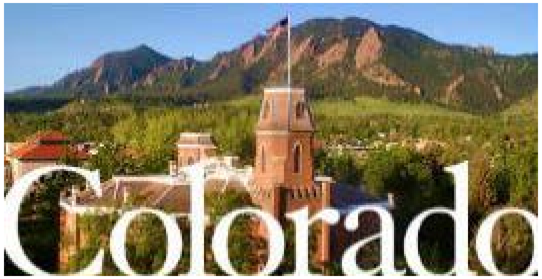
Validation and Uncertainty Quantification of MFIX-DEM Simulations of a Semicircular Fluidized Bed with Horizontal Air Jets: Preliminary Results



NATIONAL RENEWABLE ENERGY LABORATORY

PSRI

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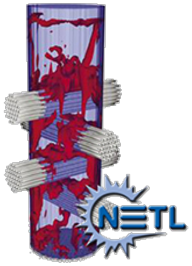
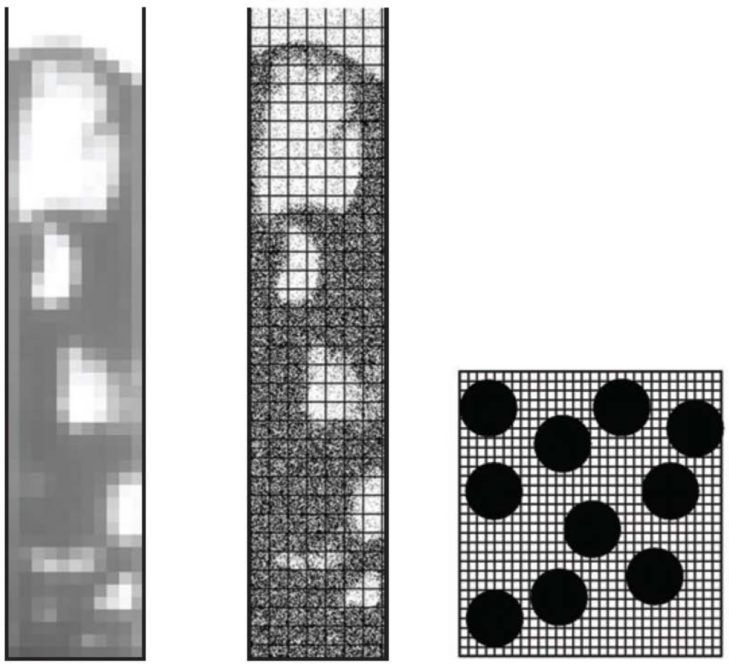
Prof. Thomas Hauser *(Univ. CO, co-PI)*
Prof. Christine Hrenya *(Univ. CO, PI)*



2017 Workshop on
Multiphase Flow Science

August 8, 2017

Background:
Numerical Methods for Studying Gas-solid Flows



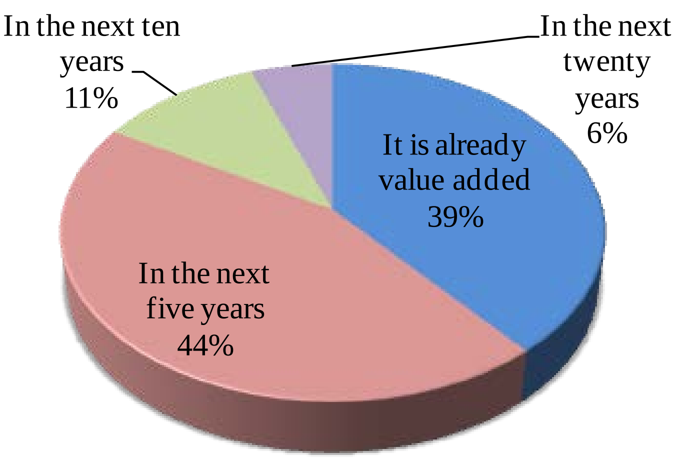
TFM CFD-DEM DNS

More detail, fewer closures →

← *Less CPU time*

van der Hoef et al. ARFM (2008)

