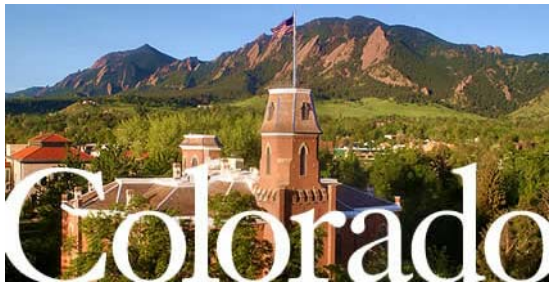
MFIX-DEM Enhancement for Industrially-Relevant Flows



2017 Crosscutting Research Project Review

Pittsburgh, PA
March 20-23, 2017

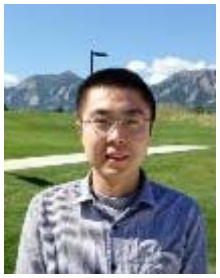
Project Leads: *Dr. Ray Cocco (PSRI, co-PI)*
Dr. Ray Grout (NREL, co-PI)
Prof. Thomas Hauser (Univ. CO, co-PI)
Prof. Christine Hrenya (Univ. CO, PI)

Project Team

University of Colorado
Chemical & Biological Engineering
DEM modeling of granular and gas-solid flows, MFIX


Prof. Christine Hrenya


Dr. William Fullmer


Dr. Peiyuan Liu

University of Colorado
Research Computing
High-performance computing, CFD


Prof. Thomas Hauser


Dr. Dane Skow


Tim Brown

NREL
Computational Science
High-performance computing, CFD


Dr. Ray Grout


Dr. Hari Sitaraman


Deepthi Vaidhynathan


Dr. Ray Cocco

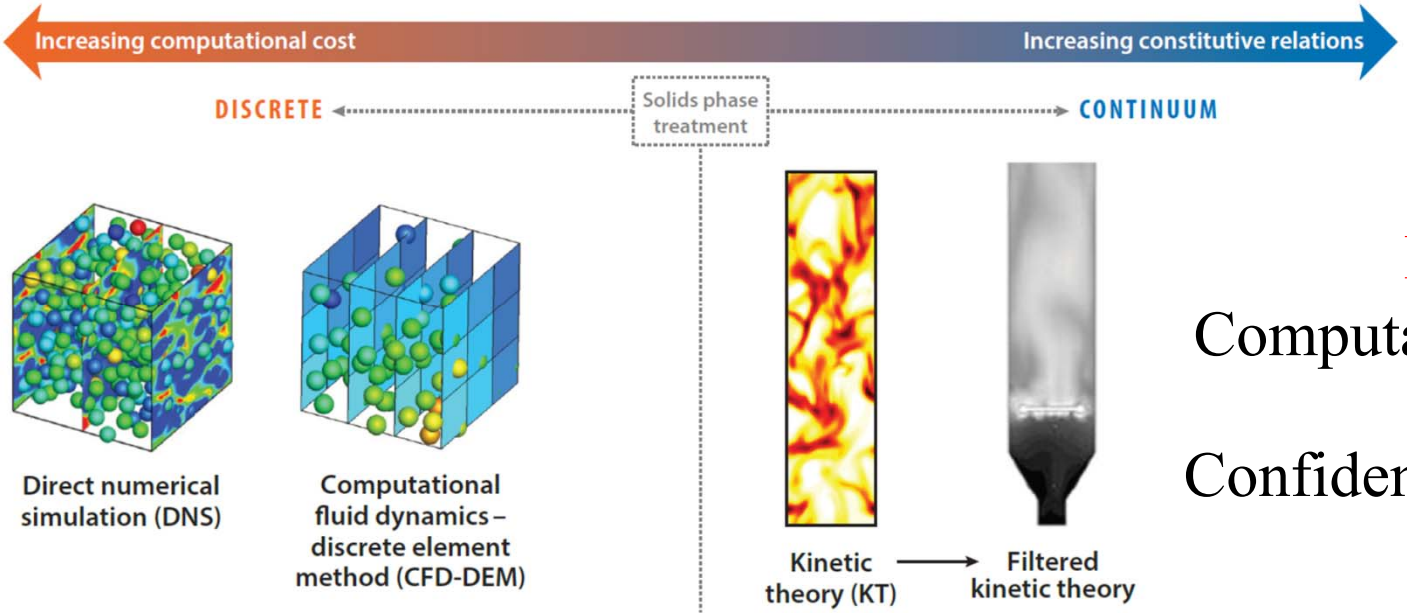

Rasa Kales


Dr. Allan Issangya


Aaron Holt

PSRI
Industrial Application and Experiments of Particle Flows

Motivation



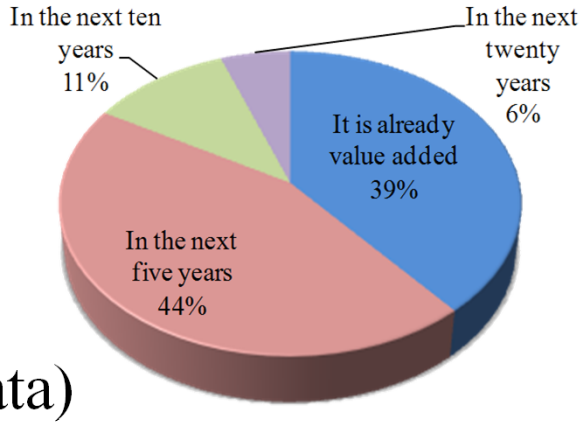
Fullmer & Hrenya
(Annu. Rev. Fluid Mech. 2017)

