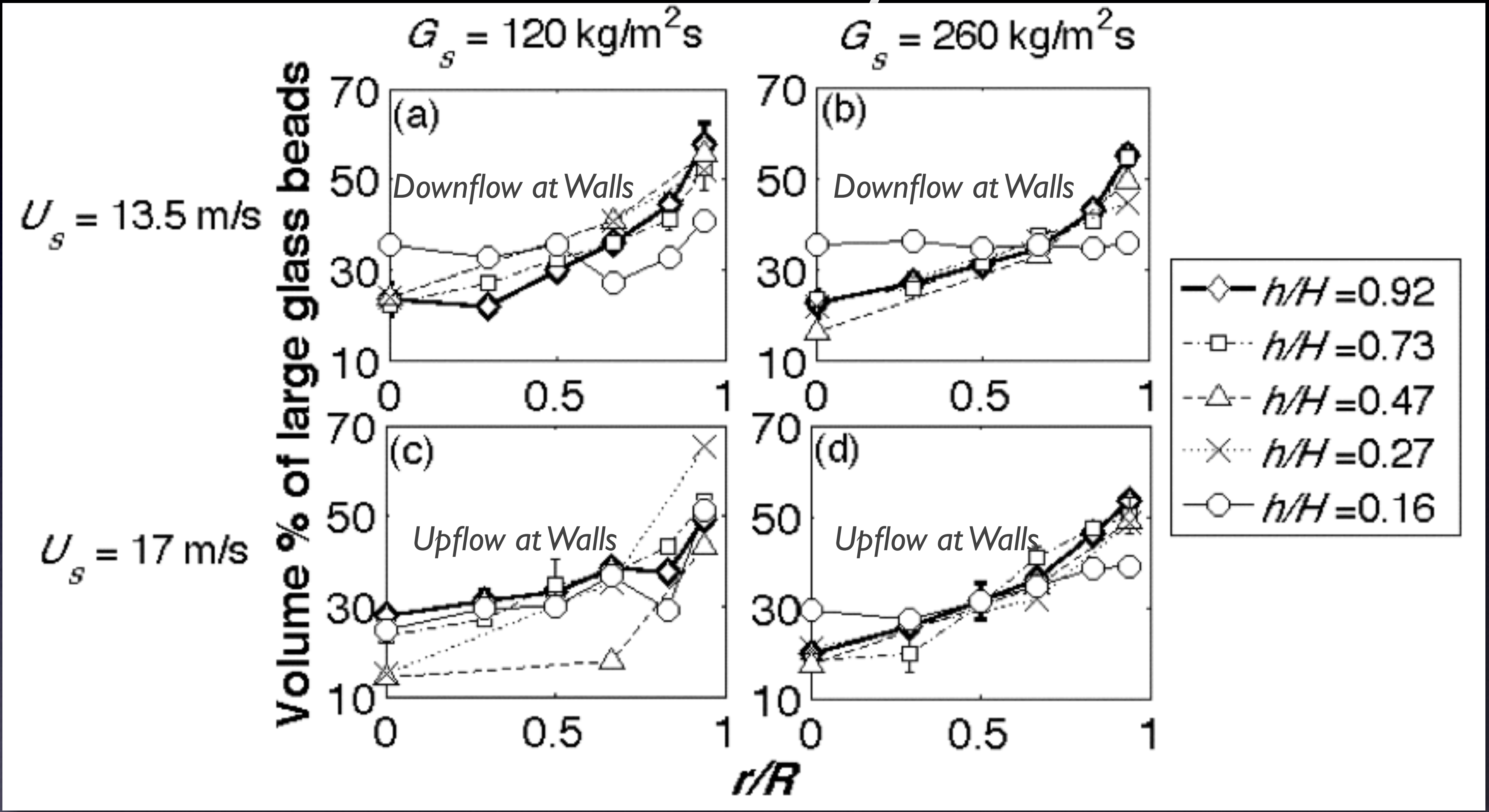


Axial Segregation with Size-Difference Binary Mixture



- *Most of the segregation occurs in the full-developed flow region*

Radial Segregation with Size-Difference Binary Mixture

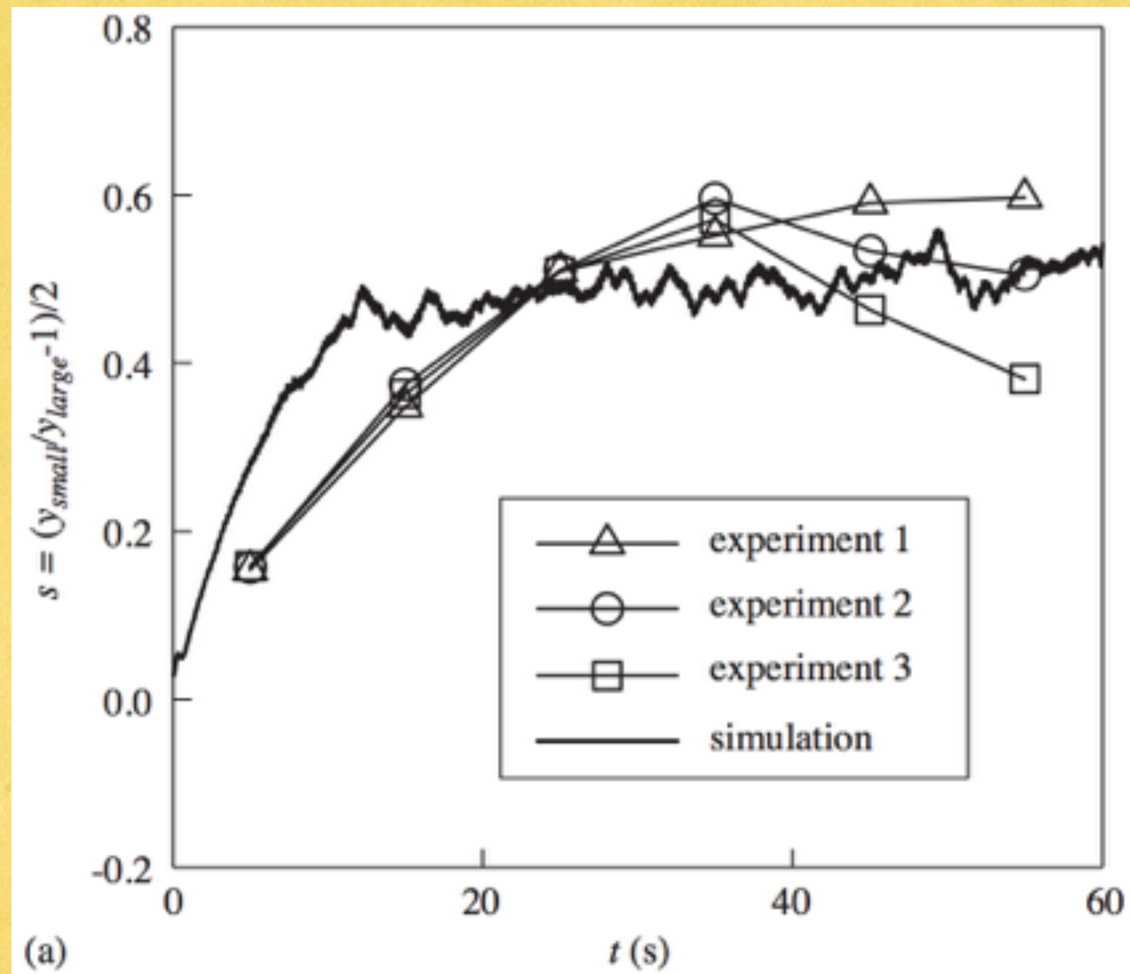


- *More segregation near the top of the riser and for downflow and upflow at the walls*

J.W. Chew, R. Hays, J.G. Findlay, S.B.R. Karri, T.M. Knowlton, R.A. Cocco, et al., Species segregation of binary mixtures and a continuous size distribution of Group B particles in riser flow, Chemical Engineering Science. 66 (2011) 4595–4604.

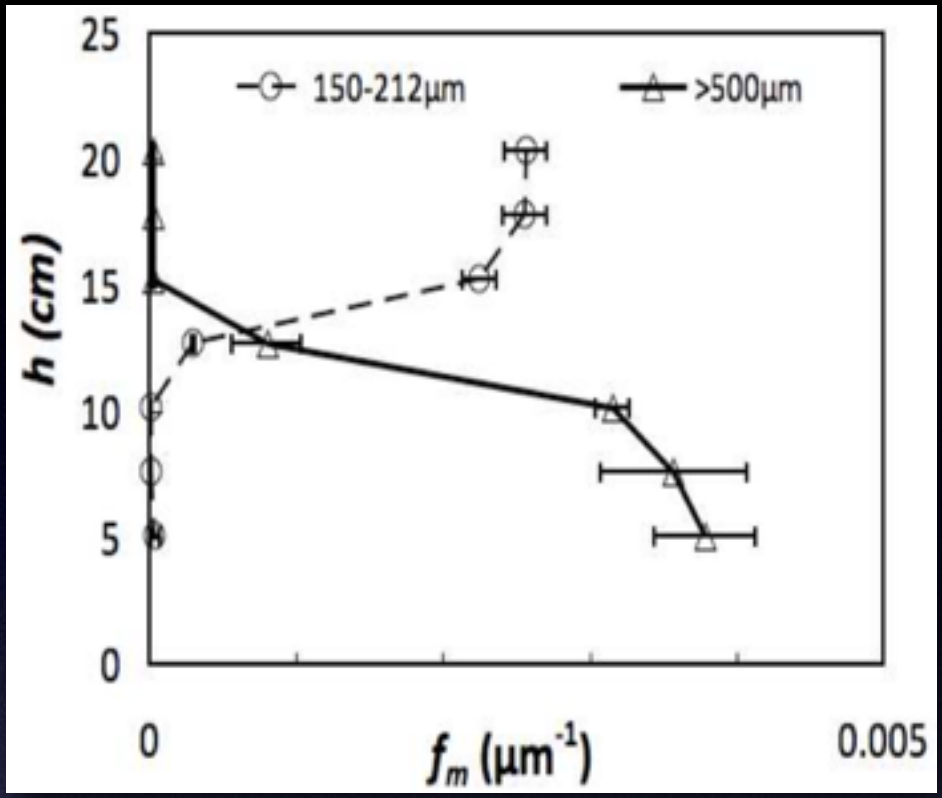
Segregation in Fluidized Beds

$$s = \frac{S-1}{S_{\max}-1} = \frac{\dfrac{\langle y_{\text{small}}\rangle}{\langle y_{\text{large}}\rangle} - 1}{\left(\dfrac{2 - x_{\text{small}}}{1 - x_{\text{small}}} - 1\right)}$$



S.D Dahl, C.M. Hrenya, Chemical Engineering Science 60 (2005) 6658–6673

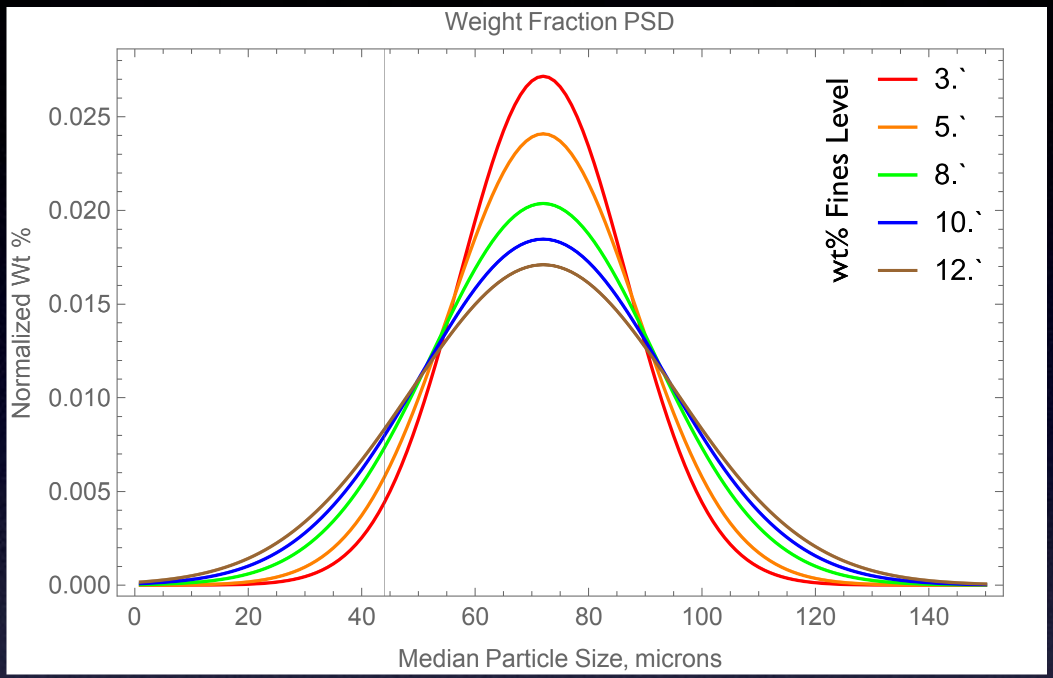
Bubbles and Segregation

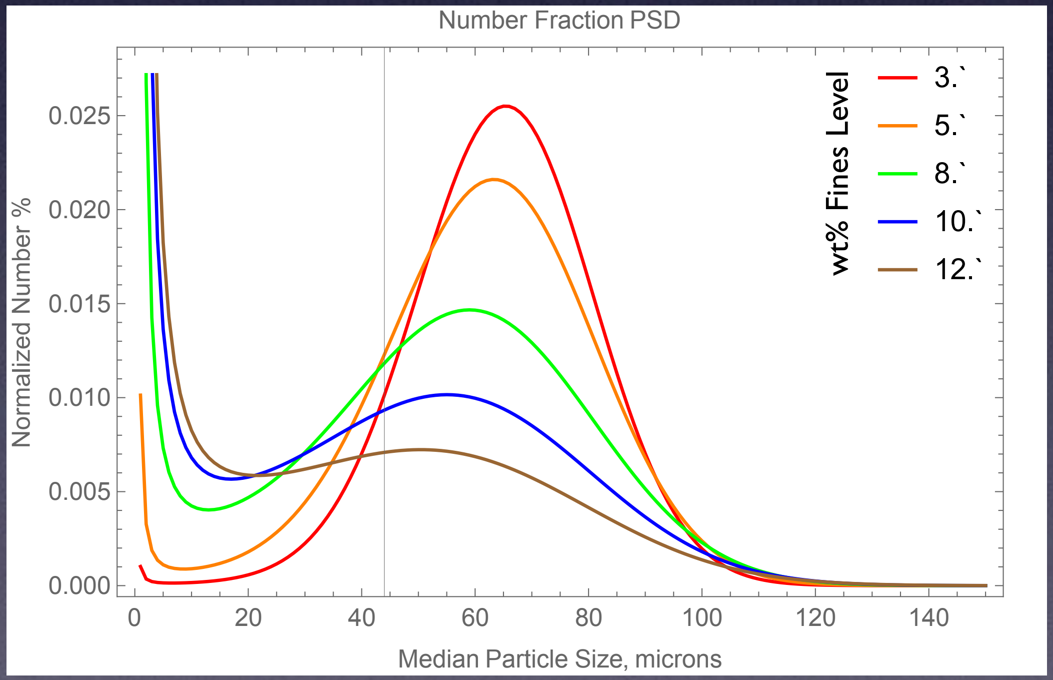


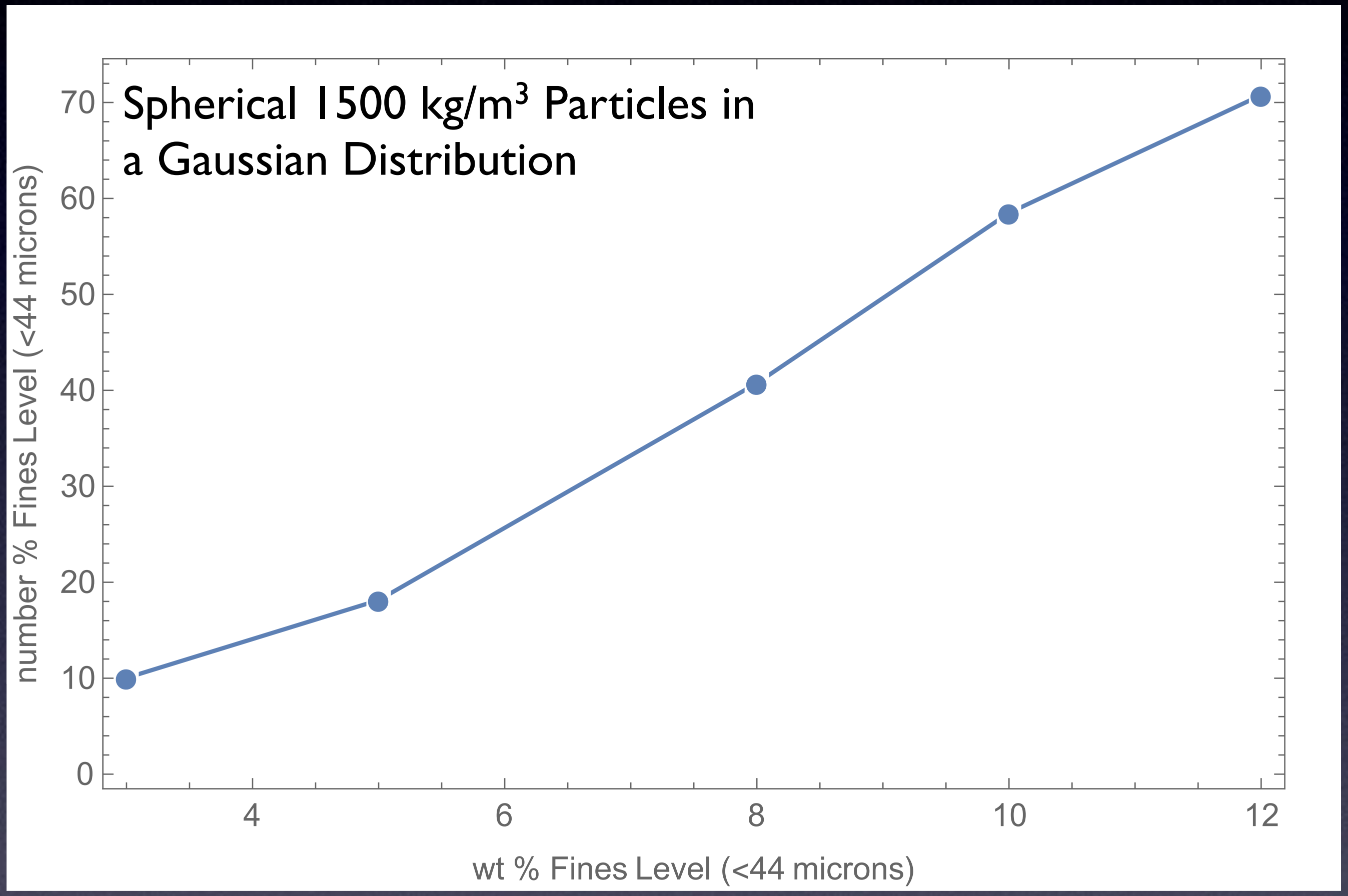
- Axial segregation profile of the finest and coarse particles with a Gaussian distribution (σ/d_{sm}=0.3)
- Bubbles limit segregation
- Bottom of the bed is limited in bubbles, thus segregation can be significant here

J. Chew, C. Hrenya, On the Link between Bubbling and Segregation Patterns in Gas-Fluidized Beds with Continuous Size Distributions, Ind. Eng. Chem. Res. (2010) 1–29.

Particle Size Distribution

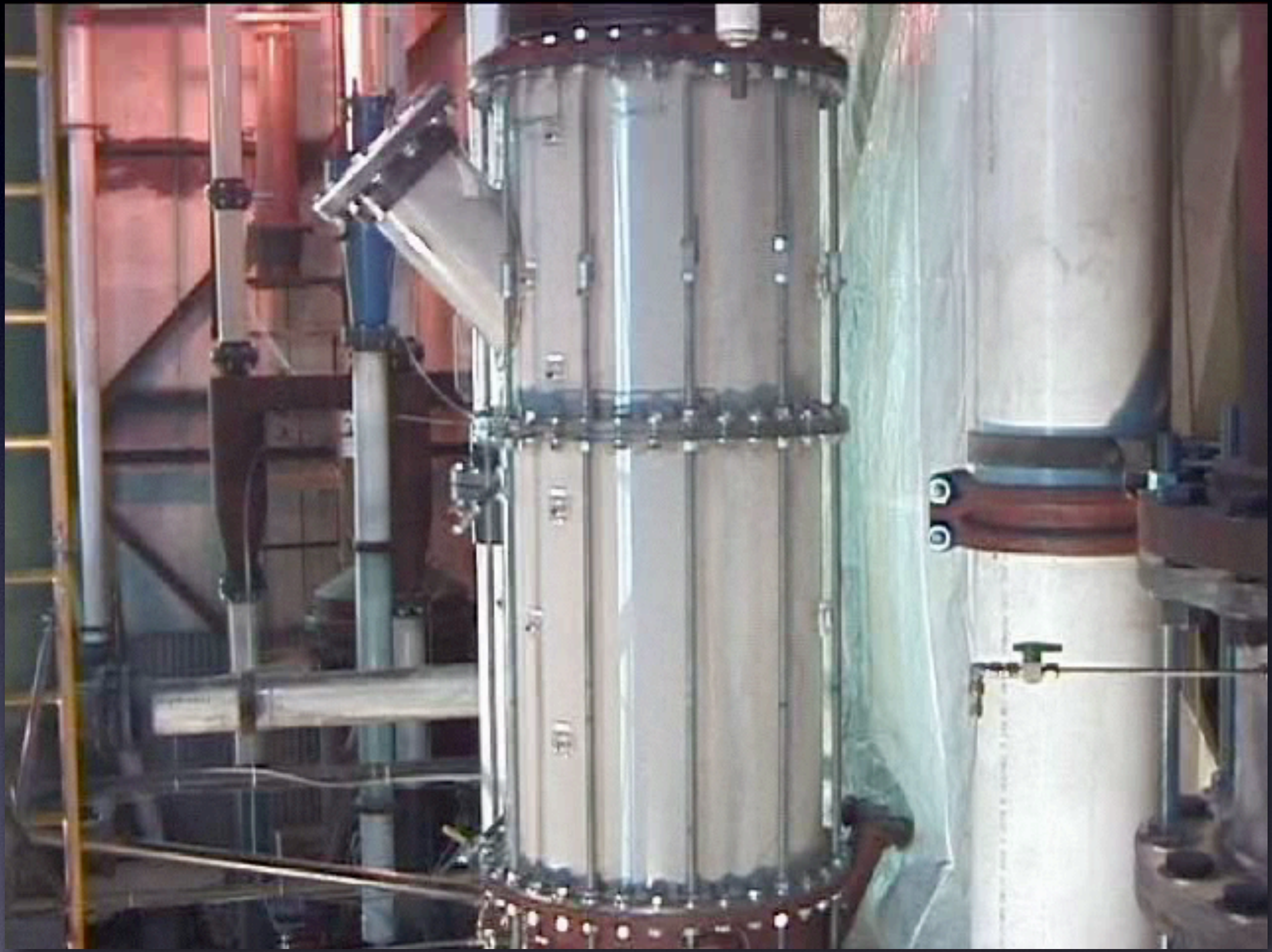






Strength in Numbers

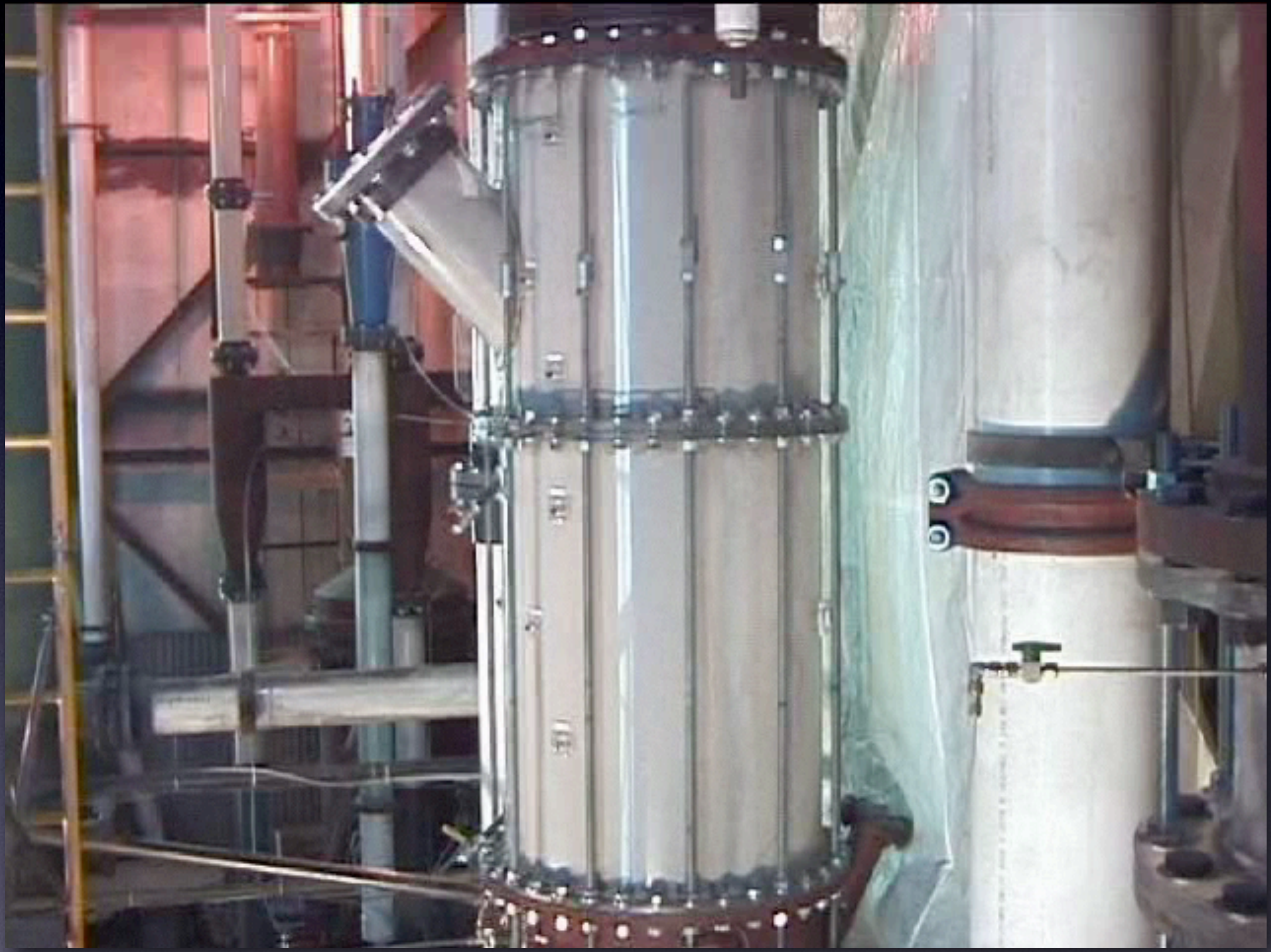
Gas Bypassing in Fluidized Beds



0.9 m ID Fluidized Bed
Ug = 0.46 m/sec with FCC powder (3% fines)

- Large regions of the bed poorly fluidized!
  - Severe bypassing of gas
- Grid pressure drop >> 1/3 bed pressure drop
- Little help in detection
  - ΔP/L was uniform
  - Entrainment rate did not change

Gas Bypassing in Fluidized Beds



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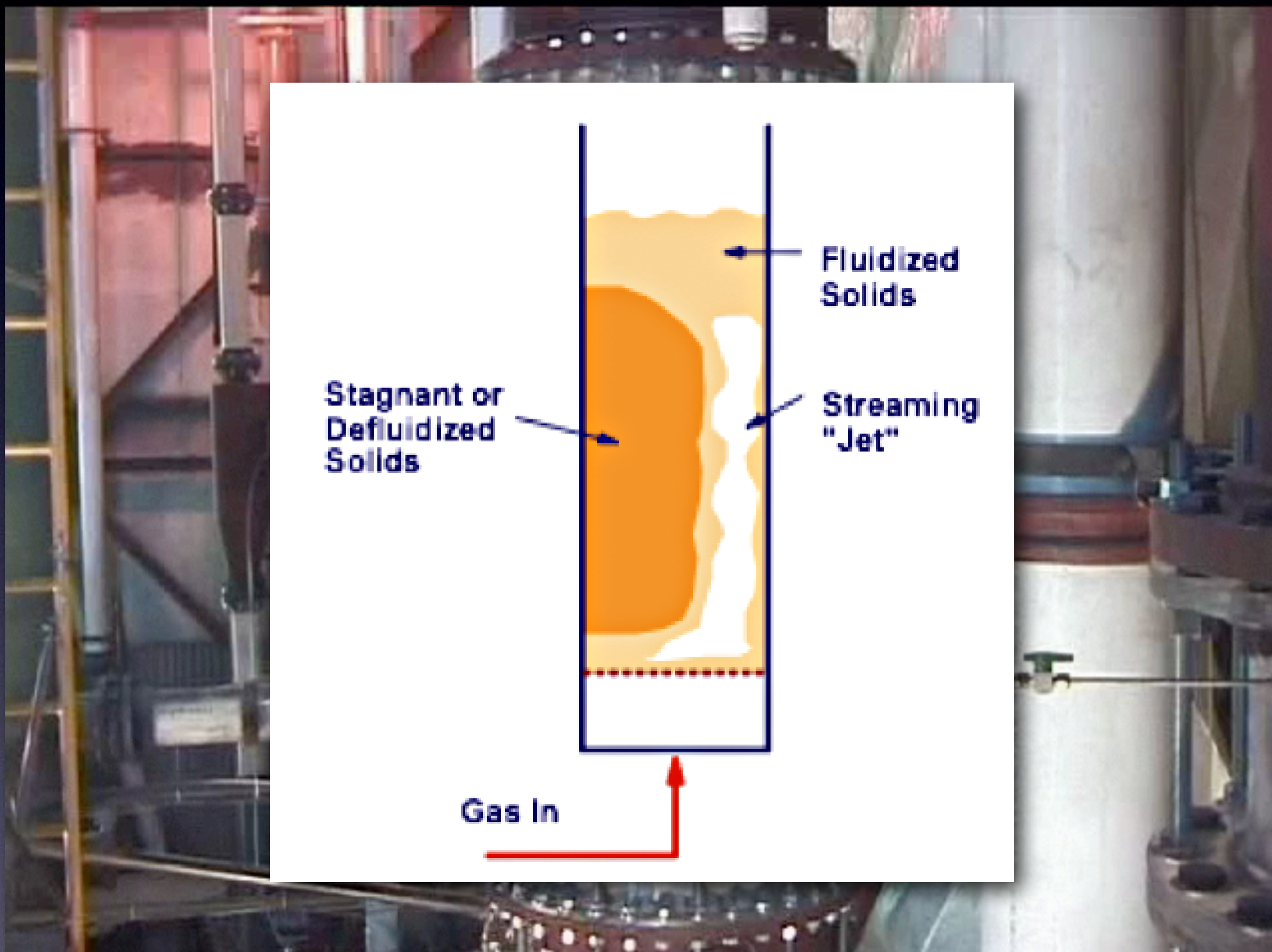

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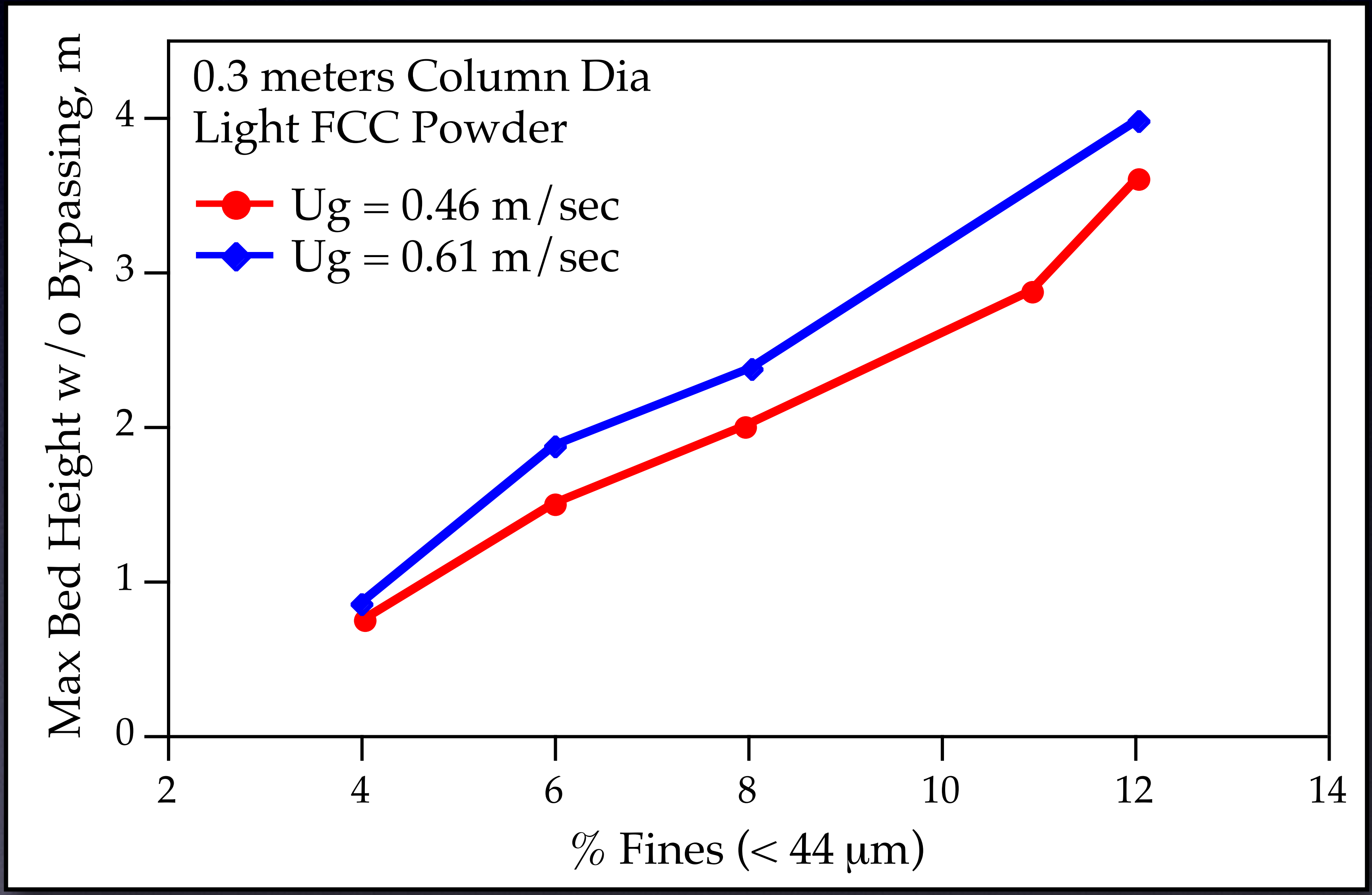
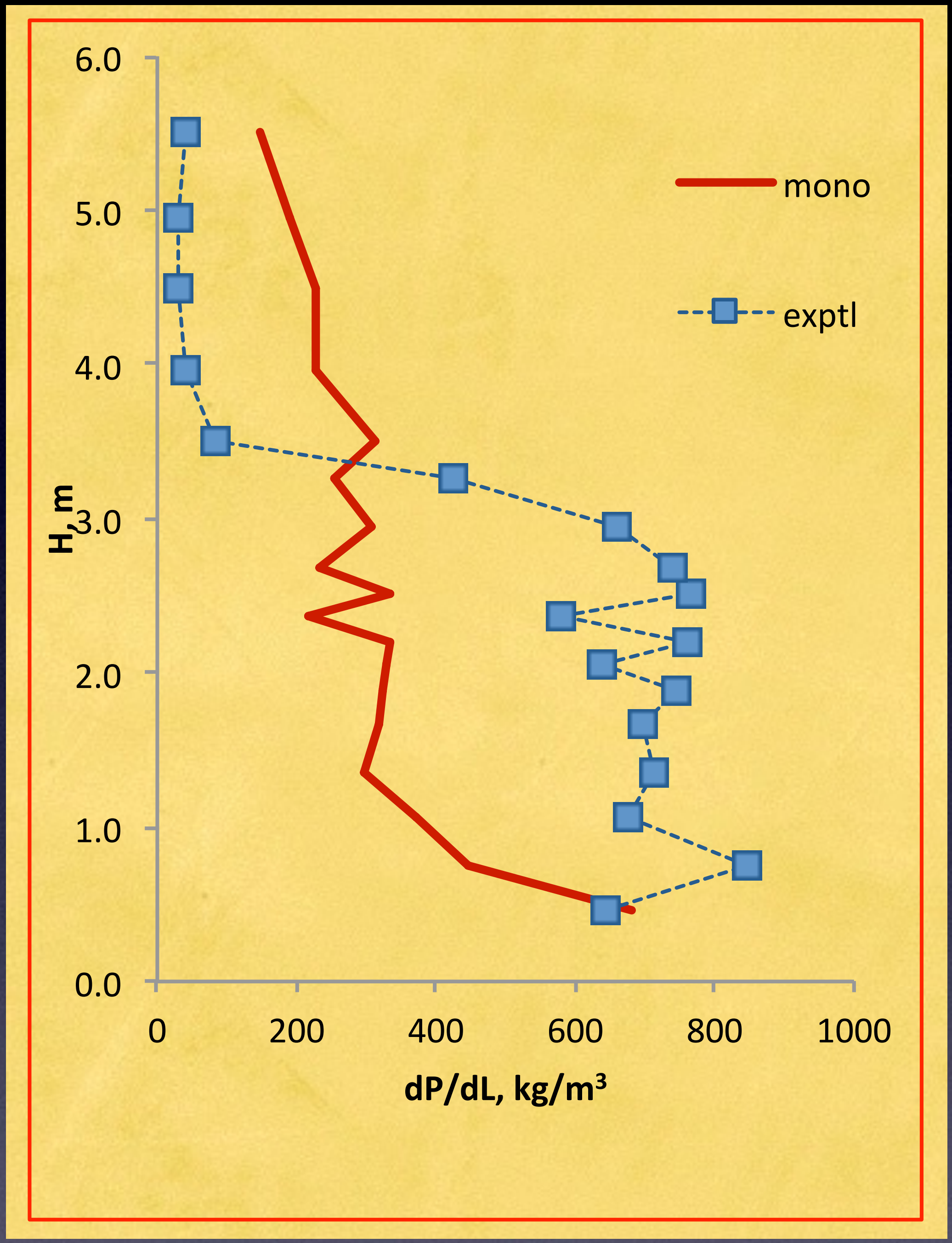
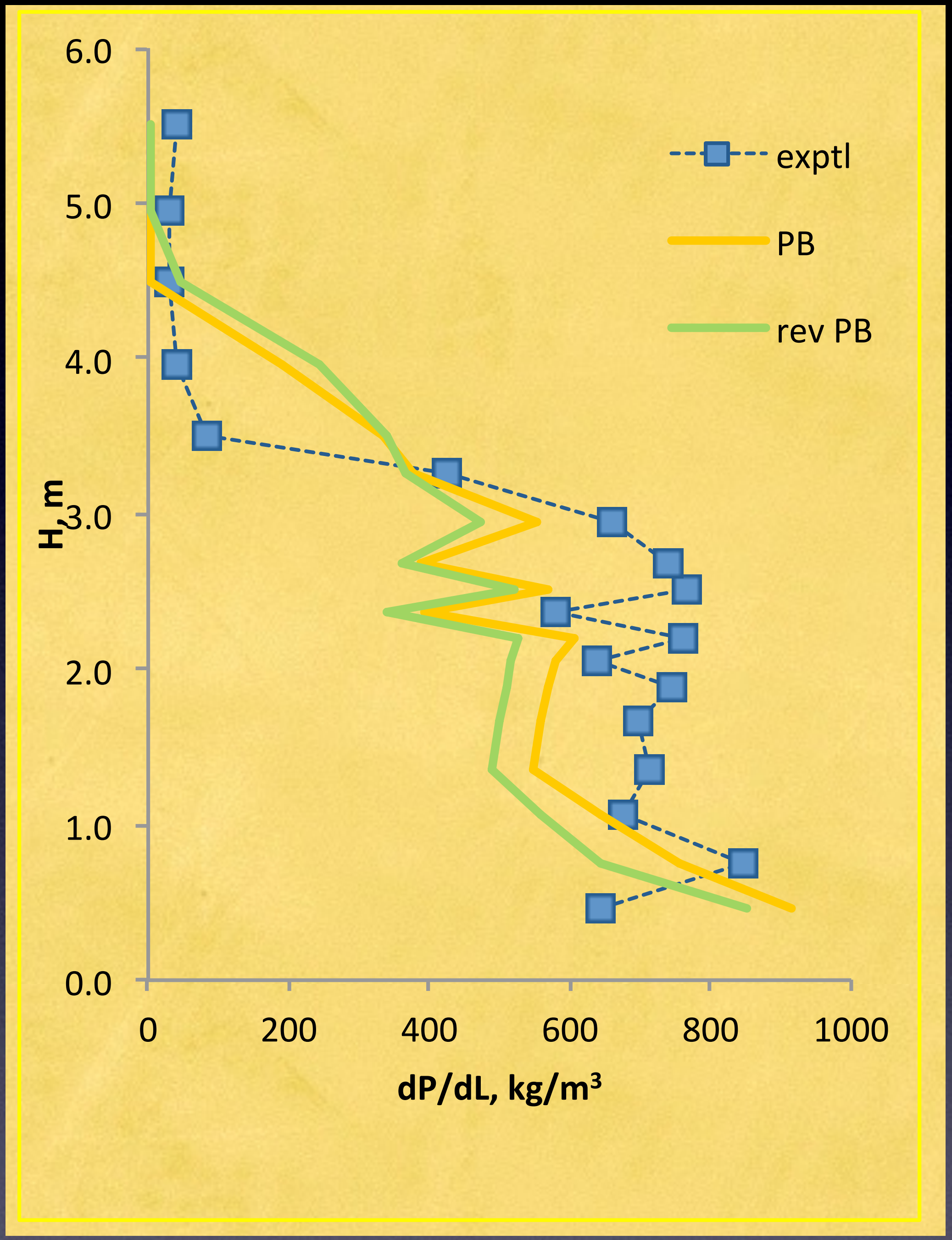
Fines Matter