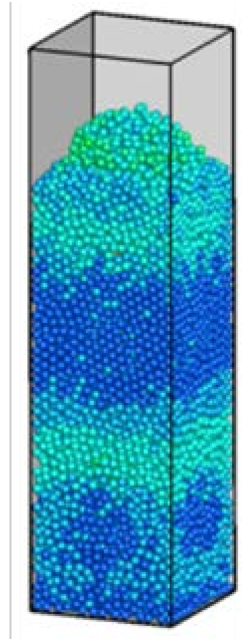
Expected value added through DEM



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

DEM: a balance between computational overhead and sources of uncertainty

Motivation



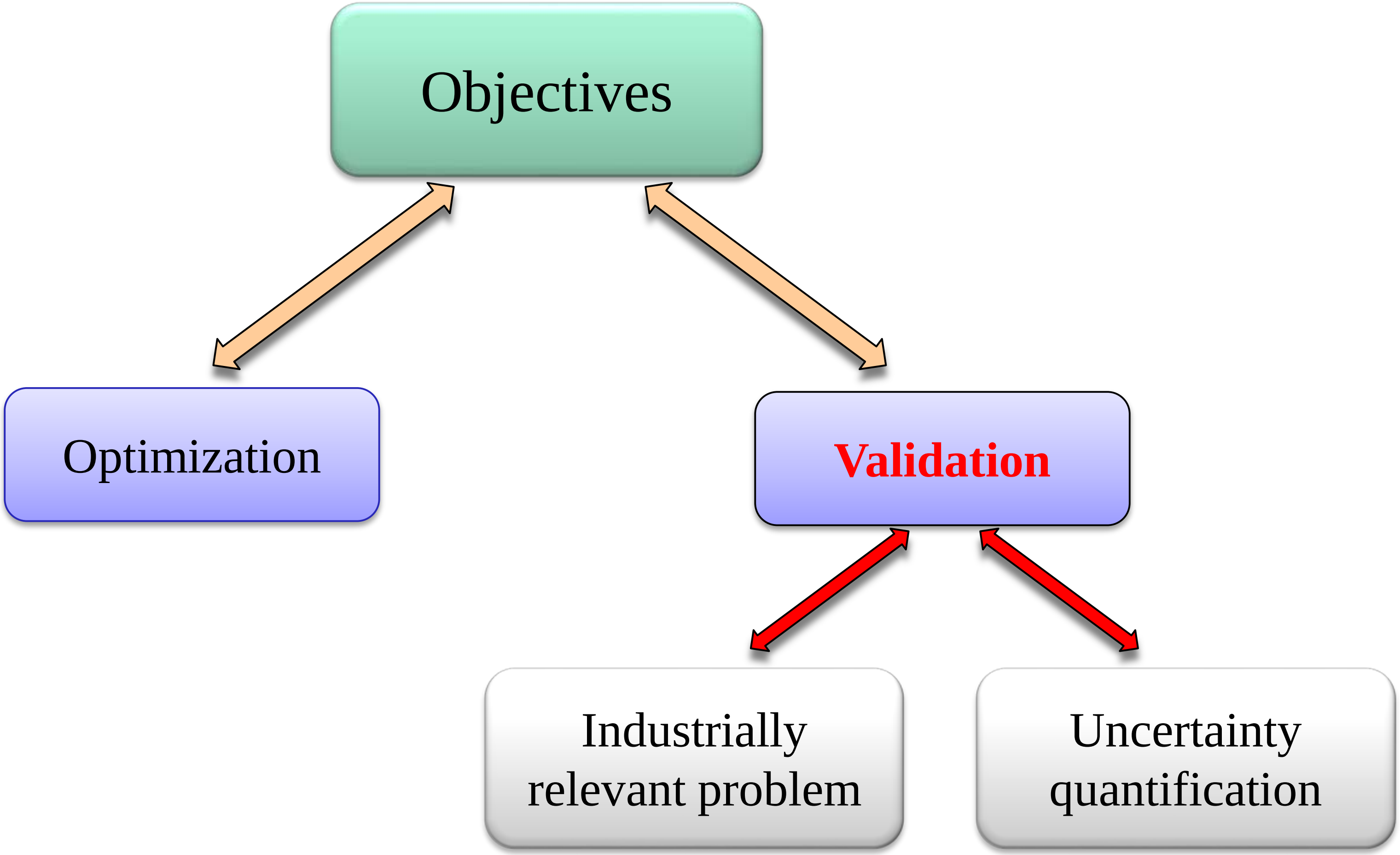
Laboratory	CFD-DEM	Industry
$N_p \sim 10^{10}$	$N_p \sim 10^4$ - 10^7	$N_p \sim 10^{14}$

Goal: DEM application toward industrially relevant flows

Challenges

- Speed ⇒ Optimization
- Results reliability ⇒ **Validation (this talk)**

Overall Project:
MFIX-DEM Enhancement towards Industrial Applications



Funding by the U.S. Department of Energy under
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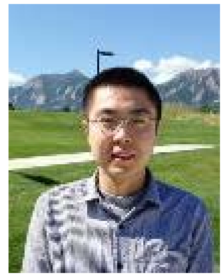
Team

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


Prof. Christine Hrenya


Dr. William Fullmer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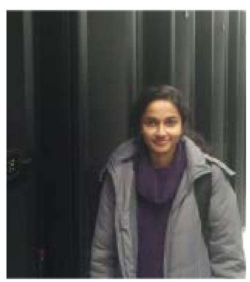
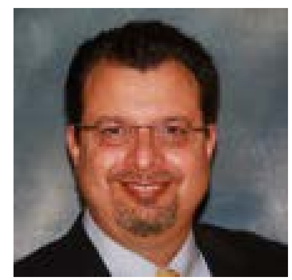
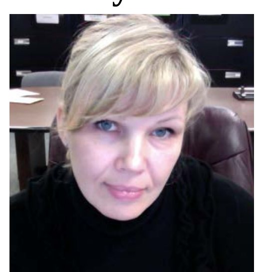
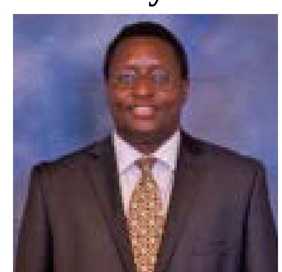