Barriers:
Computational Overhead
vs
Confidence in Predictions

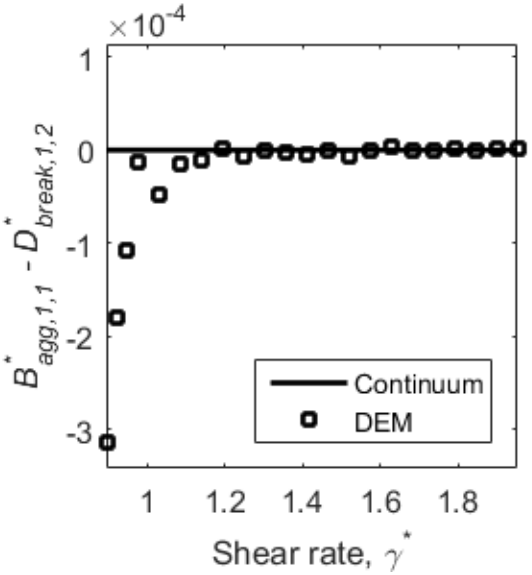
Motivation:
DEM application toward industrially-relevant systems

Potential significance of the results of the work

Expected value added through DEM:
PSRI Industrial Survey
(Cocco et al., *Chem. Eng. Prog.*, in press)

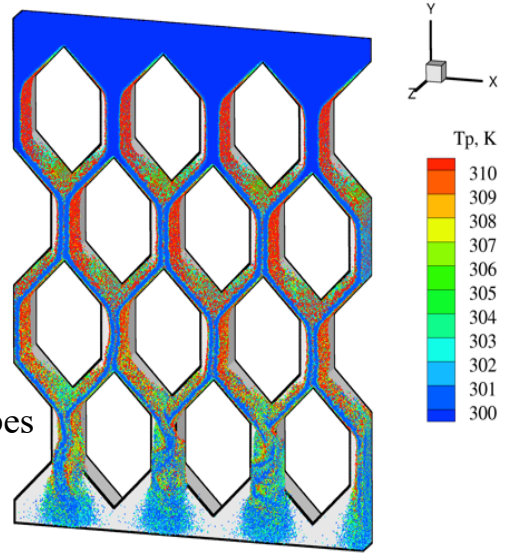


- Expanded industrial use of DEM
- Indirect: Improved physics in continuum and hybrid modeling (DEM as benchmark data)
- Direct: Aid in design/optimization of industrial components



Agglomeration balance of doublets:
Continuum Theory for Rapid, Cohesive-Particle Flows
(Kellogg, Liu, LaMarche & Hrenya, submitted)

Fully-developed characteristics:
Heat transferred to particles falling over heated tubes
(Morris et al., *Solar Energy*, 2016)



Phase I Statement of Project Objectives (SOPO)

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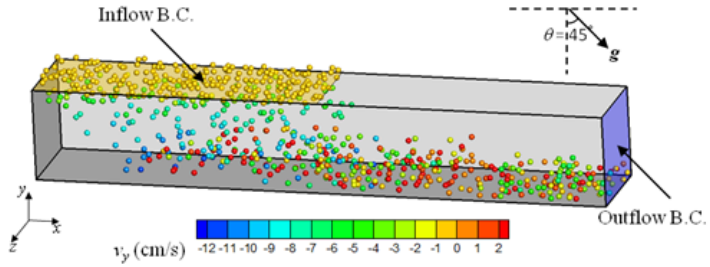
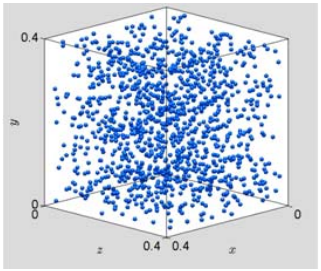
Milestone 2: Benchmark Cases