PSRI & NETL Challenge Problem

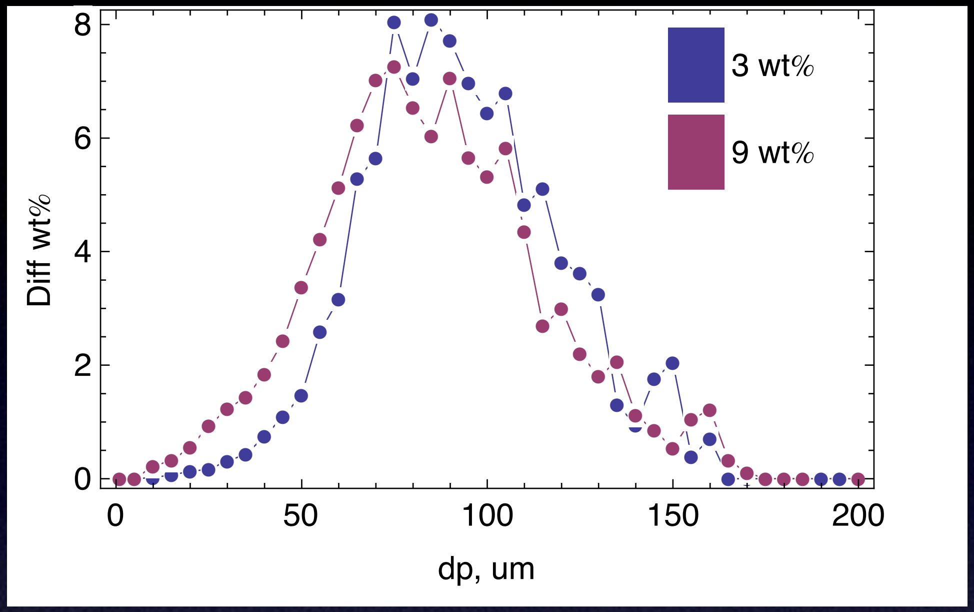




Eulerian-Eulerian with Single Particle Size

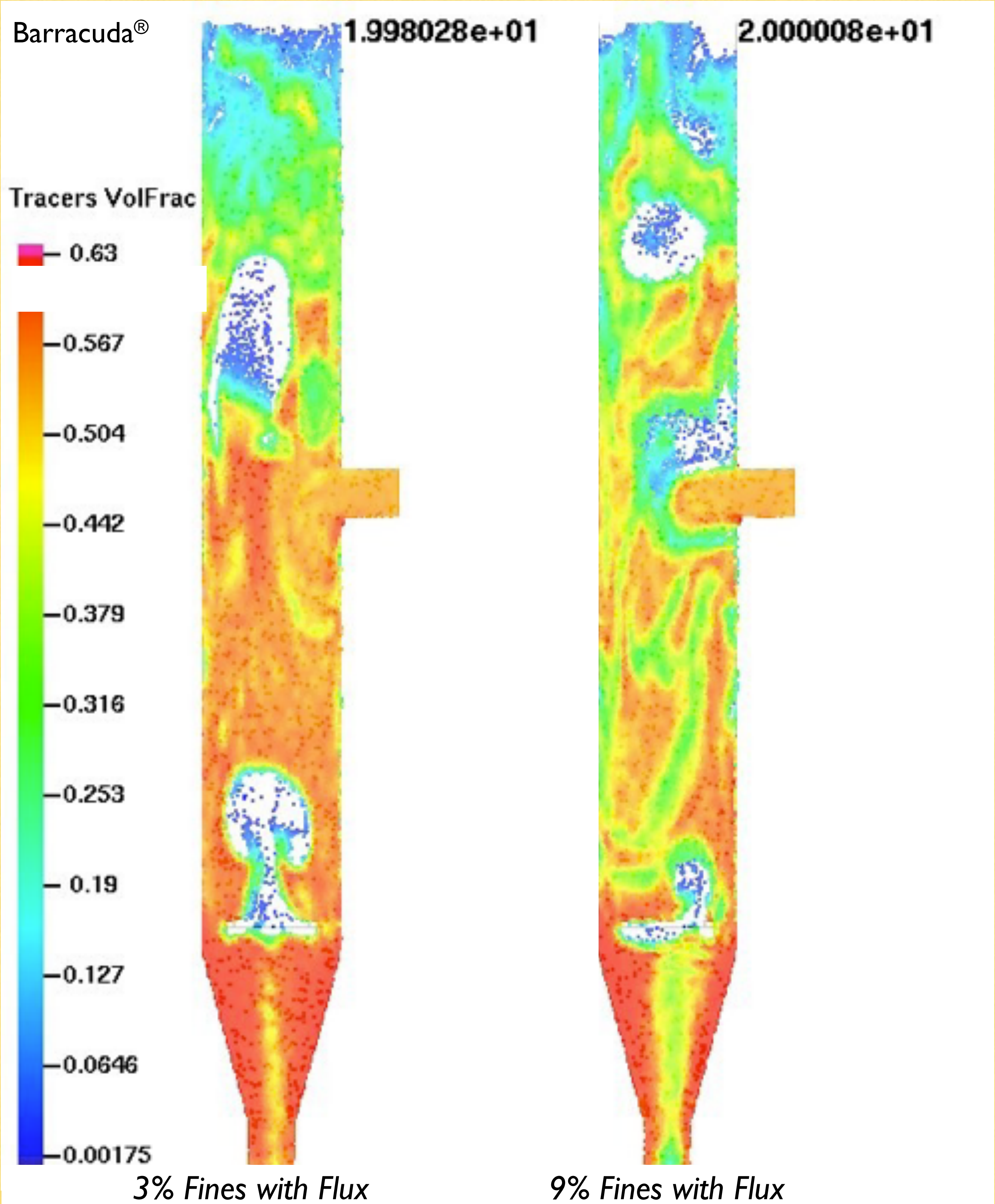
Eulerian-Eulerian with Population Balance for Particle Size Distribution

Gas Bypassing



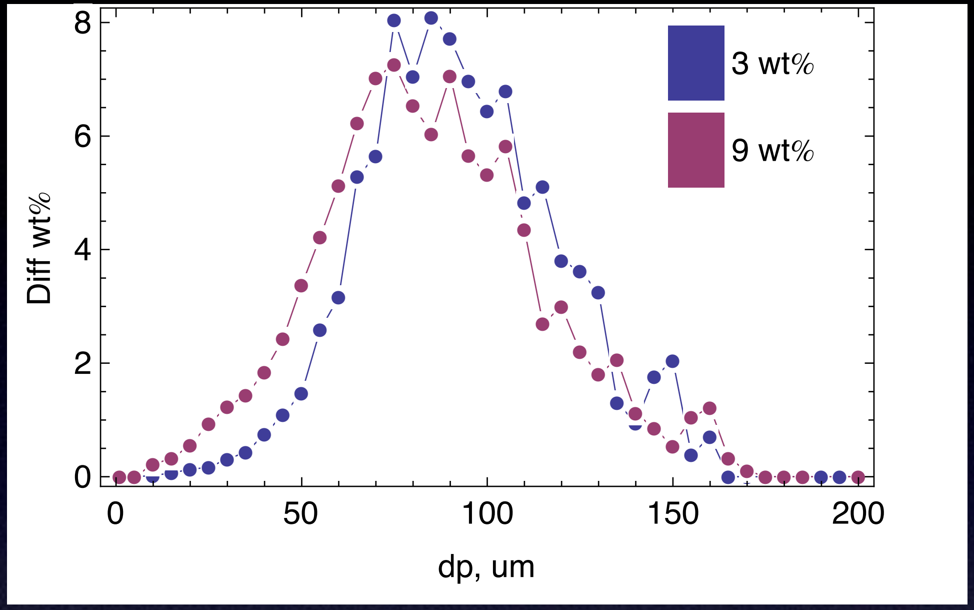
Reported	dp50, µm	% Fines, (< 44 µm)
3 wt%	80.4 µm	2.7%
8 wt%	81.0 µm	8.6%

- Significant difference in hydrodynamics due to fines level, not median particle size.
- If using one representative particle size, which one do you use?



2 ft/sec (0.6 m/sec) Superficial Gas Velocity

Gas Bypassing



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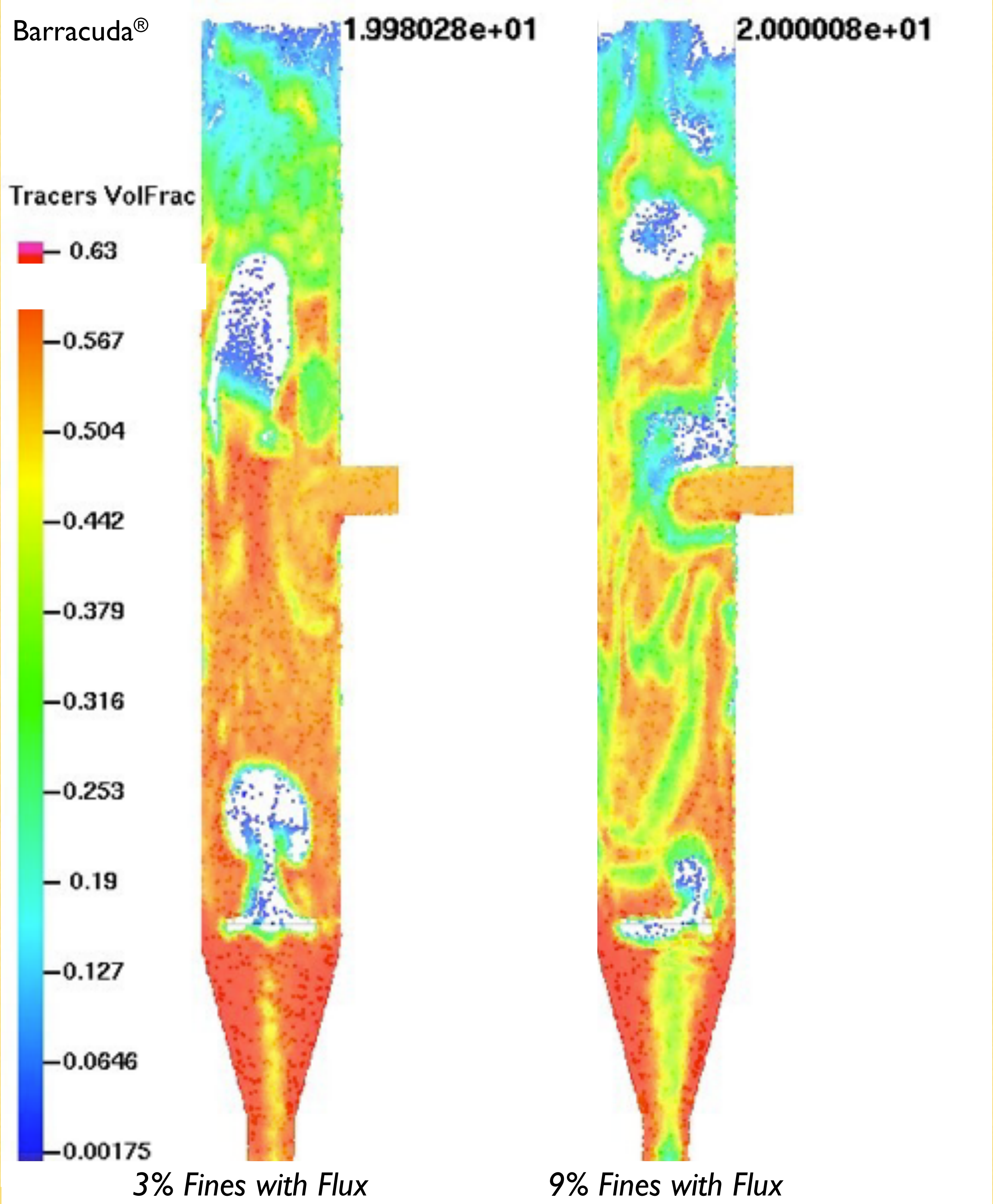

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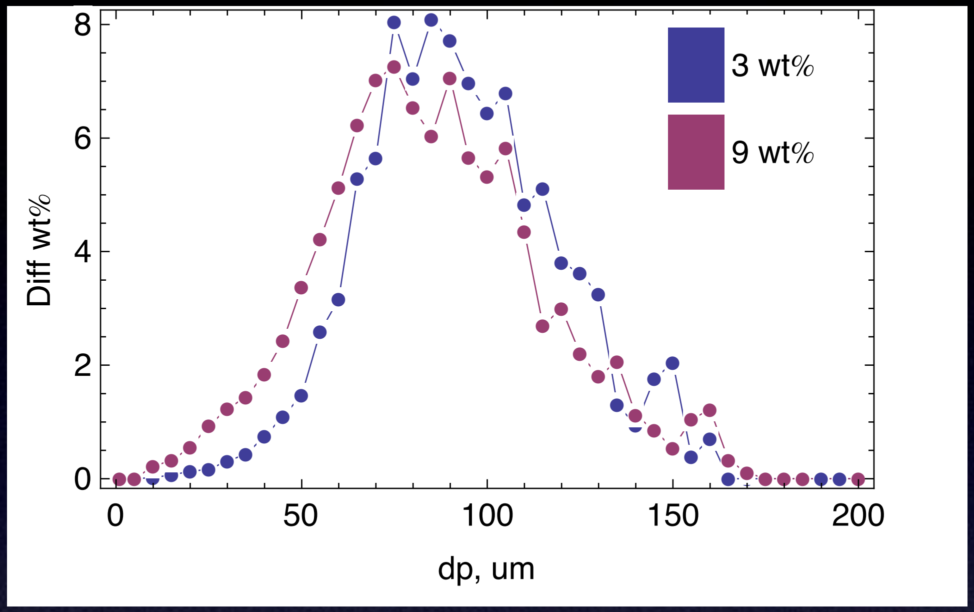

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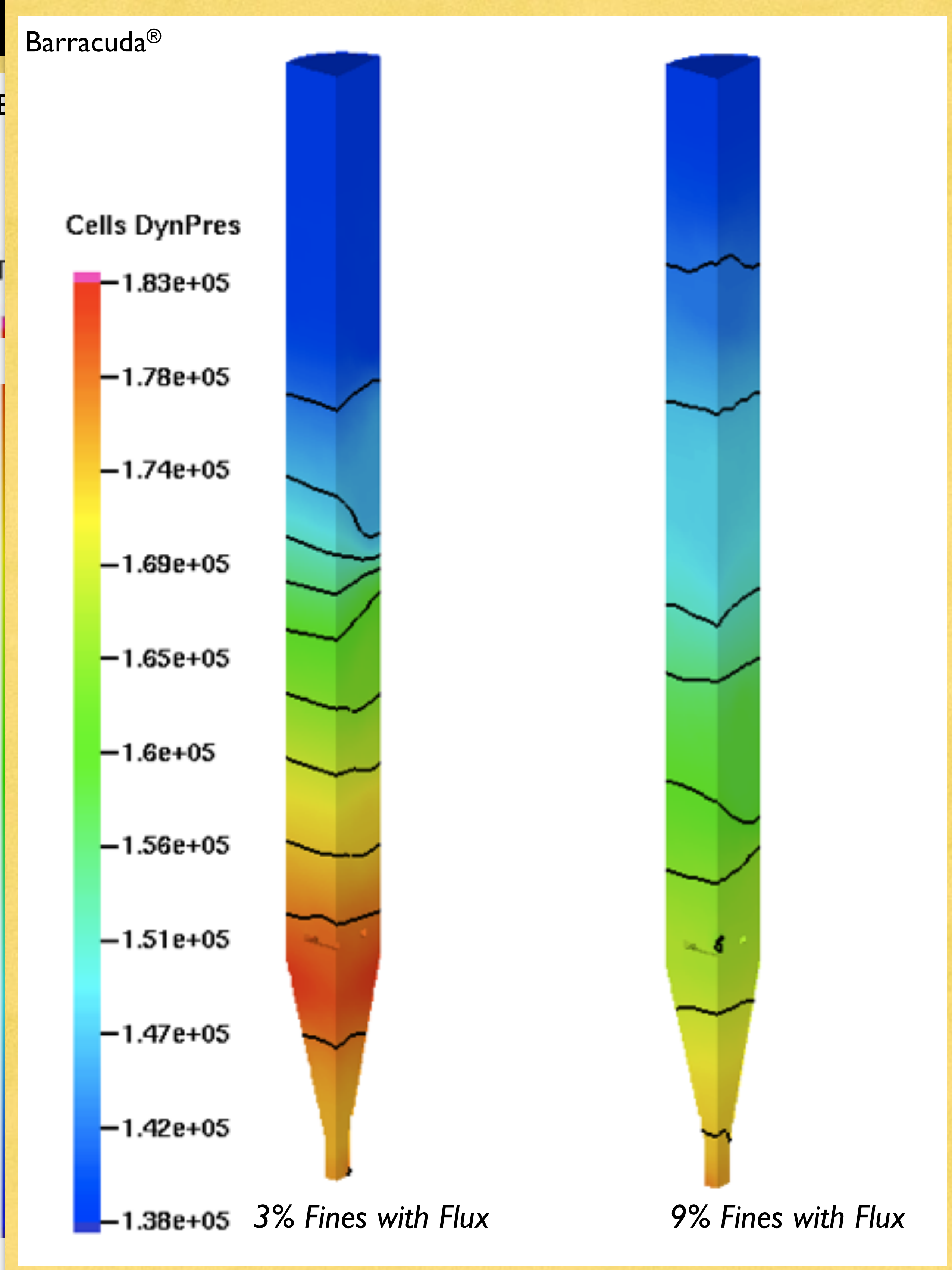

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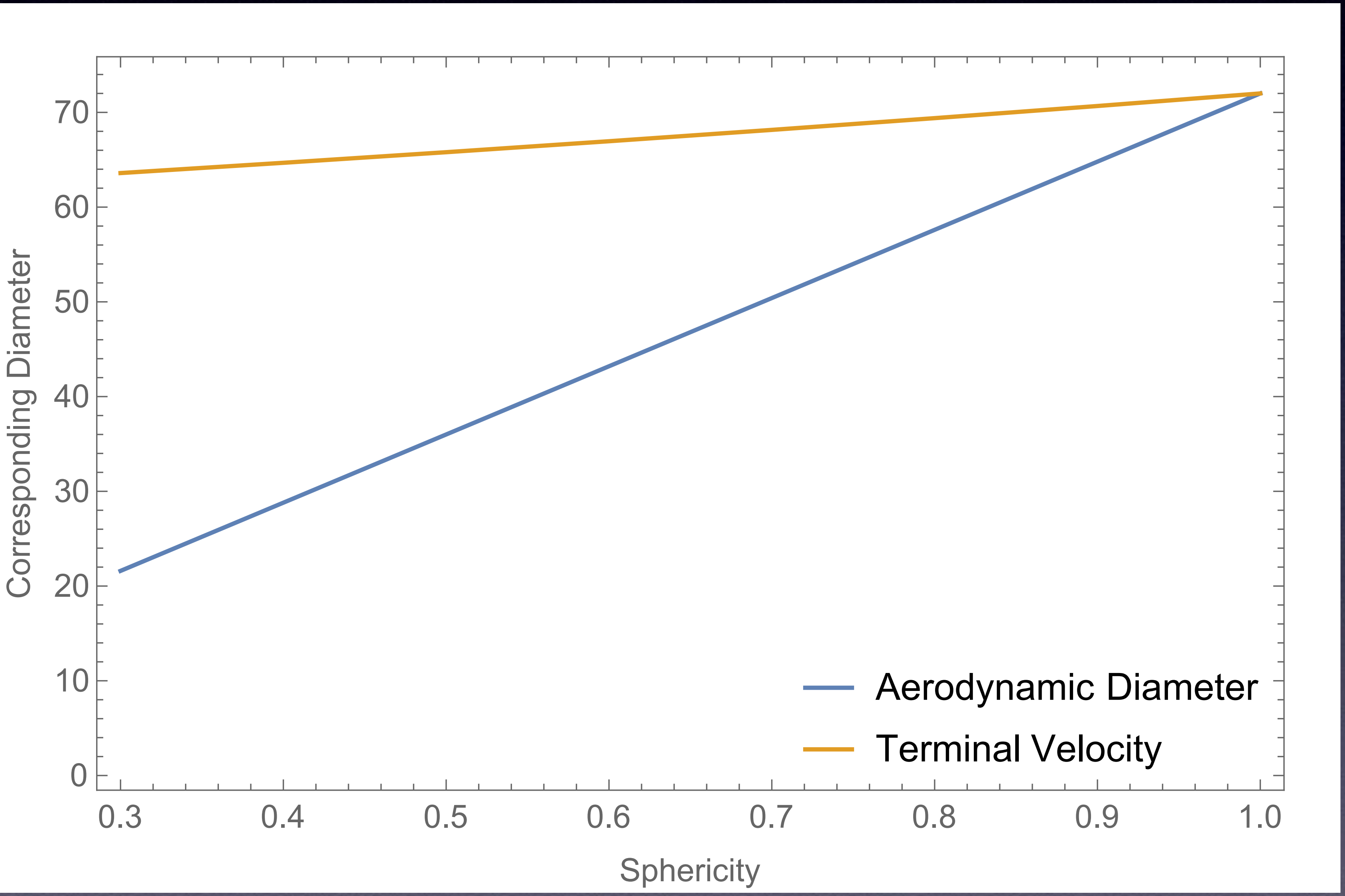
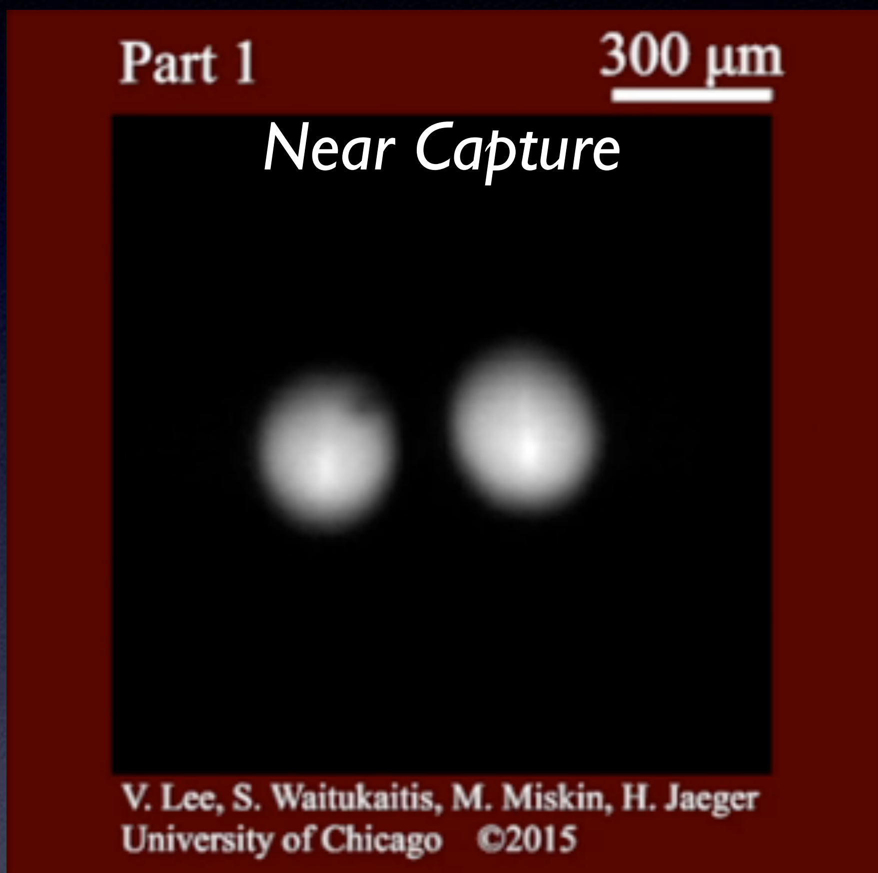
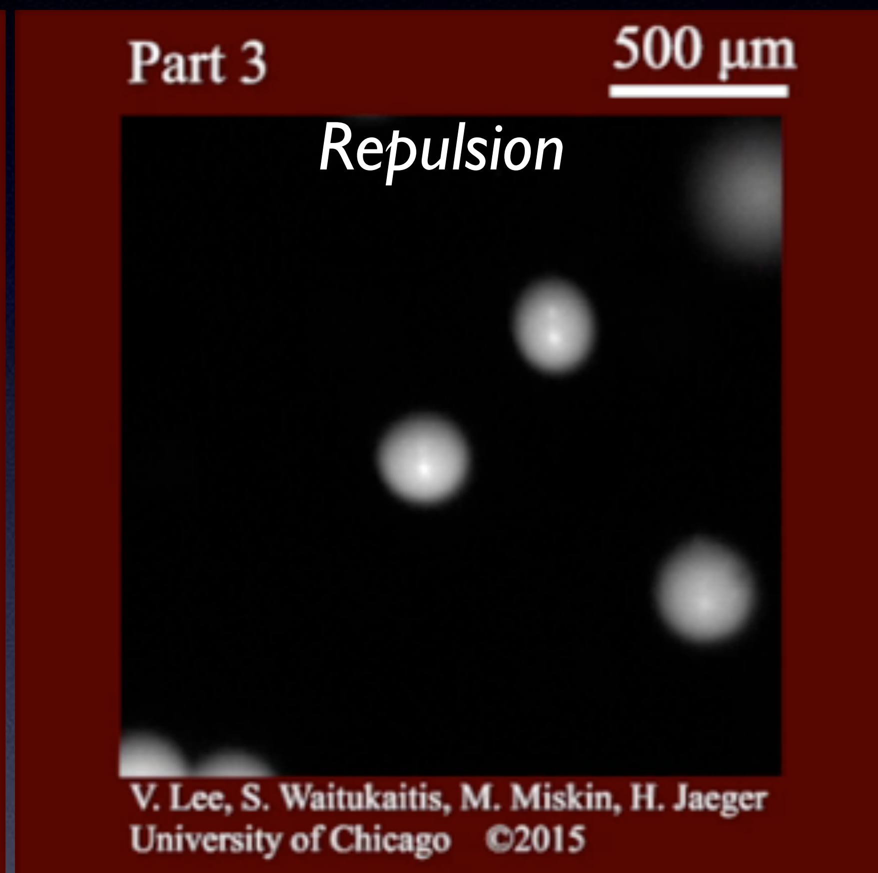
Particle Shape

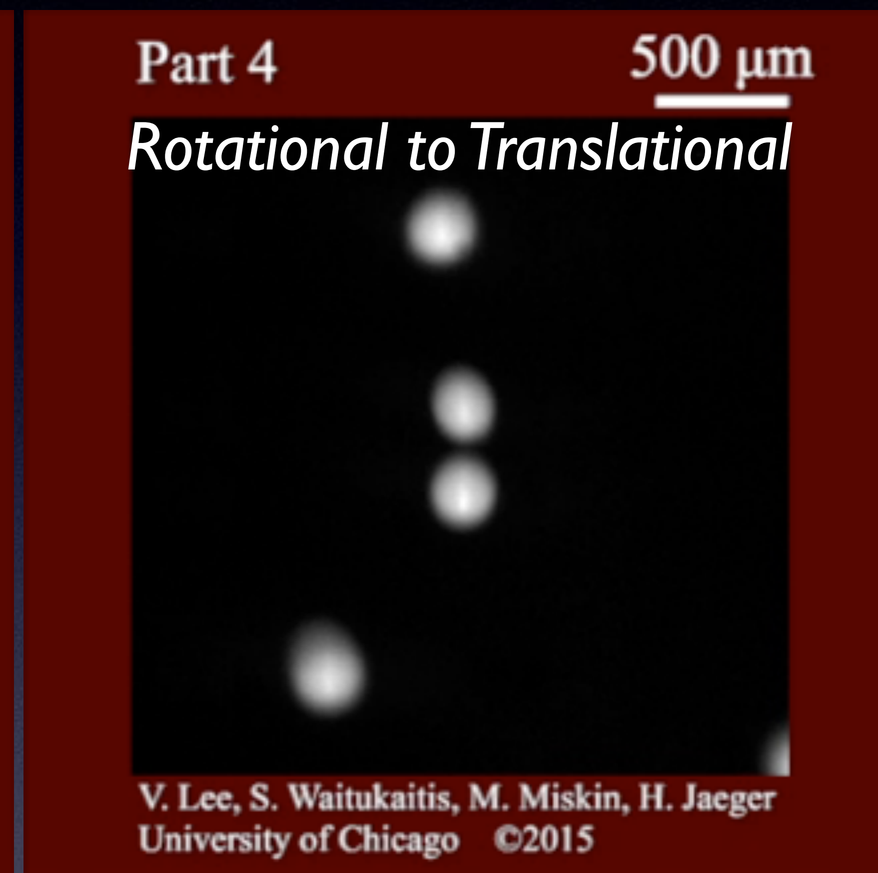
Aerodynamics



Particle-Particle Interactions







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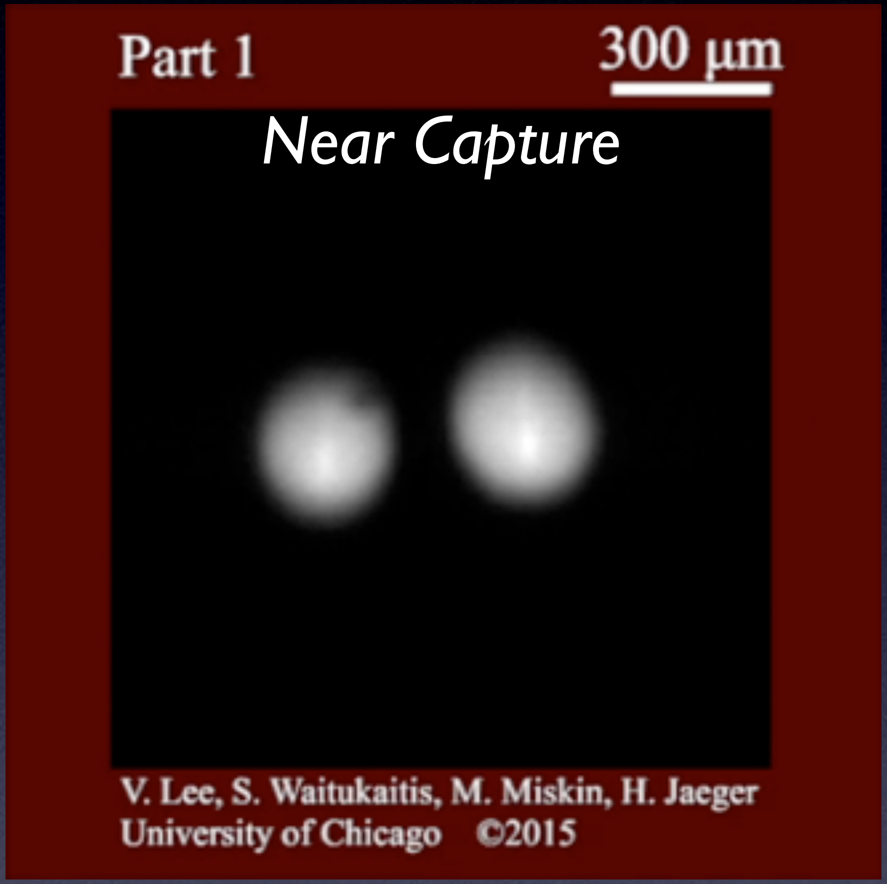

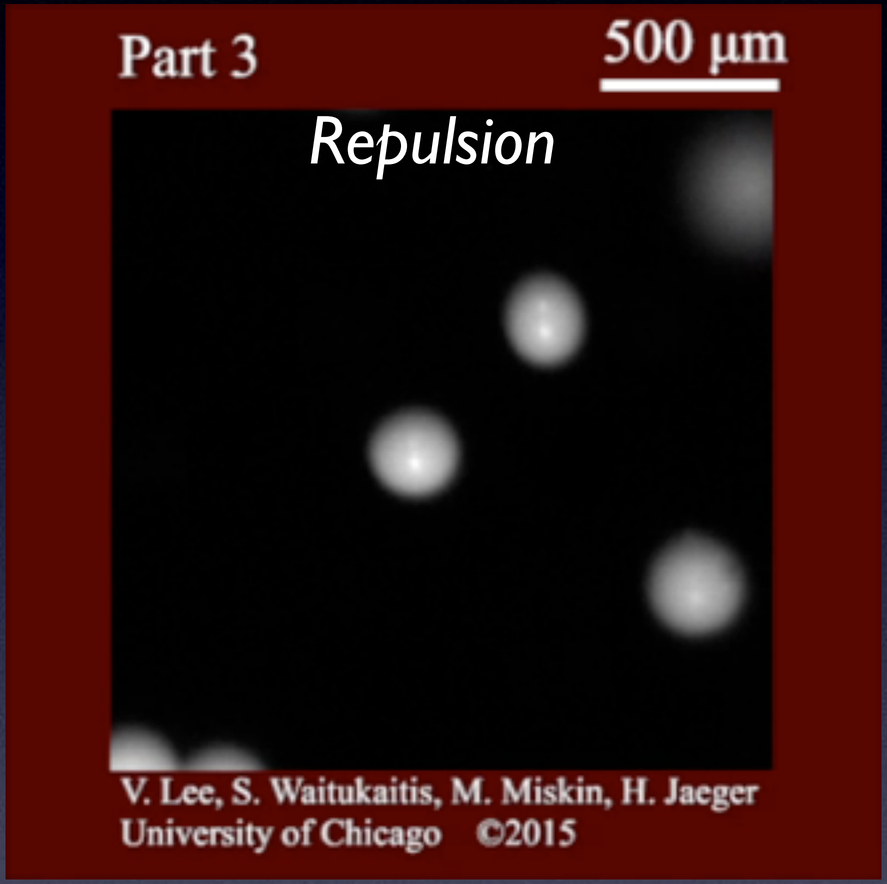

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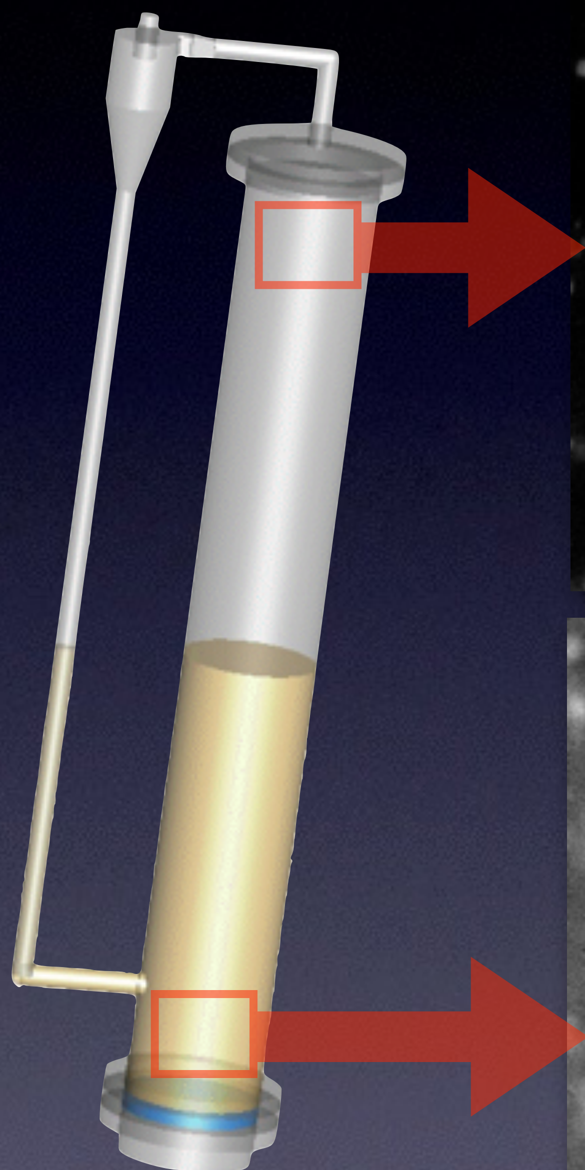
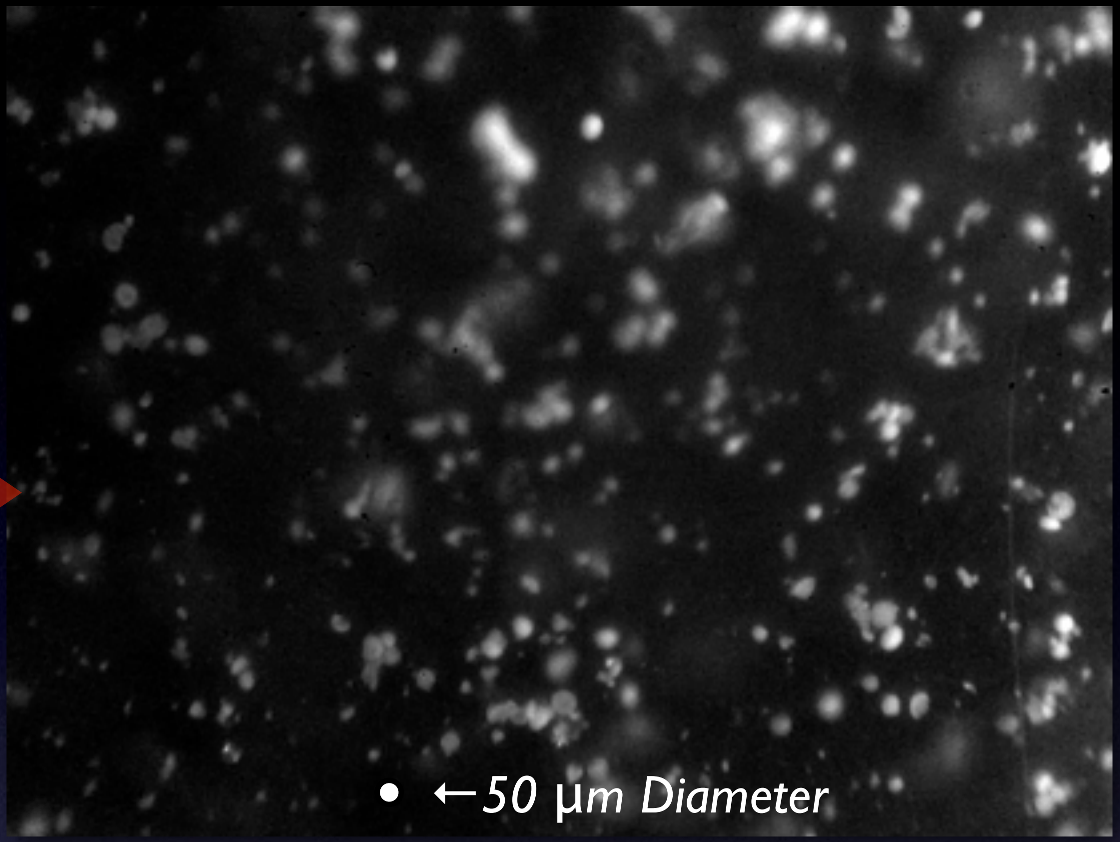
Particle Morphology and Adsorbates

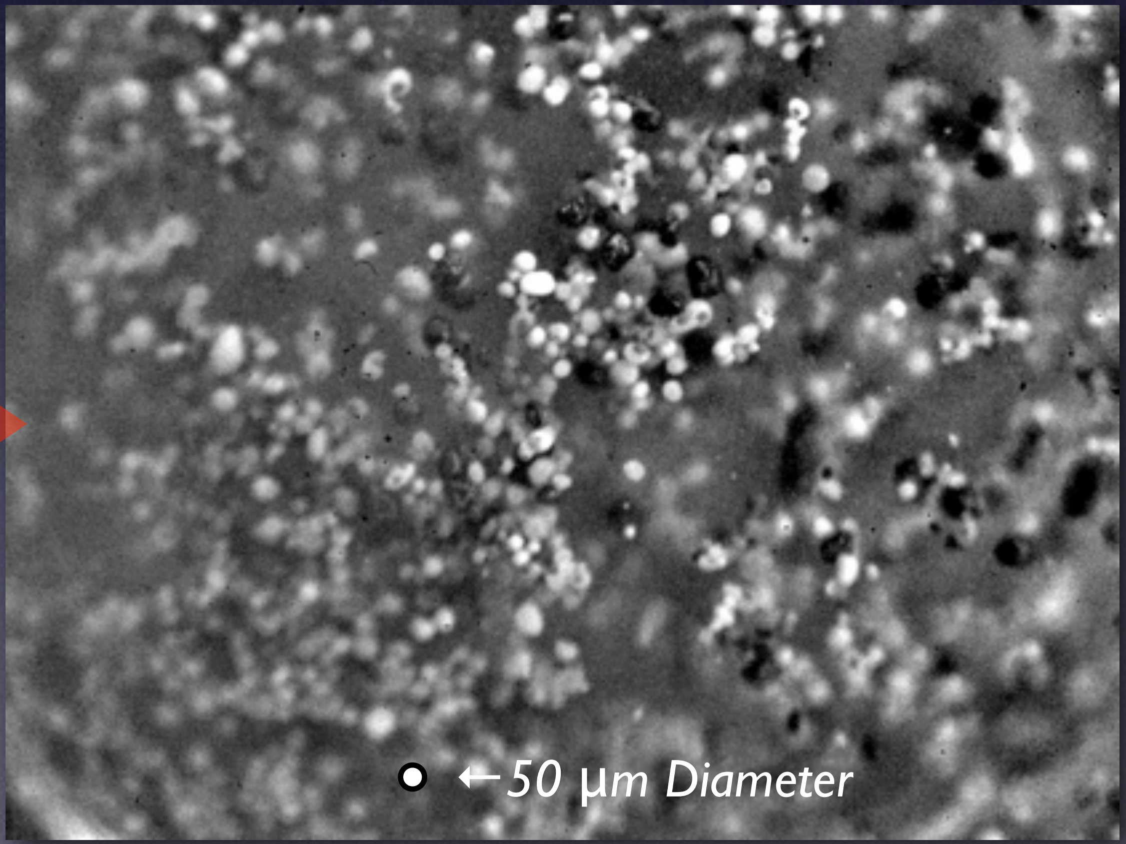
- 30% of the material in the freeboard were observed as clusters
- Average cluster size was 11 particles

FCC powder with d_{p50} of 72 microns in a 6-in (15-cm) ID fluidized bed with a superficial gas velocity of 1 ft/sec (0.3 m/sec)