Dr. Deepthi Vaidhynathan

PSRI
Industrial Application and Experiments of Particle Flows


Dr. Ray Cocco


Rasa Kales

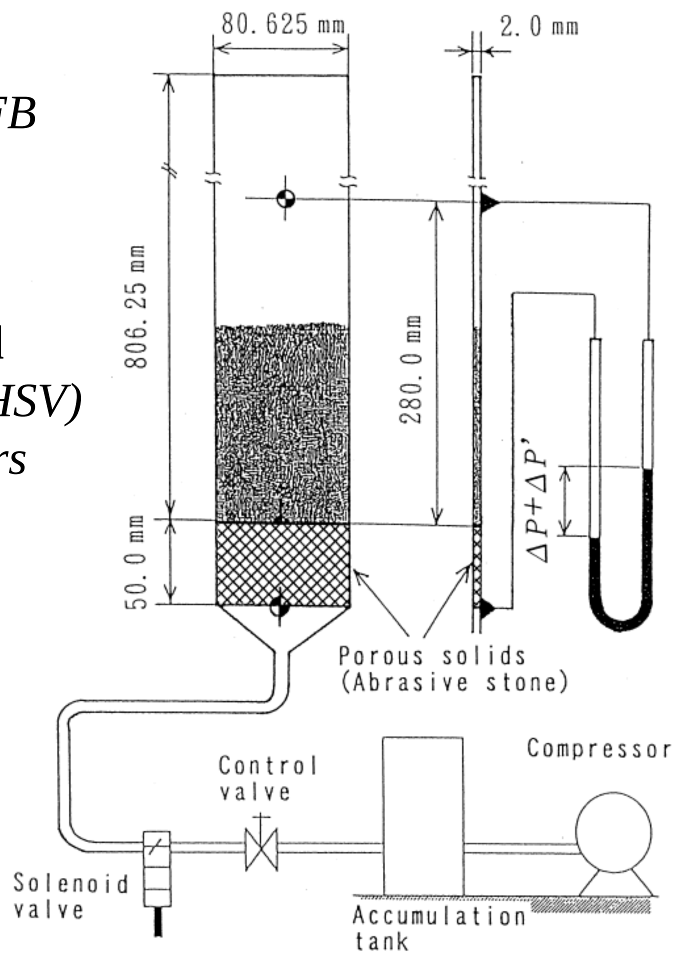

Dr. Allan Issangya

CFD-DEM Validation: Literature Survey

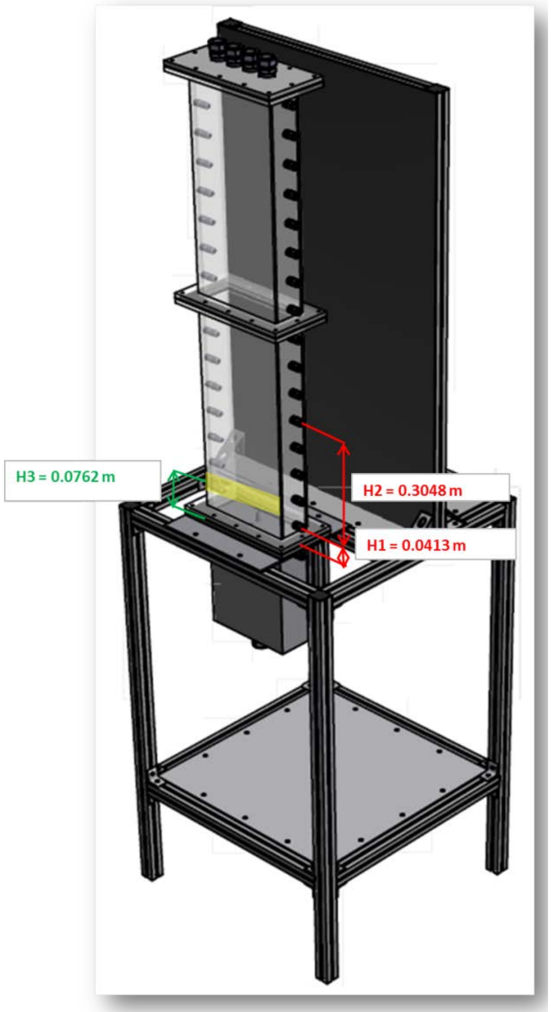
Common system
- *Small rectangular FB*
- *Group D particles*
- $N_p \sim 10^5$

Experimental method
- *High speed video (HSV)*
- *Pressure transducers*
- *PIV/MRI*

Metrics to compare
- *Flow patterns*
- *Pressure drop*
- *Velocity profiles*

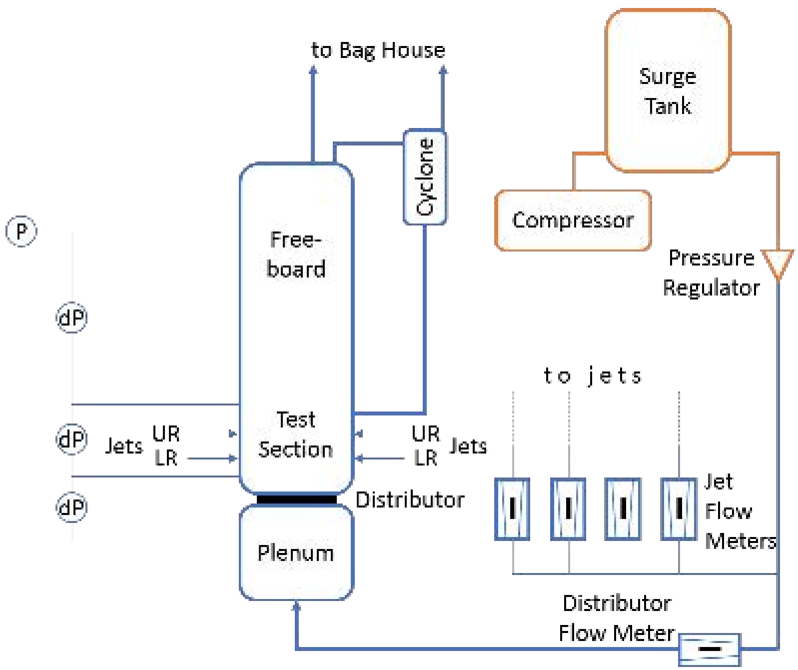


(Yuu et al., Powder Technol., 2000)



NETL Small-Scale Challenge Problem I
(Gopalan et al., Powder Technol., 2016)

Experimental setup
Semi-circular Fluidized Bed with Multiple Horizontal Jets



Dimensions	Values (cm)
Bed width, W	28.575 ± 0.159
Bed depth, D	15.169 ± 0.317
Bed height, H_s	29.14 ± 0.285
Jet diameter, d_J	0.386

Flow conditions	Values (cm/s)
Distributor flow, U	146.68 ± 9.77 (~ 1.1 Umf)
Jet velocity, U_J (cm/s)	~ 20,000