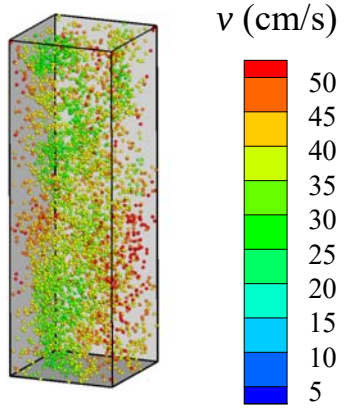
Dilute, nearly instantaneous collisions



Ramp flow

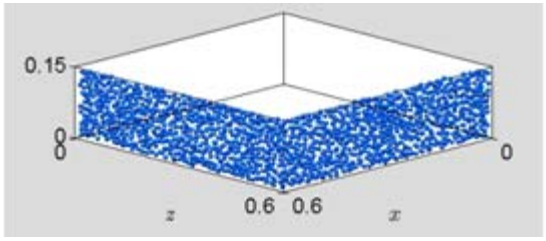


Homogeneous cooling

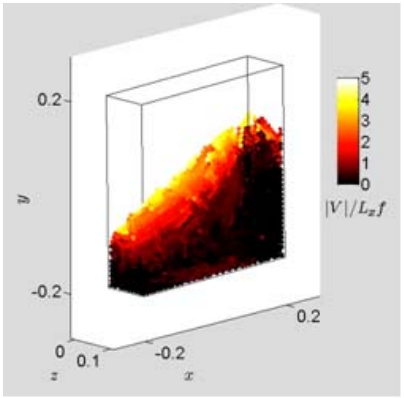


Riser flow

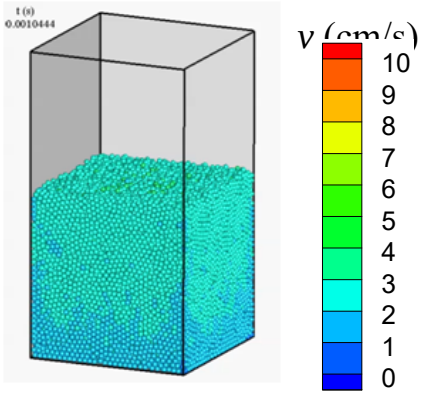
Dense, enduring contacts



Settling



Square tumbler

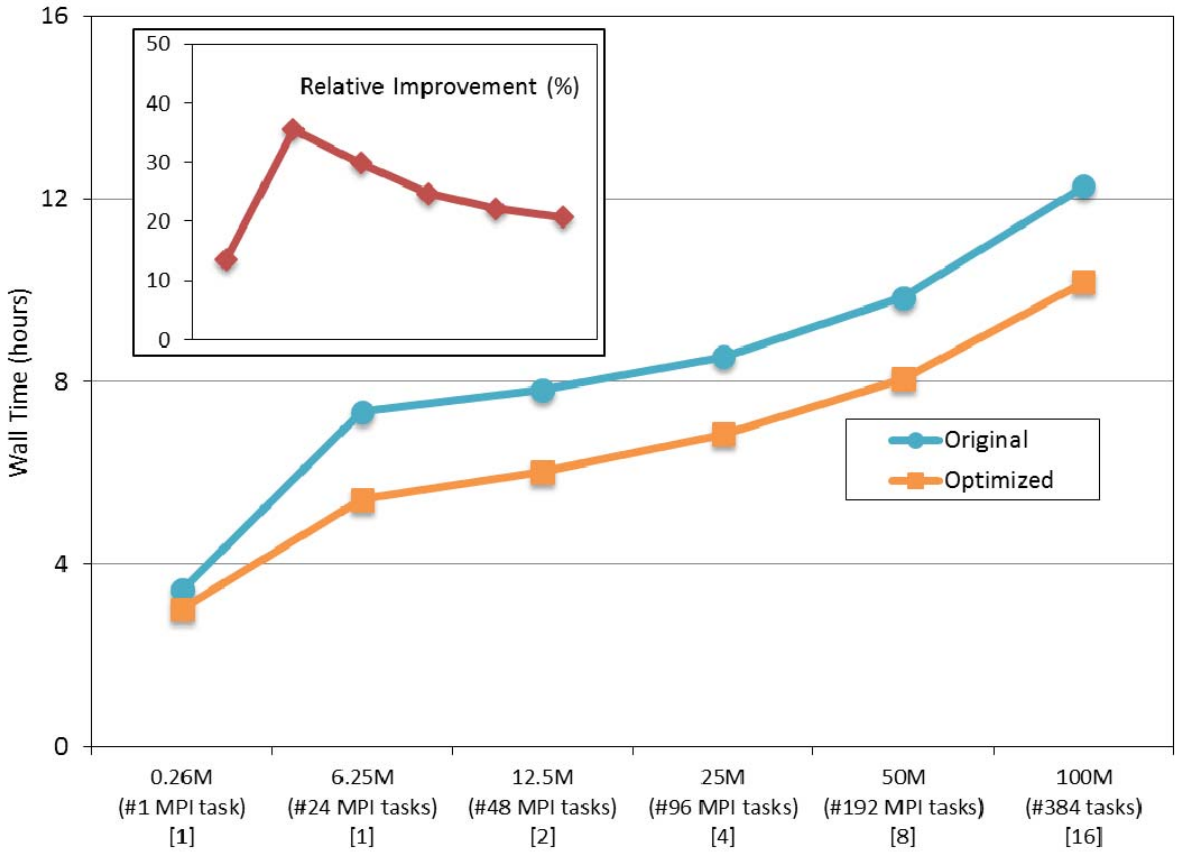


Fluidized bed

Milestone 2 report (submitted to DOE)

100M Particle Settling – Weak Scaling

- Locality-based Particle Sorting – improves neighbor search
- State-based Particle sorting – improves vectorization
- Masking – improves vectorization



Milestone 5 report (submitted to DOE)

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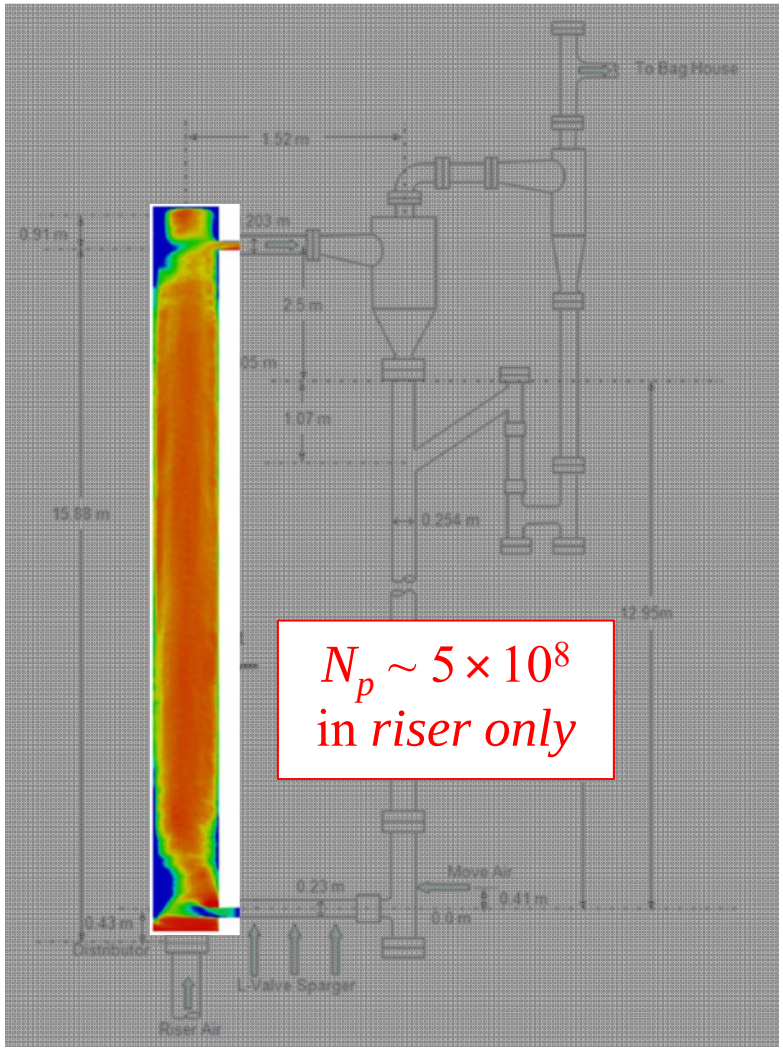
Need for CFD-DEM Validation Data