Phantom V7.1 @ 4000 fps, 20 µs exposure (NETL)





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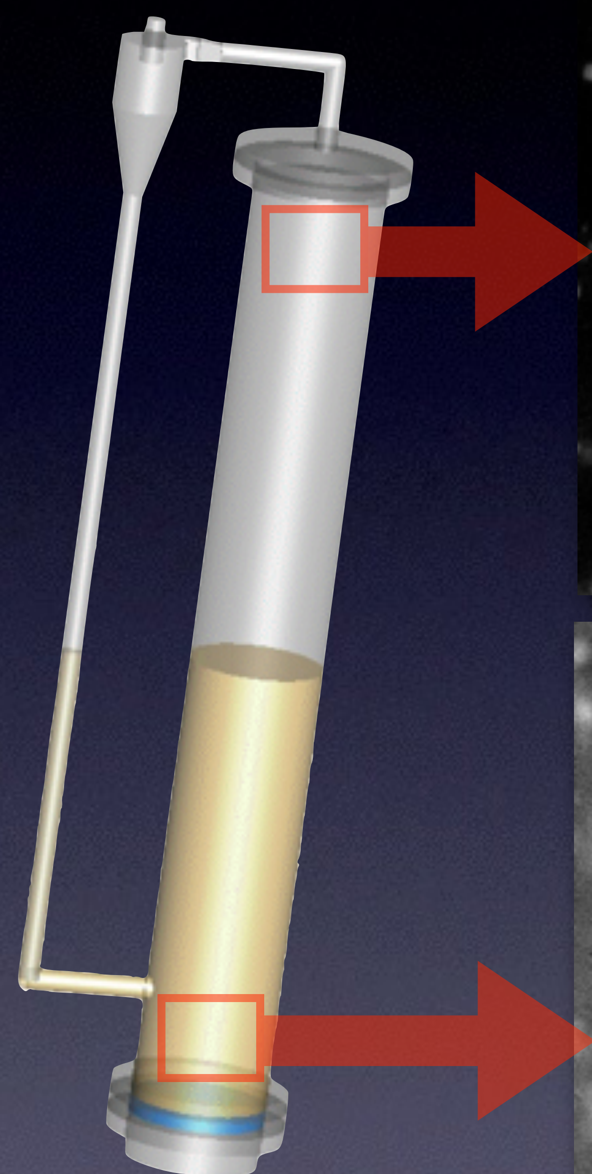

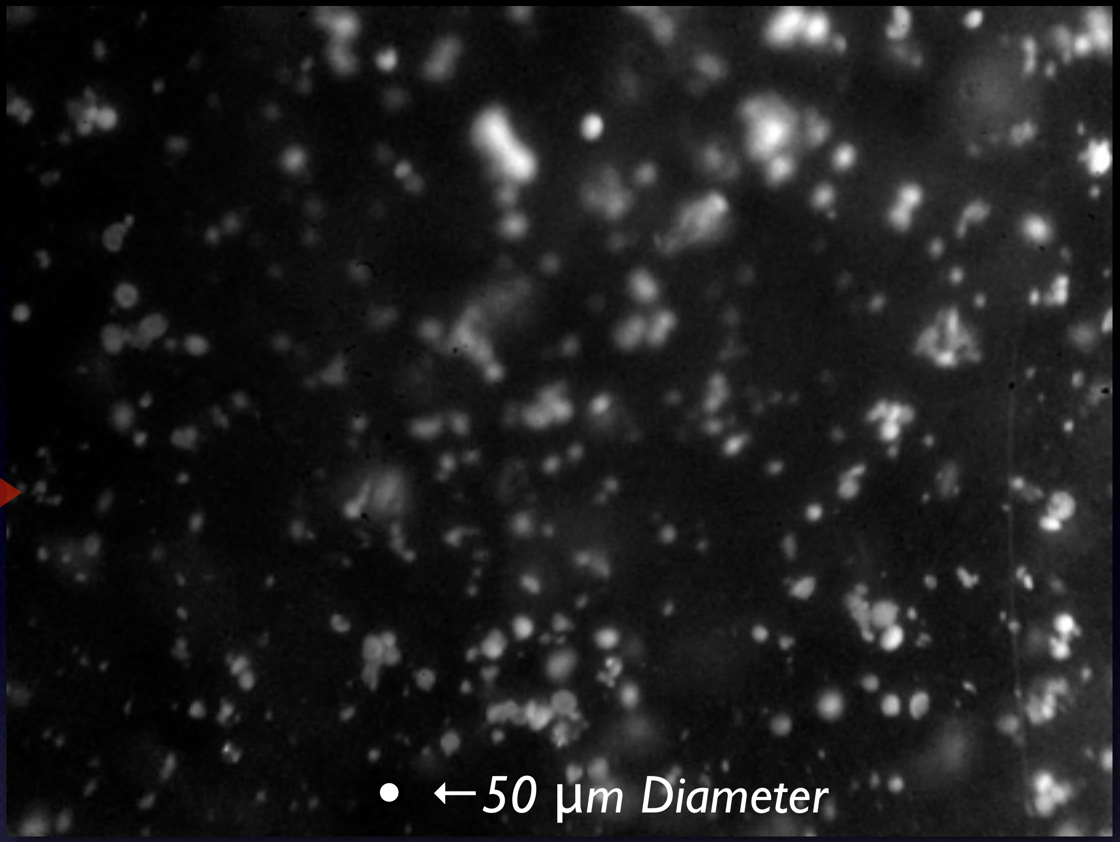

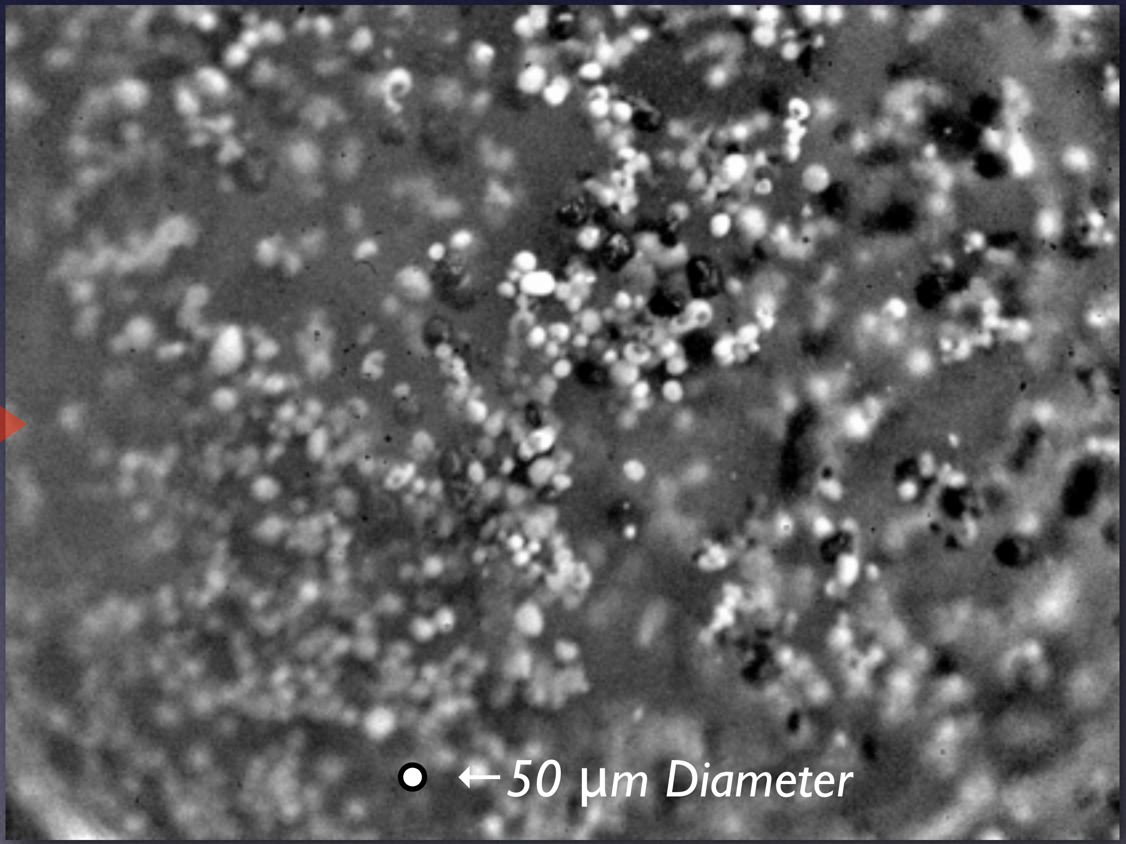

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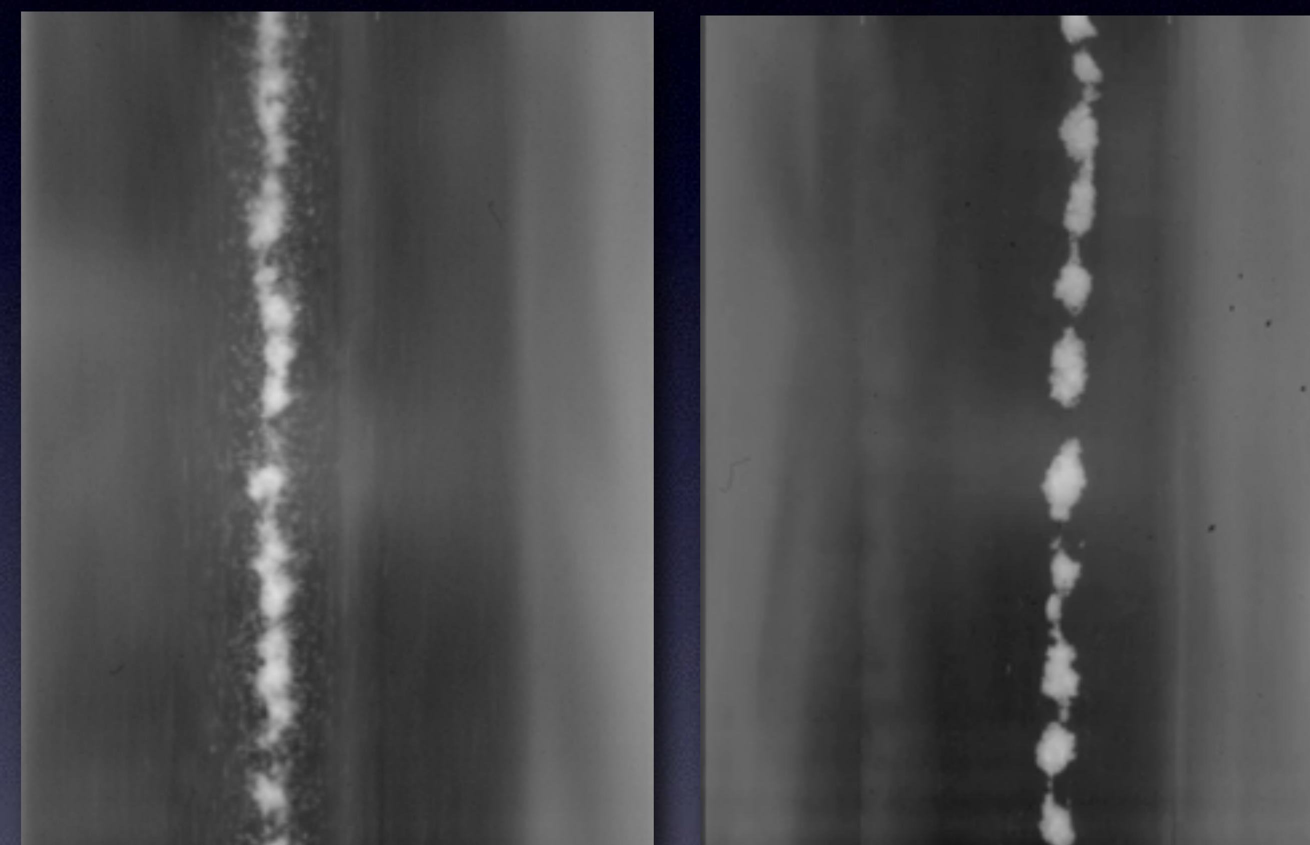
Powder Drop Experiment

- Particle clustering may not be due to hydrodynamic effects
- All commercial CFD codes for granular-fluid systems capture only hydrodynamic effects
  - Cohesive effects are ignored
    - Electrostatics
    - Van der Waals
    - Boundary layer "wetting"



University of Chicago powder drop experiment with 100 micron glass beads

Royer, J.R., Evans, D.J., Oyarte, L., Guo, Q., Kapit, E., Möbius, M.E., Waitukaitis, S.R., Jaeger, H.M., H, Nature 459 (2009) 1110-1113.

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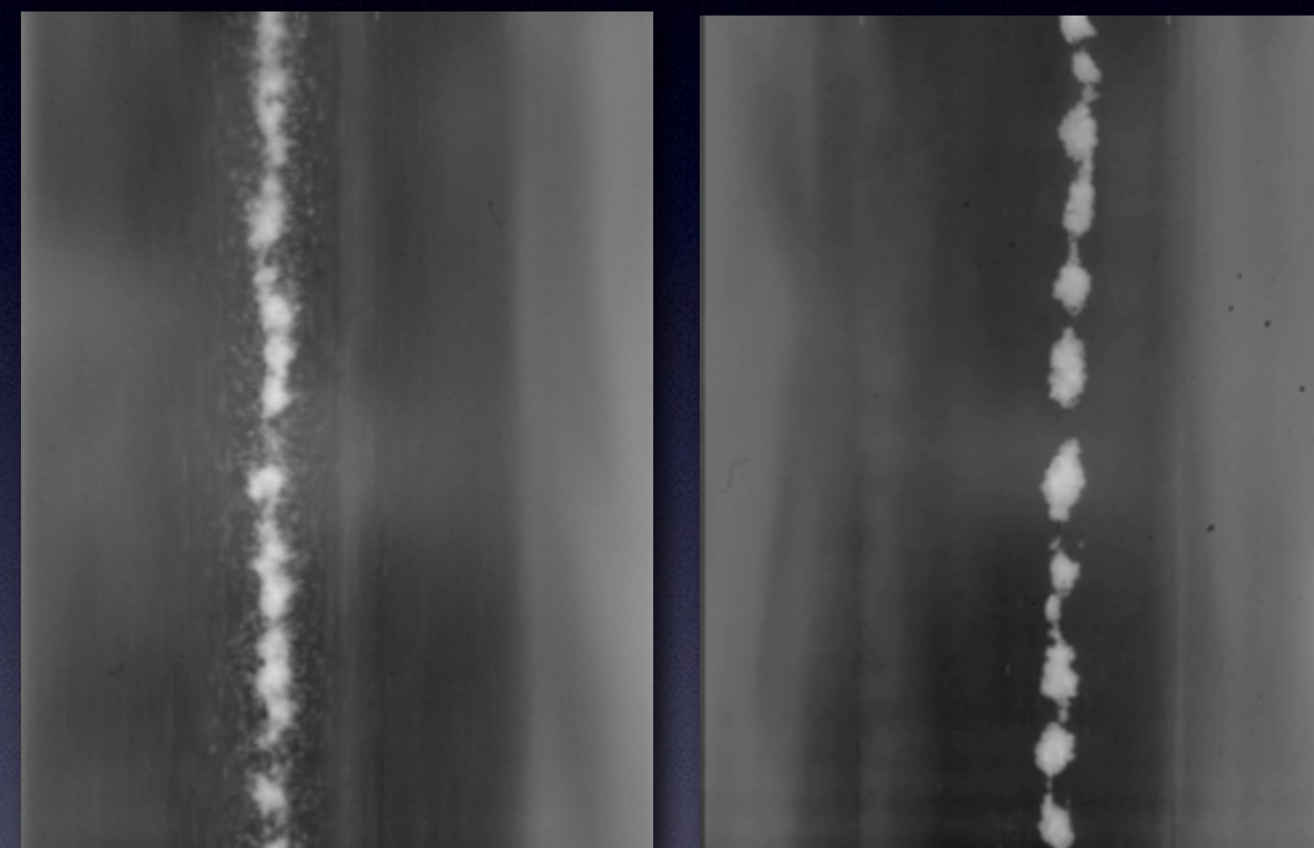

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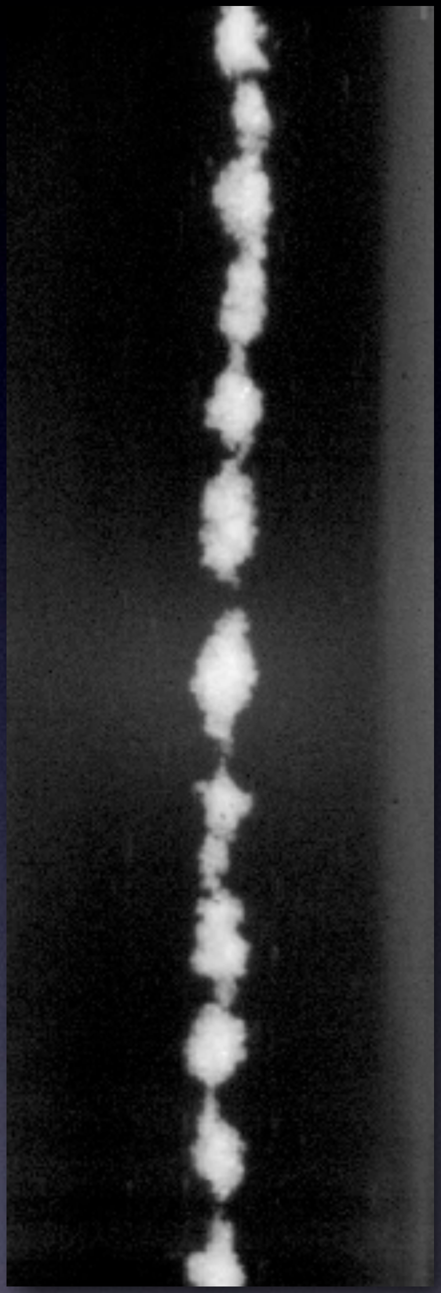
What are Holding These Clusters Together?

- Glass beads (d_{p50} = 107 μm) vs. copper powder (d_{p50} = 130 μm)
- Both performed below 1 torr
- Glass beads clustered together were the copper powder did not

Glass Beads



Copper Powder

No Change in Electrical Field

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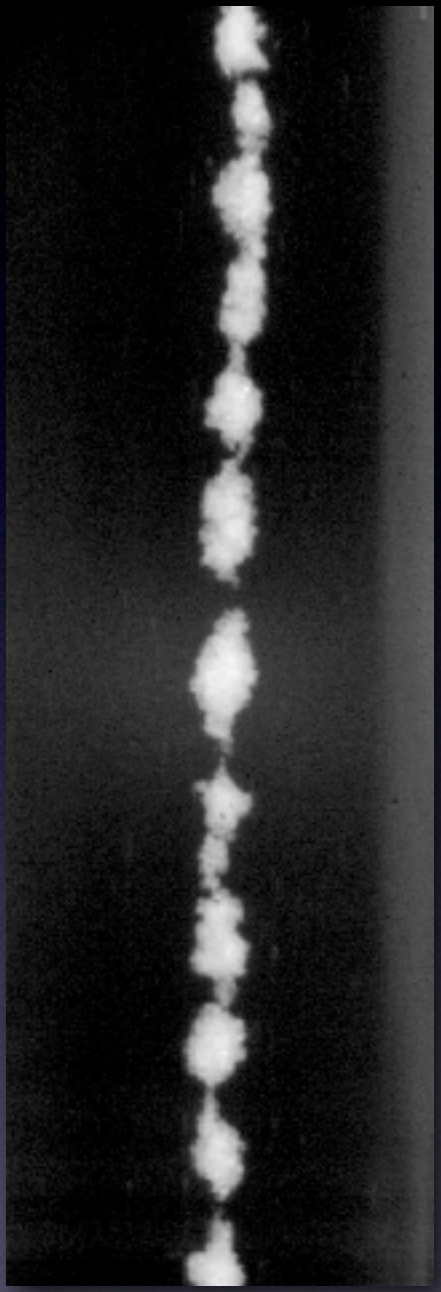
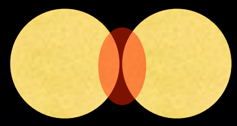


Copper Powder

No Change in Electrical Field

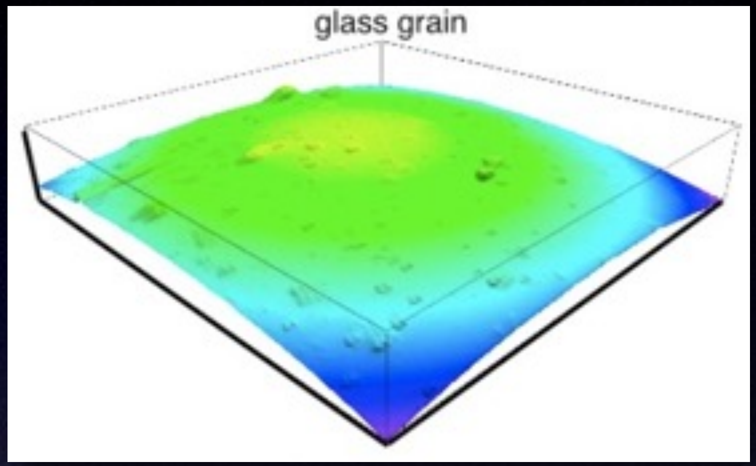
Surface Roughness and Cohesive Forces

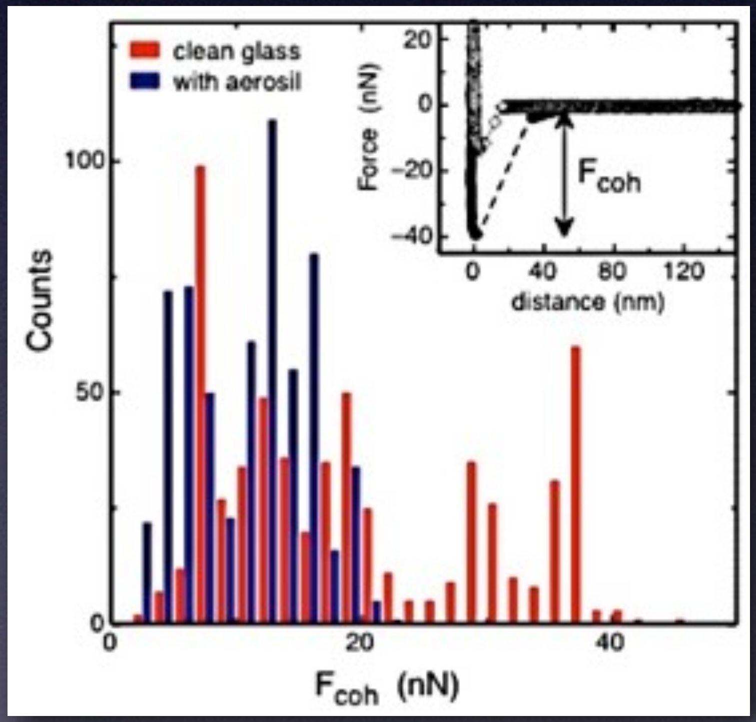
- Copper has 3.5 times more cohesive forces between two particles than the glass beads
- Surface protrusions from rough surfaces appear not to be inhibiting cohesive forces
- Oil did make the copper particles cluster



Strong Cohesive Force

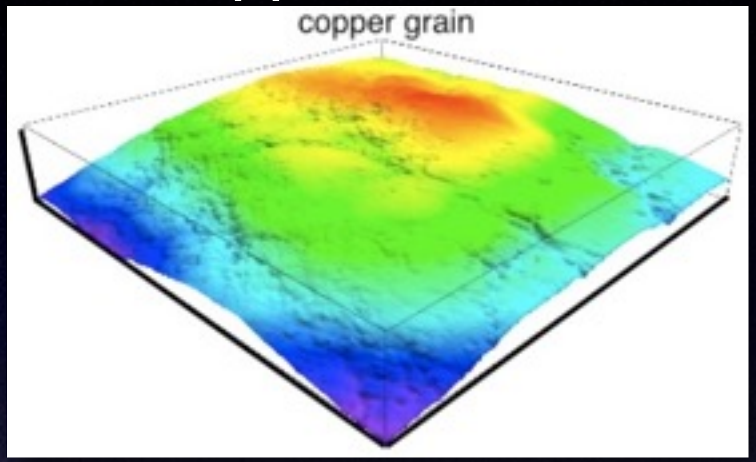
Glass Beads

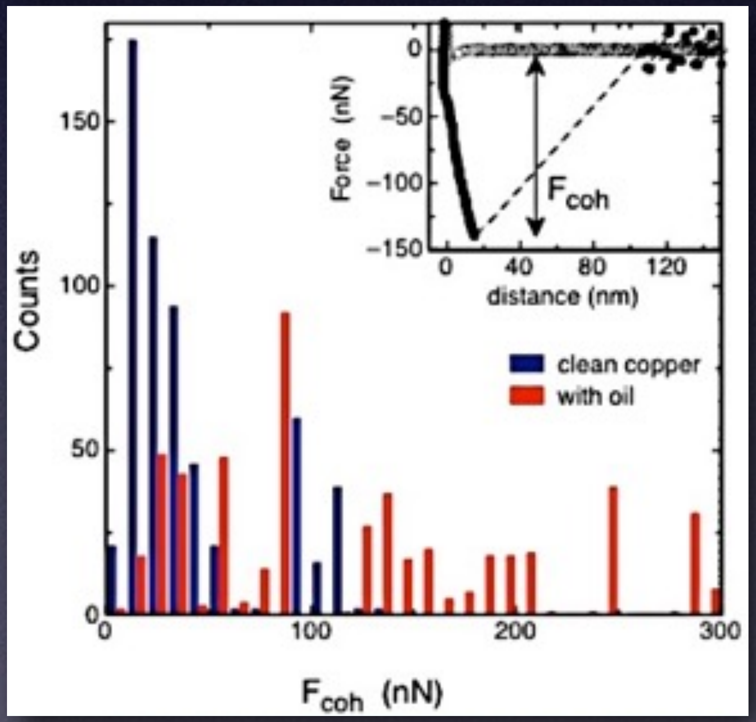




Weak Cohesive Force

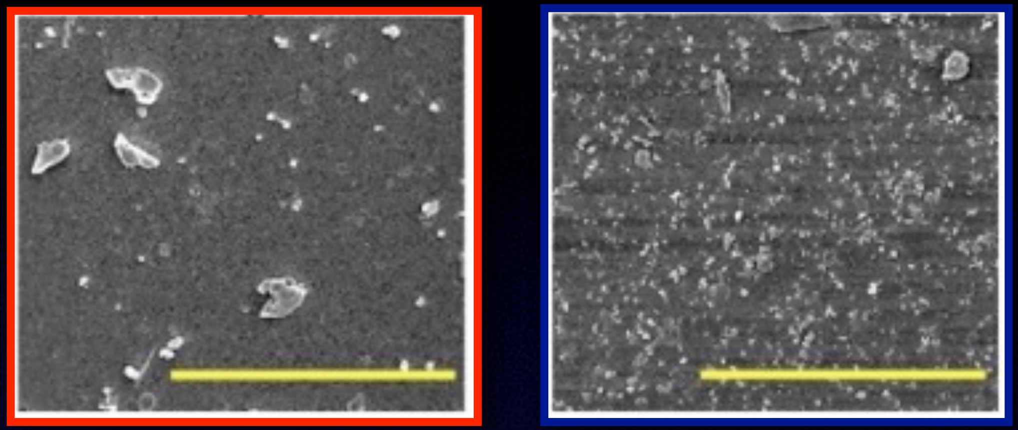
Copper Powder





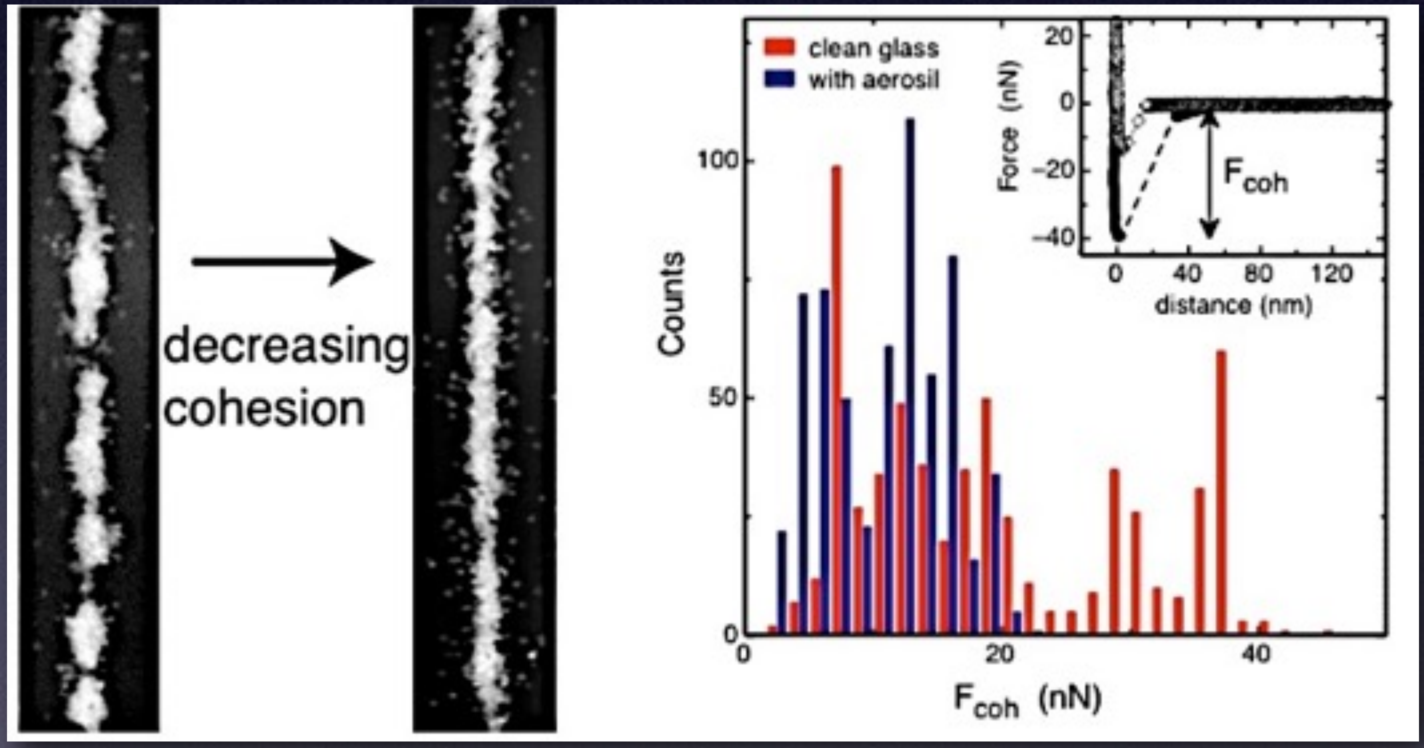
AFM Results from University of Chicago

What are Holding These Clusters Together?



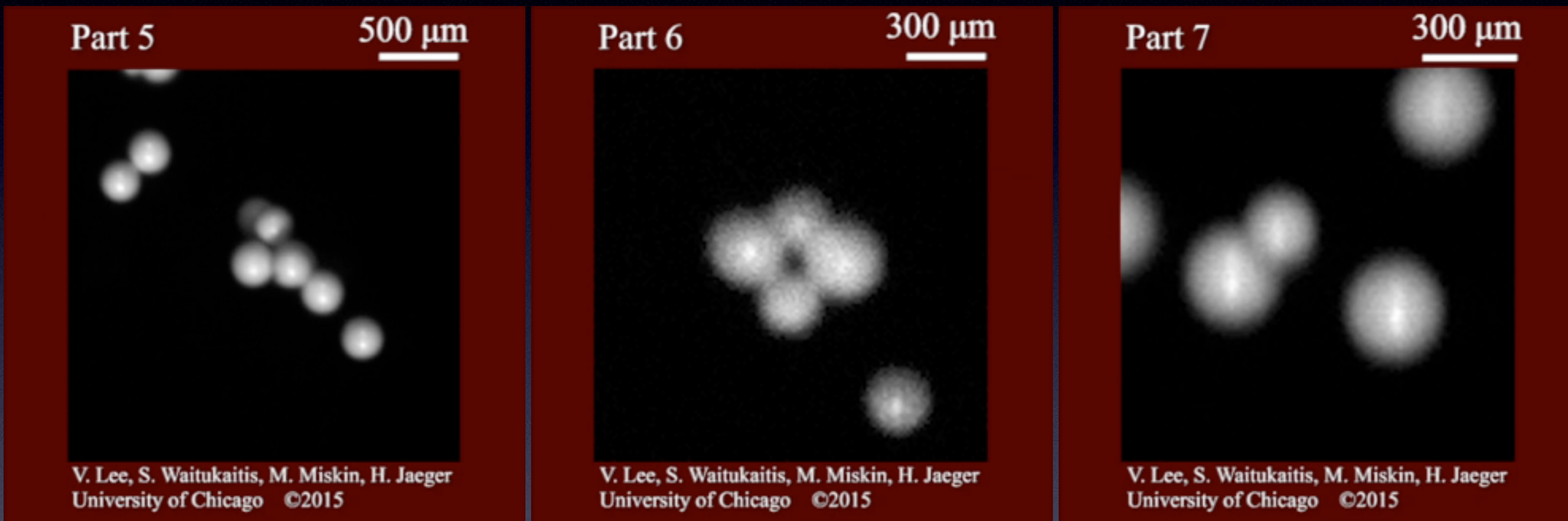
Glass Beads with and without Aerosil

- Relatively smooth surface appear to result in high cohesion
- Aerosil addition reduced cohesion
- Could this be a surface roughness factor?
- Rough surfaces results in less cohesive forces?



AFM Results from University of Chicago

Particle Clustering During Free Fall



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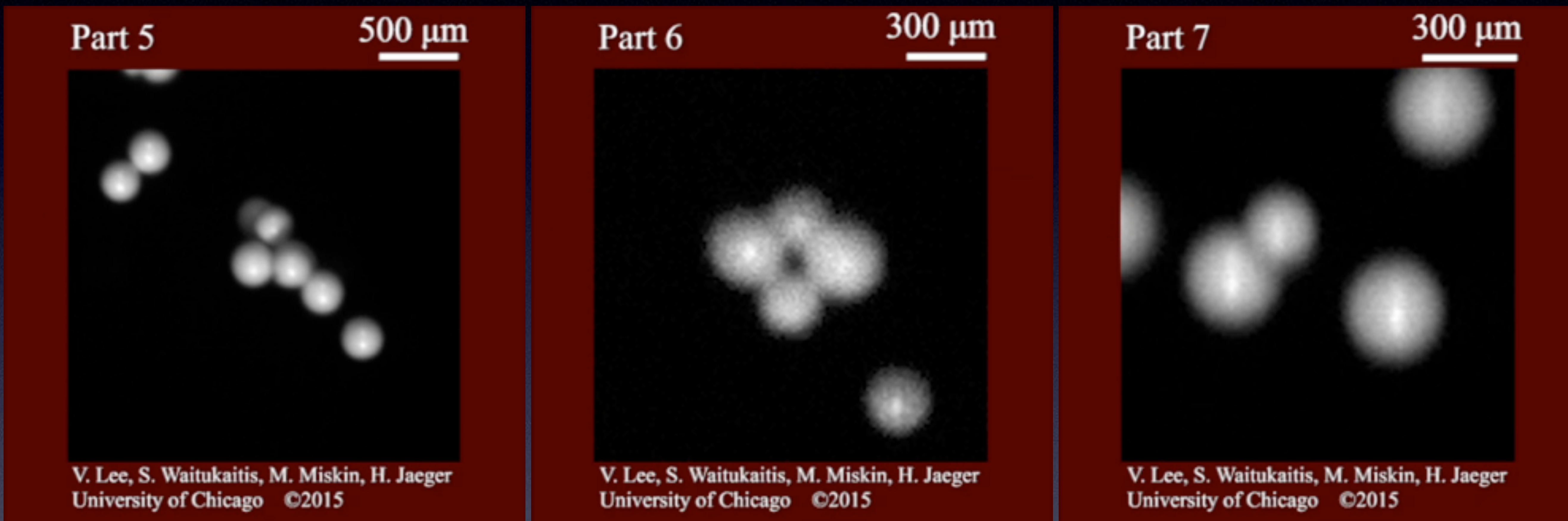

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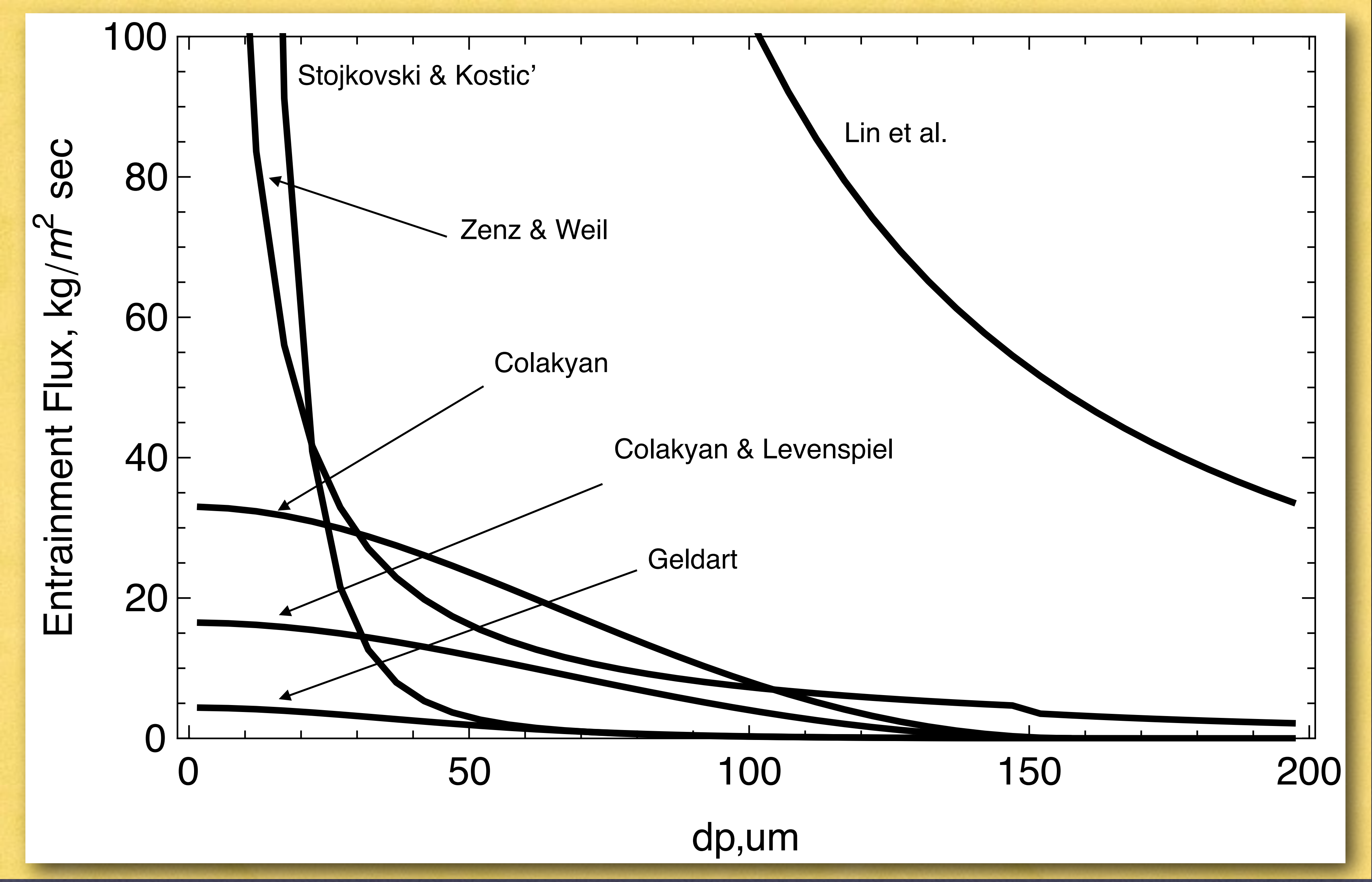
Entrainment

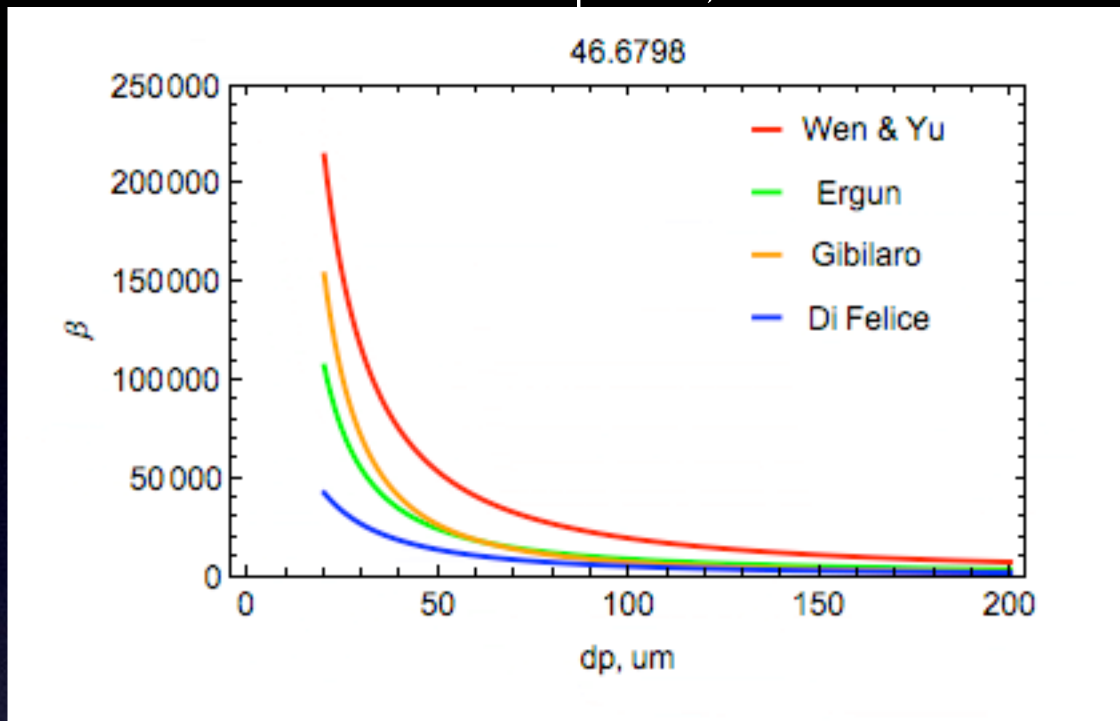


Entrainment rate calculations based on FCC catalyst powder with 9% fines in a 3-meters ID x 12-meters tall fluidized bed with a bed height of 6 meters and superficial gas velocity of 1 m/sec at room temperature

Stojkovski, V., Kostic', Z., Thermal Science, 7 (2003) 43-58.
Zenz, P.A., Weil, N.A., AIChE J., 4 (1958) 472-479.
Lin, L, Sears, J.T., Wen, C.Y., Powder Technology, 27 (1980) 105-115.
M. Colakyan, N. Catipovic, G. Jovanovic, T.J. Fitzgerald, AIChE Symp. Ser. 77 (1981) 66.
Colakyan, M., Levenspiel, O., Powder Technology, 38 (1984), pp. 223-232
Geldart, D., Cullinan, J., Georghiades, S., Gilvray, D., Pope, D.J., Trans. Inst. Chem. Eng., 57 (1979) 269-277.

