MFiX Suite Quality Assurance

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Solutions for Today | Options for Tomorrow

Outline

- **Preliminary MFiX Verification & Validation**
  - Continuous phase
  - Discrete phase
  - Particle-In-Cell (PIC)
- **VV&UQ Framework for granular & multi-phase flows**
  - Extended ASME V&V 20
  - Application
    - Hopper discharge
    - Pulsed fluidized bed
- **Challenge Problem**
- **Ongoing efforts**

Glossary

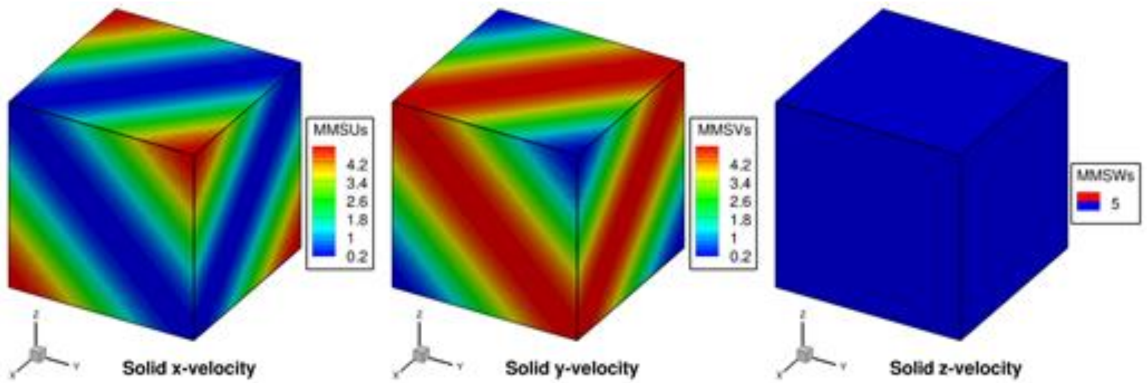
- **Code Verification:** Process of determining if the numerical algorithms are implemented correctly and verifying its order of accuracy.
- **Solution verification:** Process of determining the correctness of input data, numerical accuracy of solution and correctness of output data.
- **Validation:** Process of determining the degree to which a model corresponds to a real system.
- **Uncertainty Quantification:** Process of determining the uncertainty in numerical predictions due to inherent randomness in physical properties **(aleatory)** and lack of knowledge **(epistemic)**.
- **Control variable:** Variables in an experiment/simulation that are controlled or modified while performing a parameter sweep.
- **Response variable (Quantity of Interest)**: The observable quantity used for validation.