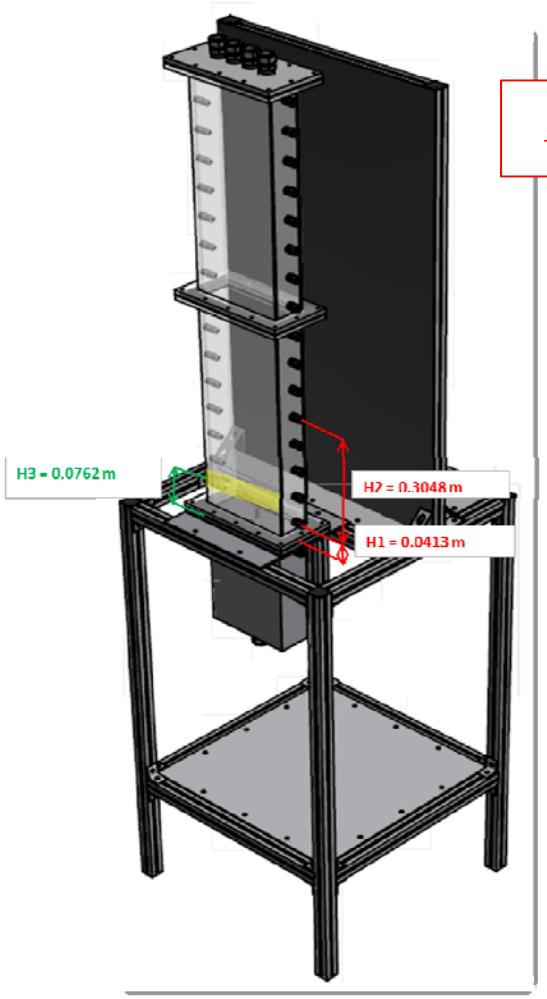
NETL/PSRI Challenge Problem III



$N_p \sim 5 \times 10^8$ in *riser only*

(Li et al., *Chem. Eng. Sci.*, 2012)

NETL Small-Scale Challenge Problem I



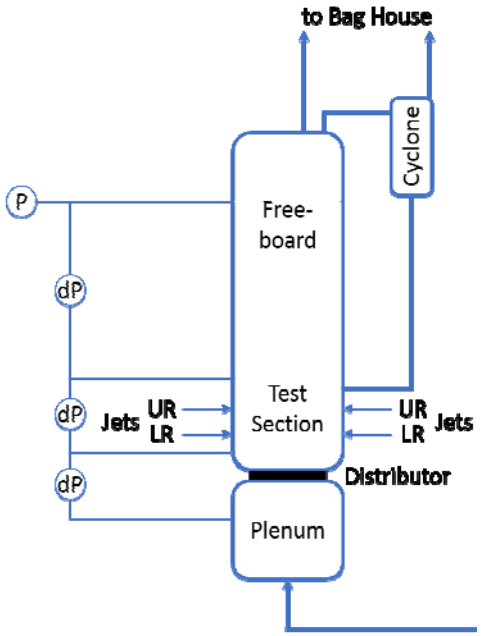
$N_p \sim 1 \times 10^5$

Rectangular FB
W = 23 cm
D = 7.6 cm
H = 122 cm

(Gopalan et al., *Powder Tech.*, 2016)

Horiz. Jet Experiments: Unit and Materials

Semi-circular Fluidized Bed with Side Jets



Characteristics:

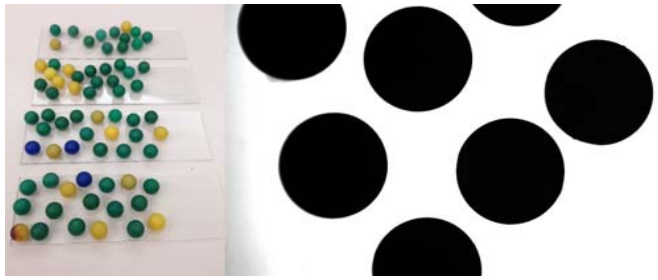
- $W = 11.25$ in
- $h_{bed} \sim W$
- $d_j \sim 4$ mm
- $U \sim U_{mf}$ $\sim$ 30-150 cm/s
- $U_j \sim 200$ m/s

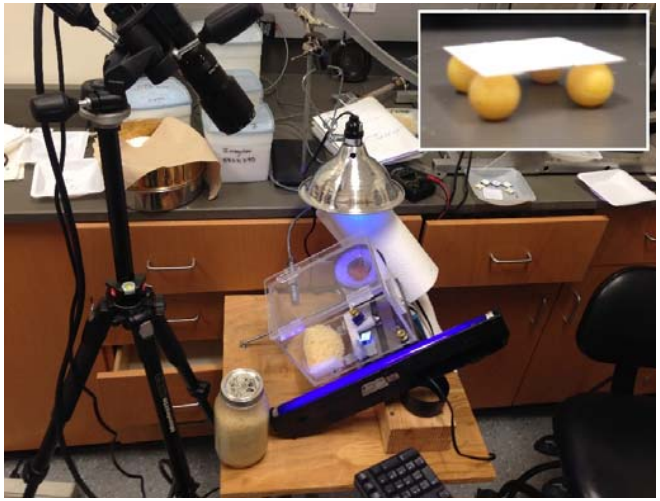
Materials

- **6.0 mm plastic:** $N_p \sim 6 \times 10^4$
- **3.0 mm ceramic:** $N_p \sim 4 \times 10^5$
- 1.6 mm mix: $N_p \sim 3 \times 10^6$
- 1.5 mm glass: $N_p \sim 4 \times 10^6$
- 1.0 mm ceramic: $N_p \sim 1 \times 10^7$
- 0.8 mm glass: $N_p \sim 3 \times 10^7$

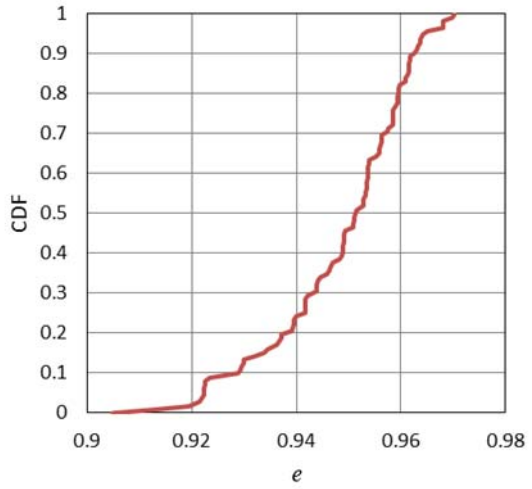
Horiz. Jet Experiments: Particle Characterization