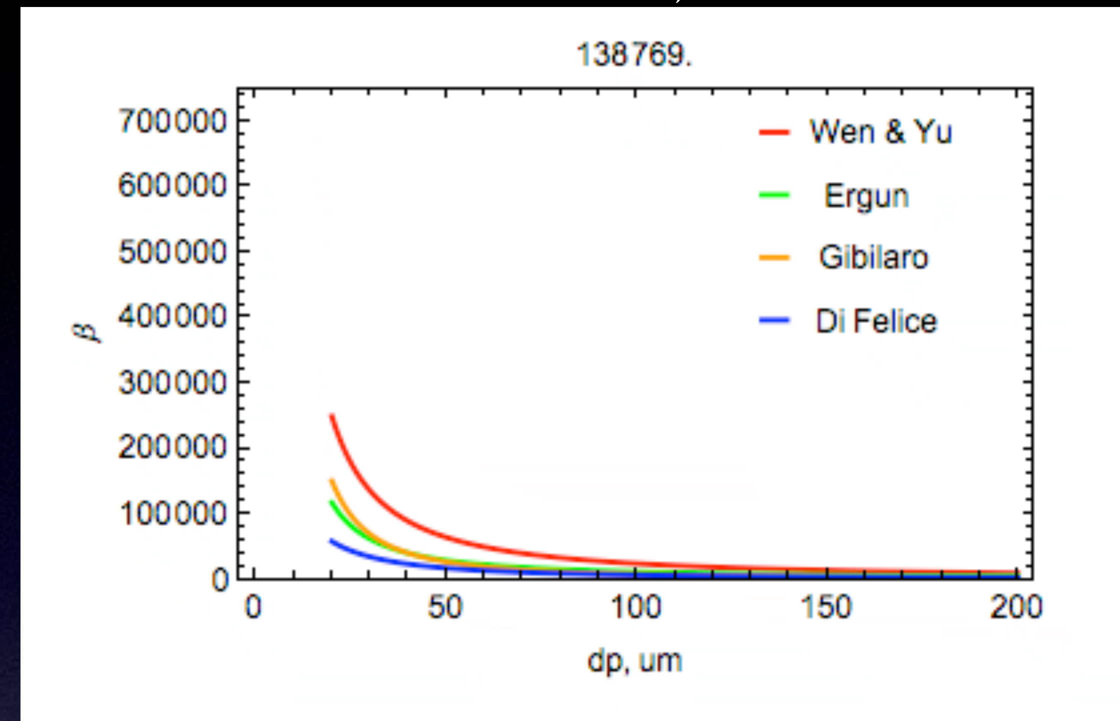
Factors Affecting Drag

Temperature, °C



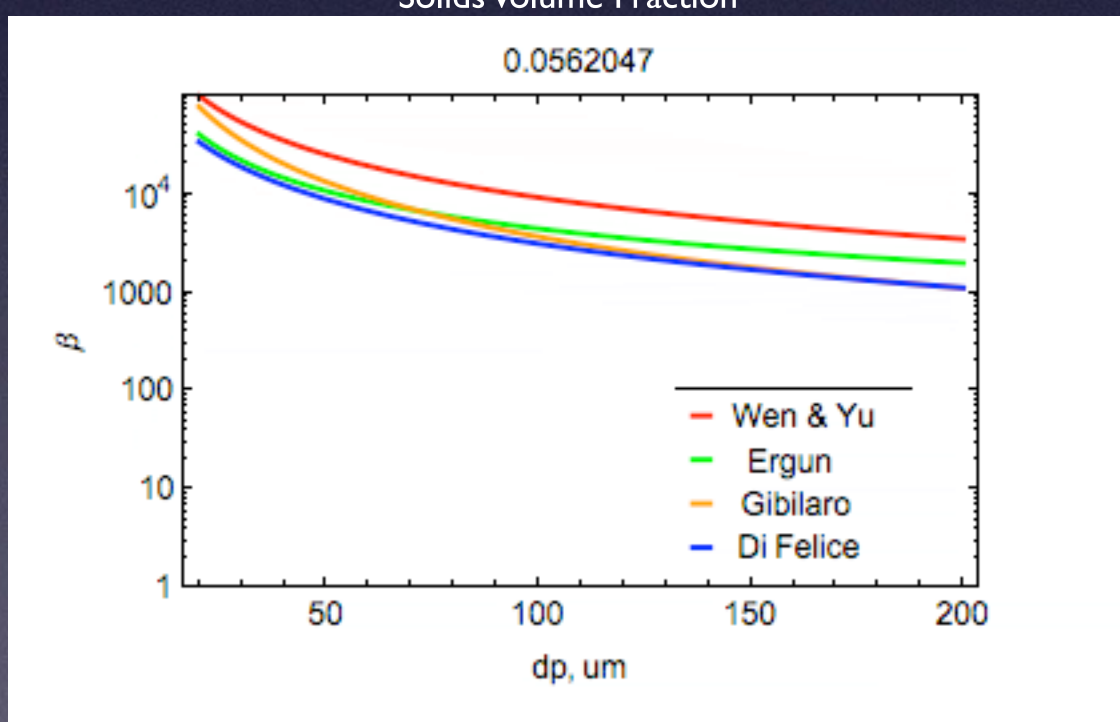
Not all correlations predict the same trend with temperature

Pressure, Pa



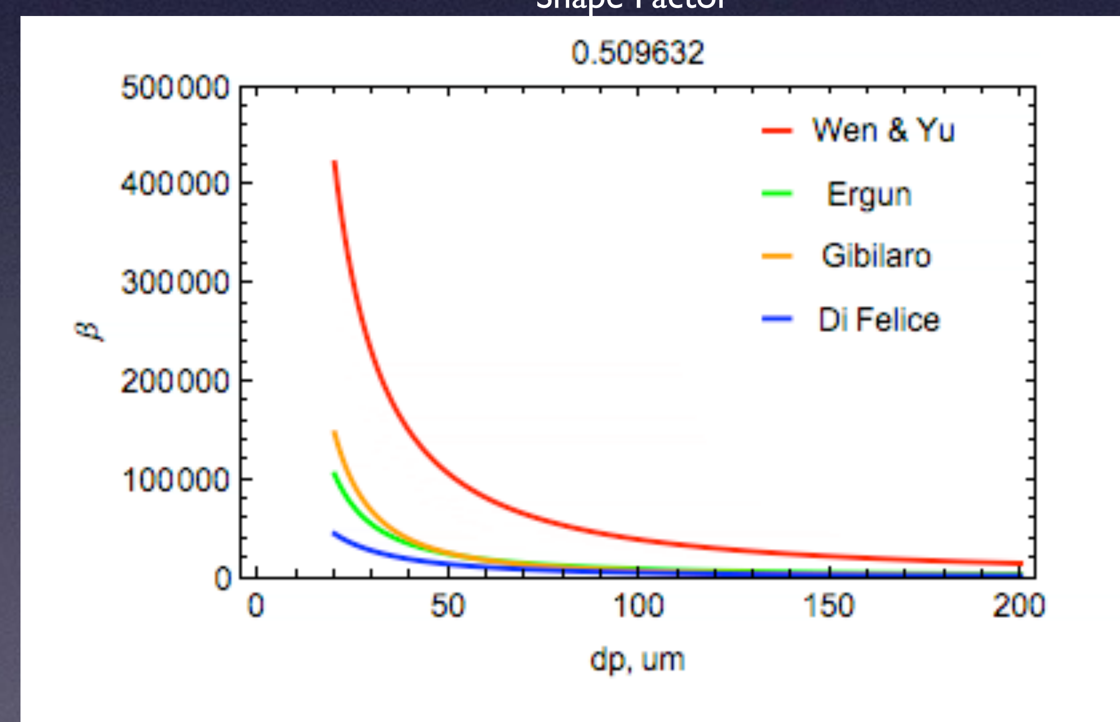
High pressures result in greater drag due to higher gas density

Solids Volume Fraction



All correlations are highly sensitive to solids volume fraction

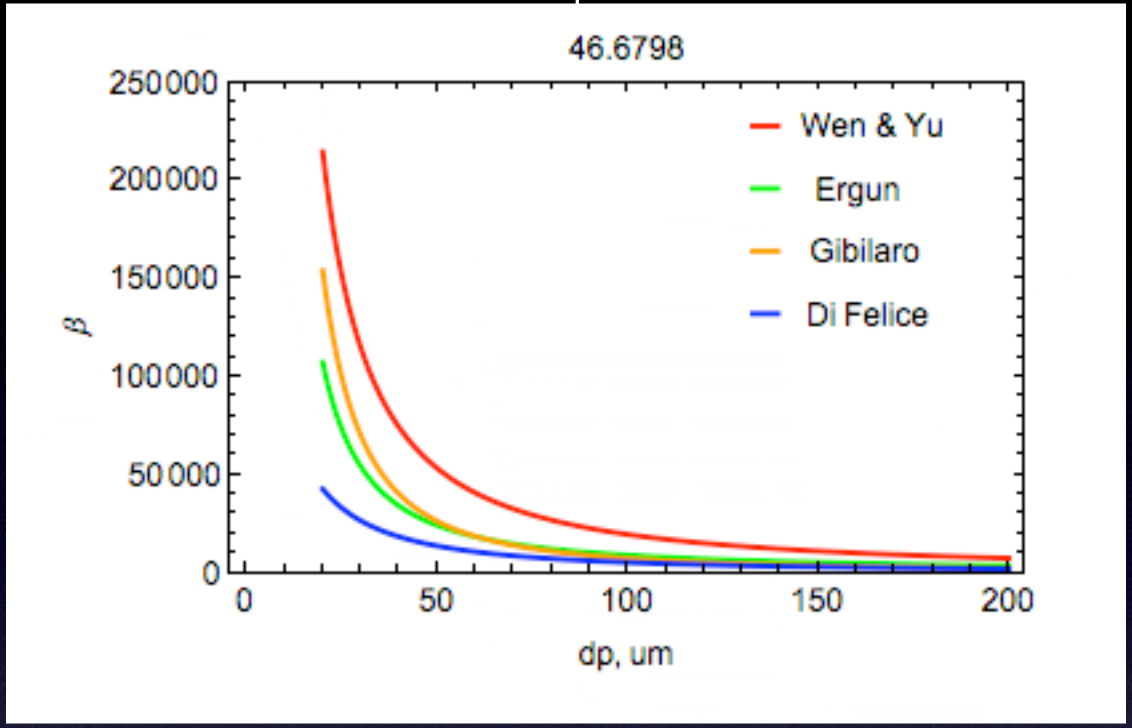
Shape Factor



The less spherical the particles, the greater the drag

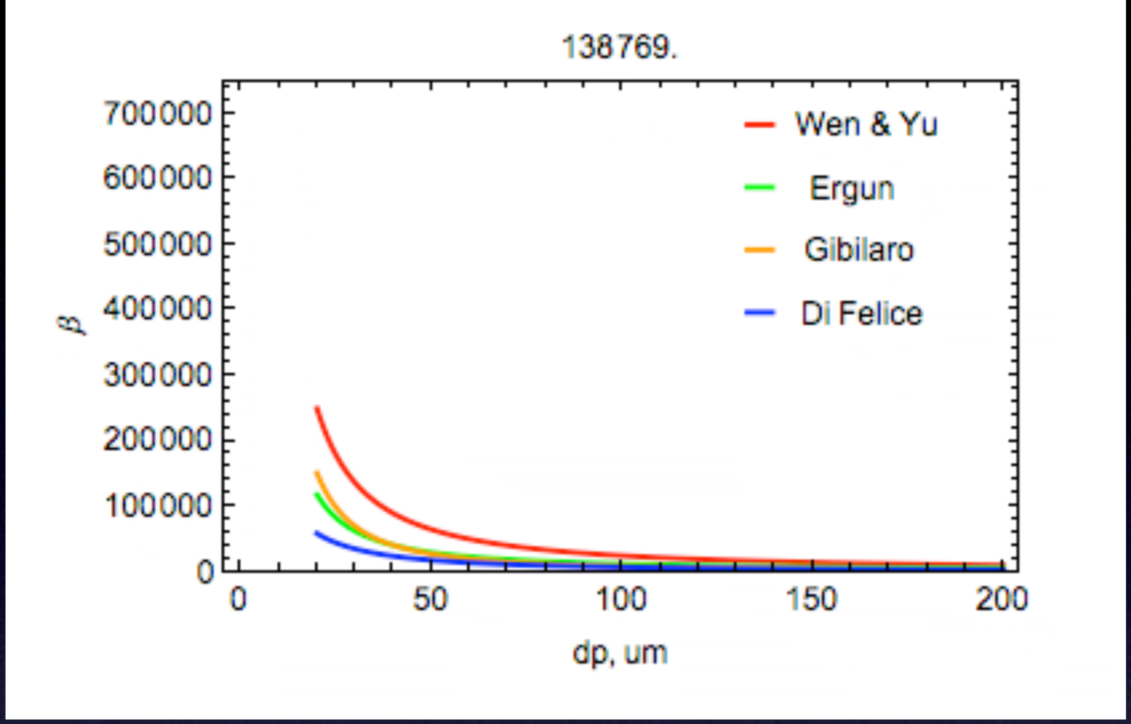
Factors Affecting Drag

Temperature, °C



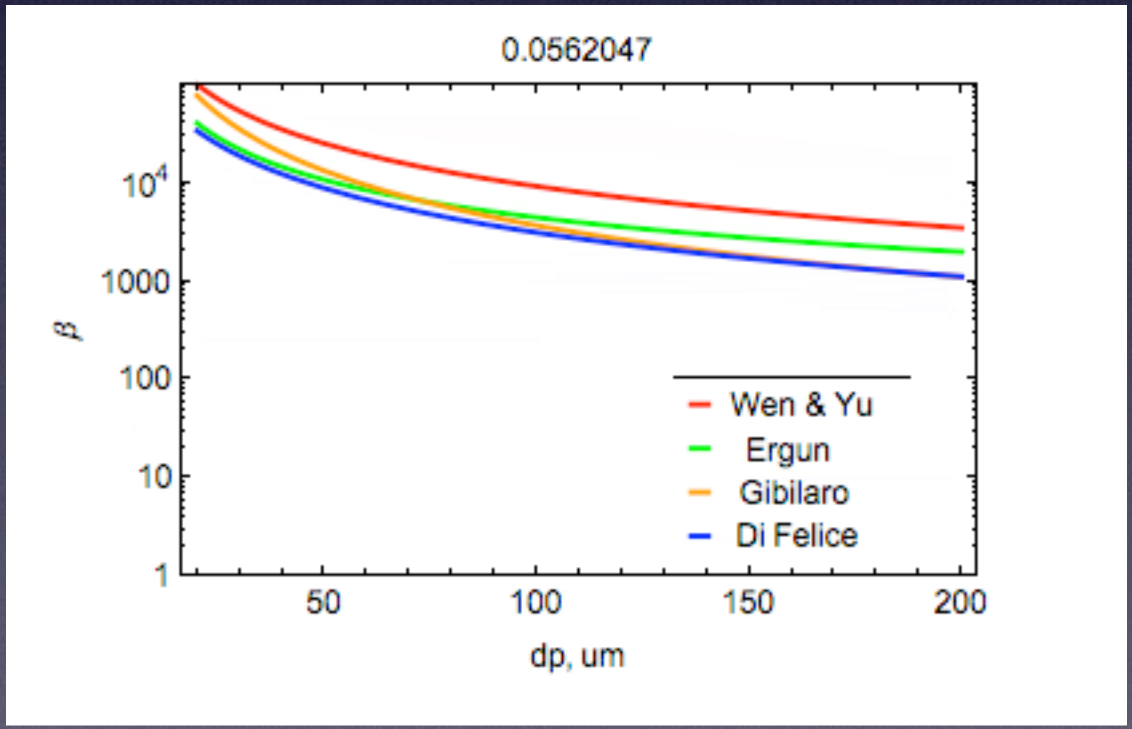
Not all correlations predict the same trend with temperature

Pressure, Pa



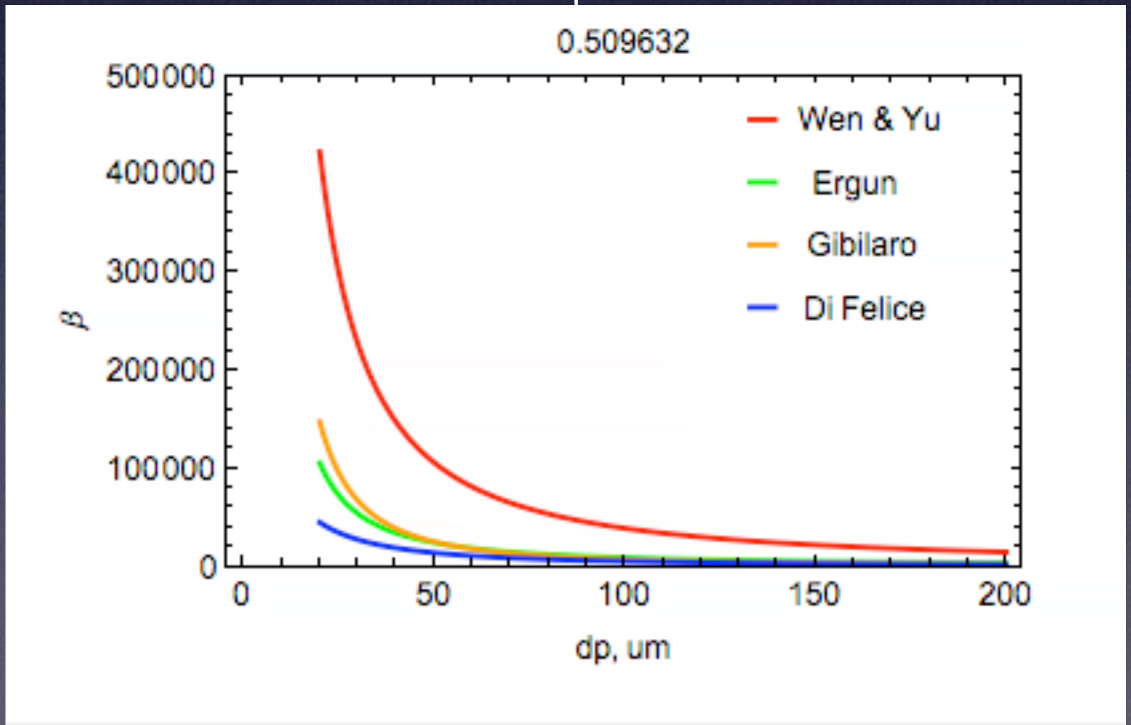
High pressures result in greater drag due to higher gas density

Solids Volume Fraction



All correlations are highly sensitive to solids volume fraction

Shape Factor



The less spherical the particles, the greater the drag

Micro-Scale Data Analysis Limited

- Particle-particle and/or particle/monolayer interactions are complex
  - Modeling, even physics, not readily available
- Process modeling needs to use
  - Sub-grid models for what we don't understand
    - Large scale validation for model development

The Multi-scale Validation Paradox

Fundamentals	Model Fitting	Model Development
Micro-scale	*Meso-scale*	*Macro-scale*
1 to 100's Particles	Millions to Billions of Particles	Trillions of Particles
10^{-6} to 10^{-4} m	10^{-2} to 10^{-1} m	10^{-1} to 10^{2} m
Experiments are cheap	Experiments are inexpensive	Experiments are expensive
Simulations are cheap	Simulations are cheap	Simulations are expensive
Analysis are expensive	Analysis are inexpensive	Analysis are cheap

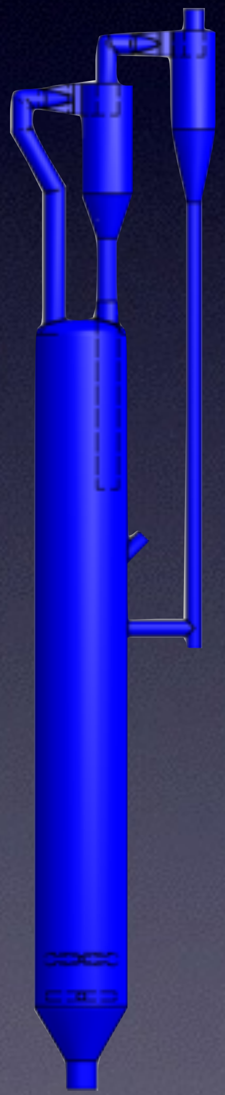
PSRI/NETL Challenge Problem

Circulating Fluidized Bed

- NETL's 12-in (30-cm) ID x 52-ft (16-m) tall CFB
- Geldart Group A and B material
- Gas jet in riser

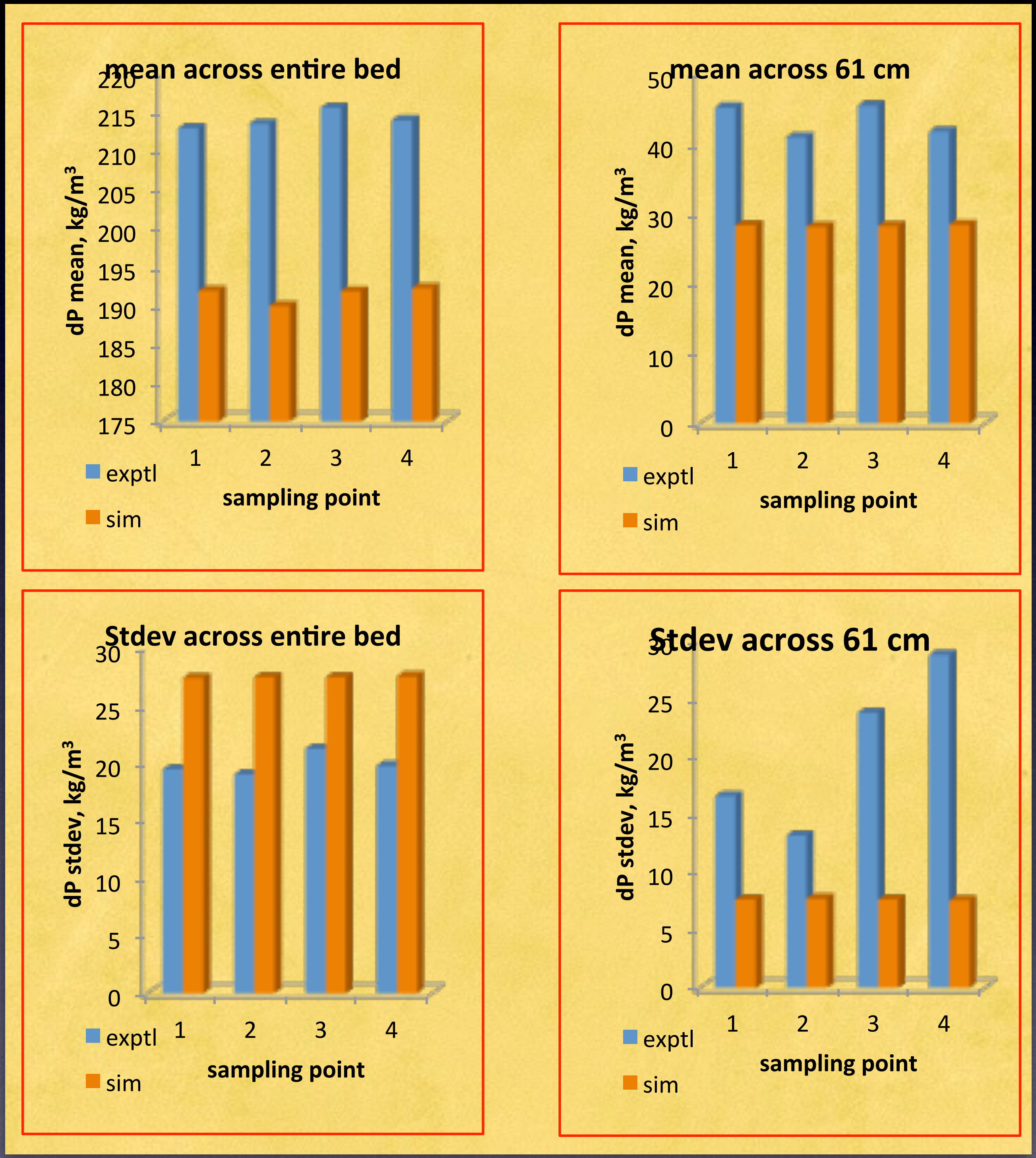
Bubbling Fluidized Bed

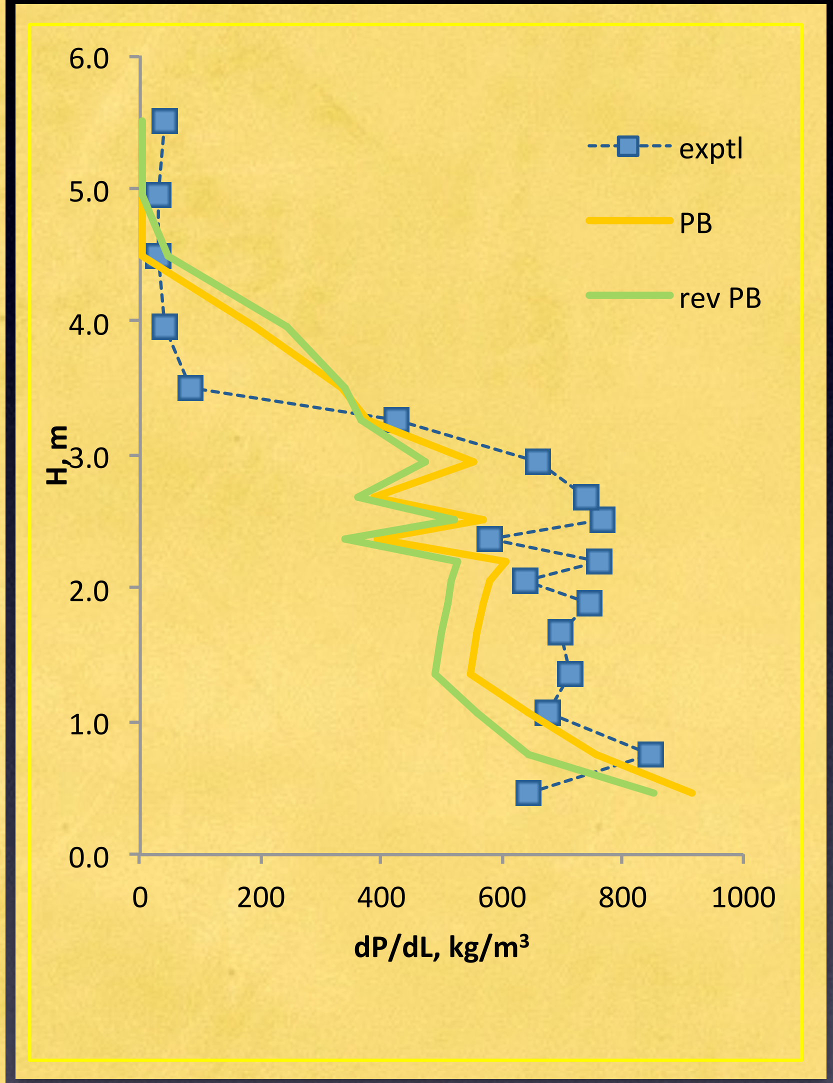
- PSRI's 3-ft (92-cm) ID x 20-ft (6-m) tall BFB
- FCC Powder with different fines levels
- 3% and 12% fines
- Gas bypassing present in low fines case



BFB Modeling Results: Modeler BFB1

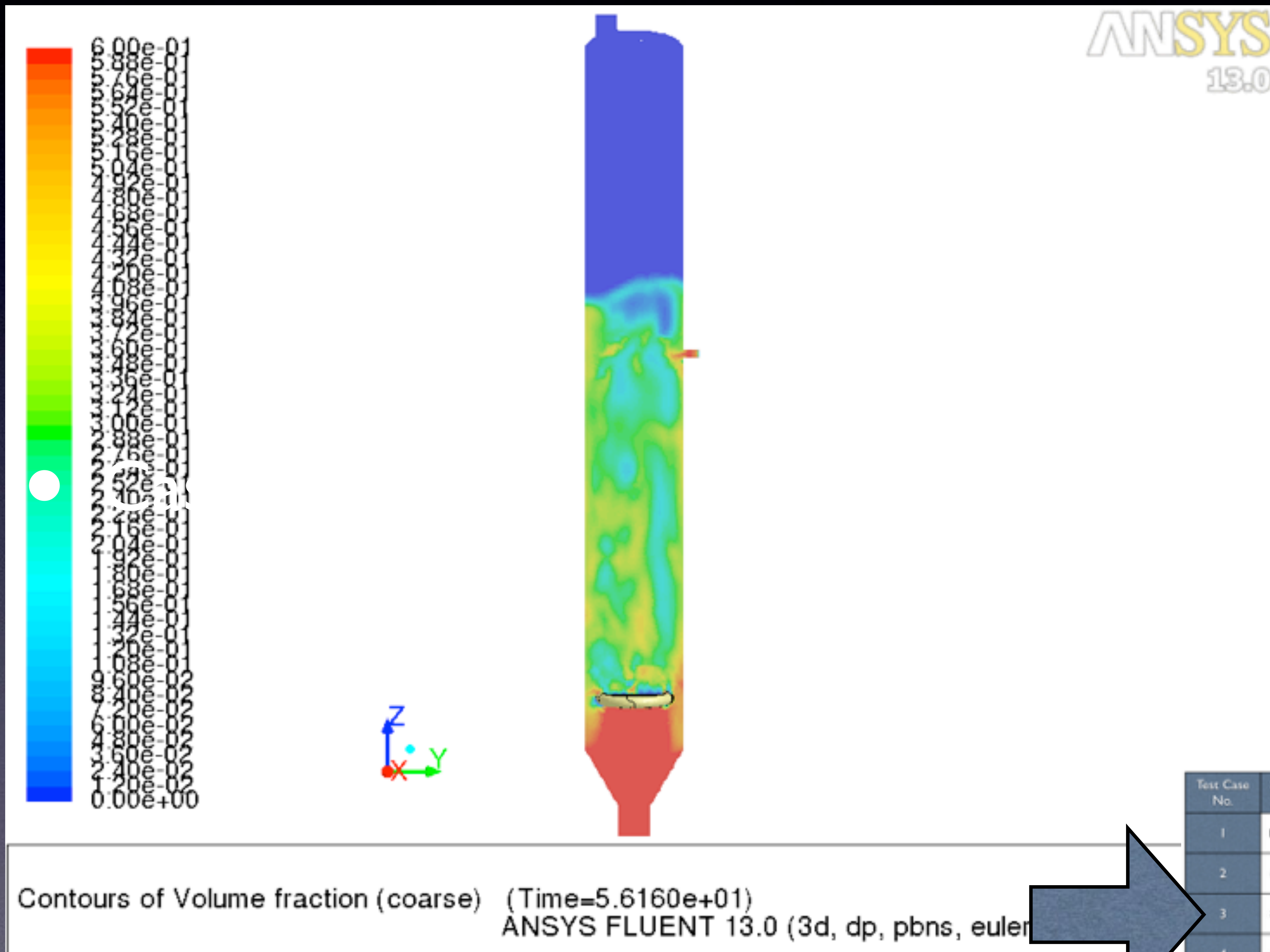
with PB for PSD





BFB Modeling Results: Modeler BFB1

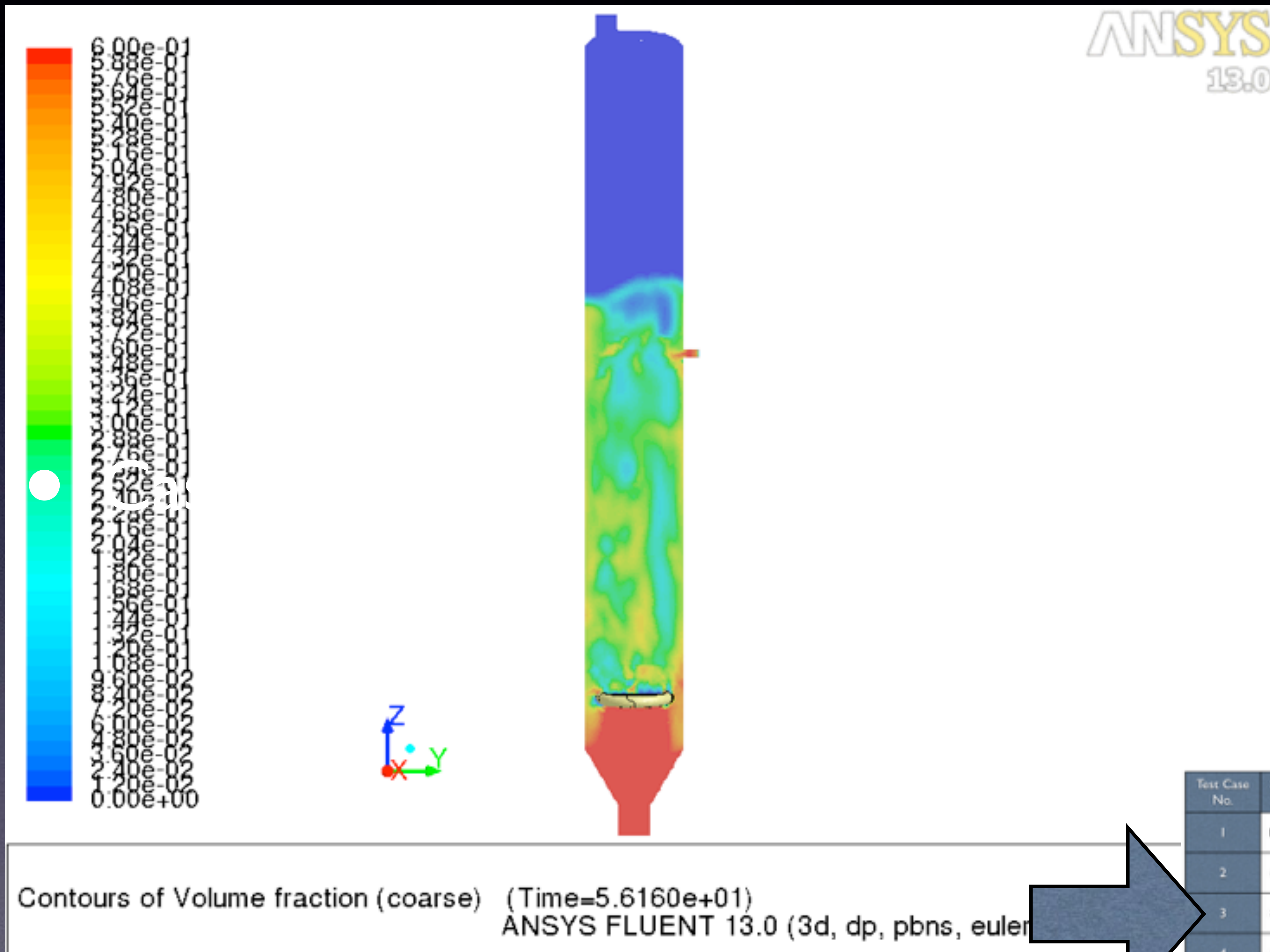
with PB for PSD



Test Case No.	Static Bed Height	FCC Fines Content	Superficial Gas Velocity	Fluidization Behavior
1	12 ft (3.6 m)	3%	1 ft/sec (0.3 m/sec)	Gas Bypassing
2	4 ft (1.2 m)	3%	1 ft/sec (0.3 m/sec)	Uniform
3	8 ft (2.4 m)	3%	2 ft/sec (0.6 m/sec)	Gas Bypassing
4	8 ft (2.4 m)	12%	2 ft/sec (0.6 m/sec)	Uniform

BFB Modeling Results: Modeler BFB1

with PB for PSD



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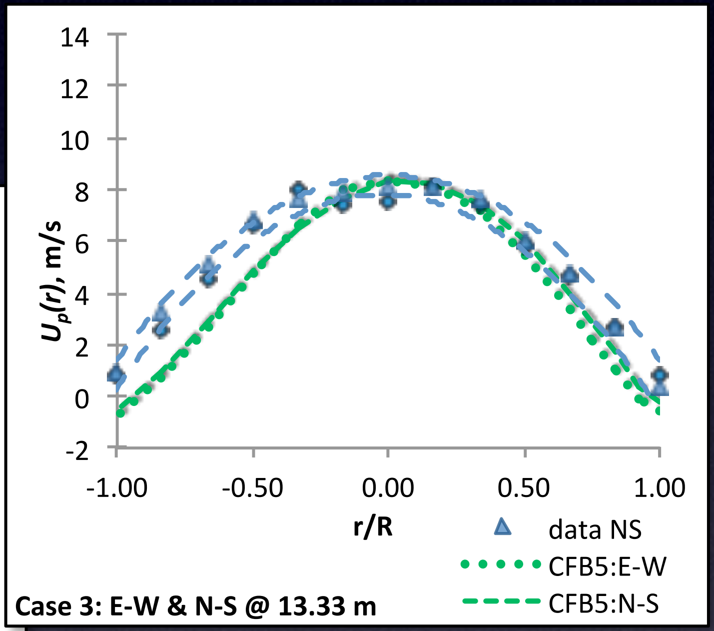
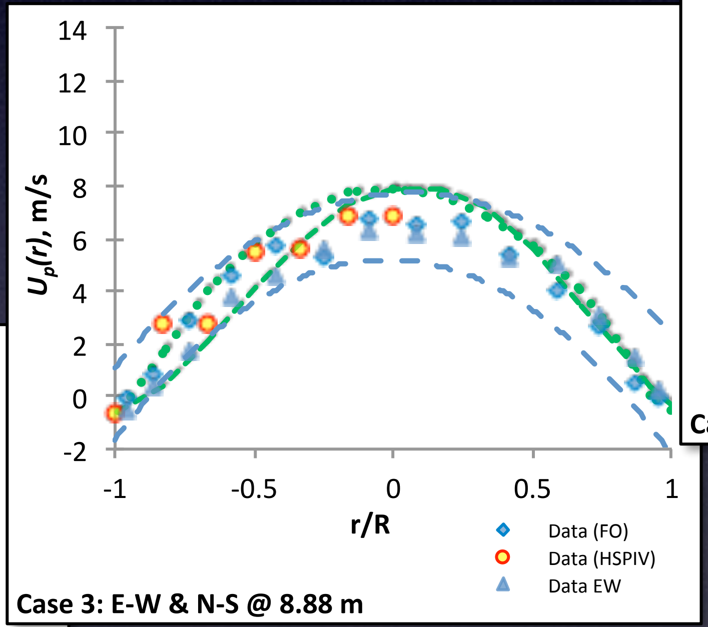
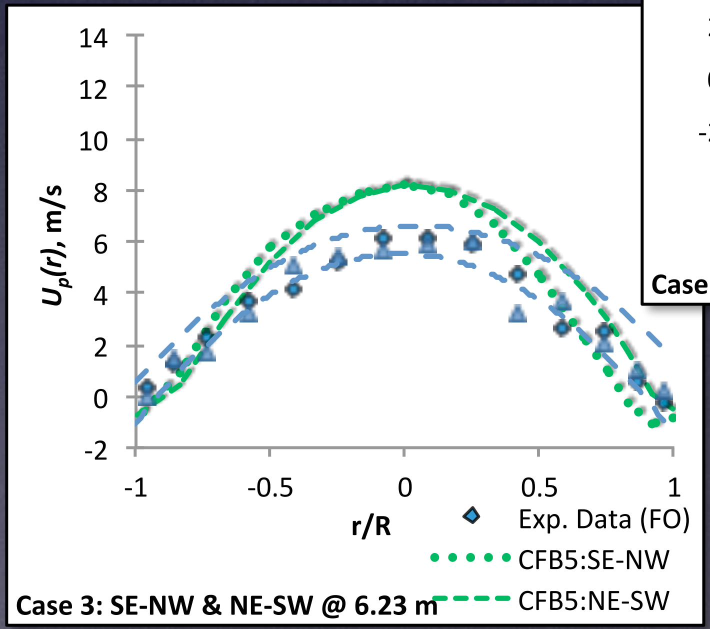
CFB Modeling Results: Modeler CFB5