Materials

Materials

6.0 mm plastic: $\boldsymbol{N_p \sim 6 \times 10^4}$

3.0 mm ceramic: $N_p \sim 4 \times 10^5$

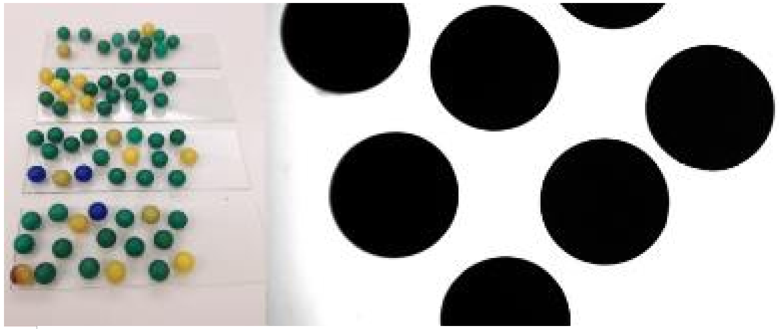
1.6 mm mix: $N_p \sim 3 \times 10^6$

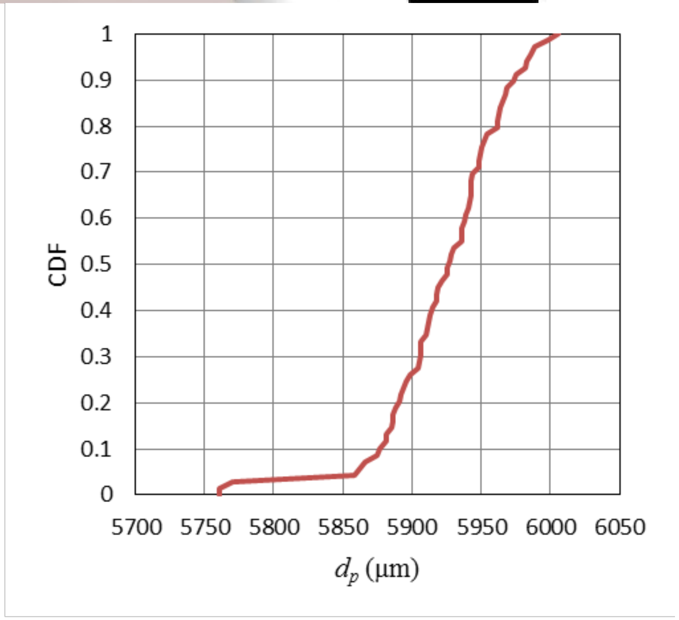
1.5 mm glass: $N_p \sim 4 \times 10^6$

1.0 mm ceramic: $N_p \sim 1 \times 10^7$

0.8 mm glass: $N_p \sim 3 \times 10^7$

Particle size characterization

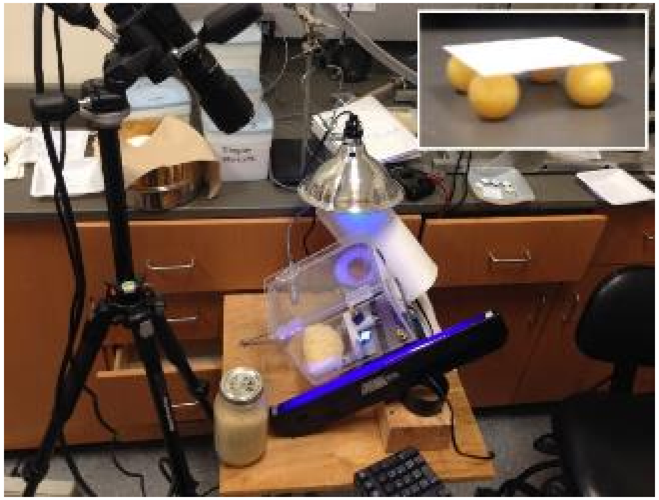


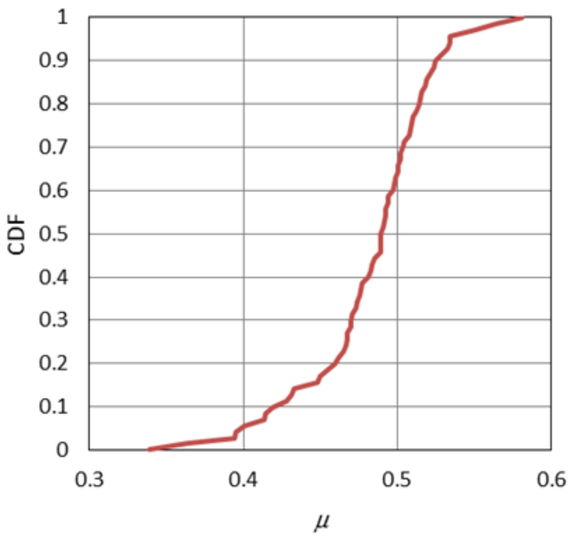


(LaMarche et al., Chem. Eng. J., 2017)