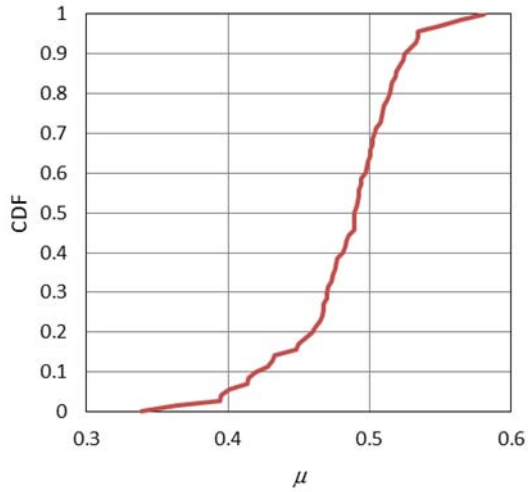
Methods





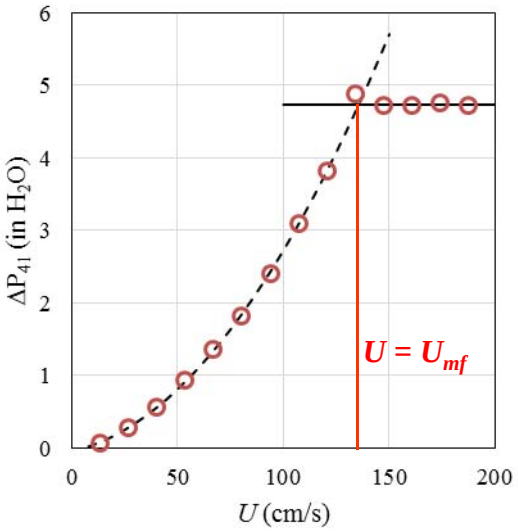
Results





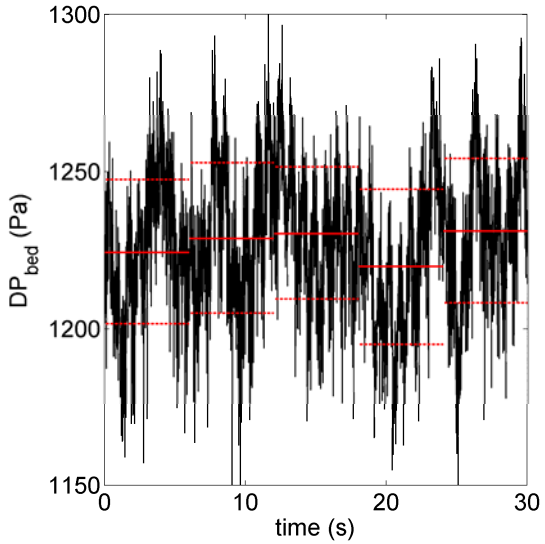
Horiz. Jet Experiments: Pressure Drop

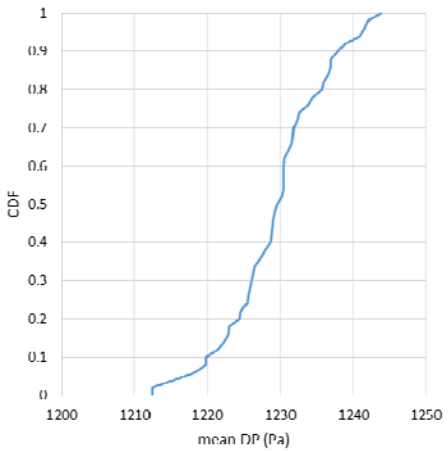
Fluidization Curve

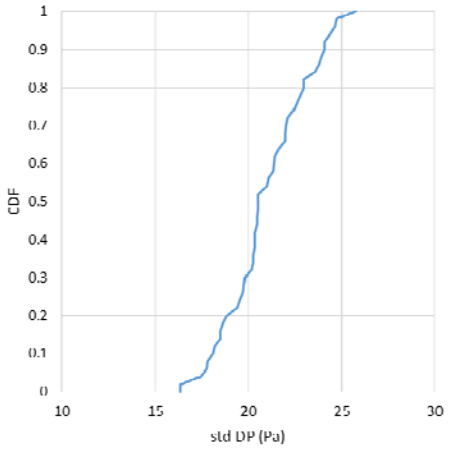


U_{mf} = 135 cm/s
Bed operated at:
$U \sim$ 90% & 110% of U_{mf}

DP Results