Radial Profile: Case 3 $u_p(r)$ - HDPE

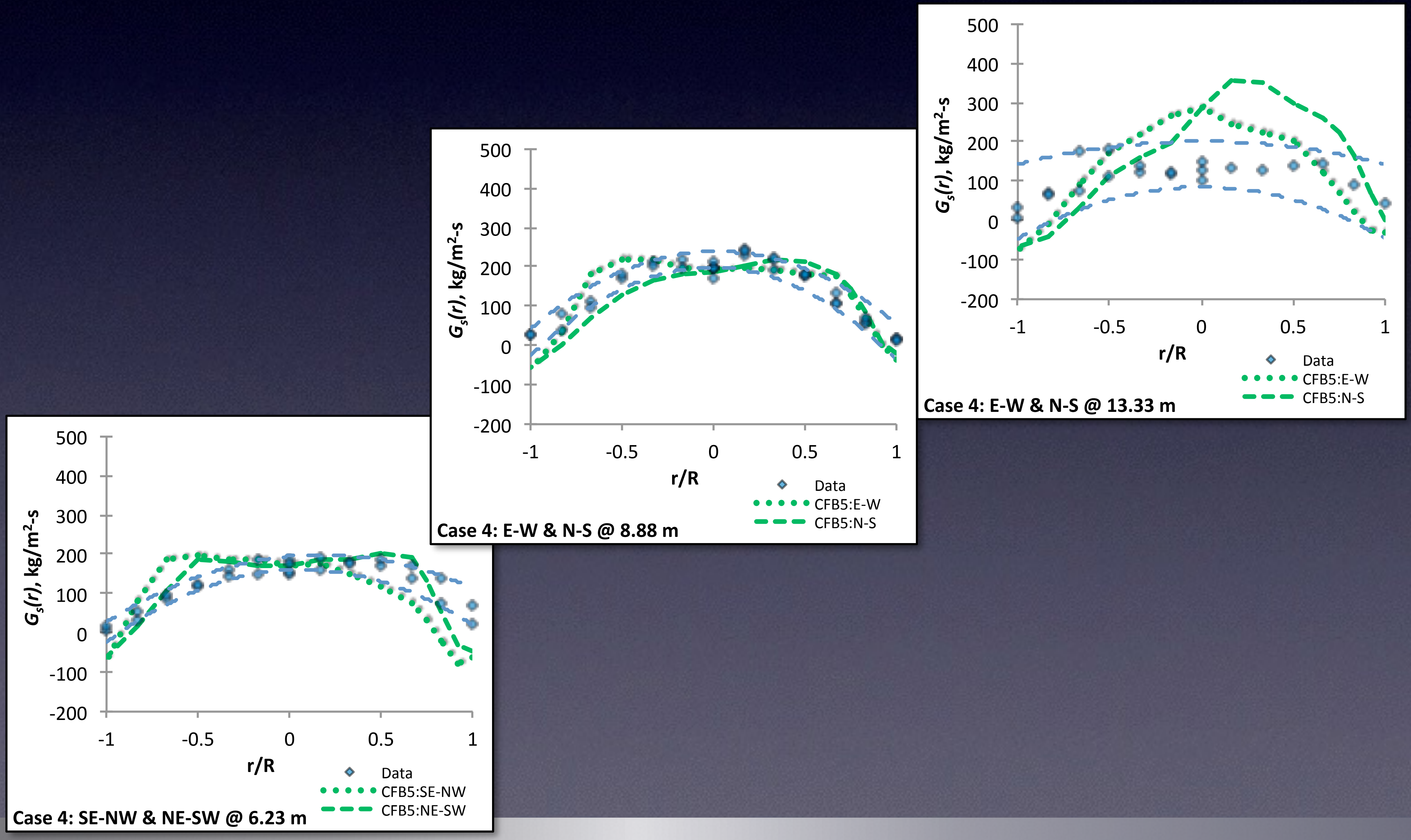






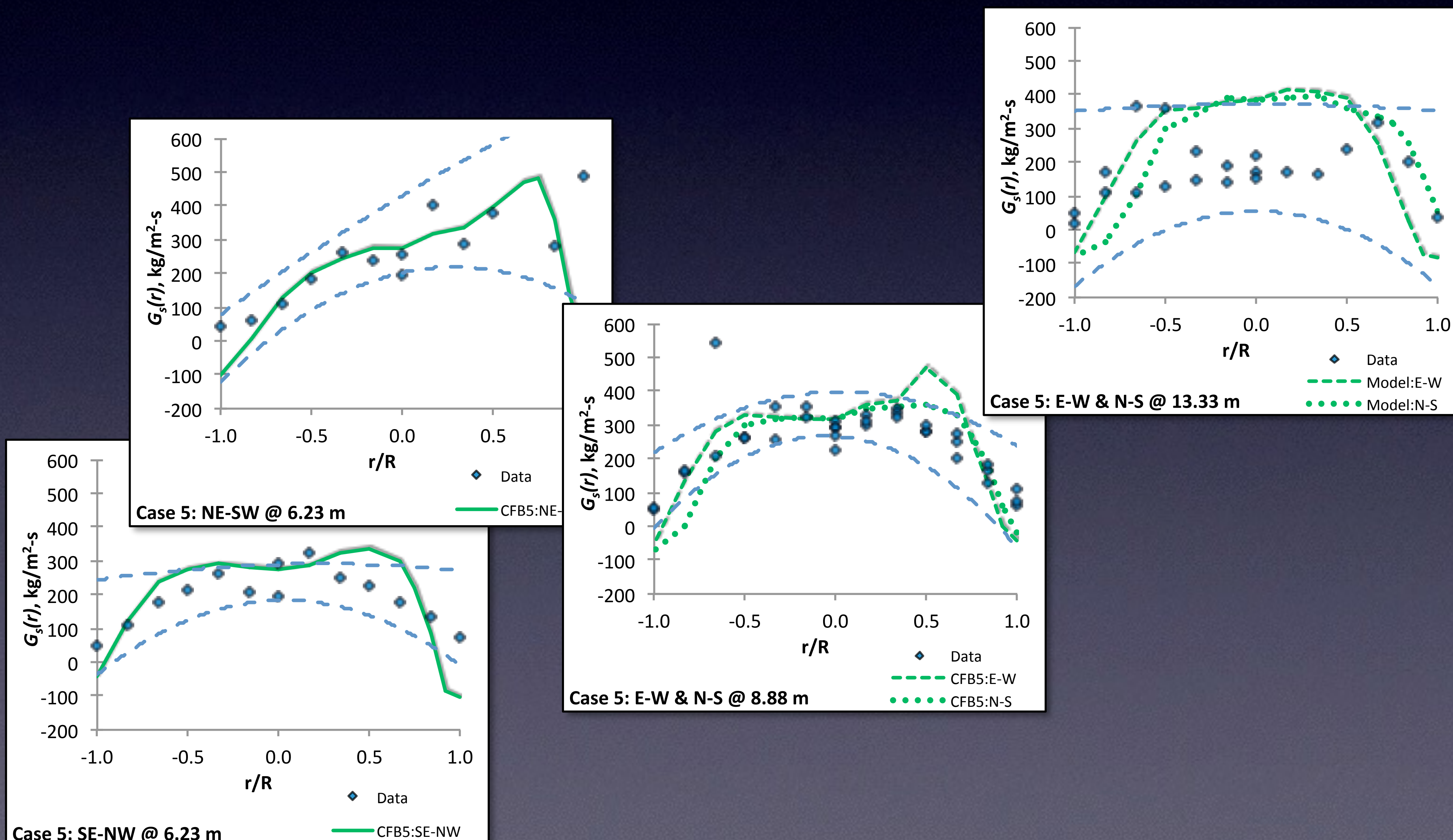
CFB Modeling Results: Modeler CFB5

Radial Profile: Case 4 $G_s(r)$ - HDPE



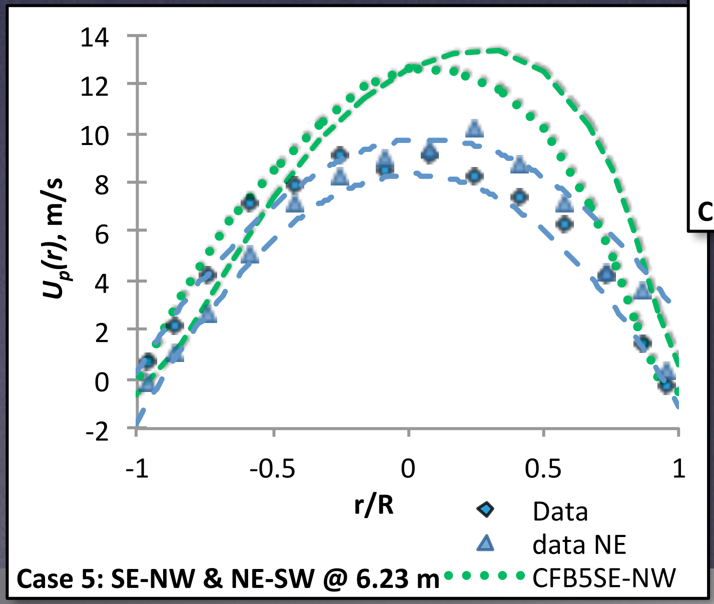
CFB Modeling Results: Modeler CFB5

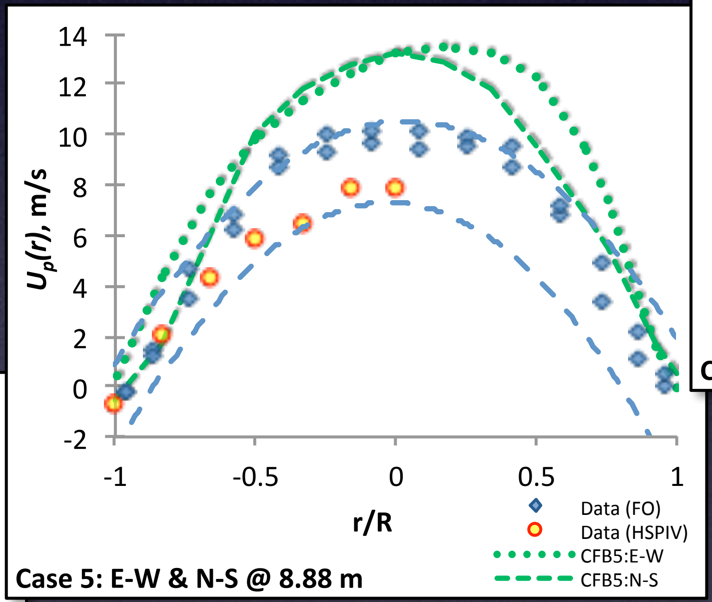
Radial Profile: Case 5 $G_s(r)$ - HDPE

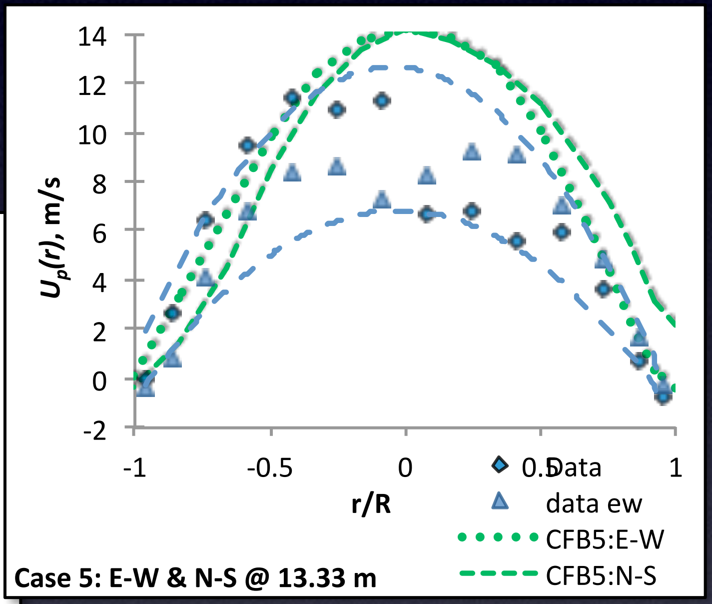


CFB Modeling Results: Modeler CFB5

Radial Profile: Case 5 $u_p(r)$ - HDPE





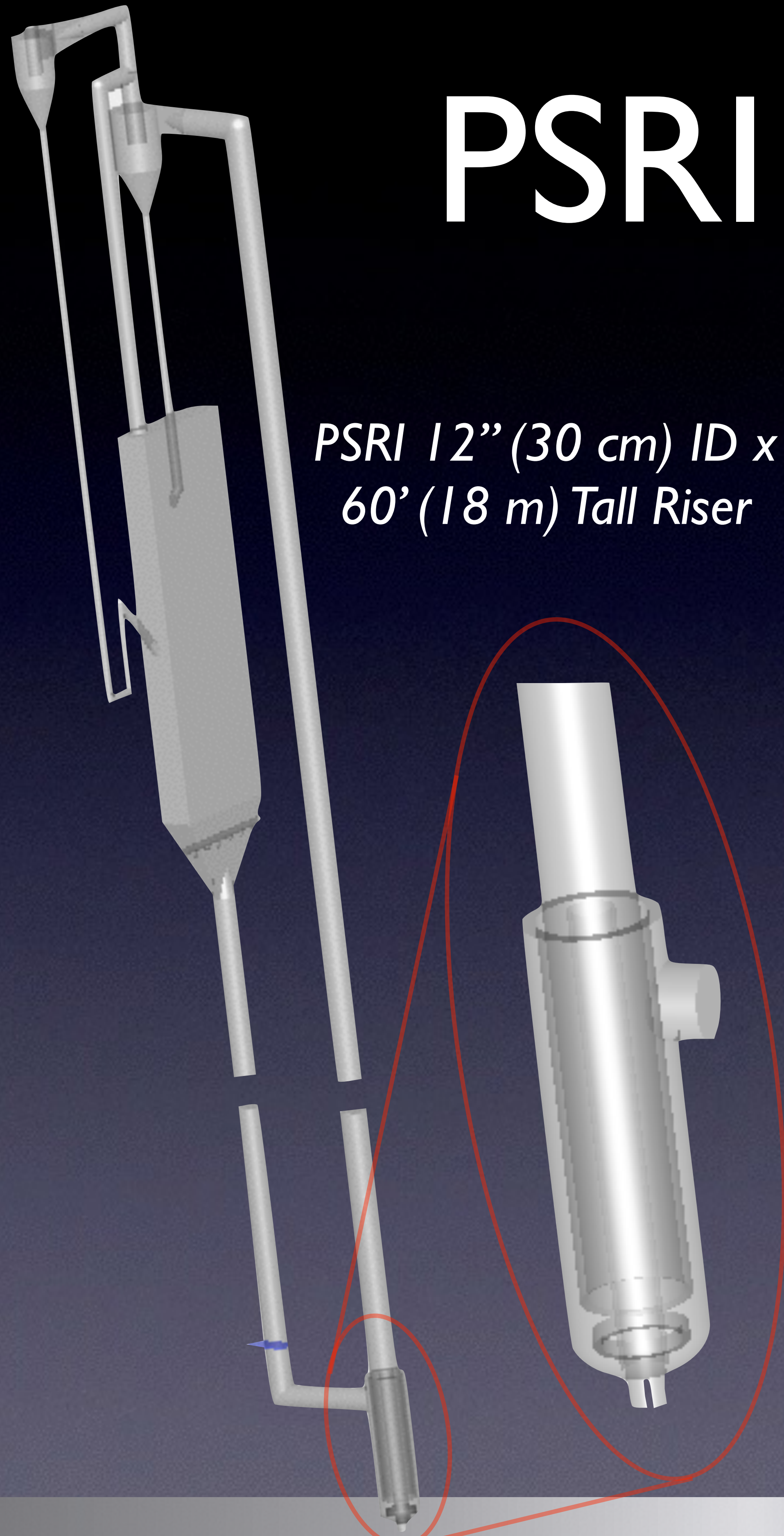


PSRI
Particulate Solid Research, Inc.

Applying the Fundamentals

PSRI Riser

PSRI 12" (30 cm) ID x 60' (18 m) Tall Riser

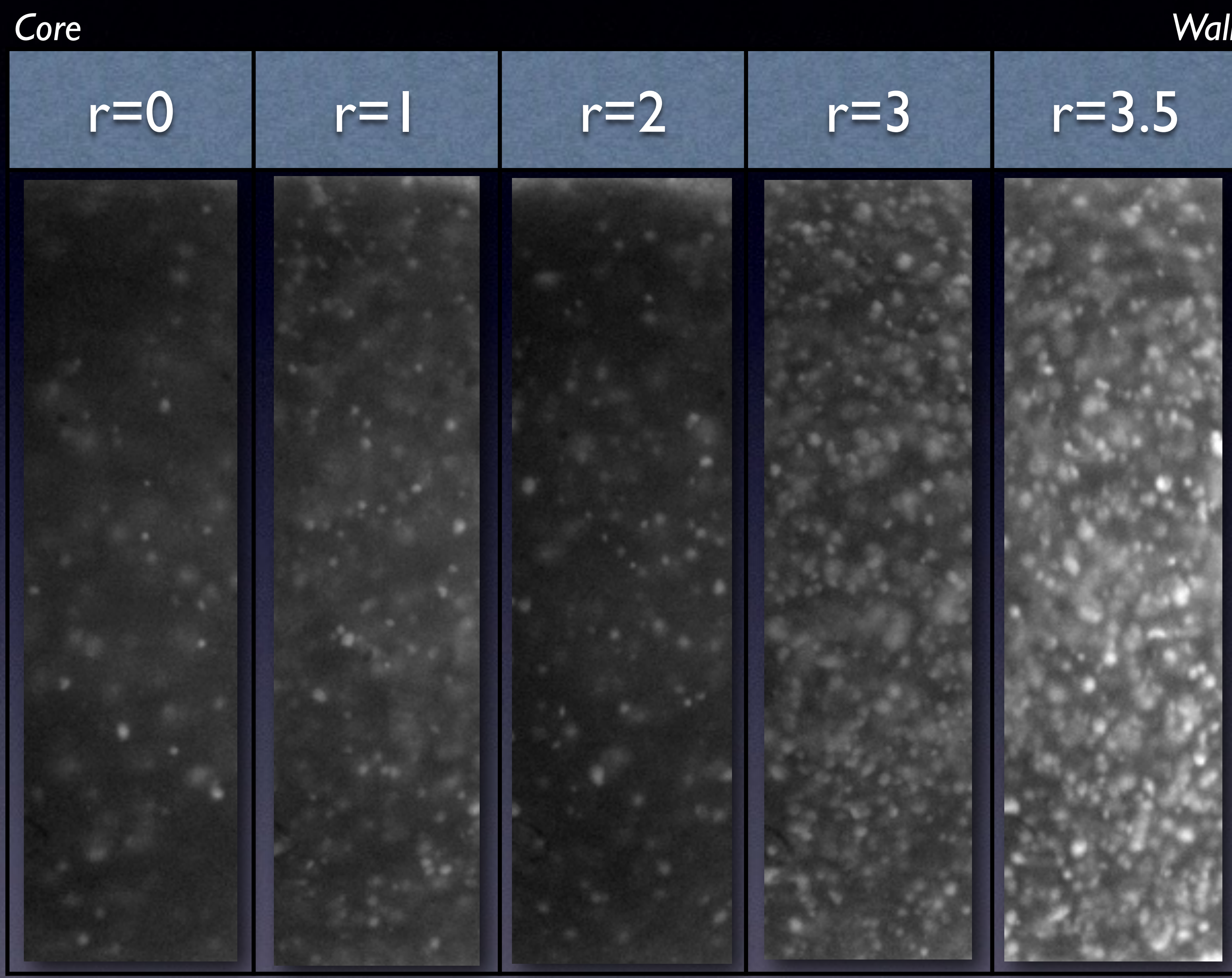


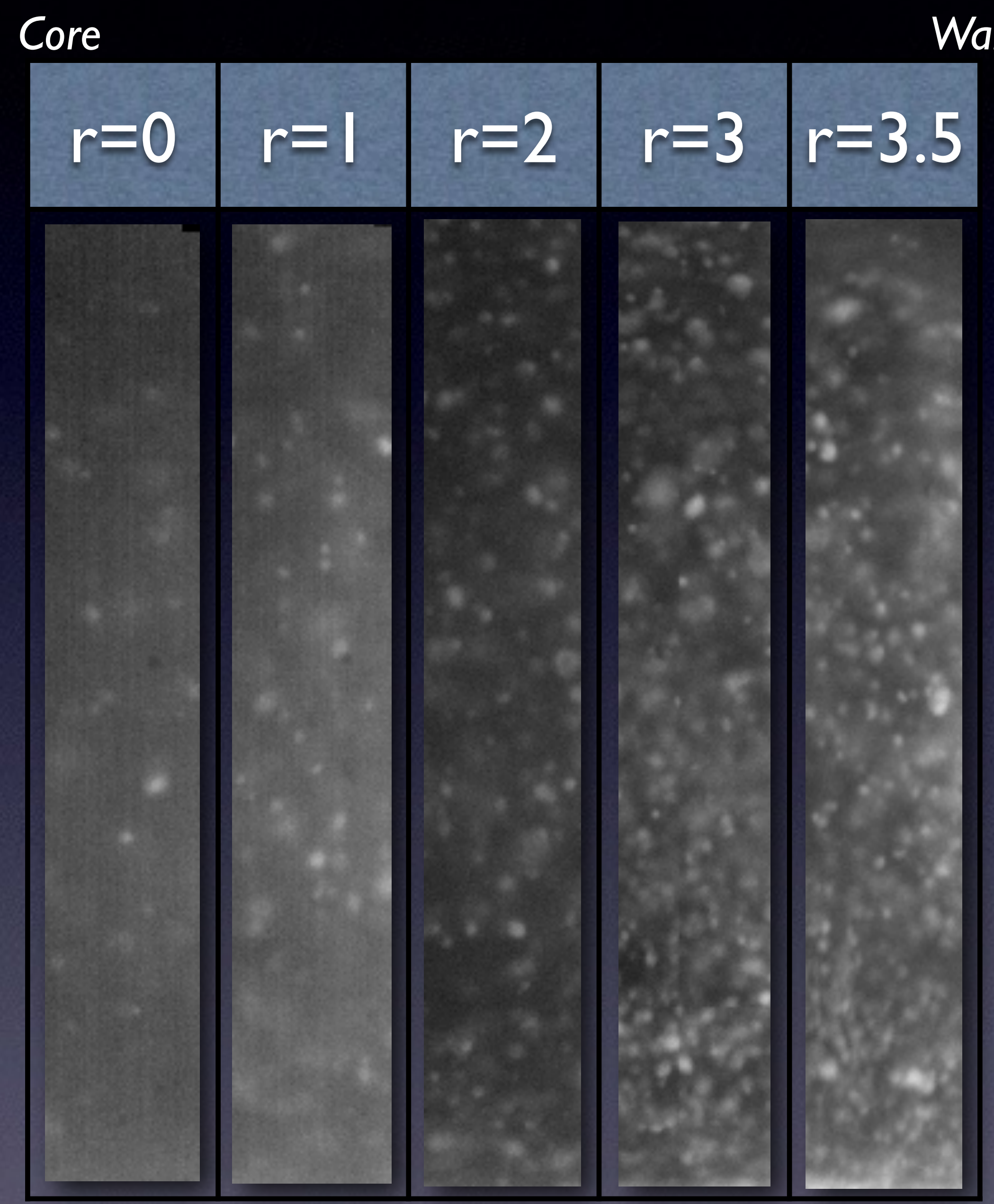
Risers have been designed to provide symmetric profiles

Imaging the Core-Annulus Profile

30 ft/sec & 10 lb/ft^2-sec
9.1 m/sec & 50 kg/m^2-sec

60 ft/sec & 80 lb/ft^2-sec
18.3 m/sec & 400 kg/m^2-sec



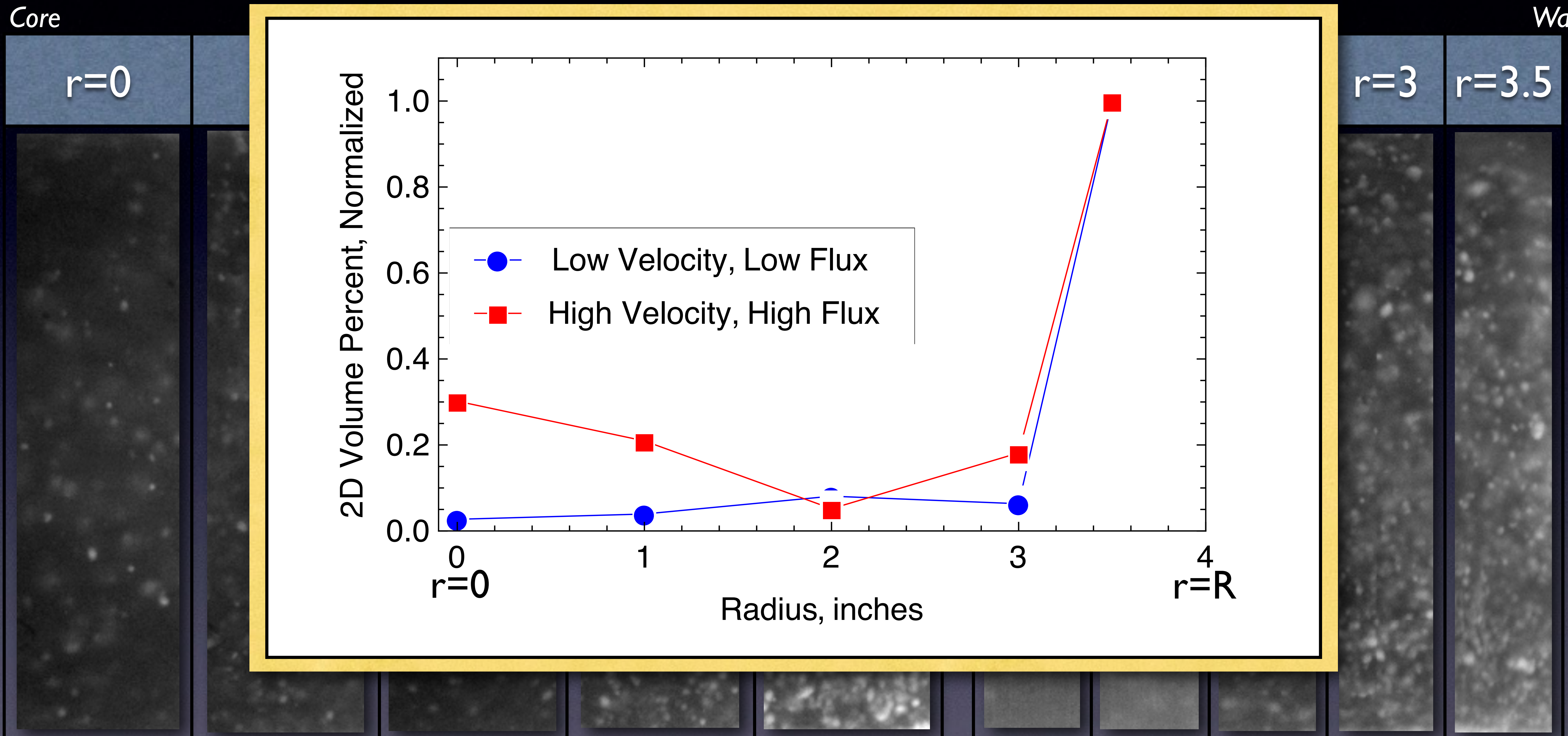


FCC Catalyst in PSRI's 8-Inch (20-cm) Dia x 72-Foot (22-m) Tall Riser
Slower particle velocities means we can use higher resolutions

Imaging the Core-Annulus Profile

30 ft/sec & 10 lb/ft^2-sec
9.1 m/sec & 50 kg/m^2-sec

60 ft/sec & 80 lb/ft^2-sec
18.3 m/sec & 400 kg/m^2-sec



FCC Catalyst in PSRI's 8-Inch (20-cm) Dia x 72-Foot (22-m) Tall Riser
Slower particle velocities means we can use higher resolutions

Not Just Core Annulus Profile

	Low Flux 10 lb/ft^2-sec (50 kg/m^2-sec)	High Flux 80 lb/ft^2-sec (400 kg/m^2-sec)
Low Velocity 30 ft/sec (9.1 m/sec)		
High Velocity 60 ft/sec (18.2 m/sec)		

PSRI's 8-inch (20-cm) dia x 72-feet (22-m) tall riser with FCC powder

Not Just Core Annulus Profile

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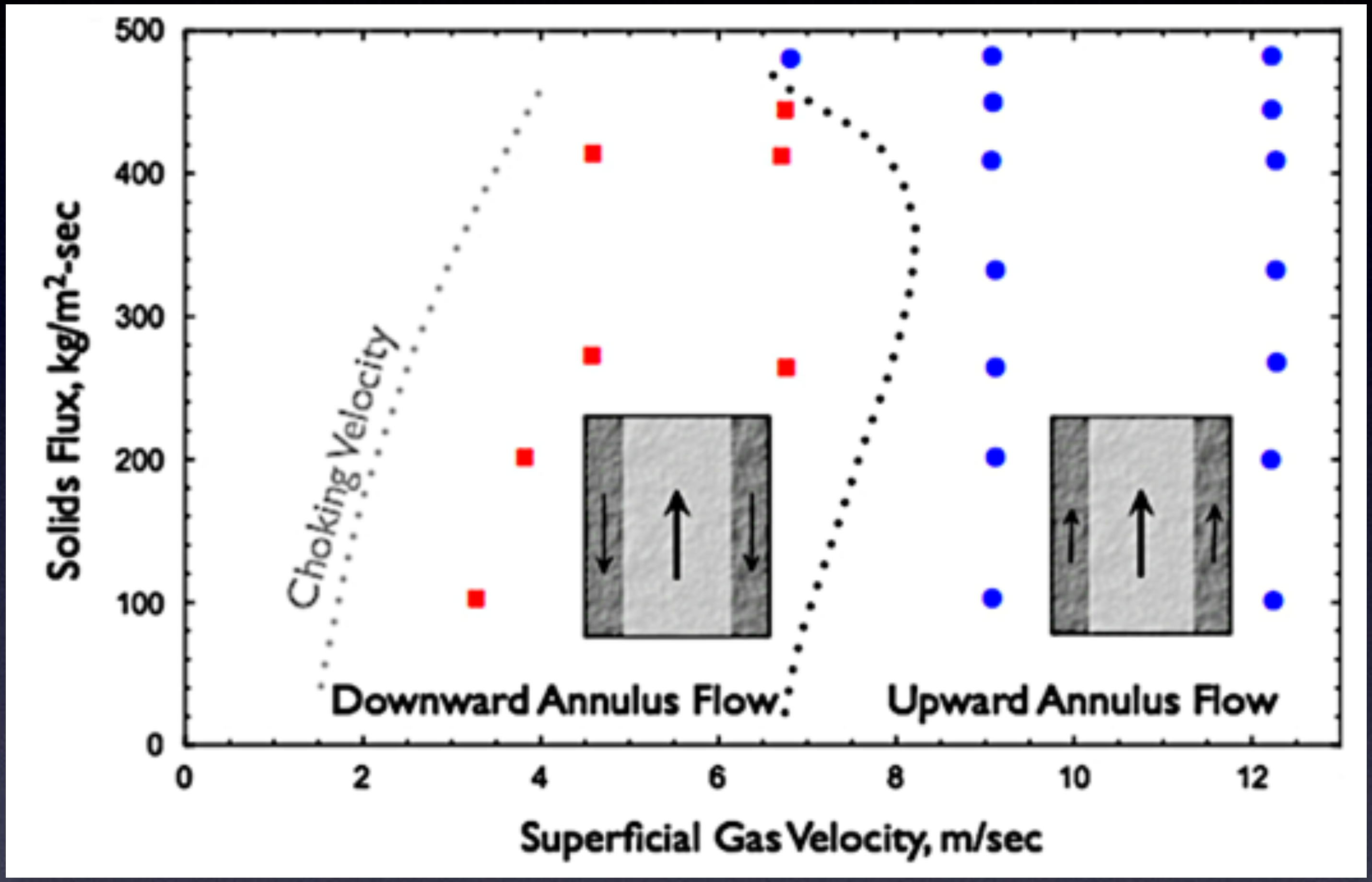
Low Velocity 30 ft/sec (9.1 m/sec)		
High Velocity 60 ft/sec (18.2 m/sec)		

PSRI's 8-inch (20-cm) dia x 72-feet (22-m) tall riser with FCC powder

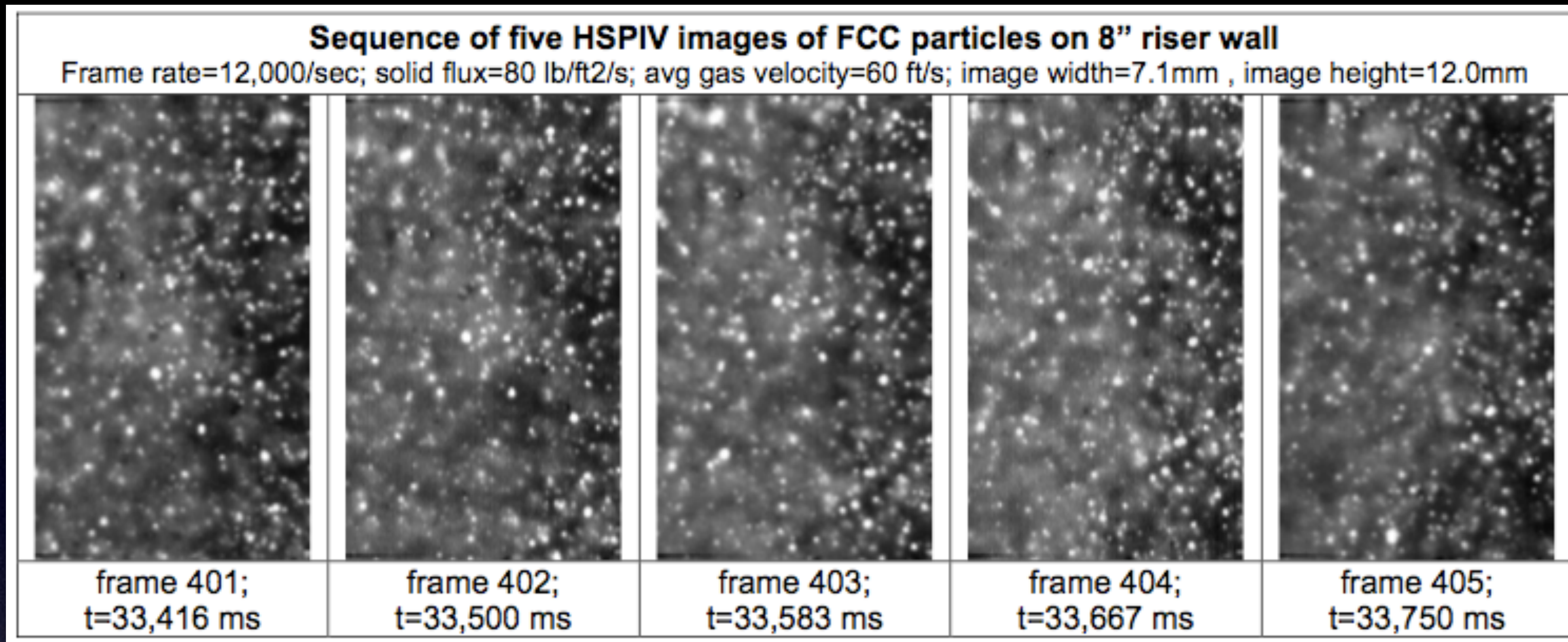
Level of Down Flow is Important

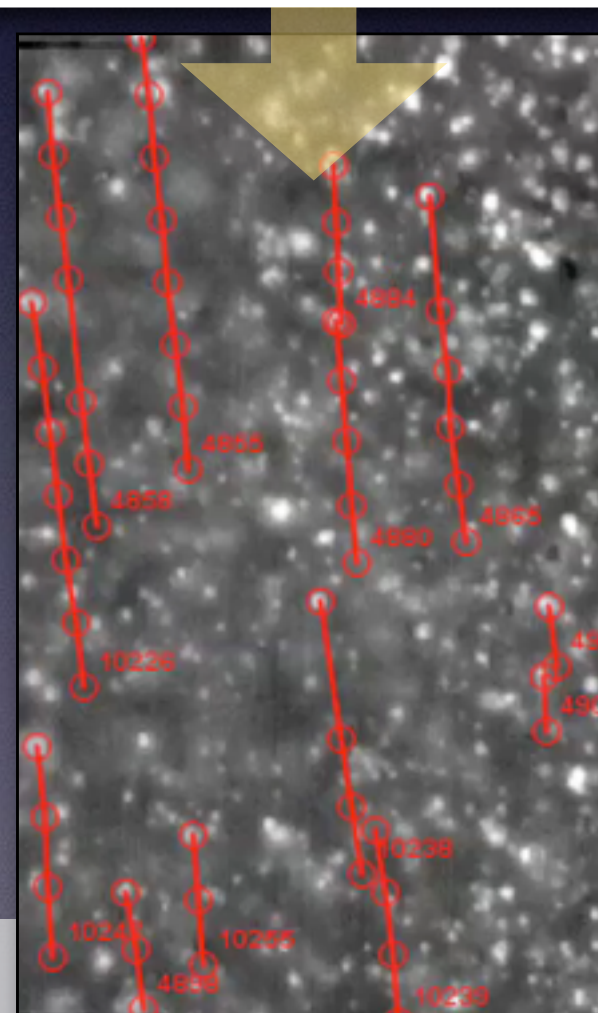


- Degree of backmixing depends if we have up flow or down flow at the wall
  - For FCC, coking is an issue with backmixing

J. McMillan, F. Shaffer, B. Gopalan, J.W. Chew, C. Hrenya, R. Hays, et al., Particle Cluster Dynamics During Fluidization, Chemical Engineering Science. 100 (2013) 39–51

PIV Measurements: NETL's HSPIV



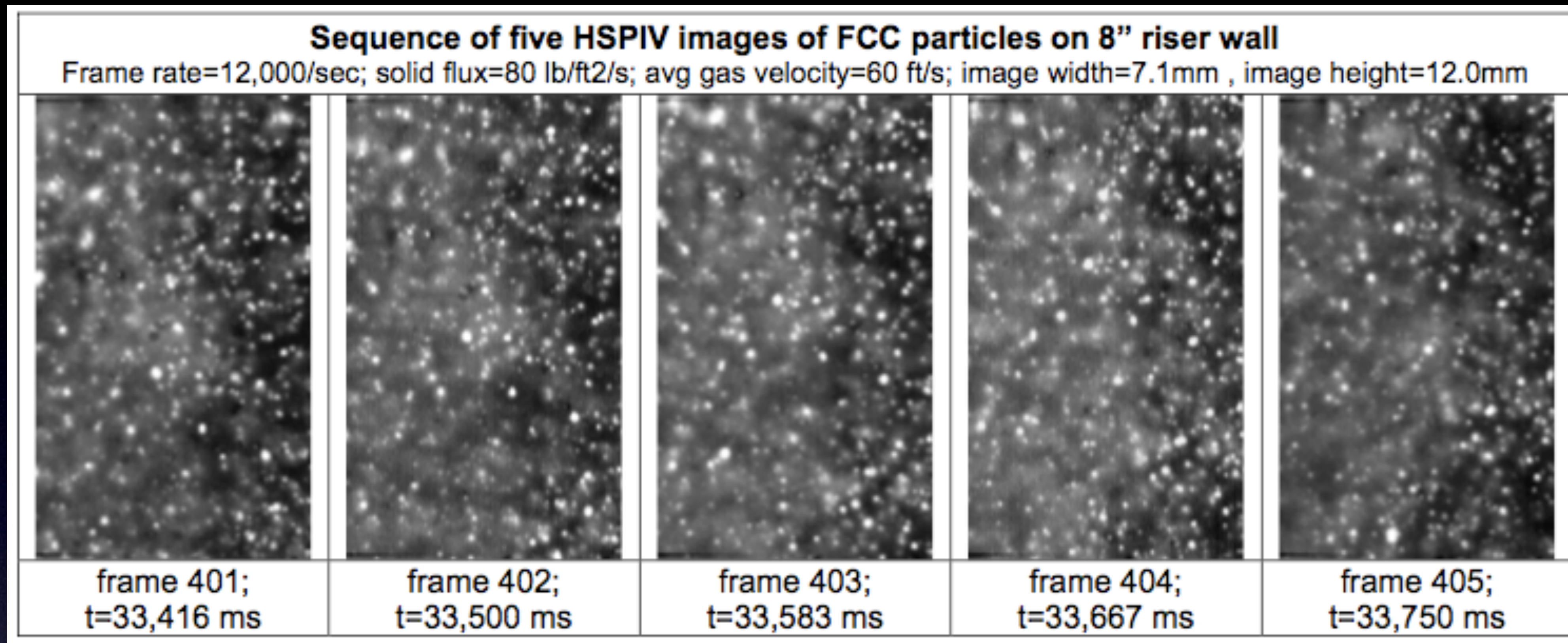


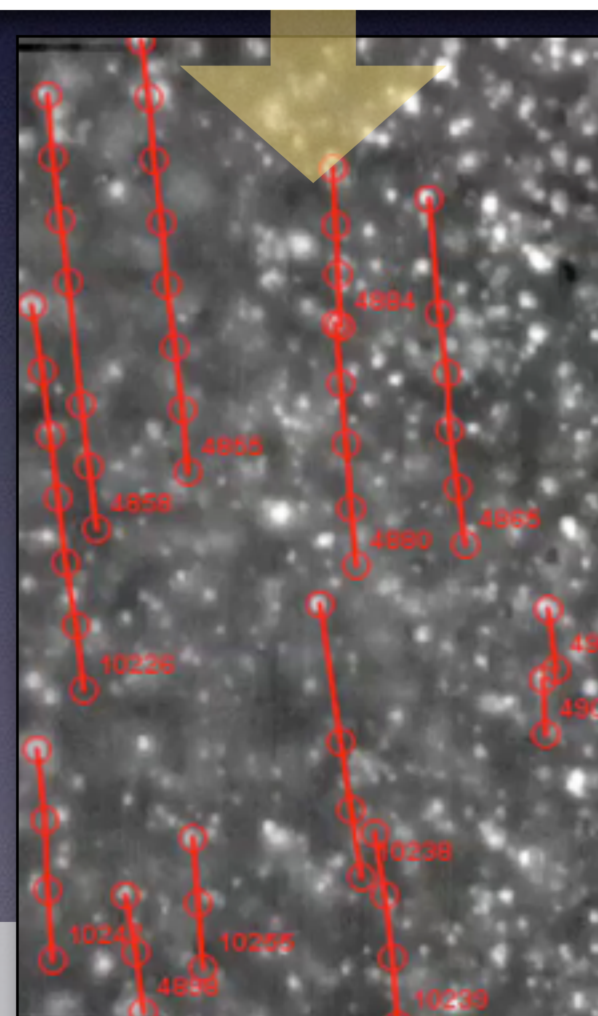
Tracking is based on at least 5 subsequent frames

PSRI's 8-inch (20-cm) dia x 72-feet (22-m) tall riser with FCC powder

F. Shaffer, B. Gopalan, R.W. Breault, R. Cocco, S.B.R. Karri, R. Hays, et al., High speed imaging of particle flow fields in CFB risers, (2013) 1–14.