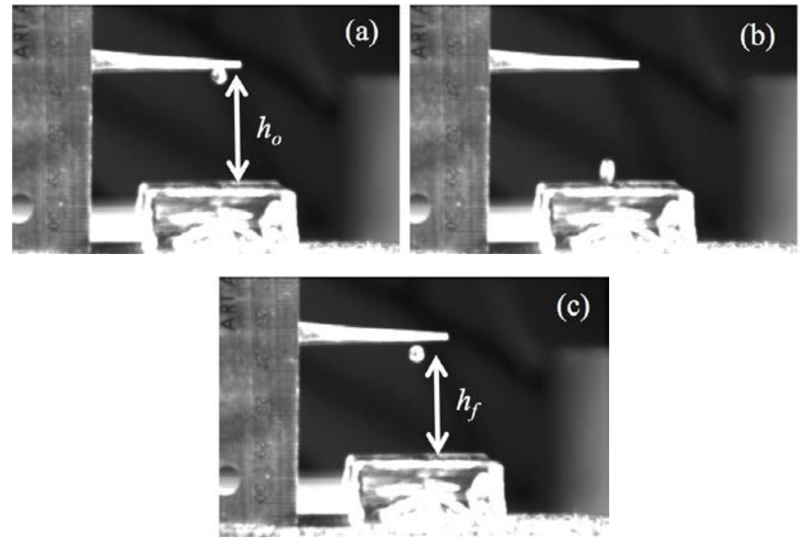
Materials

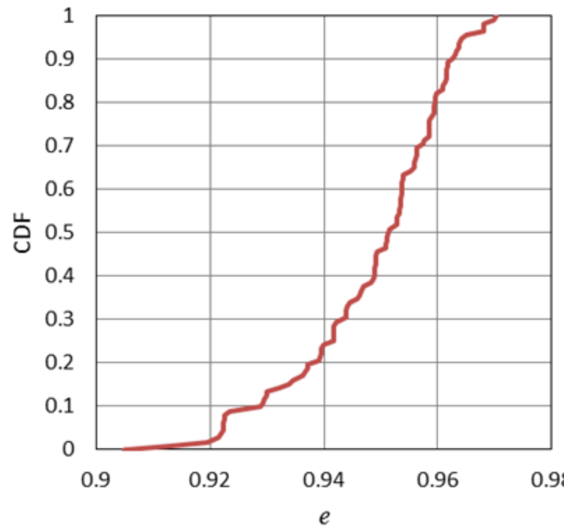
Sliding friction measurement





Coefficient of restitution measurement

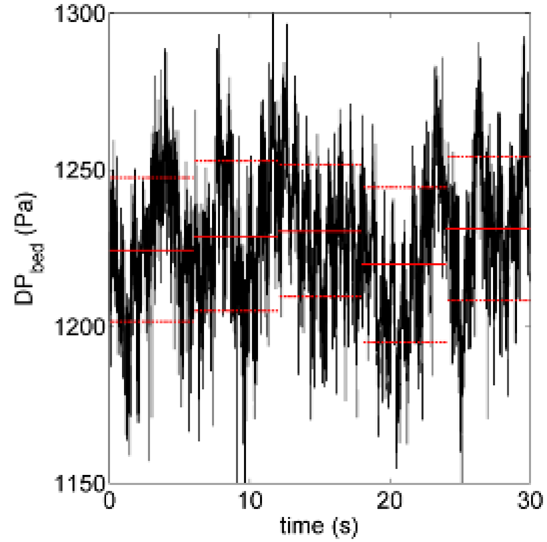


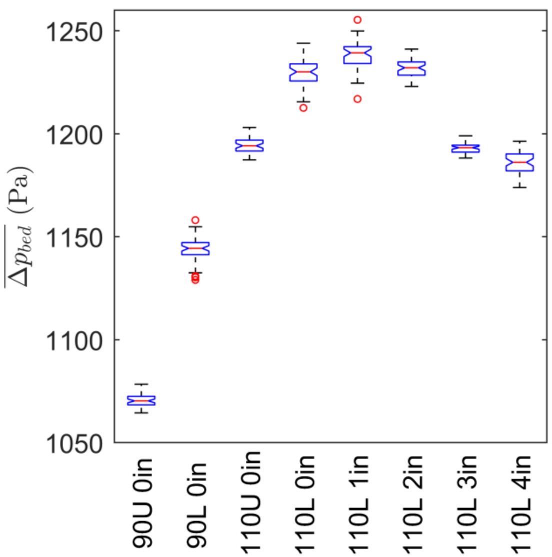


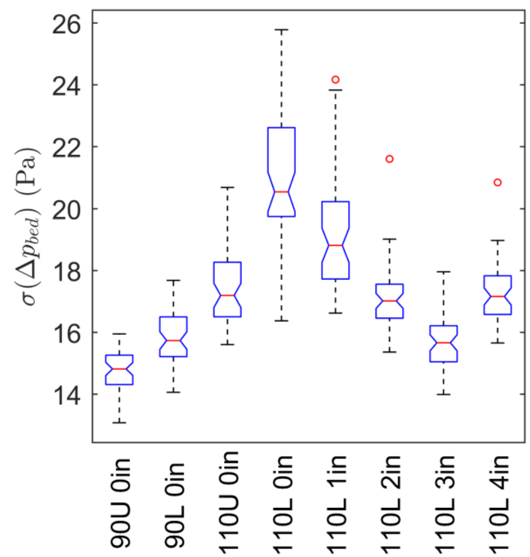
(LaMarche et al., Chem. Eng. J., 2017)

Experimental Results (SRQs)