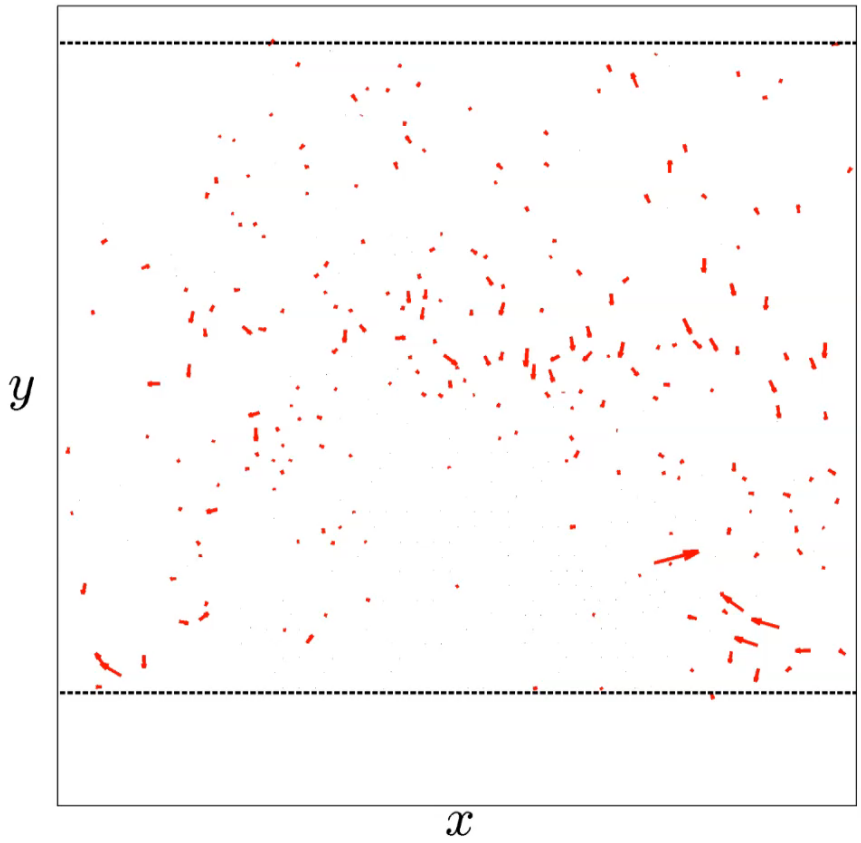




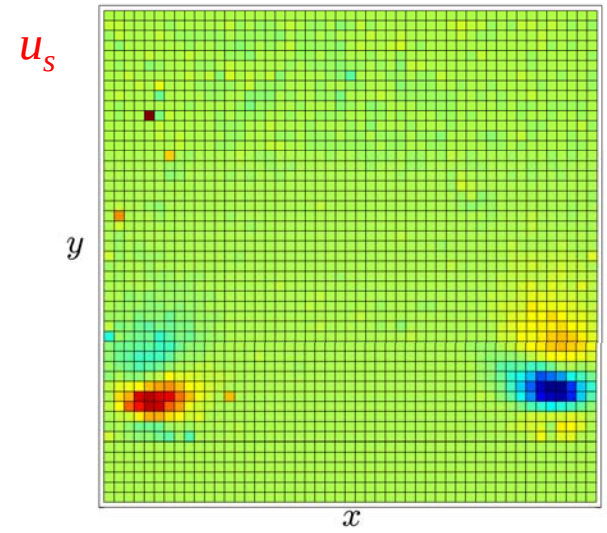
Horiz. Jet Experiments: HSV and PT

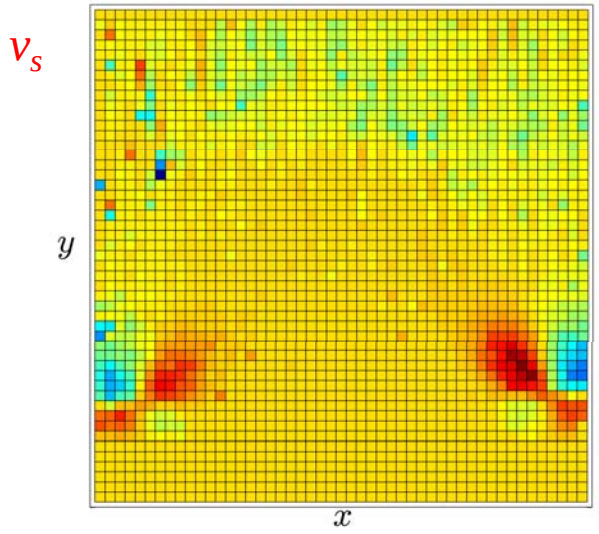
Raw HSV Data

Particle Tracking (PT) Analysis



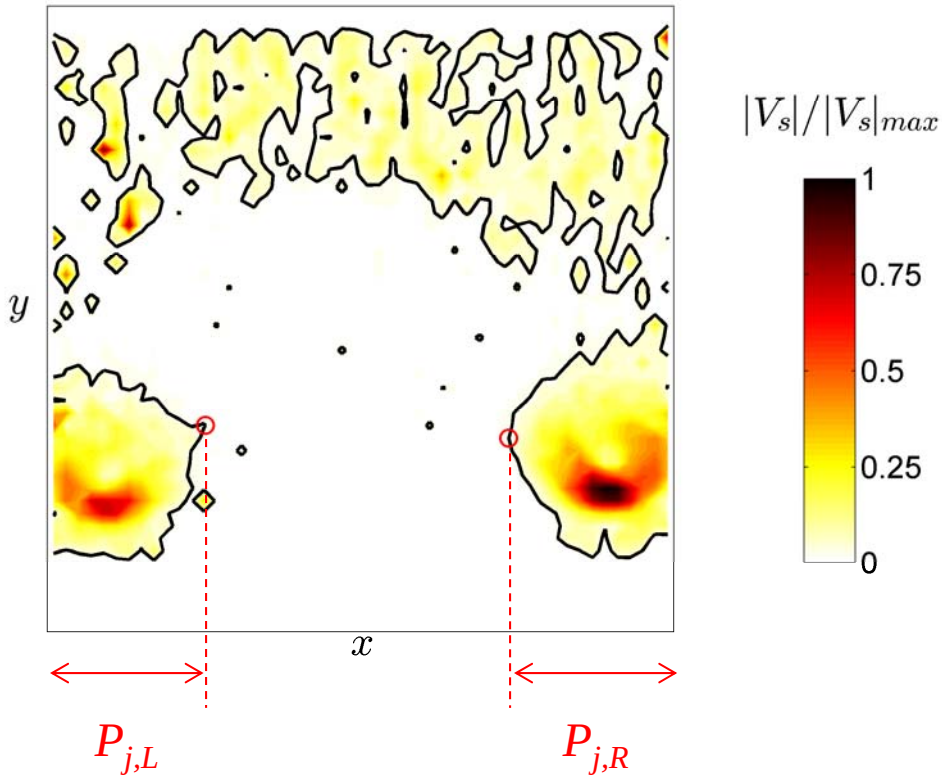
Horiz. Jet Experiments: PT Post-processing





Jet Penetration Results

5% Isoline



Milestone 6b report (submitted to DOE)