PIV Measurements: NETL's HSPIV





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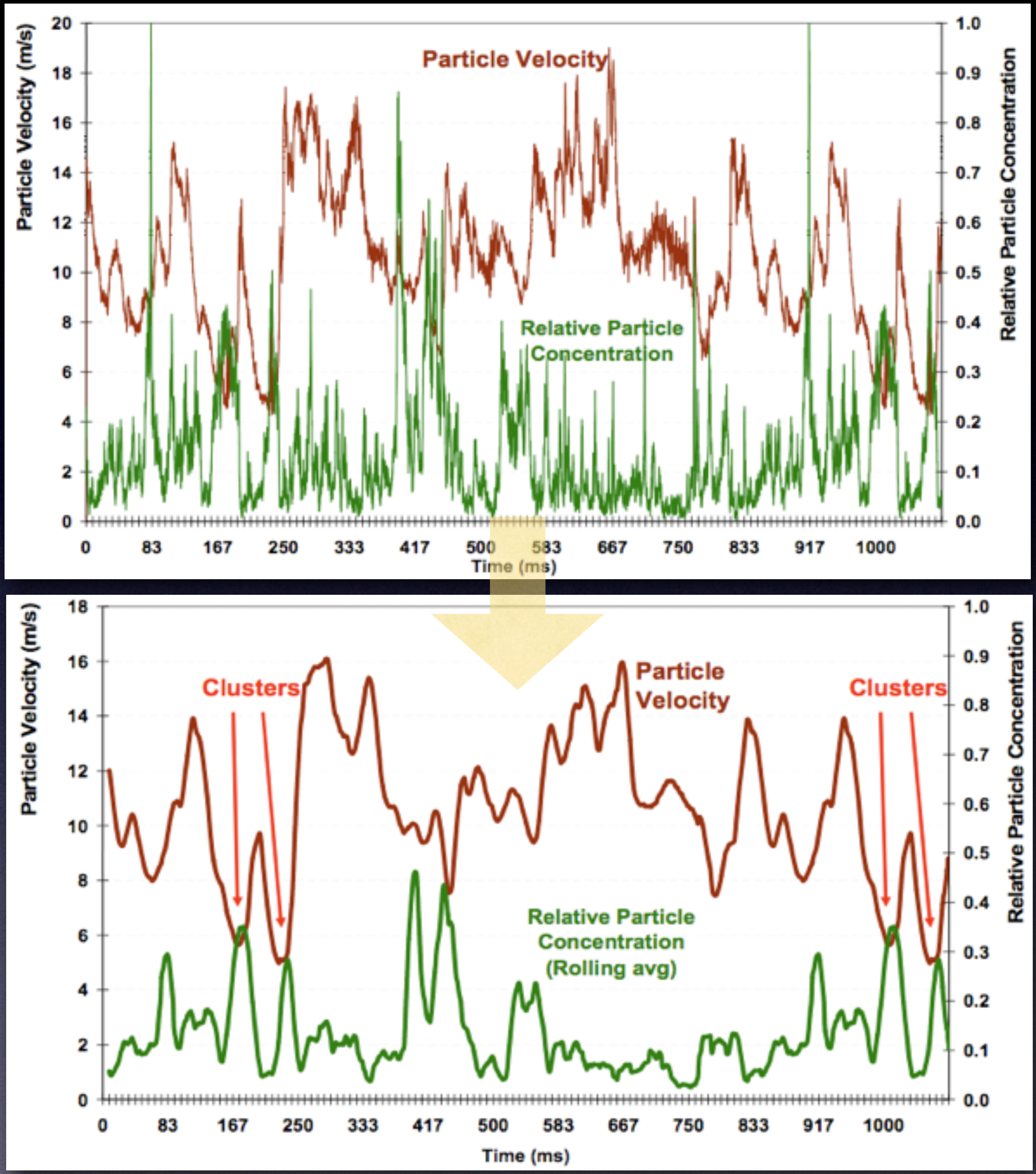
PSRI's 8-inch (20-cm) dia x 72-feet (22-m) tall riser with FCC powder

F. Shaffer, B. Gopalan, R.W. Breault, R. Cocco, S.B.R. Karri, R. Hays, et al., High speed imaging of particle flow fields in CFB risers, (2013) 1–14.

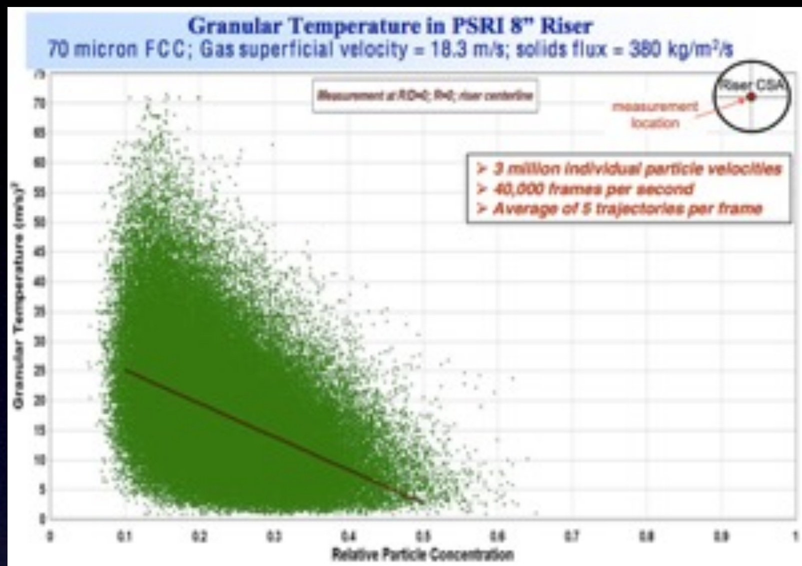
Cluster Velocities

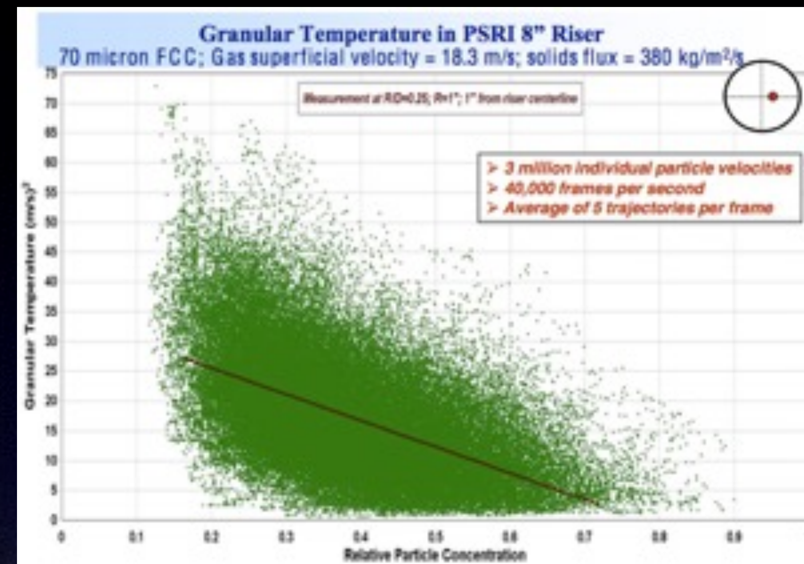
- Clusters determined by lower velocities AND higher solids concentrations
- Cluster Velocities measured at 12 to 24 ft/sec (3.7 to 7.3 m/sec)
  - 50% lower than the mean particle velocity

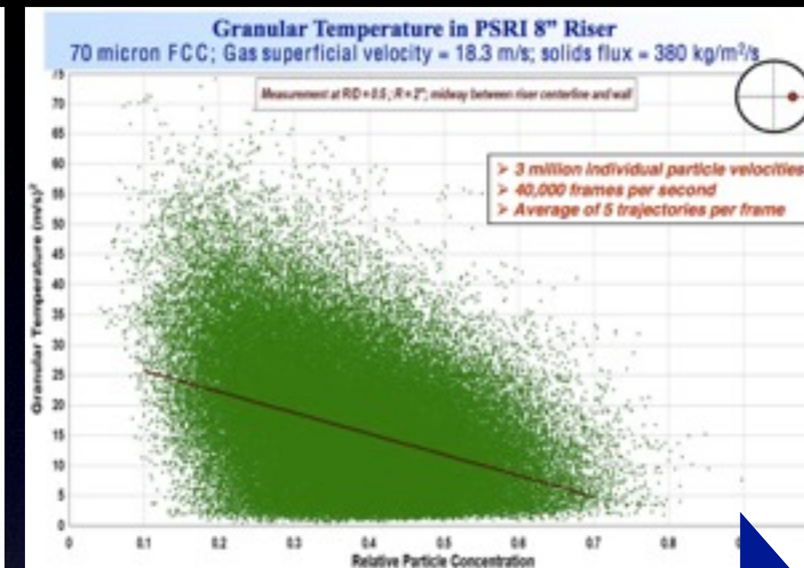


Granular Temperature

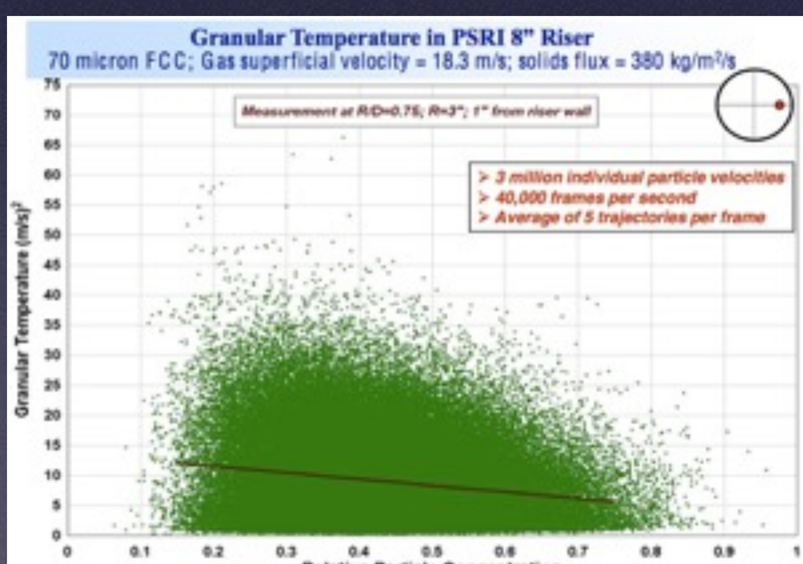
Measuring Granular Temperature in a 0.2-m Diameter x 22-m Tall Riser with FCC Catalyst Powder

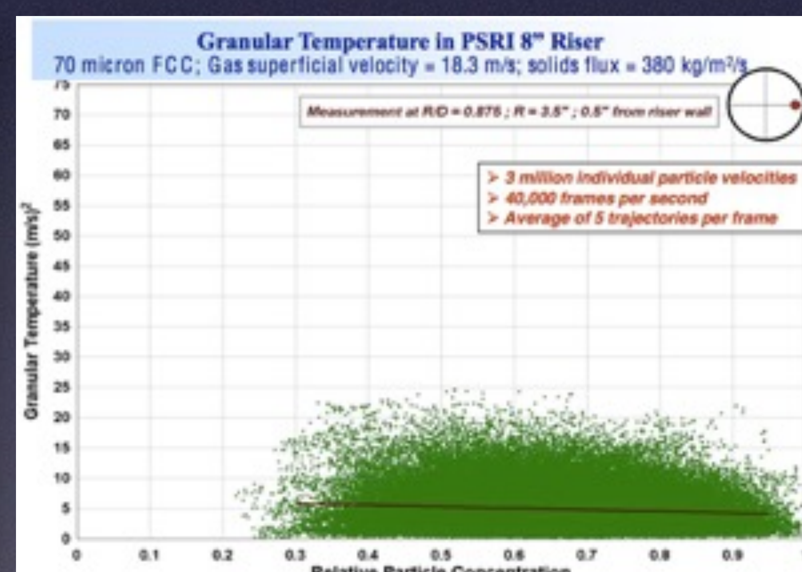


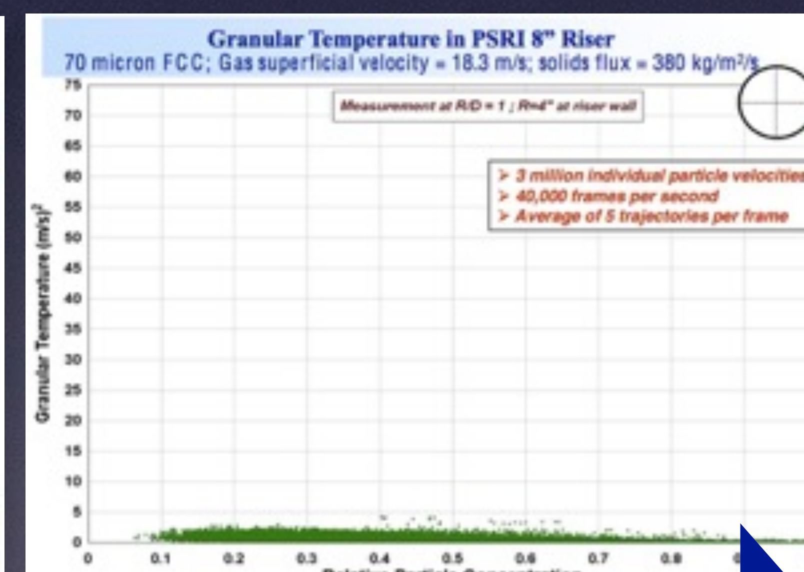




Core

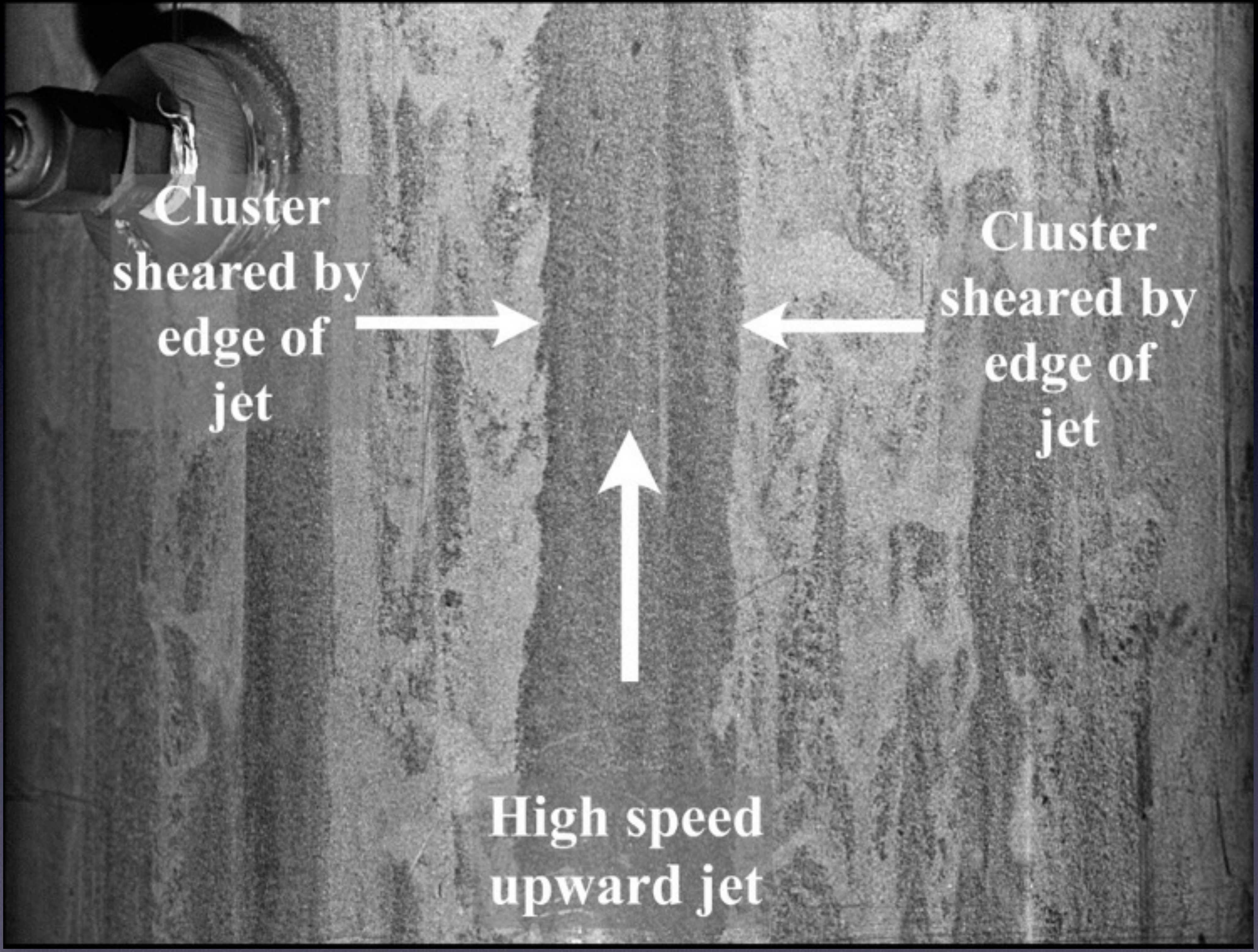






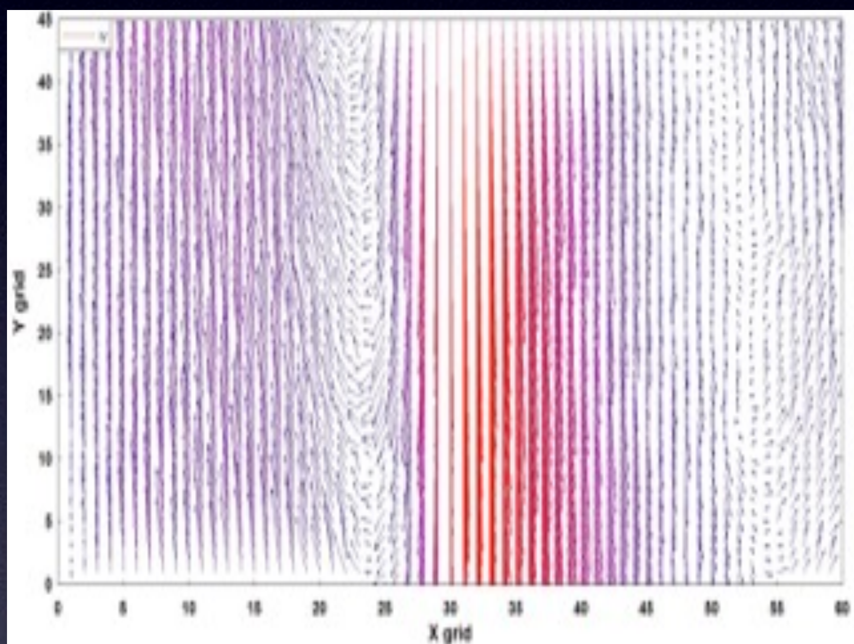
Wall

Clusters and Streamers

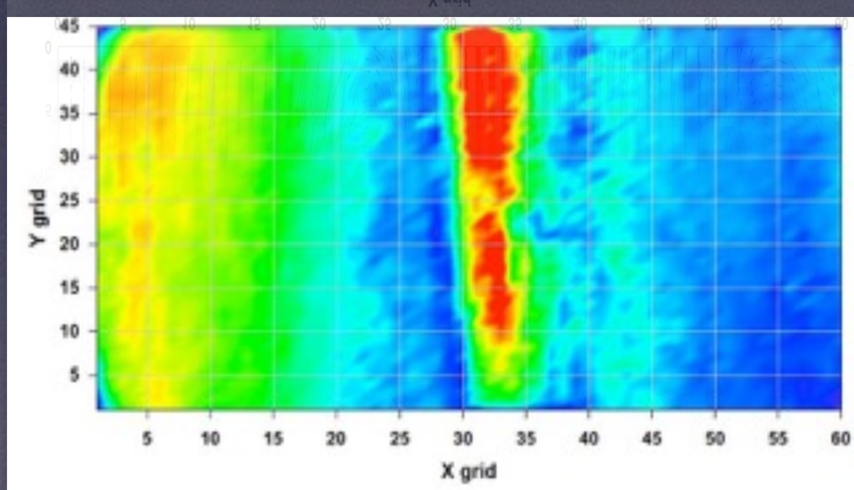


Quantifying Riser Hydrodynamics

Particle Tracking of In-Situ Images



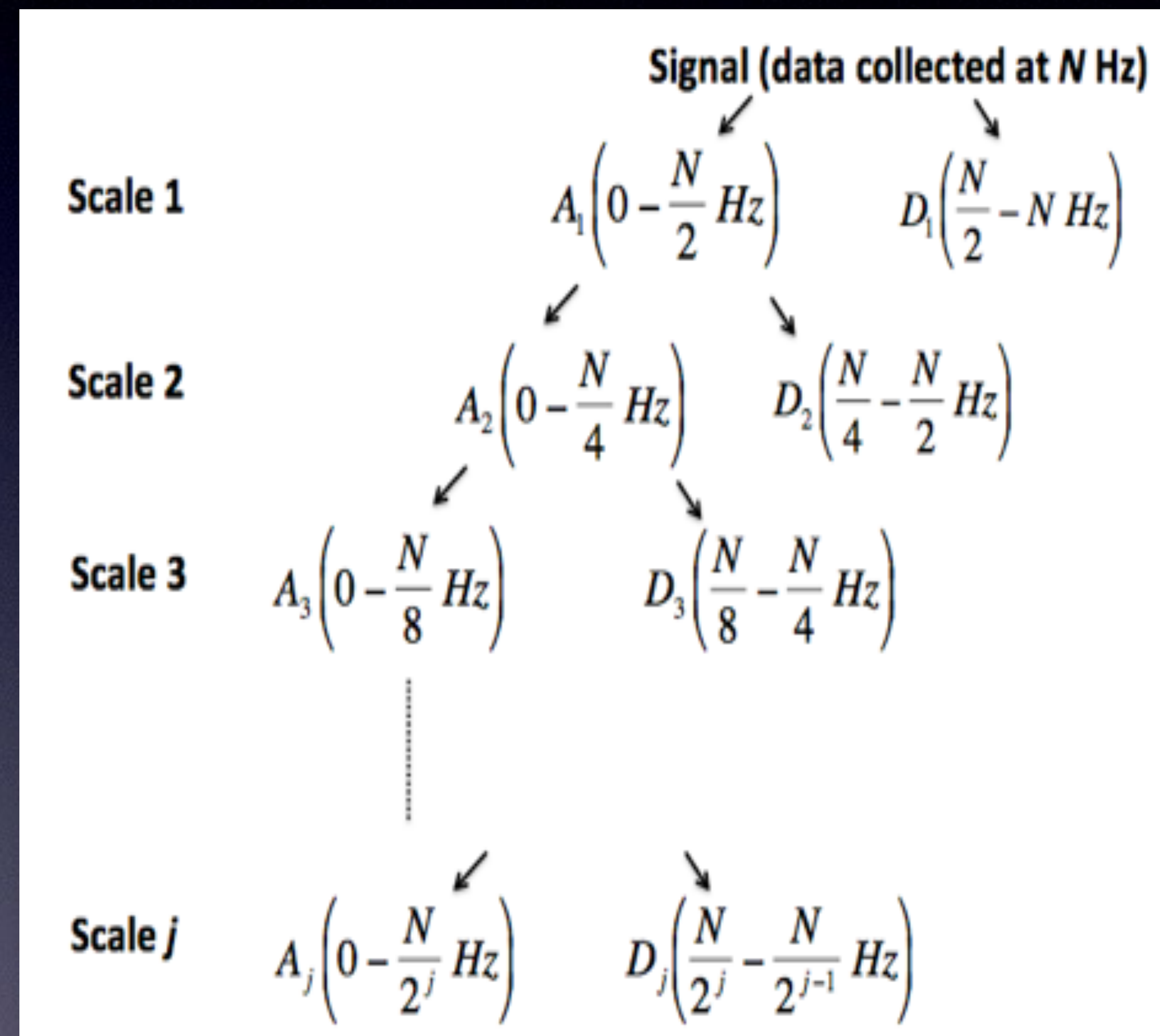
Velocity Vector Map Derived from In-Situ Images



Contour Plot of Fluctuating Velocity (RMS)

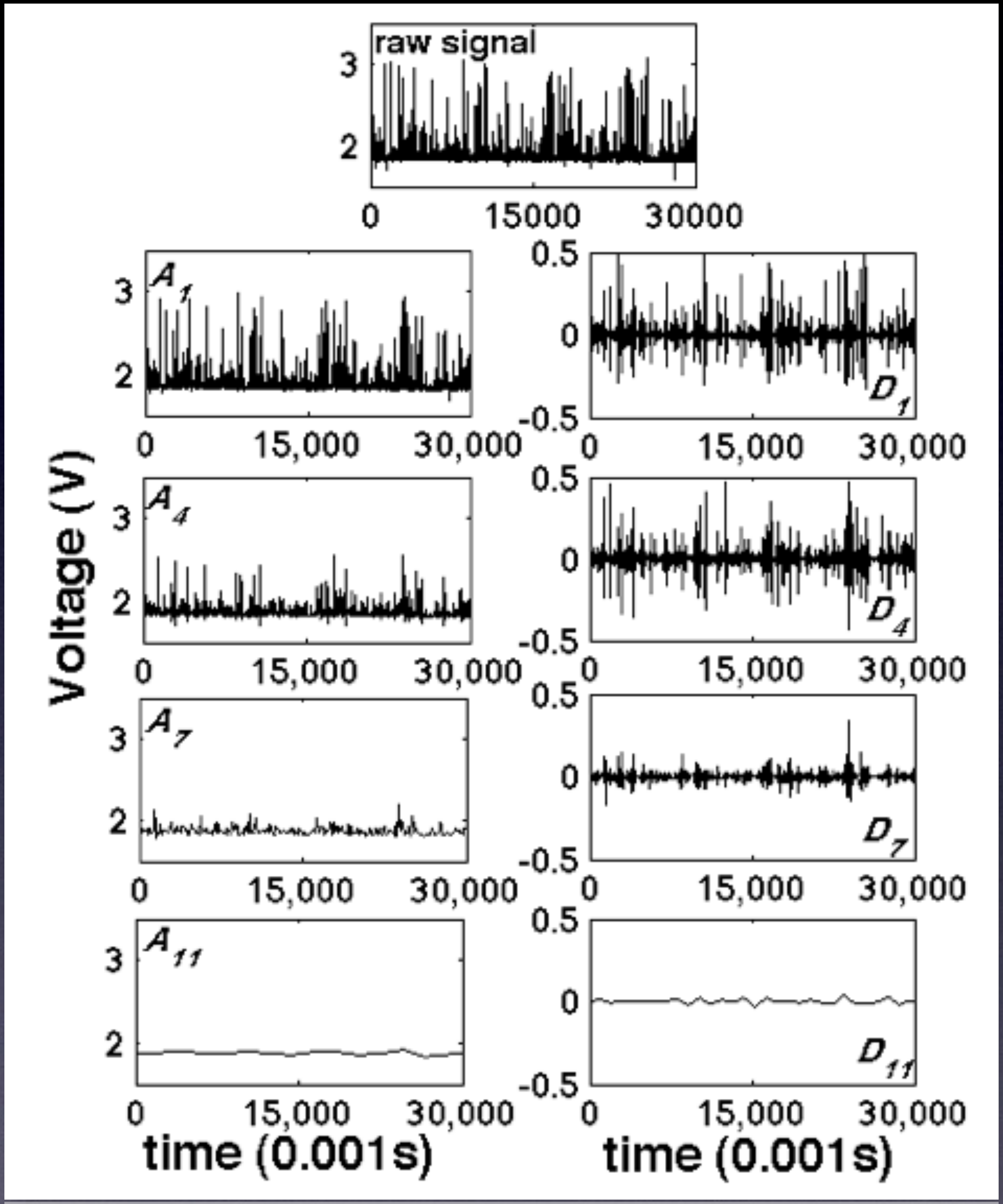
Wavelet Decomposition

- Wavelet decomposition provides a means of extracting different frequency ranges of data signals by repeatedly breaking down the signal into higher-frequency details (D) and lower-frequency approximations (A)
- Both Matlab and Mathematica have wavelet decomposition tools



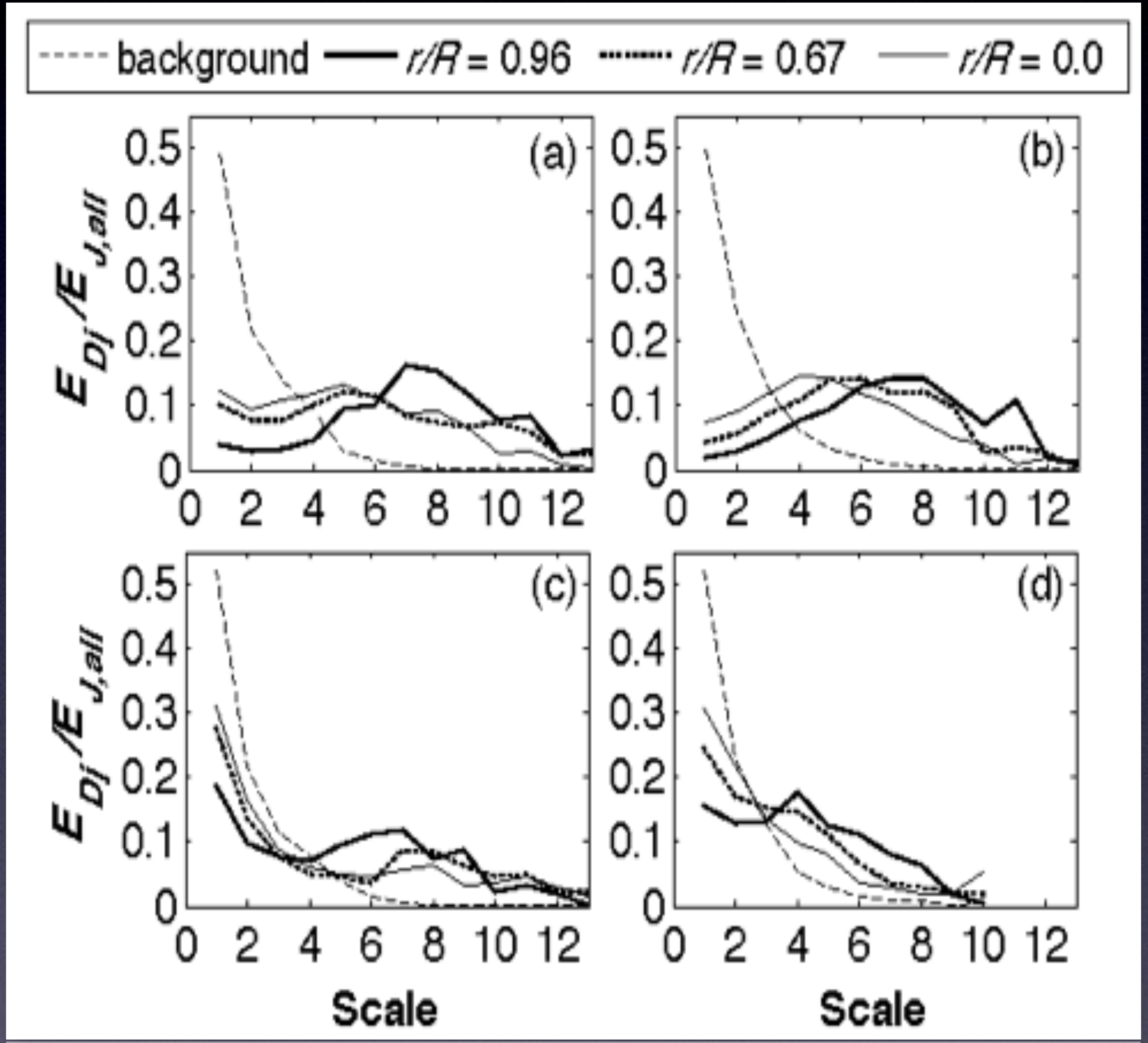
Wavelet Decomposition

- Wavelet decomposition can be used with acoustic, pressure or fiber optic data in risers and fluidized beds
- For this riser study, fiber optic data were used.
- By normalizing the energies of the high-frequency details (D), the micro, meso and macro scale events can be discerned
  - Periodicity is not a requirement for wavelet decomposition



Application of Wavelet Decomposition to Riser Hydrodynamics

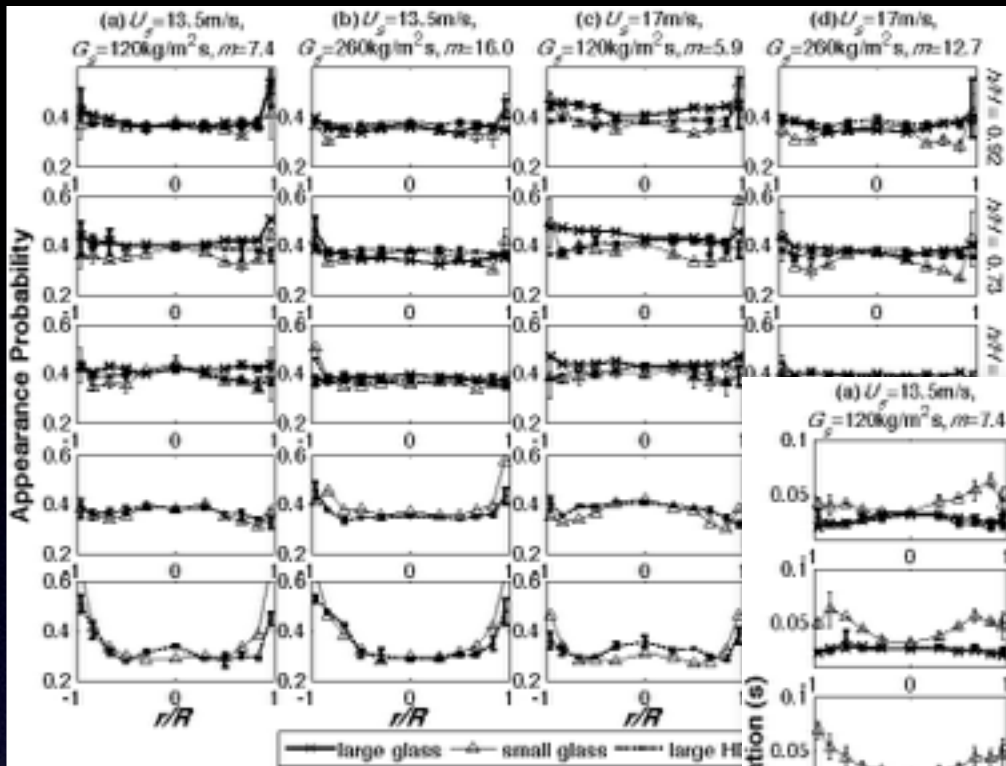
- Unlike previous work where the demarcation between scales was arbitrary, here demarcation was based on the resulting features
  - Micro-scale is 0 to 5 scale
  - Meso-scale is 5 to 11 scale
    - Clusters
  - Macro is > 11 scale
- Cluster can now be tracked according to appearance, duration and frequency

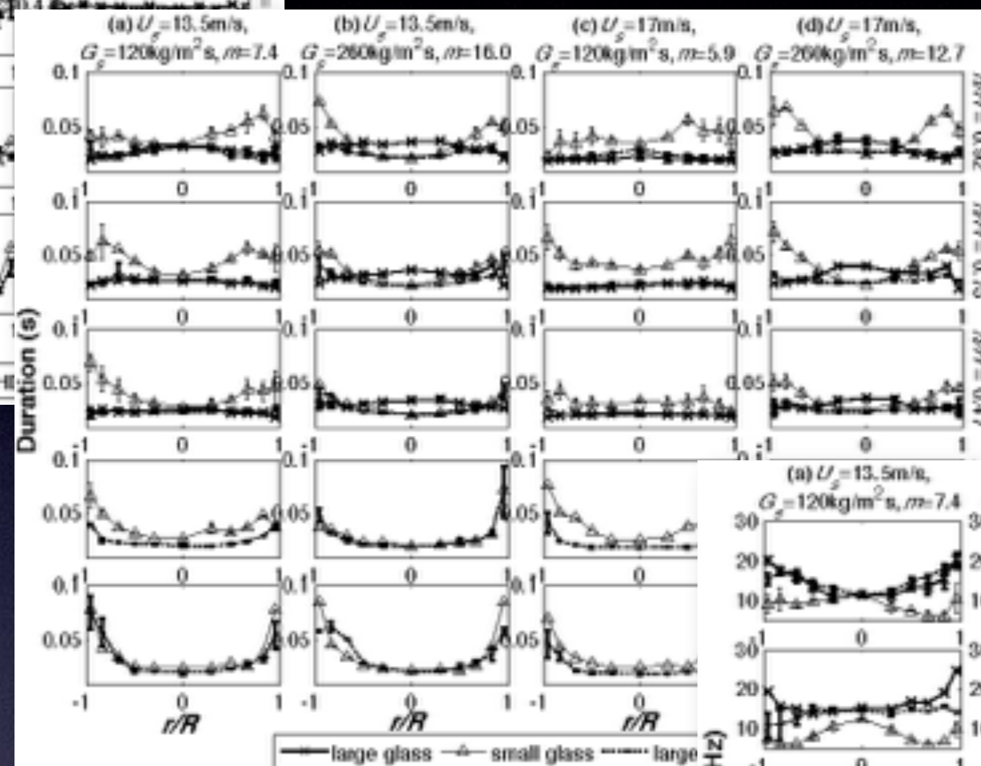


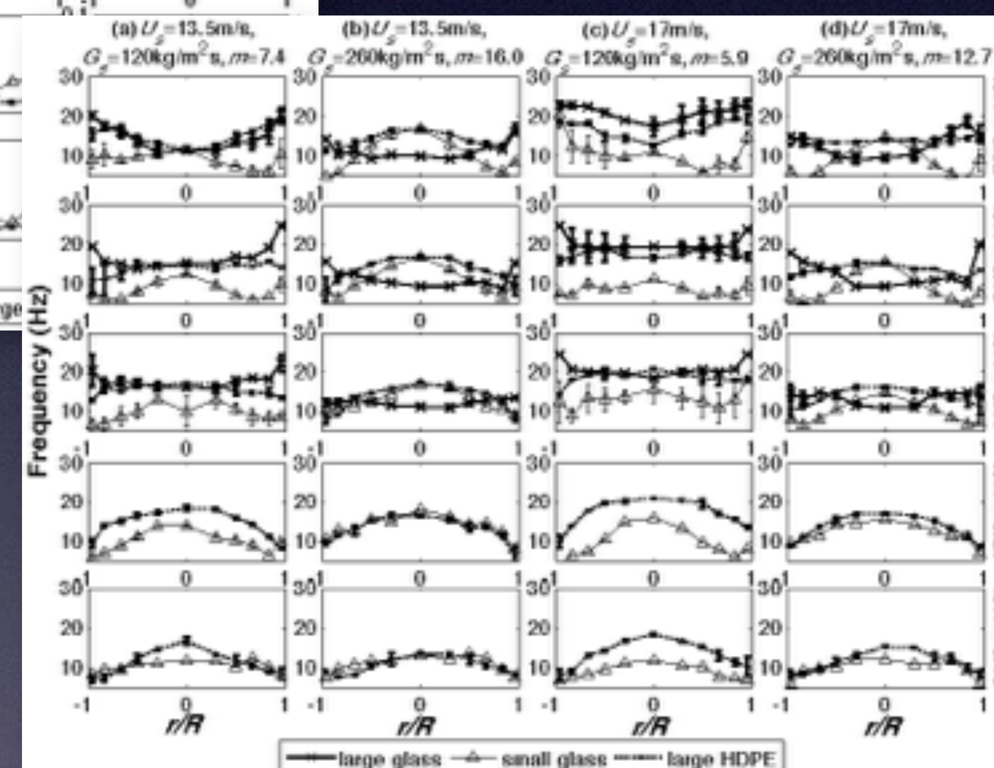
T. Yang, L. Leu, Multiresolution analysis on identification and dynamics of clusters in a circulating fluidized bed, AIChE Journal. 55 (2009).

Clusters in Riser

- Cluster appearance probability is only dependent on riser position







- Cluster duration and frequency are dependent on operating conditions and materials as well

The role of clusters is complex and dependent on particle size, density, coefficient of restitution (elasticity), friction and shape

J.W. Chew, R. Hays, J.G. Findlay, T.M. Knowlton, S.B.R. Karri, R.A. Cocco, et al., Cluster characteristics of Geldart group B particles in a pilot-scale CFB riser. II. Polydisperse systems, Chemical Engineering Science. 68 (2012) 82–93.
J.W. Chew, R. Hays, J.G. Findlay, T.M. Knowlton, S.B.R. Karri, R.A. Cocco, et al., Cluster characteristics of Geldart Group B particles in a pilot-scale CFB riser. I. Monodisperse systems, Chemical Engineering Science. 68 (2012) 72–81.
J.W. Chew, D.M. Parker, R.A. Cocco, C.M. Hrenya, Cluster characteristics of continuous size distributions and binary mixtures of Group B particles in dilute riser flow, Chemical Engineering Journal. 178 (2011) 348–358.