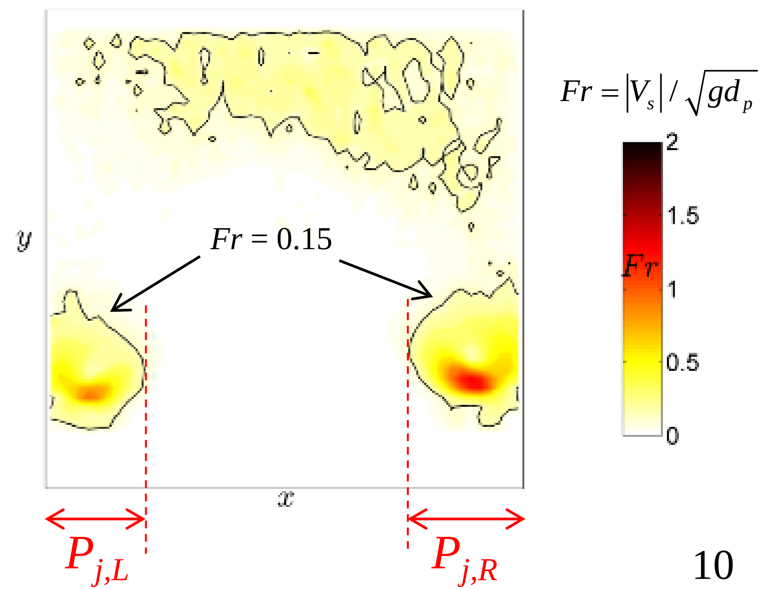
Bed pressure drop





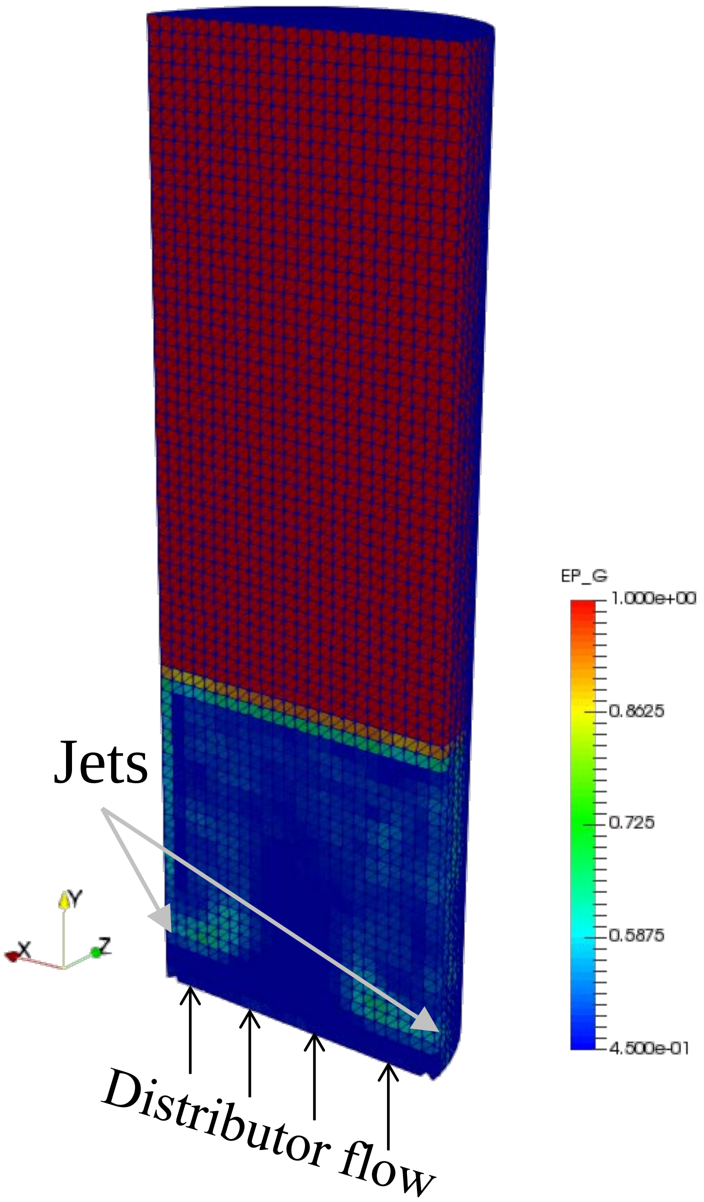


Jet penetration depth

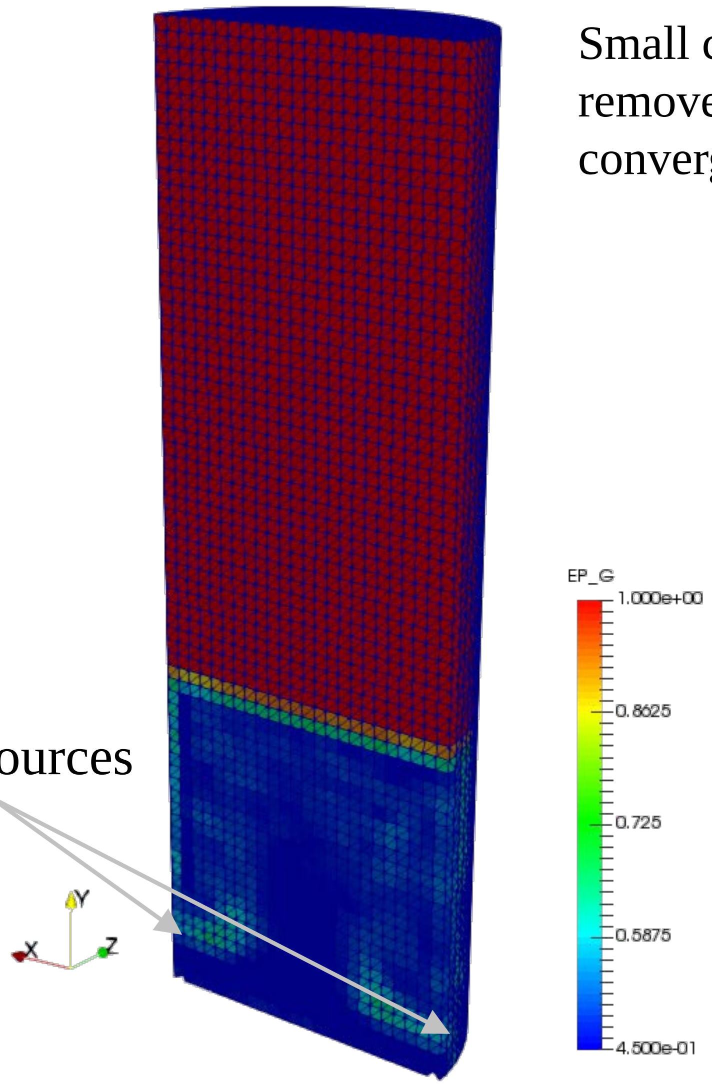


CFD-DEM Simulation Conditions: Base Case

Parameters (base case)	Values
Dimensions	
Static Height, H (cm)	85.725
Bed width, W (cm)	28.575
Bed depth, D (cm)	15.169
Static bed height, H_s (cm)	29.14015
Total number of particles, N_p	54459
Particle properties	
Diameter, d_p (cm)	0.5924
Density, ρ_p (g/cm^3)	1.0435
Spring constant, k (dyne/cm)	10^6
Sliding friction coefficient, μ_s	0.4821
Restitution coefficient, e	0.9482
Gas properties (compressible)	
Viscosity, μ_g (g·cm^{-1}·s^{-1})	1.80×10^{-4}
Superficial velocity, U (cm/s)	146.6825568
Jet diameter, D_J (cm)	0.38608
Jet height, H_J (cm)	5.1460 (L), 5.4559 (R)
Jet protrusion, D_z (cm) (from top face)	1.6669 (L), 1.7463 (R)
Jet protrusion, D_s (cm) (from side walls)	0.6072 (L), 0.6072 (R)
Jet velocity, U_J (cm/s)	20000.8537 (L), 19400.3746 (R)
Jet gas mass flow rate, $\dot{m} = \pi\rho_g U_j D_j^2/4$ (g/s)	2.7388 (L), 2.6566 (R)
Drag model	Wen_Yu



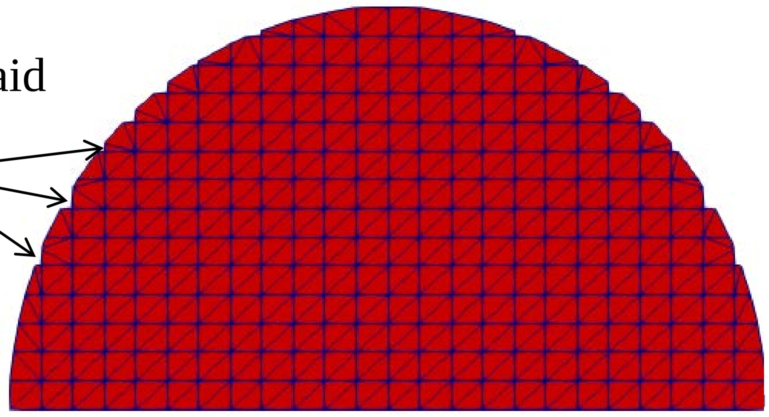
Simulating Bed Geometry with Cartesian Cut-Cells



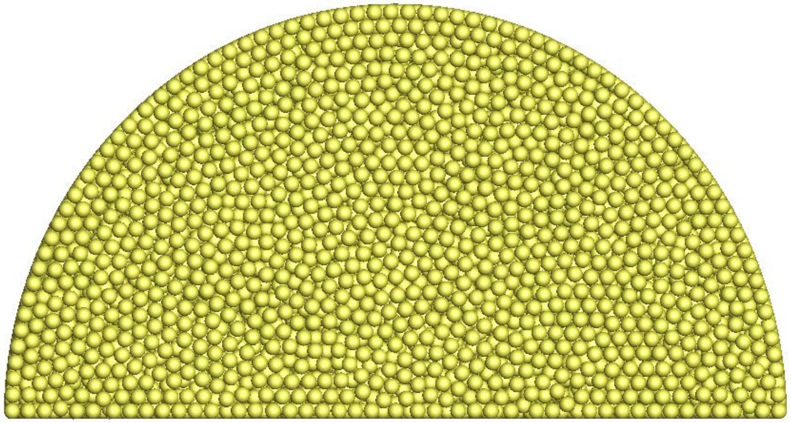
Point sources

Jet diameter < CFD cell size

Small cells removed to aid convergence



Top view (CFD cells)