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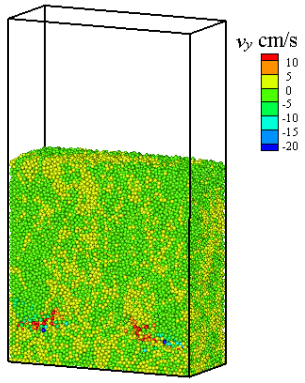
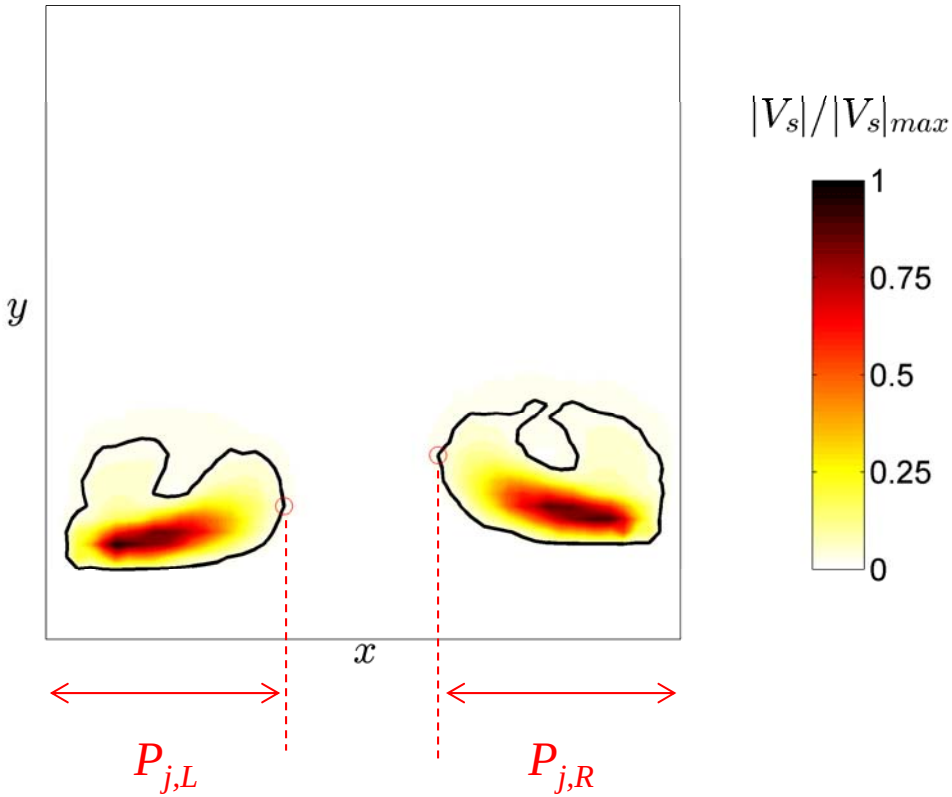
CFD-DEM+UQ: Base Case

CFD-DEM Model Description

- Rectangular geometry
- Point sources for jets
- Incompressible
- No shear- or particle-induced turbulence models
- Uniform inflow
- No-slip wall BC for gas
- $\Delta x \sim 2\, d_p$



Jet Penetration Depth:
<u>same</u> analysis as exp data



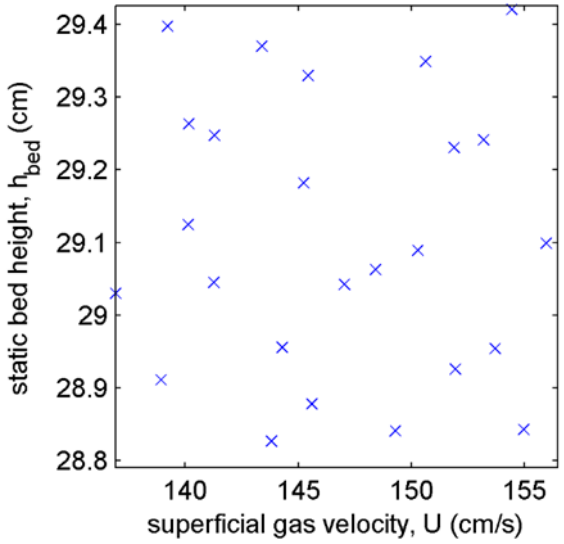
CFD-DEM+UQ: PIRT

Parameter Identification and Ranking Table

	Input Uncertainties				SRQ Ranking		
Parameter	lower bound	base case	upper bound	type	$P_{i,L}$	$P_{i,R}$	ΔP
Bed							
U (cm/s)	136.9	146.7	156.5	e	100.0	100.0	100.0
$U_{i,L}$ (m/s)	189.2	200.9	212.5	e	2.2	1.1	1.2
$U_{i,R}$ (m/s)	182.8	194.4	205.9	e	0.5	4.9	1.0
h_{bed} (cm)	28.8	29.1	29.4	e	0.3	1.1	29.9
A (cm^2)	333.1	340.4	347.8	e	-	-	-
Left Jets							
$A_{i,L}$ (cm^2)	0.1168	0.1171	0.1174	e	-	-	-
$y_{i,L}$ (cm)	5.067	5.146	5.225	e	0.0	0.0	0.0
$z_{i,L}$ (cm)	1.588	1.667	1.746	e	0.0	0.0	0.0
$d_{i,L}$ (cm)	-0.3175	0.000	0.3175	e	-	-	-
Right Jets							
$A_{i,R}$ (cm^2)	0.1168	0.1171	0.1174	e	-	-	-
$y_{i,R}$ (cm)	5.377	5.456	5.535	e	0.0	0.0	0.0
$z_{i,R}$ (cm)	1.667	1.746	1.826	e	1.5	18.2	2.1
$d_{i,R}$ (cm)	-0.3175	0.000	0.3175	e	-	-	-
Particle-phase Properties							
d_p (μm)	5761	5924	6006	a	1.8	4.9	6.8
ϕ (-)	0.931	0.943	0.948	a	0.0	0.0	0.0
ρ_p (g/cm^3)	1.042	1.0435	1.045	e	0.2	0.3	1.2
e_{pp} (-)	0.819	0.948	0.990	a	3.3	9.4	0.6
μ_{pp} (-)	0.338	0.482	0.581	a	2.8	6.3	2.2
e_{pw} (-)	0.905	0.948	0.970	a	0.0	1.0	0.1
μ_{pw} (-)	0.338	0.482	0.581	a	0.4	0.6	2.7
Gas-phase Properties							
ρ_g (g/cm^3 × 10^3)	1.1104	1.1697	1.2290	e	7.3	10.6	3.3
μ_g (g/cm-s × 10^5)	1.7	1.8	1.9	e	2.3	2.9	0.5