Macro-scale Experiments are Cost Limited

- For model development, this work is practical. However, it is too expensive and time consuming for "fitting"

The Multi-scale Validation Paradox

Fundamentals	Model Fitting	Model Development
Micro-scale	*Meso-scale*	*Macro-scale*
1 to 100's Particles	Millions to Billions of Particles	Trillions of Particles
10^{-6} to 10^{-4} m	10^{-2} to 10^{-1} m	10^{-1} to 10^{2} m
Experiments are cheap	Experiments are inexpensive	**Experiments are expensive**
Simulations are cheap	Simulations are cheap	**Simulations are expensive**
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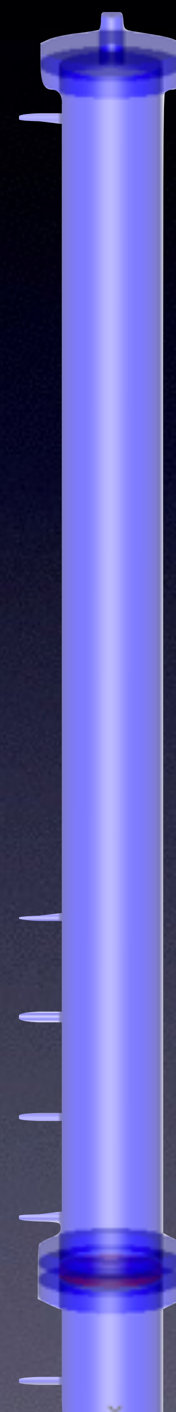
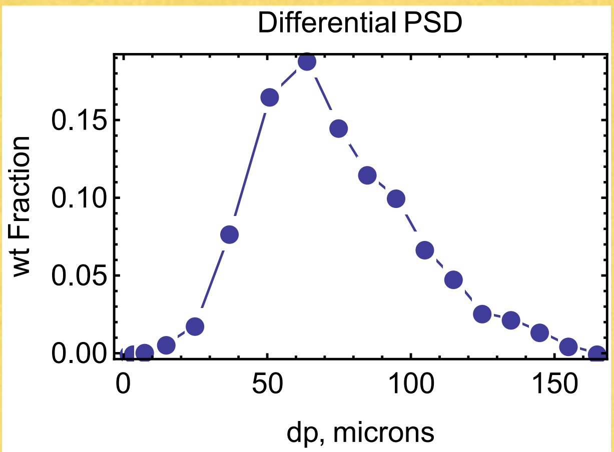
PSRI Modeling Methodology



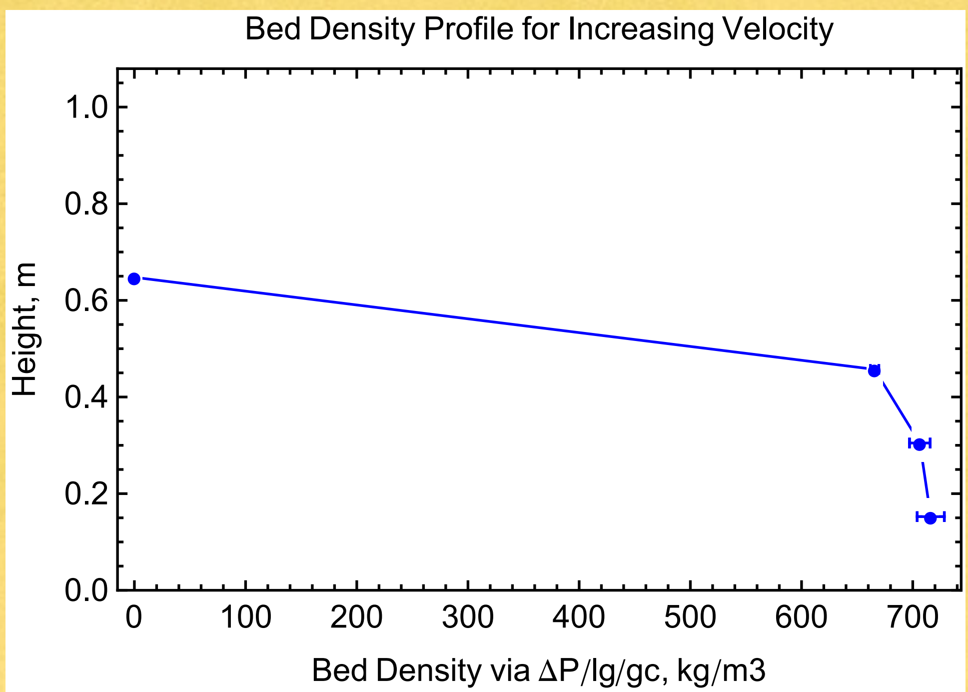
- Needs to be small scale
- Quantifiable and reproducible data

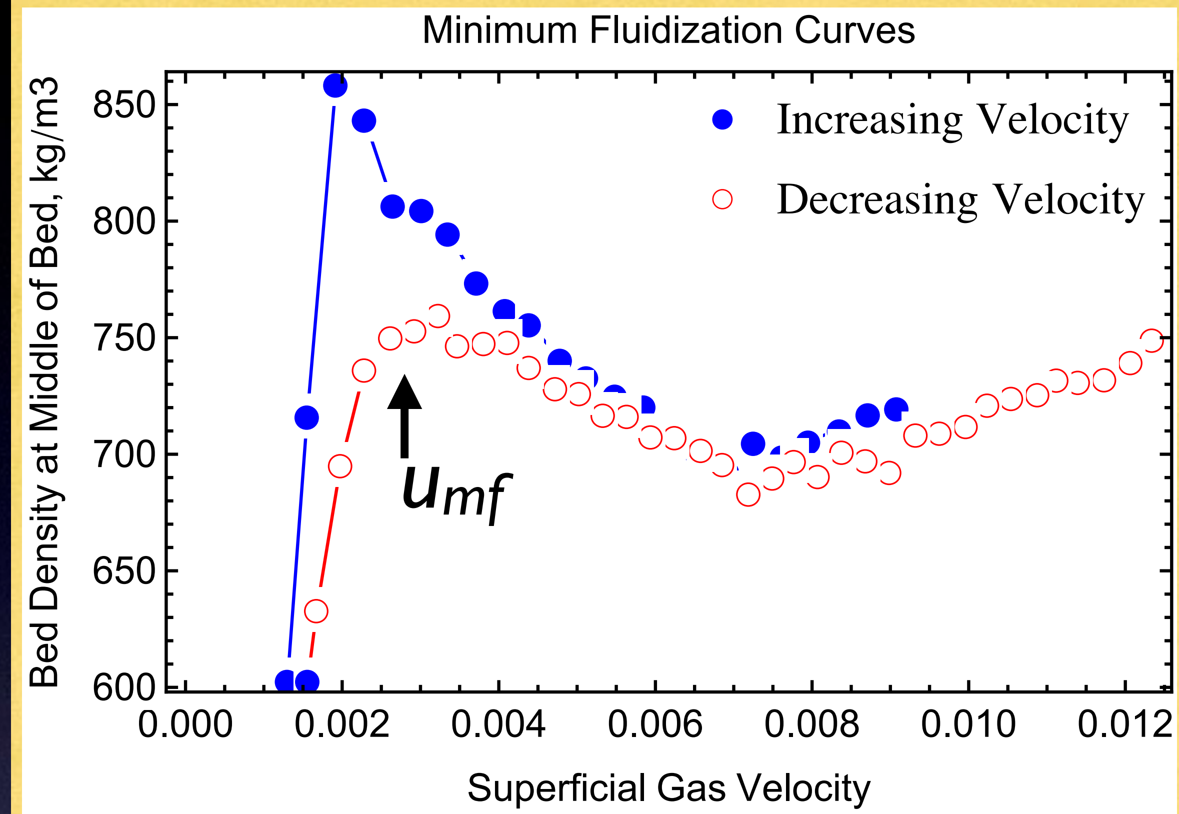
- U_{mf}, U_{mb} and bed density determined
  - Experimentally
  - Computationally

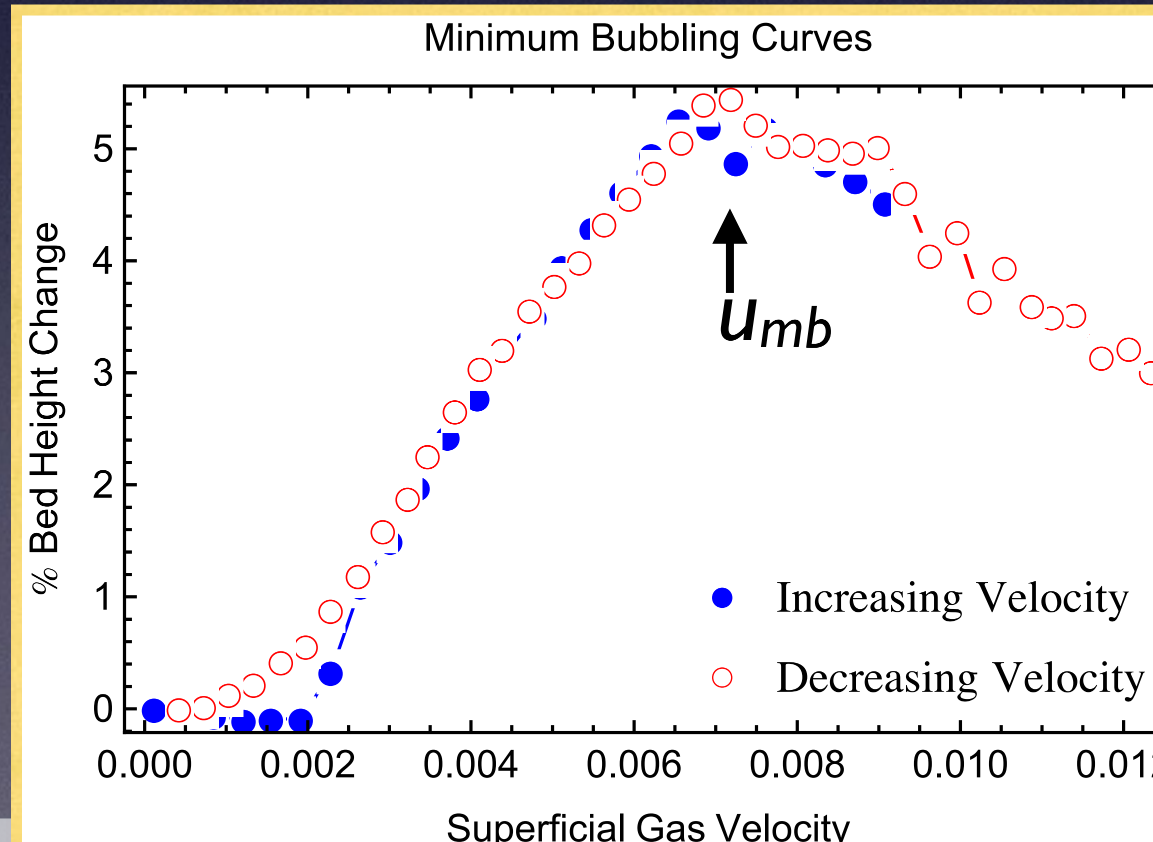
U_{mf}, U_{mb} and Bed Density for FCC eCat Powder



Properties	Results
Material	FCC eCat
Bulk Density, kg/m3	881.41026
Particle Density,kg/m3	1610.5769
Median Particle Size, um	67.3
Sauter Mean Particle Size,um	64.734484

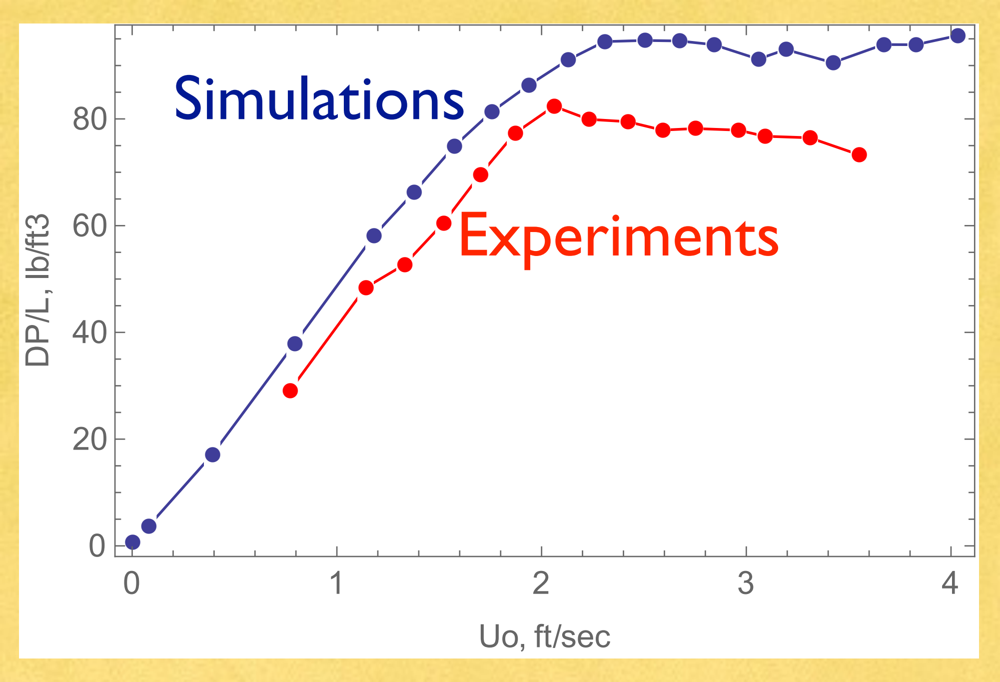


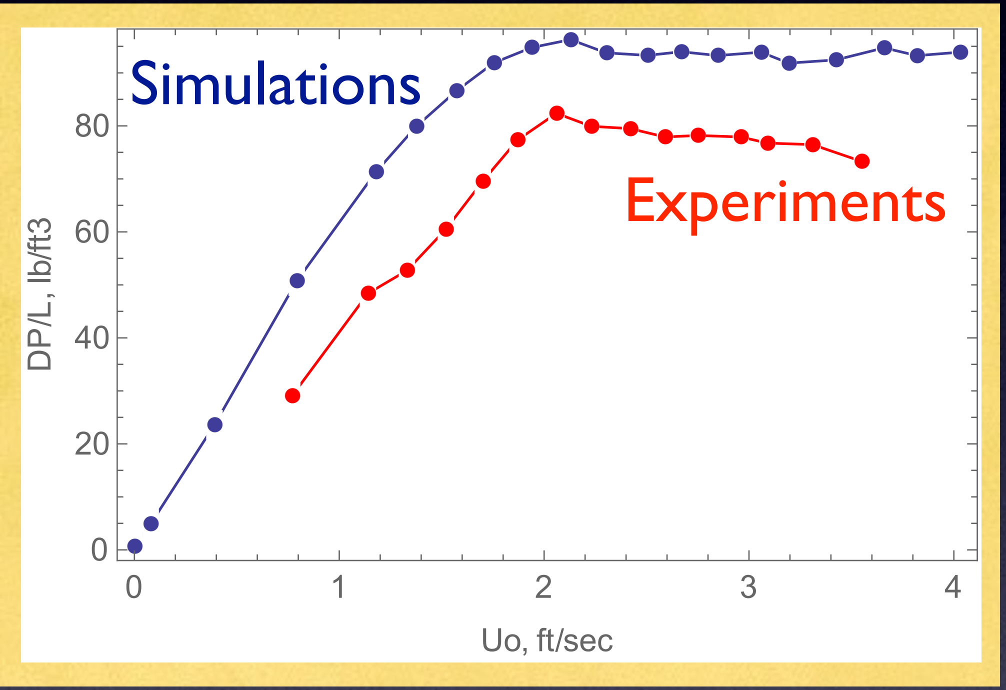




	MKS	FPS
Umf with Increasing Velocity	0.0020421848	0.0067
Umb with Increasing Velocity	0.0065532797	0.0215
Ave Bed Density	696.08707	43.435833
Umf with Decreasing Velocity	0.0033934813	0.011133333
Umb with Decreasing Velocity	0.0071933675	0.0236

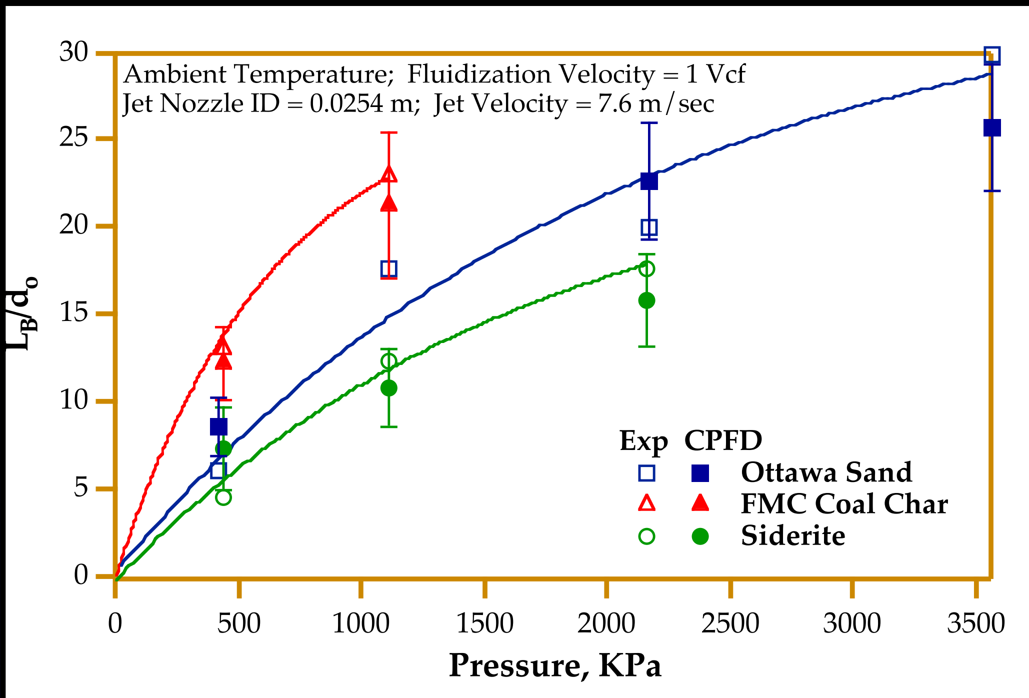
Comparison of Experimental and Computational Results



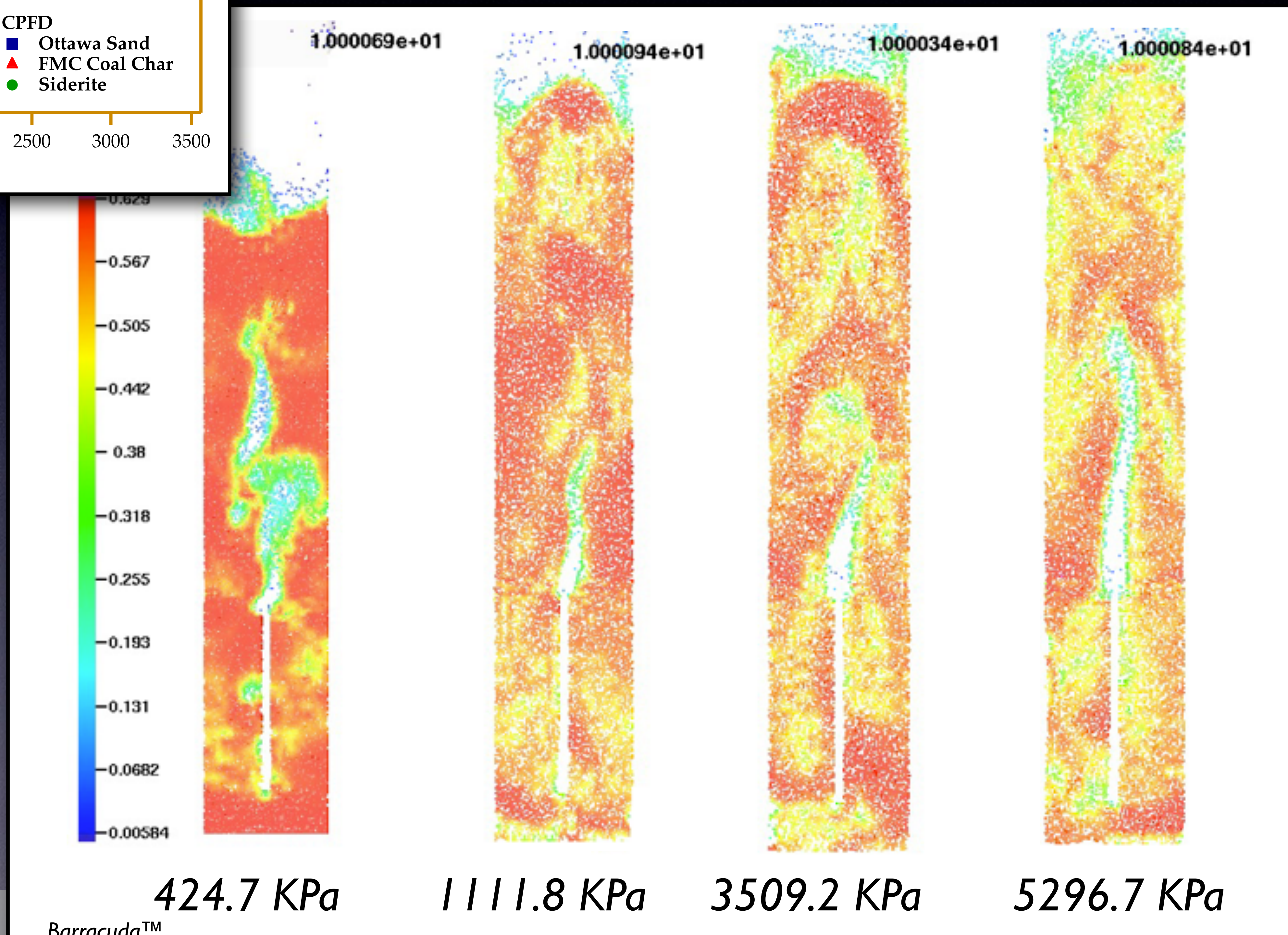


- Drag parameters are varied until bed density and U_{mf} "match" experimental data
- Method is CPU intensive

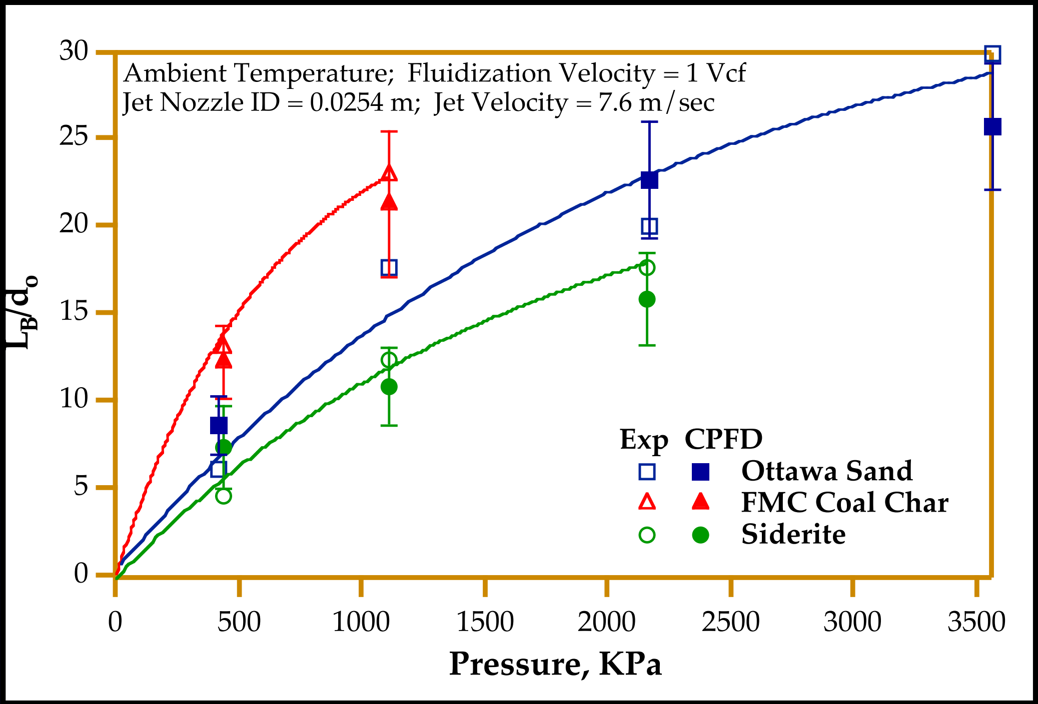
Validating with Jet Penetration Lengths

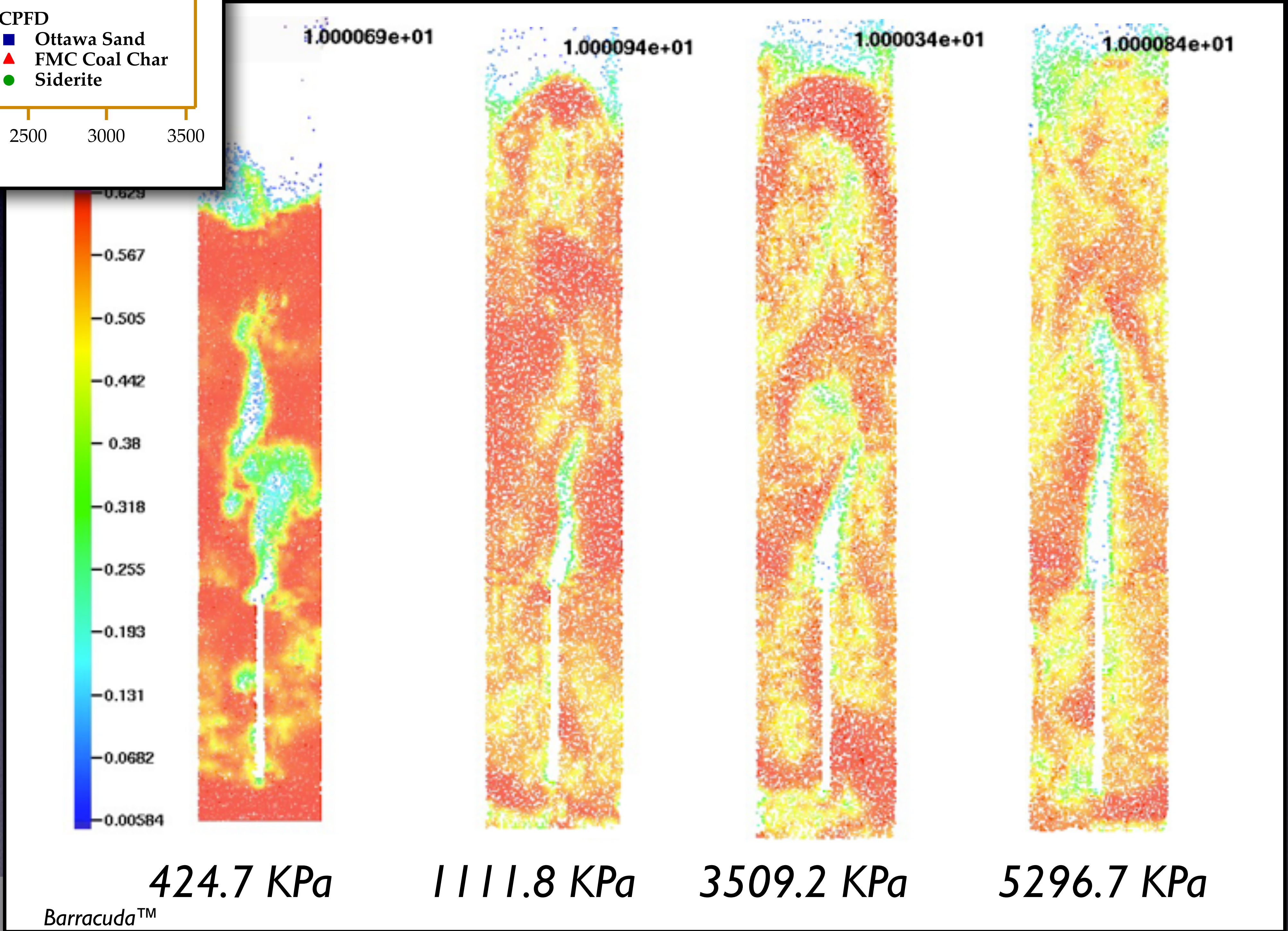


- Most jet penetration correlations do not apply to high pressure



Validating with Jet Penetration Lengths

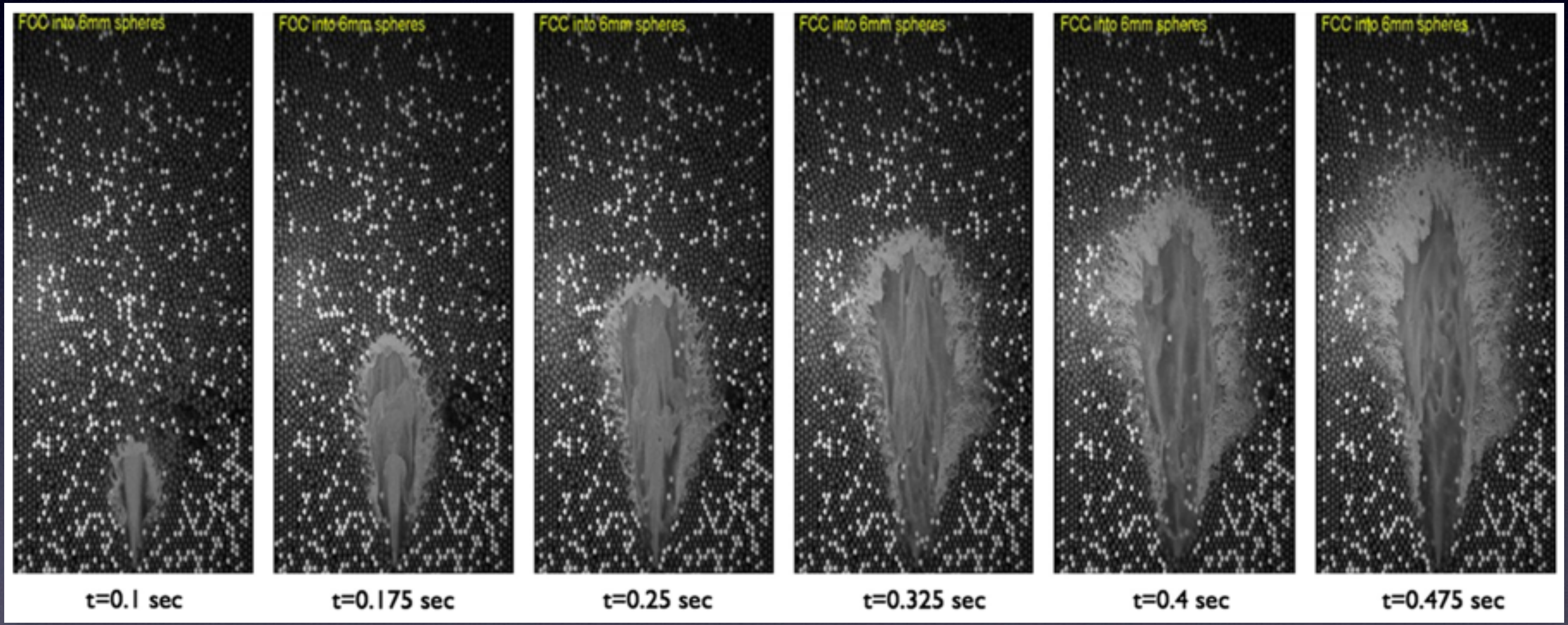




- Most jet penetration correlations do not apply to high pressure

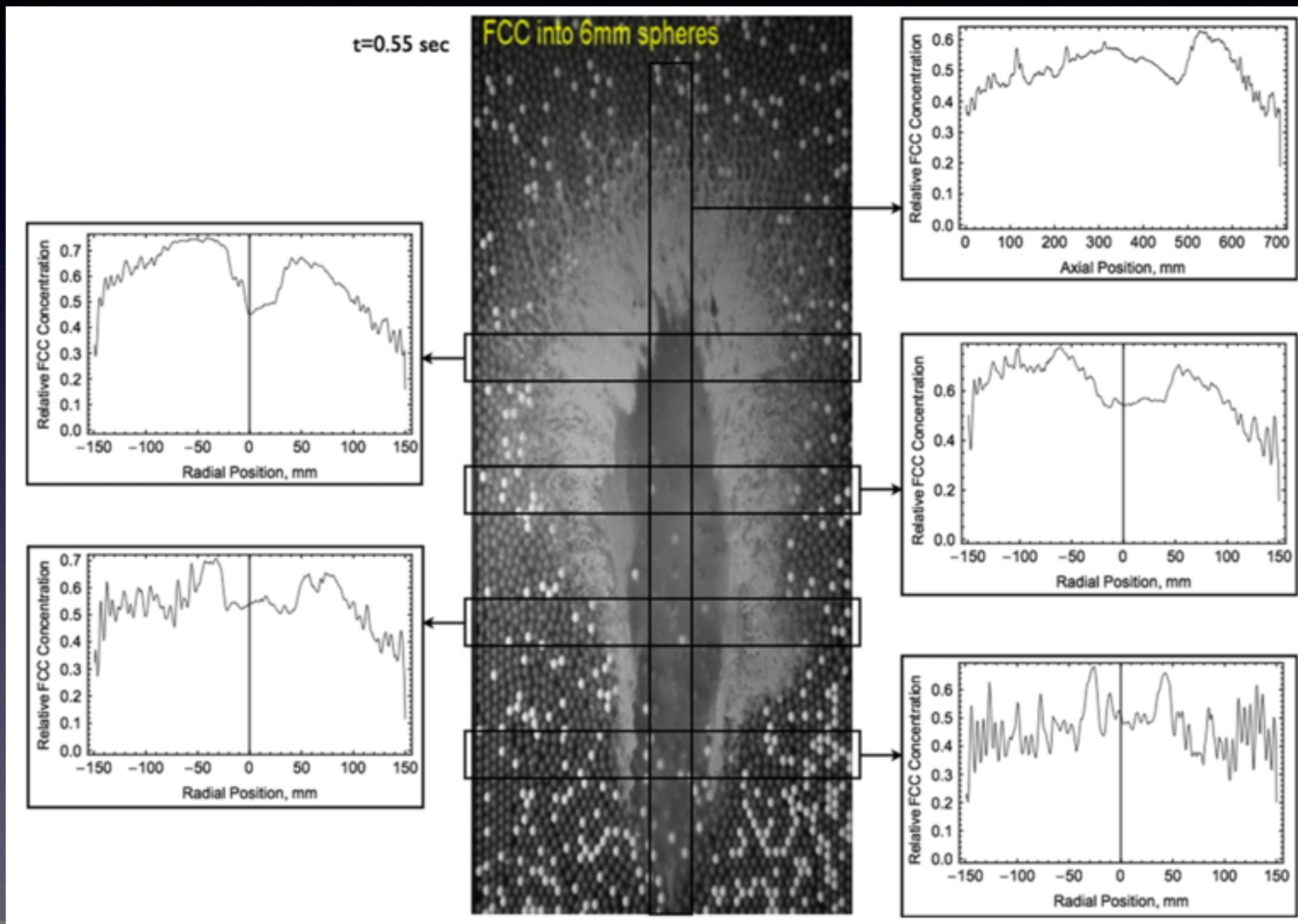
PSRI Particulate Solid Research, Inc.

Fluidization of Geldart Group D Powders



J. McMillan, F. Shaffer, B. Gopalan, J.W. Chew, C. Hrenya, R. Hays, et al., Particle Cluster Dynamics During Fluidization, Chemical Engineering Science. 100 (2013) 39–51

Fluidization of Geldart Group D Powders

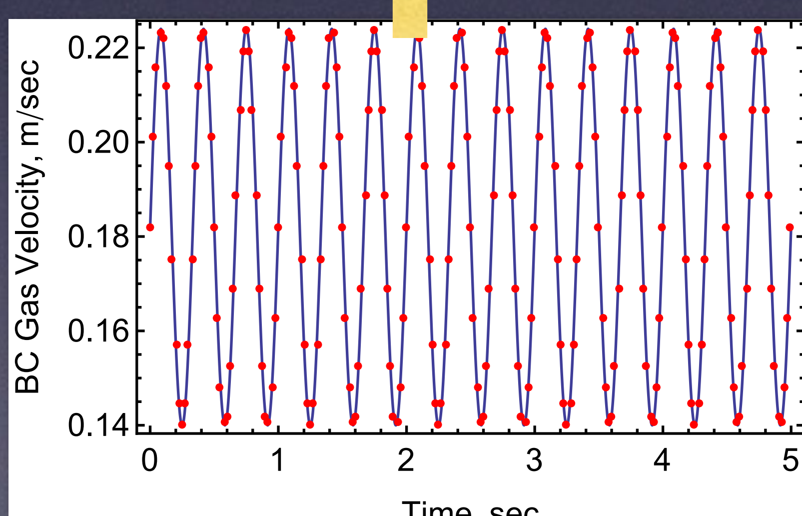


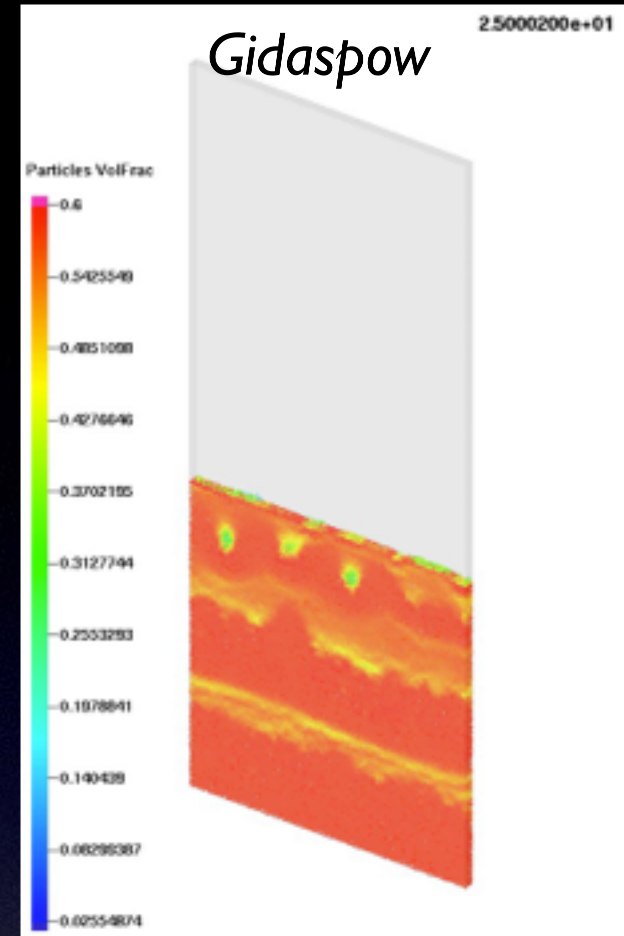
Applying the Fundamentals

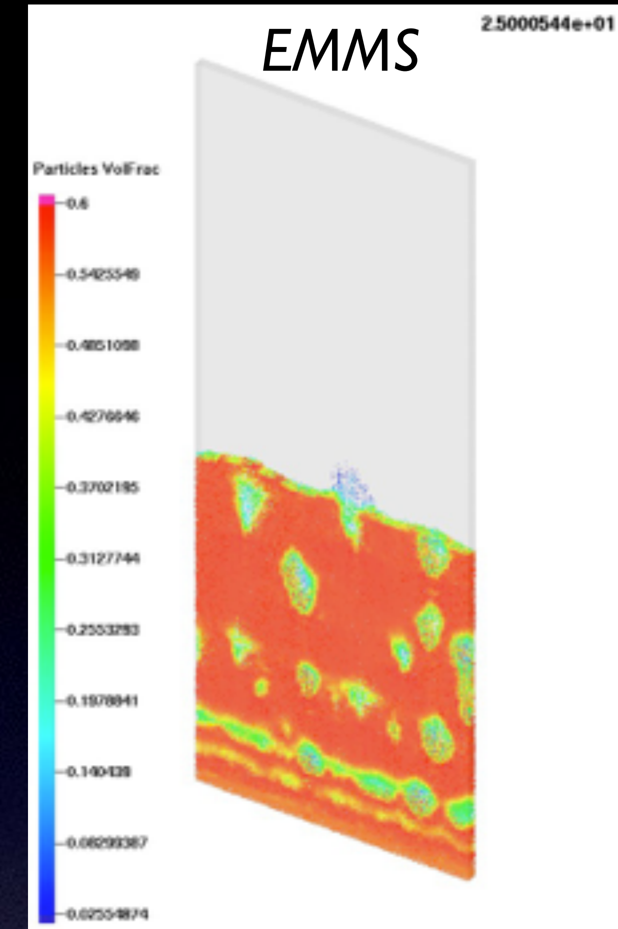
Other Experiments

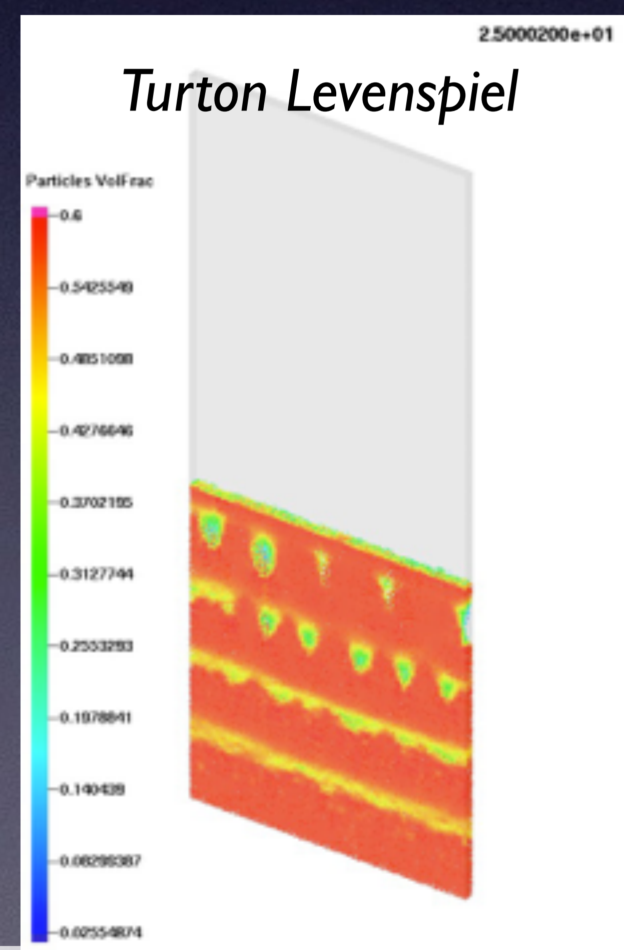
UCL 2D Bed Oscillation Experimental Study