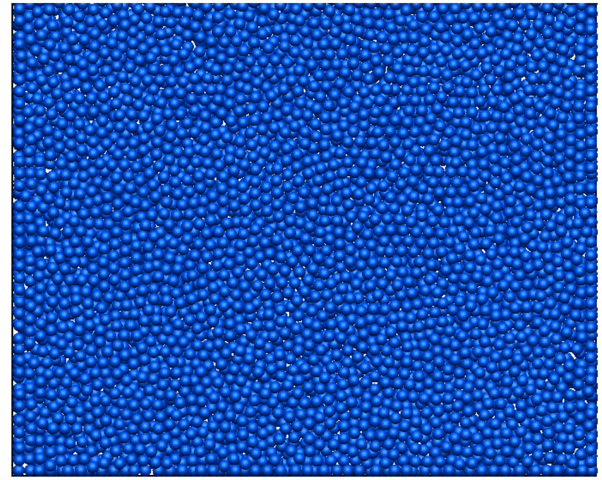


Top view (particles)

MFIX-2016-1 used to perform the simulations

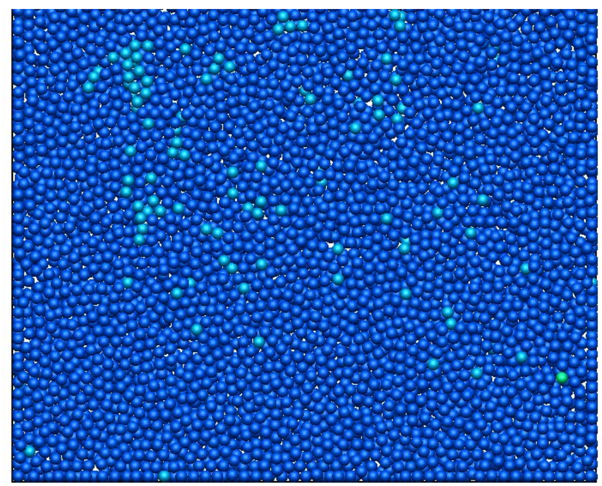
Results Comparison for the Base Case: Flow Patterns

Experiment

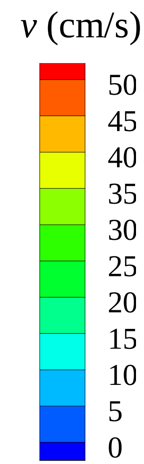


CFD-DEM

Considering true bed geometry in CFD-DEM leads to better agreement



CFD-DEM (rectangular)

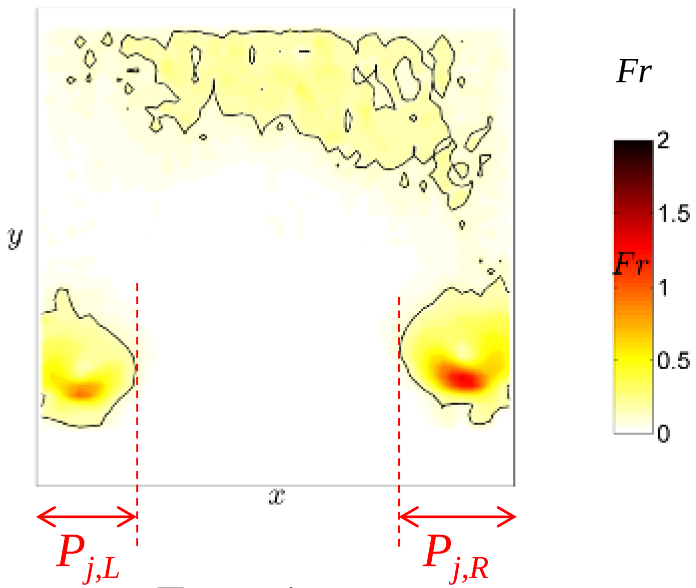


Results Comparison for the Base Case: Pressure Drop and Jet Penetration Depth

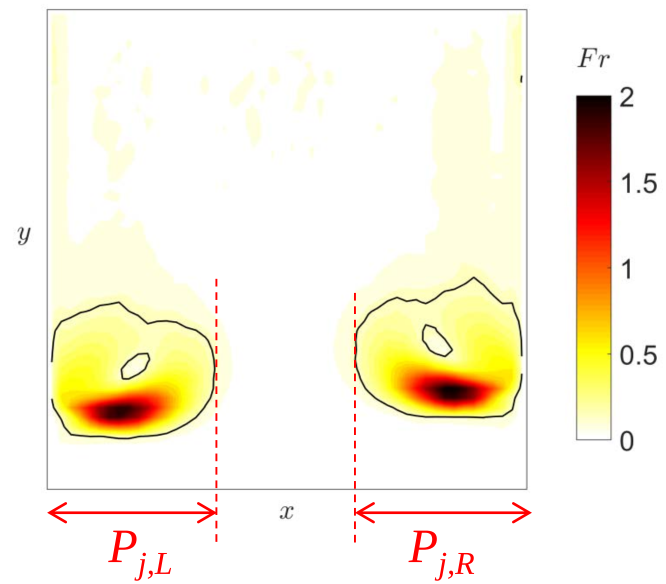
Pressure drop	Mean (Pa)	Std (Pa)
Experiment	1229.6	22.06
CFD-DEM	1421.3	109.9

Jet penetration	Left (cm)	Right (cm)
Experiment	8.034	8.770
CFD-DEM	9.398	9.620

CFD-DEM results in reasonable agreement with ameasurements



Experiment



CFD-DEM

Local Sensitivity to Uncertainties in Input Parameters

Input uncertainties

Parameter	**Lower bound**	**Base case**	**Upper bound**
Bed width, W (cm)	28.4160	28.5750	28.7340
Bed height, H_s (cm)	28.7909	29.1402	29.4259

CFD-DEM

$\overline{\Delta p_{bed}}$ (Pa)

Parameter	**Lower bound**	**Base case**	**Upper bound**
Bed width, W (cm)	1422.7	1421.3	1424.8
Bed height, H_s (cm)	1399.6	1421.3	1442.5