1. $> 10^{1.5}$ Important
2. $10^{1.5} - 10^{1.0}$ Mildly Important
3. $10^{1.0} - 10^{0.5}$ Marginal
4. $10^{0.5} - 10^{0.0}$ Mildly Insignificant
5. $< 10^{0.0}$ Insignificant

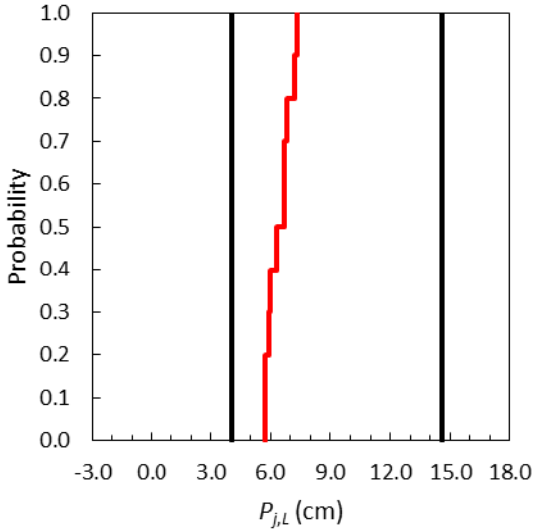
Sampling

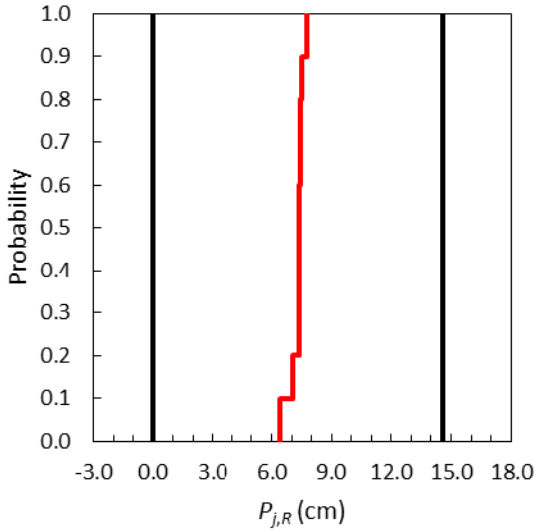


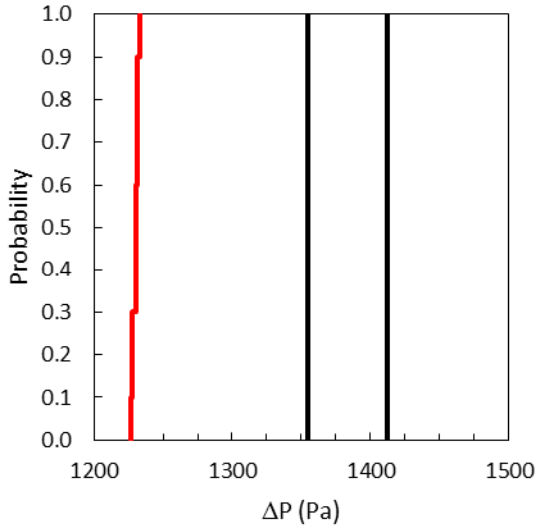
Milestone 7 report (submitted to DOE)

CFD-DEM+UQ: Results

Empirical CFDs of the *experimental results (red line)*
with the *CFD-DEM propagated UQ in the SRQs (black lines)*

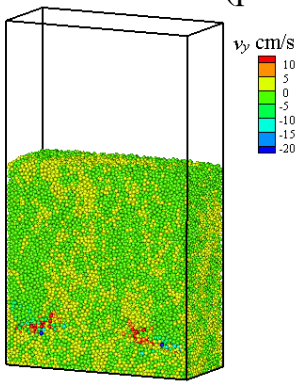


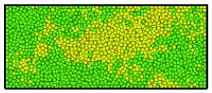




Phase-II CFD-DEM+UQ: *Very* Preliminary Results

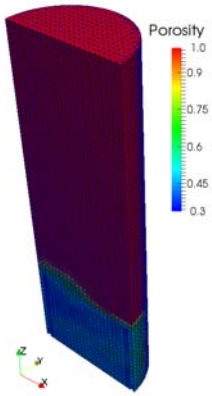
Rectangular geometry w/ point-source jets
(previous)

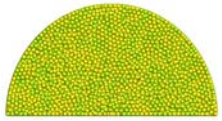




Bottom view

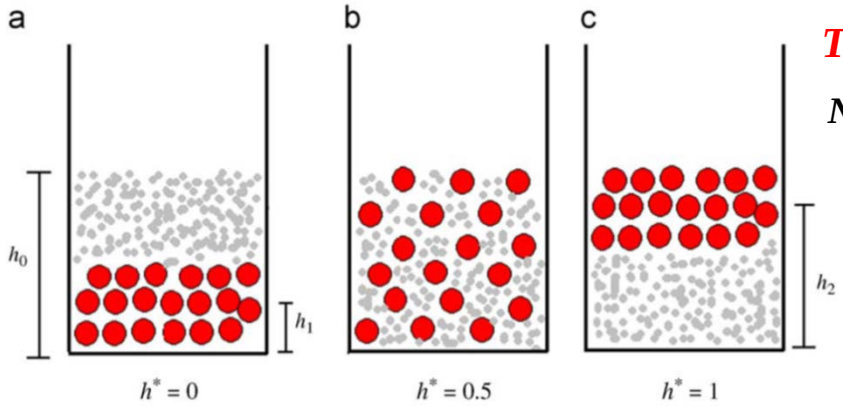
Semi-elliptical geometry w/ cut-cells & point-source jets
(in progress)





Bottom view

Phase-II Outlook



Task 8: Very, Very Small Scale Problem

$N_p \sim O(3)$

Task 9: Countercurrent Air Flow Stripper Unit

thank you for your attention