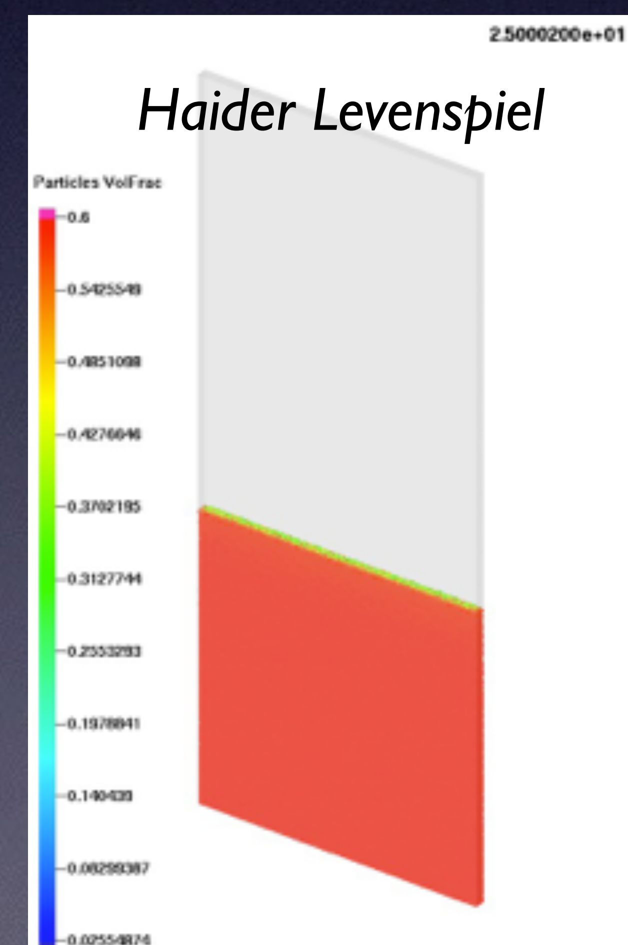
4 cm x
40 cm x
100 cm







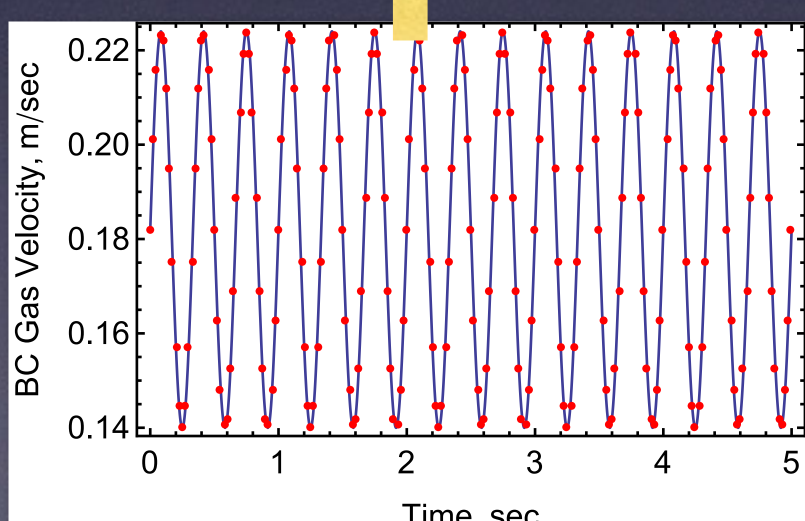


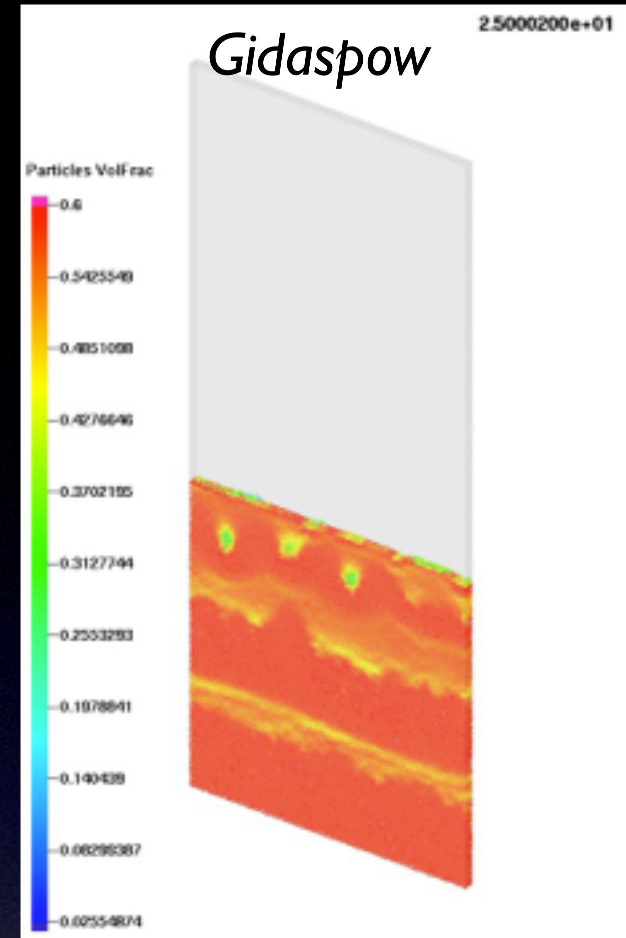


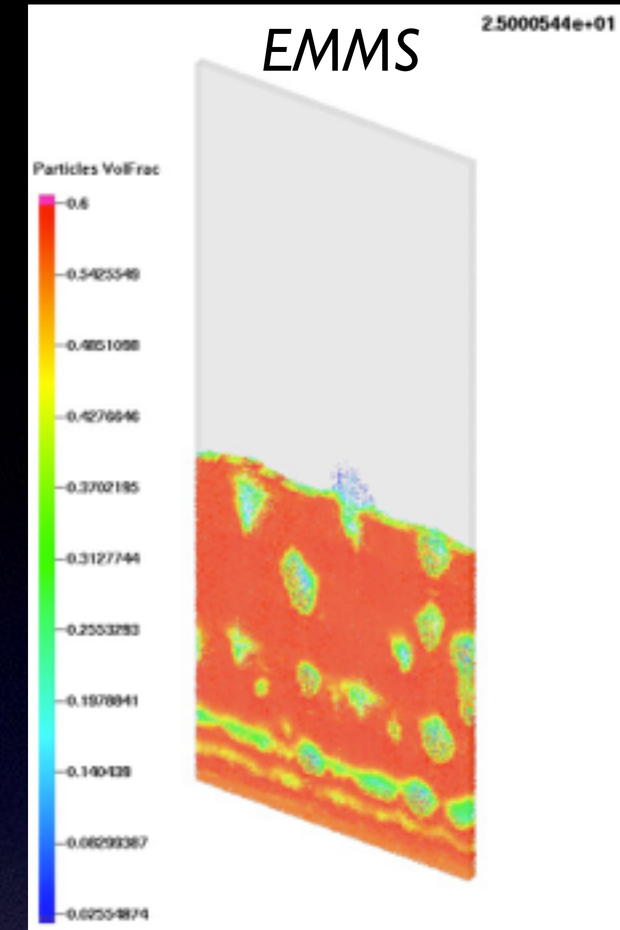
Other Experiments

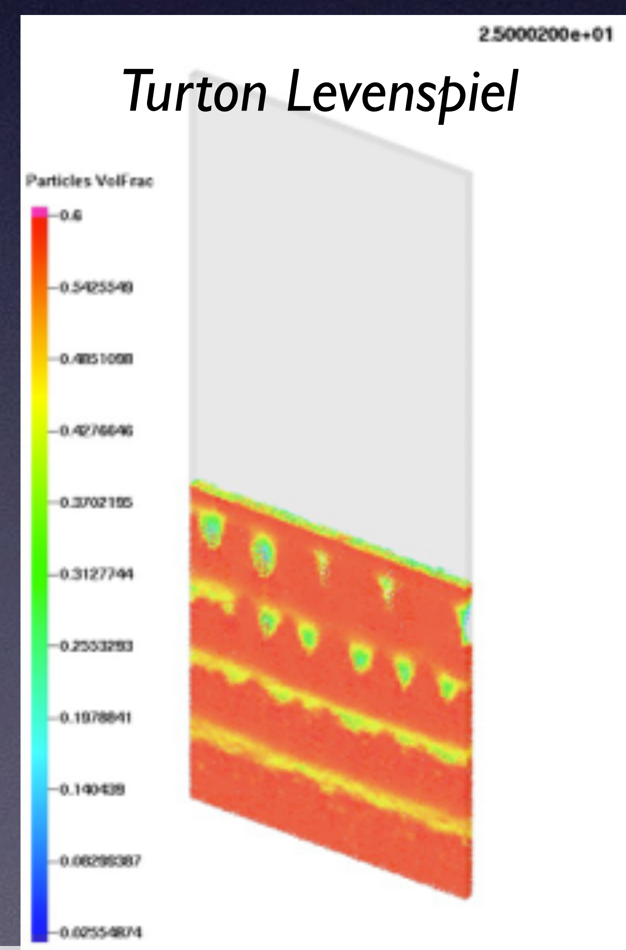
UCL 2D Bed Oscillation Experimental Study

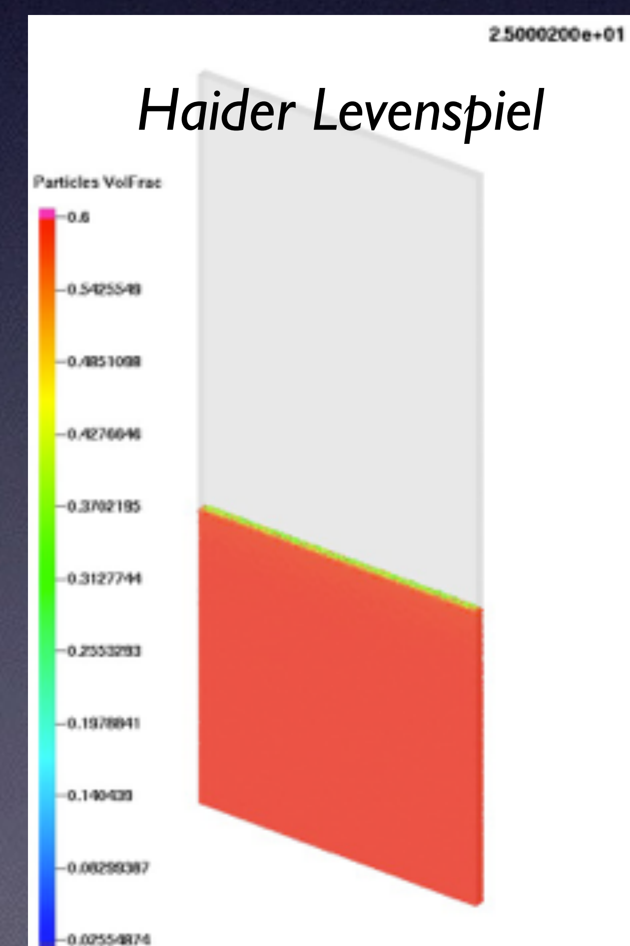
4 cm x
40 cm x
100 cm







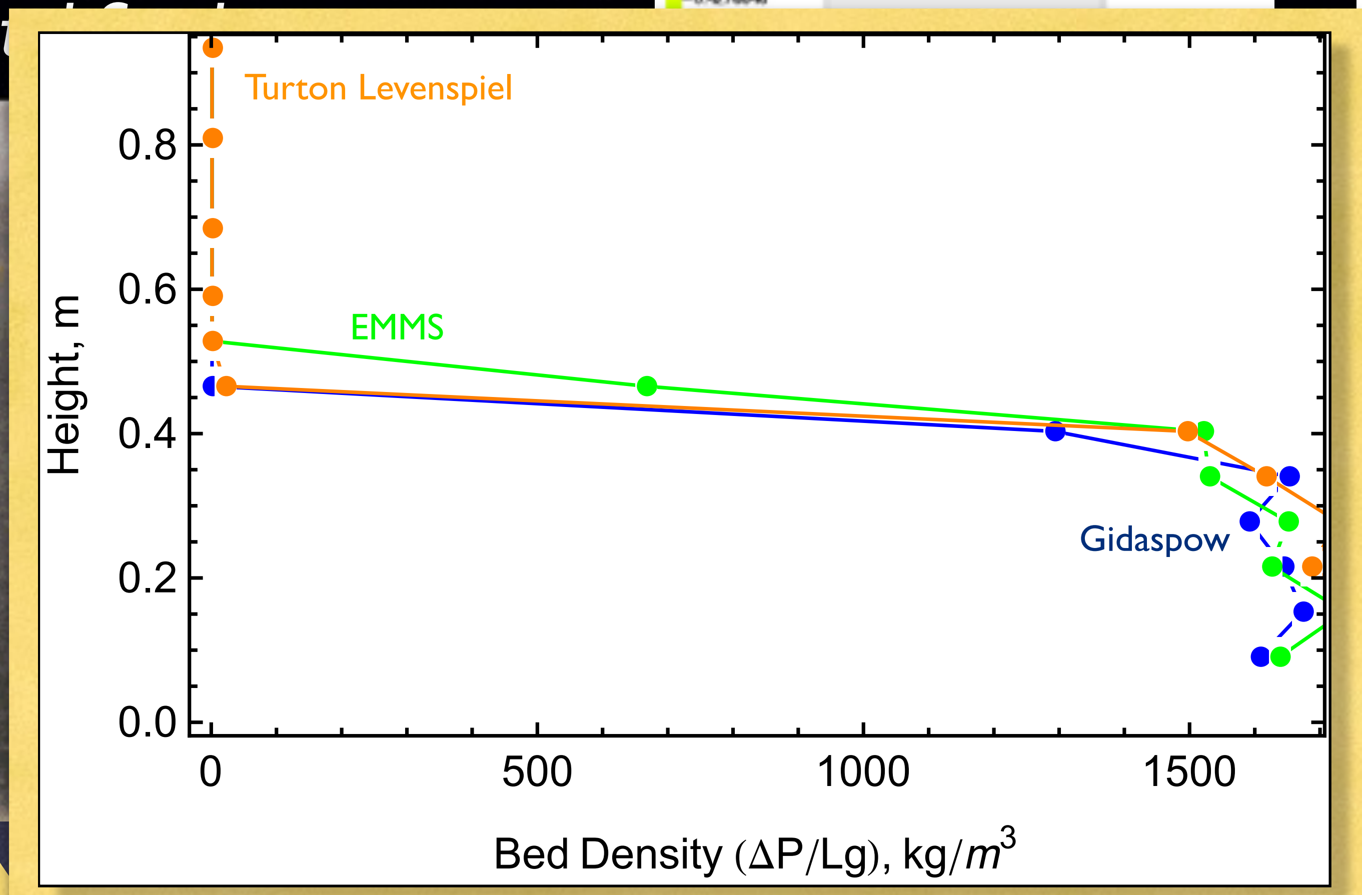


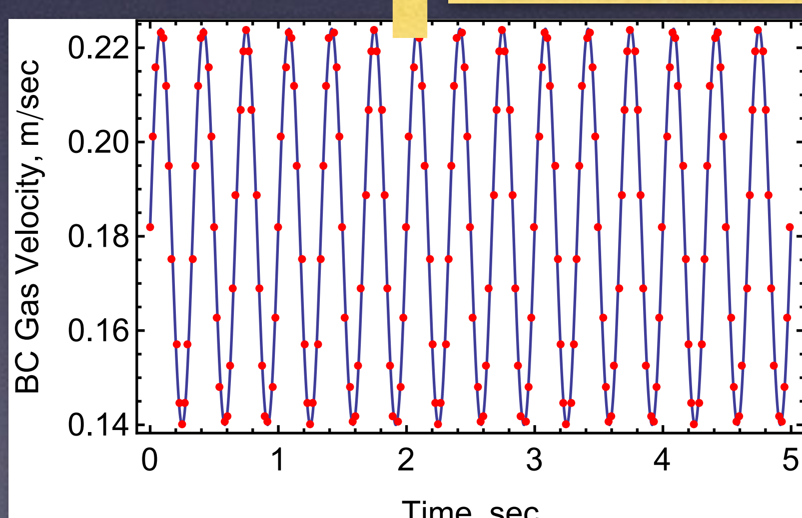


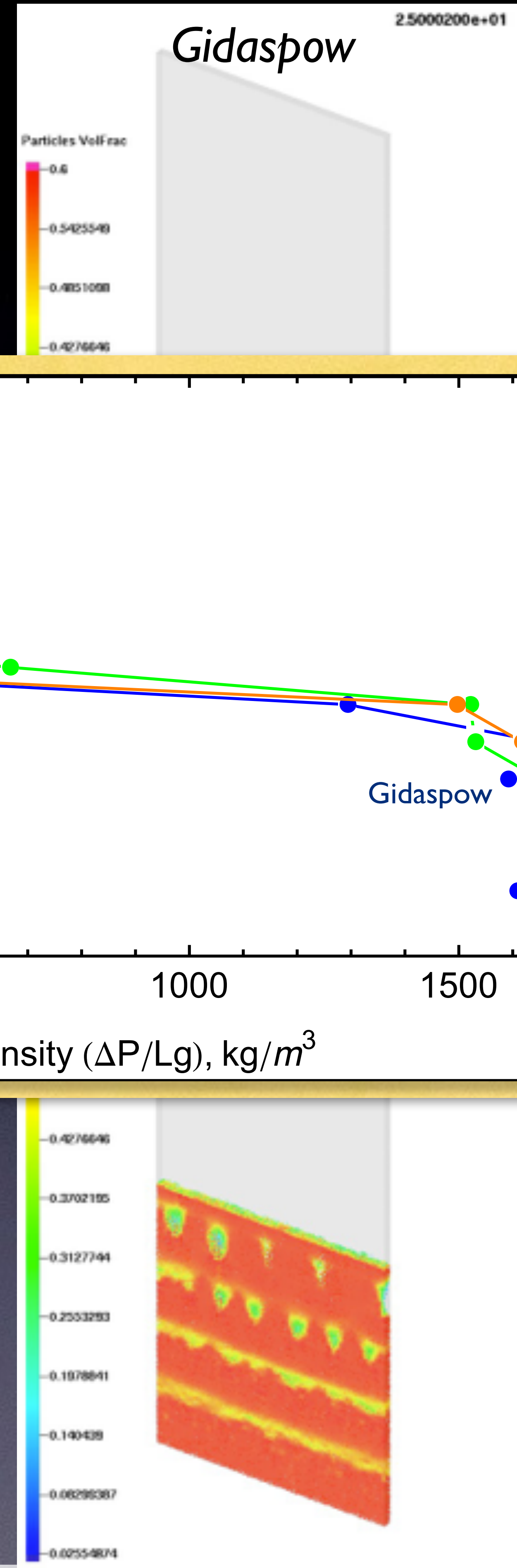
Other Experiments

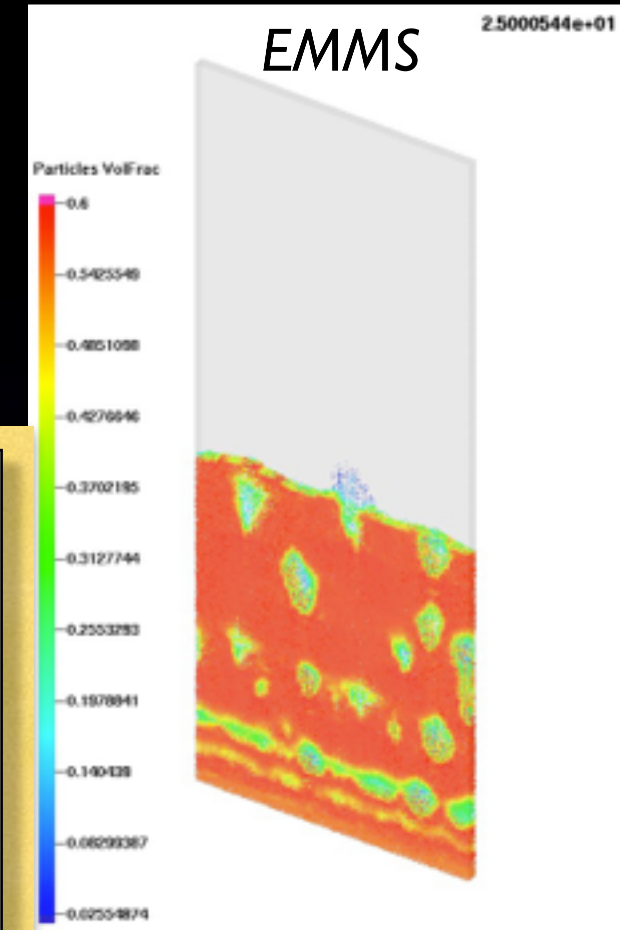
UCL 2D Bed Oscillation Experiment

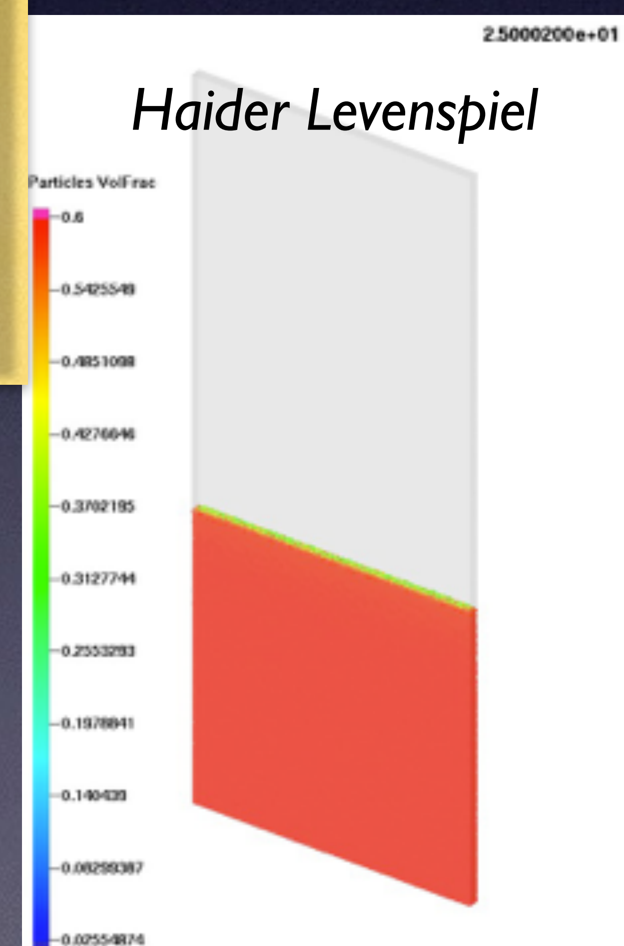
4 cm x
40 cm x
100 cm



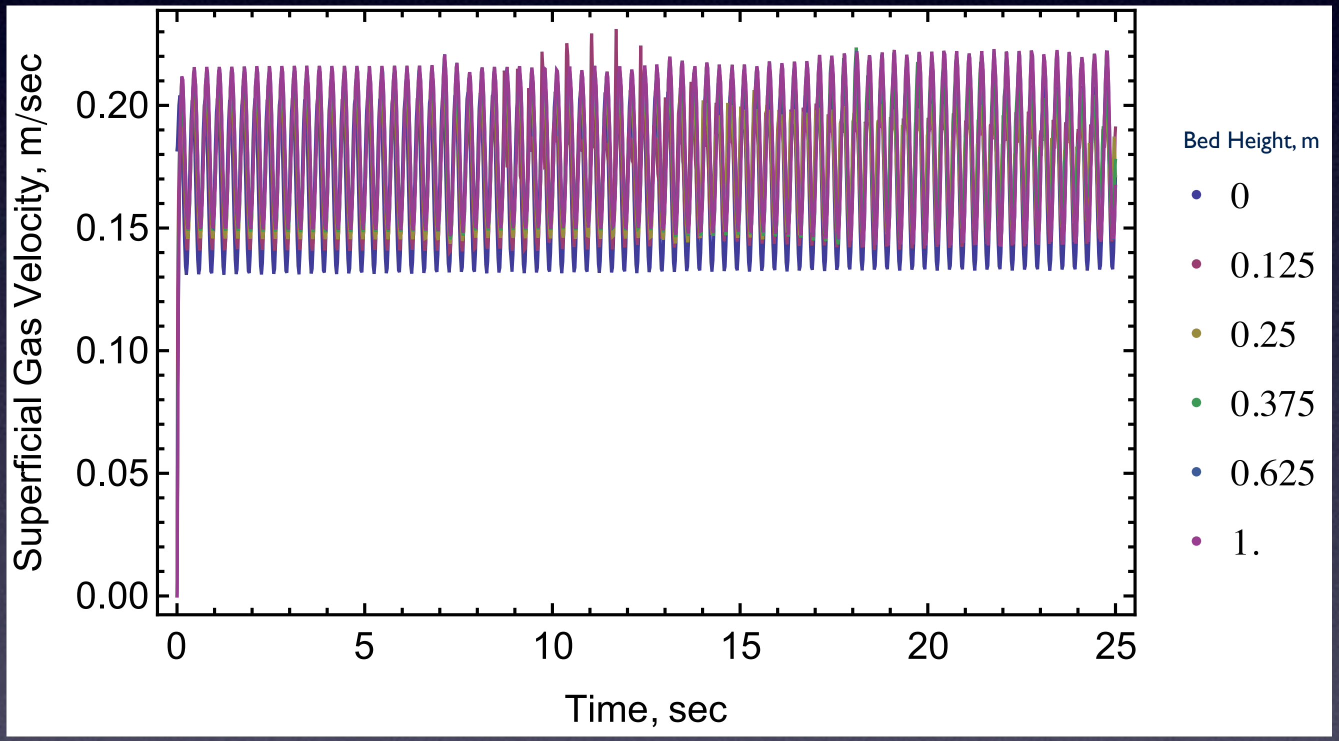


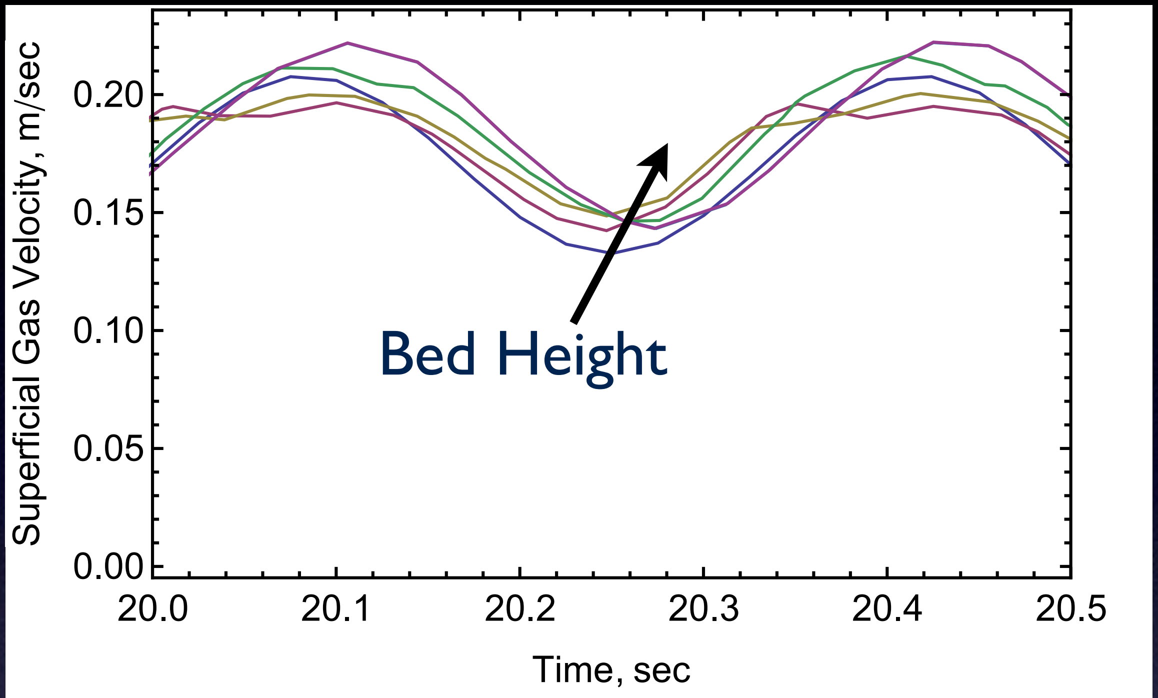


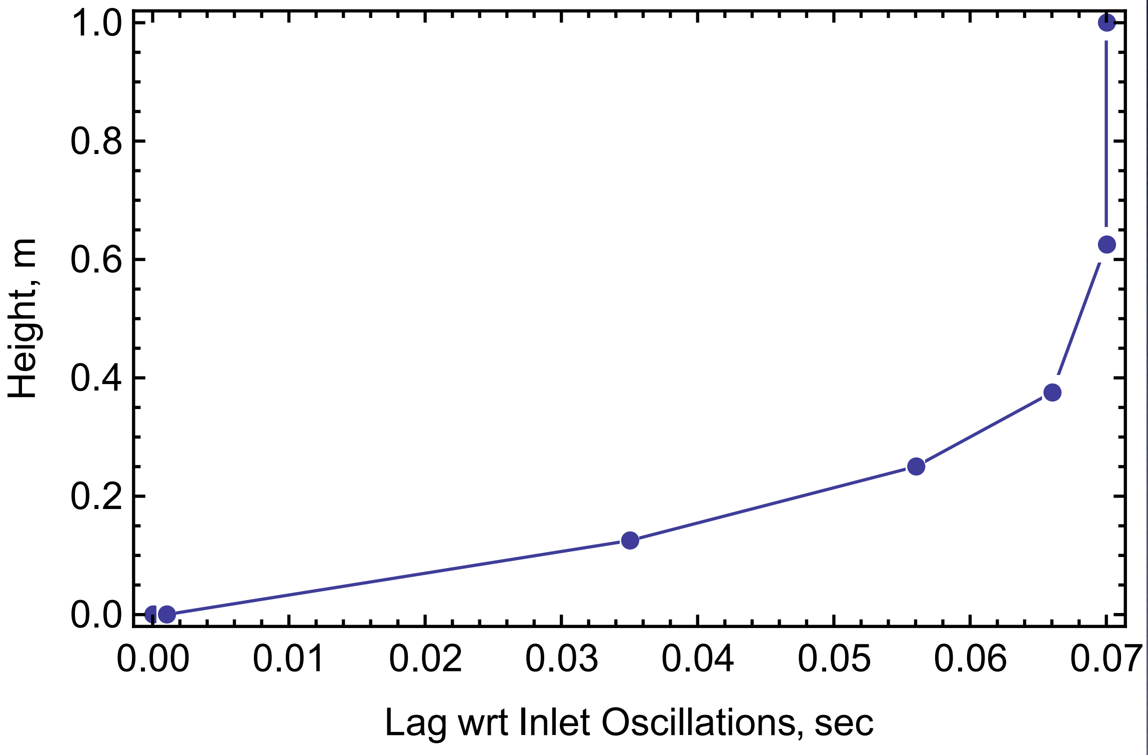




"Phase Shift" As Gas Flows Through Bed

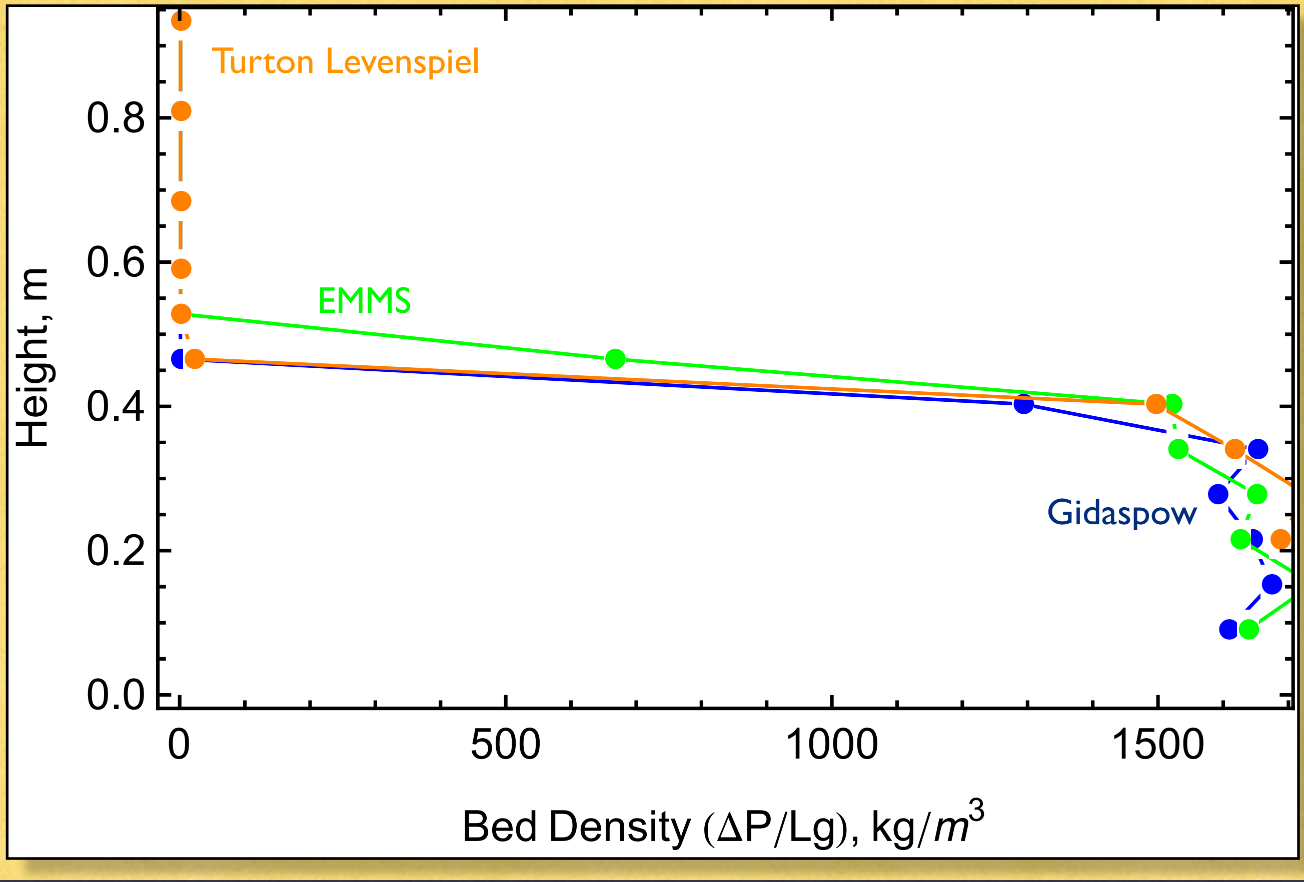


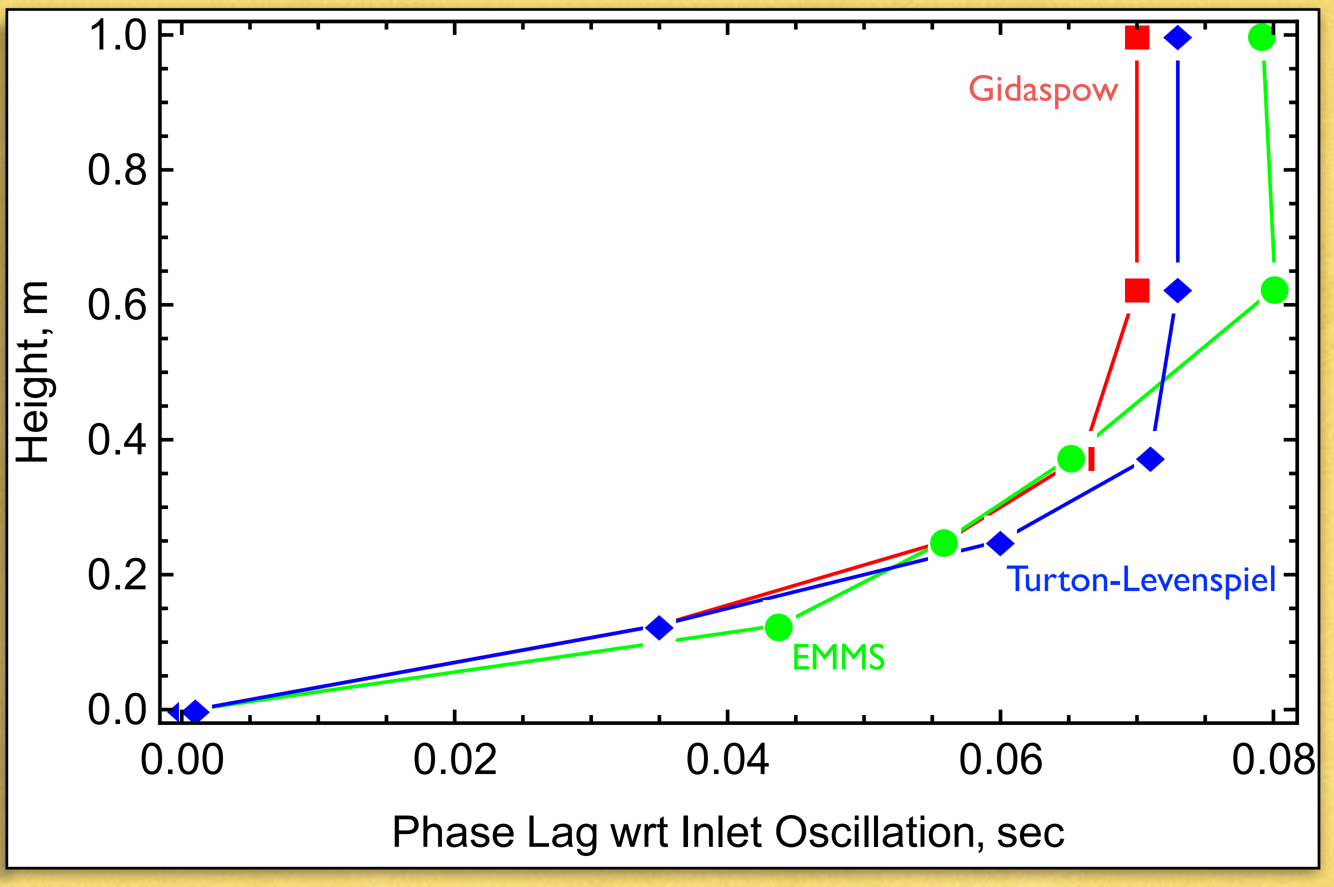




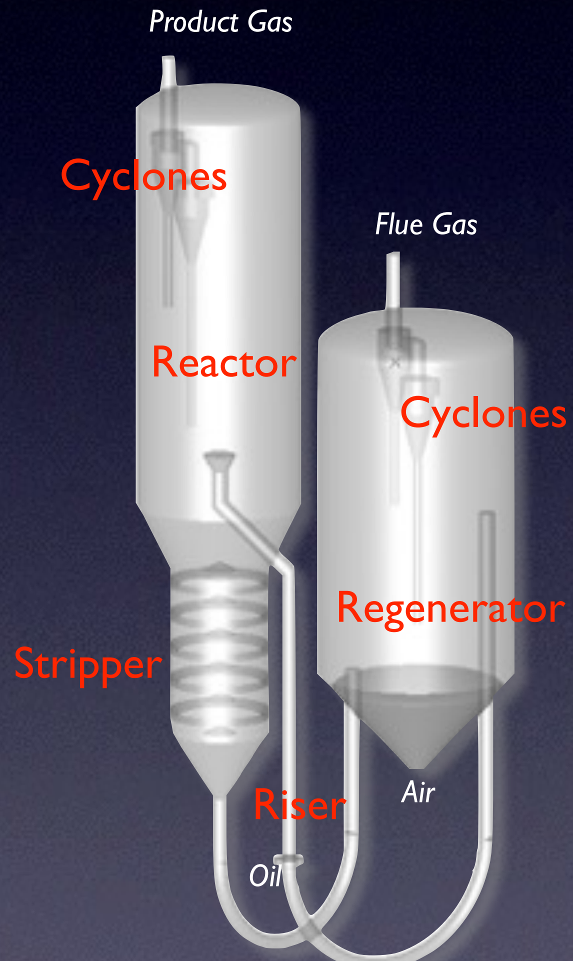
Cross-correlation used to determine how the gas fluctuation periods shift with increasing axial position

Discerning Drag with Phase Shifts in Gas Velocity?

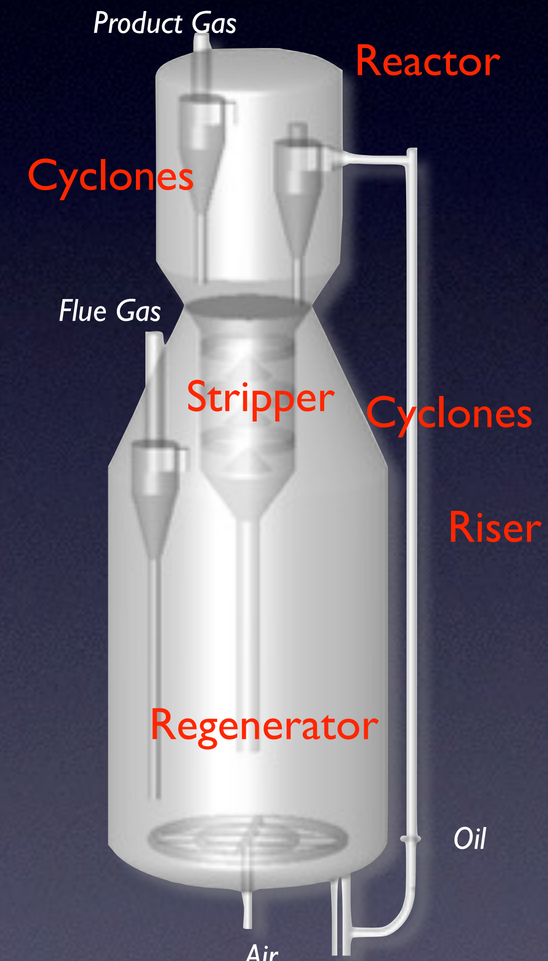




What About CFB Risers?



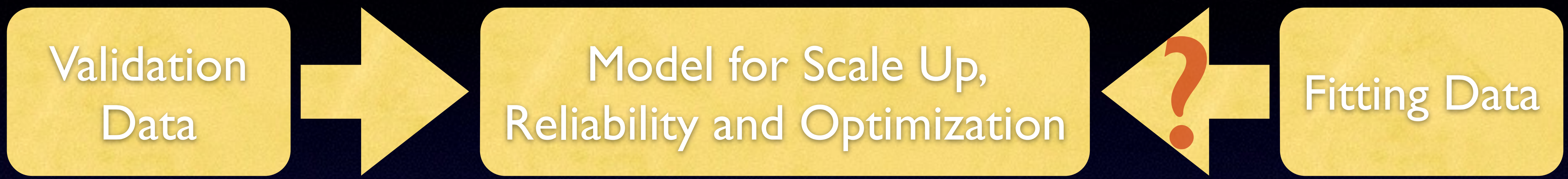
ExxonMobil IV*



KBR Stack*

*Based on D. Kunii, O. Levenspiel, Fluidization Engineering, 2nd, Butterworth-Heinemann, 1991

Question



- Do we need to develop experimental methods for model “fitting”
  - As well as continued efforts with model development
- Do we need to completely understand particle interactions or can we come up with clever experiment(s) to bridge that gap?