Square "error" relative to the base case

$$\left|\delta Y_i^{(j)}\right|^2 = \left(Y_i^{(j+)} - Y_i^{(0)}\right)^2 + \left(Y_i^{(j-)} - Y_i^{(0)}\right)^2$$

Parameter	$\left\|\delta Y_i^{(j)}\right\|^2$ (Pa^2)
Bed width, W (cm)	13.81
Bed height, H_s (cm)	922.25

H_s more important than W in affecting $\overline{\Delta p_{bed}}$

(Abdul-Razzak et al. 2002)

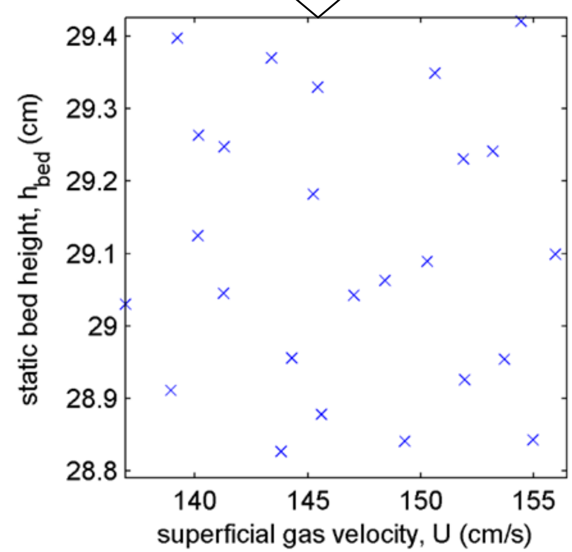
Next Step: UQ tests

Parameter Identification and Ranking Table

Input Uncertainties					SRQ Ranking		
Parameter	lower bound	base case	upper bound	type	Pj,L	Pj,R	ΔP_mean
Bed							
U (cm/s)	136.9132	146.6826	156.4519	e	100.000000	100.000000	37.385600
Uj,L (m/s)	189.2253	200.8537	212.4821	e	15.032656	1.459381	1.581862
Uj,R (m/s)	182.8222	194.3746	205.9270	e	0.520213	38.775714	2.029440
hbed (cm)	28.7909	29.1402	29.4259	e	0.072480	1.439458	56.249878
W (cm)	28.4160	28.5750	28.7340	e	0.337803	2.042138	0.842206
D (cm)	14.8520	15.1690	15.4860	e	1.121335	2.948648	0.101814
Umf (cm/s)	126.0000	135.6000	145.2000	e	1.884692	0.762066	100.000000
Left Jets							
Aj,L (cm2)	0.1168	0.1171	0.1174	e			
yj,L (cm)	5.0667	5.1460	5.2254	e	0.000000	0.000000	0.000000
zj,L (cm)	1.5875	1.6669	1.7463	e	0.000000	0.000000	35.085184
dj,L (cm)	-0.3175	0.0000	0.3175	e			
Right Jets							
Aj,R (cm2)	0.1168	0.1171	0.1174	e			
yj,R (cm)	5.3765	5.4559	5.5353	e	0.000000	0.000000	0.000000
zj,R (cm)	1.6669	1.7463	1.8256	e	0.000000	0.000000	0.000000
dj,R (cm)	-0.3175	0.0000	0.3175	e			
Particle-phase Properties							
dp (μm)	5761.2441	5923.7773	6005.5477	a	2.590285	4.866265	4.125328
ϕ	0.9309	0.9427	0.9478	a	0.000000	0.000000	0.000000
ρp (g/cm3)	1.0420	1.0435	1.0450	e	0.086299	1.085820	1.412422
epp	0.8187	0.9482	0.9900	a	1.798462	6.265876	16.935445
μpp	0.3384	0.4821	0.5812	a	0.214815	7.750162	16.360982
epw	0.9050	0.9482	0.9703	a	0.217821	0.966280	0.554787
μpw	0.3384	0.4821	0.5812	a	0.734406	1.558998	0.592837
Gas-phase Properties							
rg (g/cm3 x 103)	1.1104	1.1697	1.2290	e			
mg (g/cm-s x 105)	1.7	1.8	1.9	e	0.263699	2.550182	1.441958
T (K)	277.4	293.0	303.5	e	0.967773	0.846740	0.422388

$> 10^{1.5}$	Important
$10^{1.5} – 10^{1.0}$	Mildly Important
$10^{1.0} – 10^{0.5}$	Marginal
$10^{0.5} – 10^{0.0}$	Mildly Insignificant
$< 10^{0.0}$	Insignificant

LHS Sampling



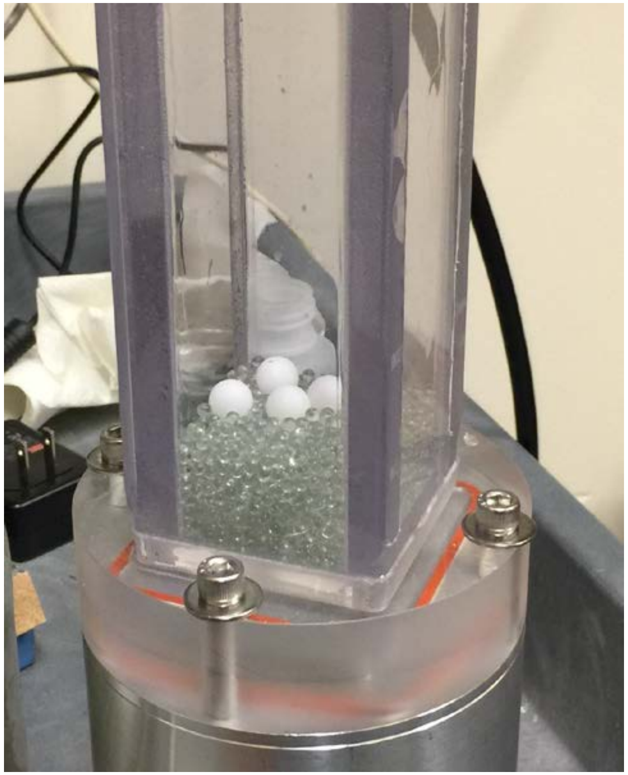
Summary

So far

- Performed experiments and material characterization
- Measured SRQs for direct comparison
  - Pressure drop
  - Jet penetration depth
- Established the PIRT

Next steps

- UQ for important parameters in PIRT (~10^4 simulations)
- Explore simpler systems with ~10^3 particles (VVSSP)



Acknowledgements

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