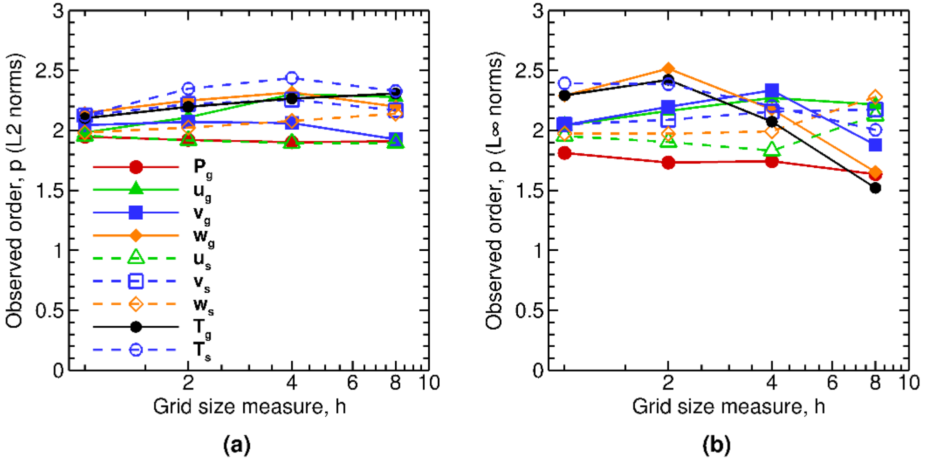
MFiX DEM MFiX PIC MFiX TFM MFiX Exa

MFiX-FLD V&V

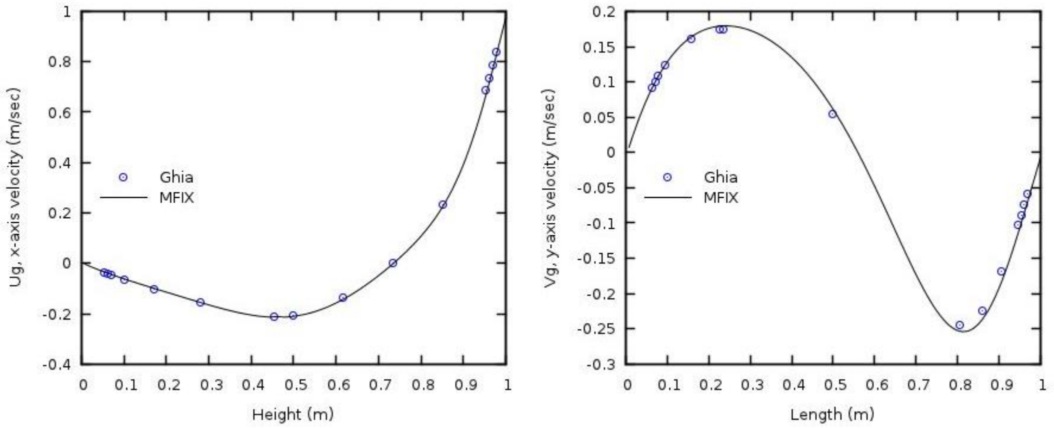
Continuous phase

Method of Manufactured Solutions

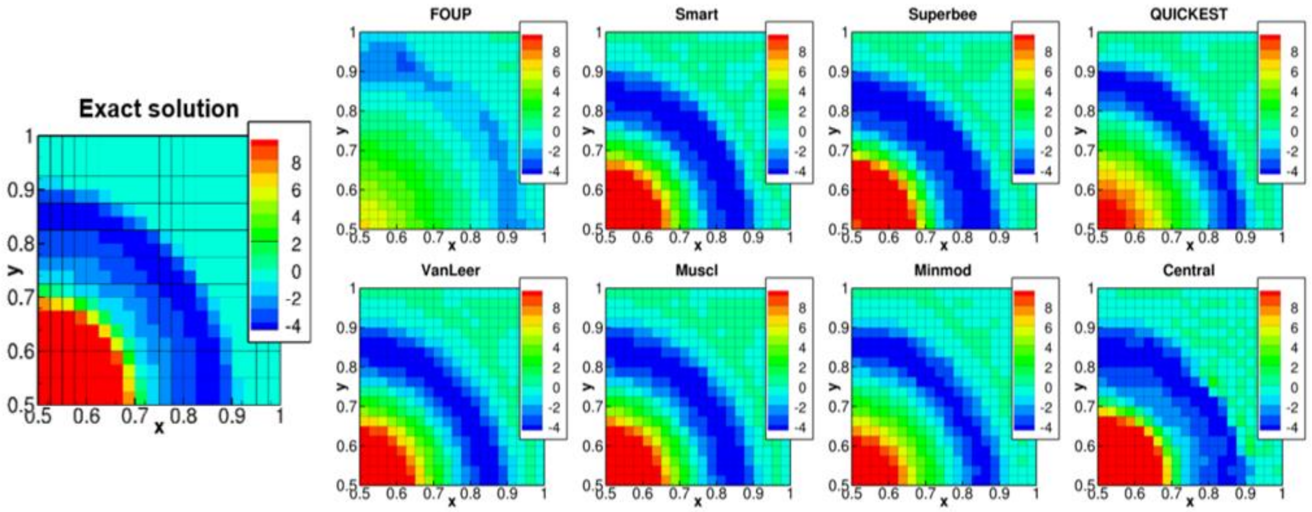




Lid-driven cavity



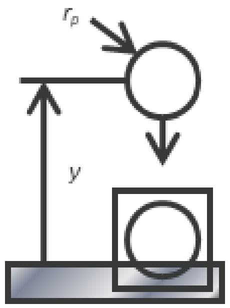
Gresho vortex



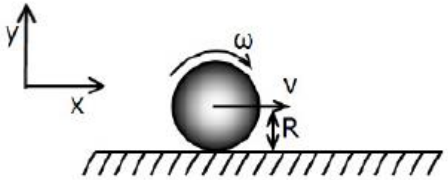
MFiX-DEM V&V

Discrete phase

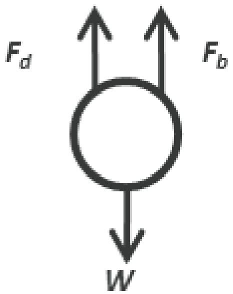
Particle-wall collision



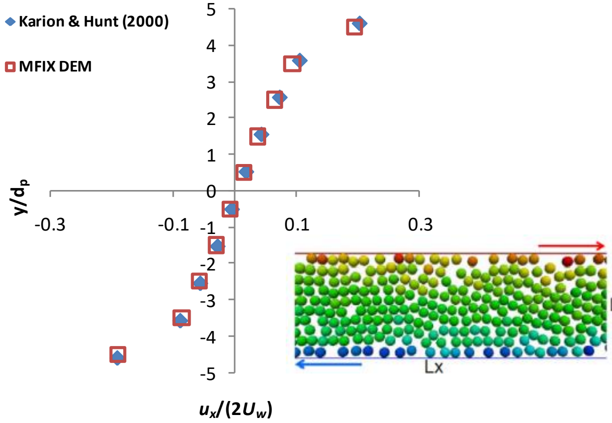
Rolling on rough wall



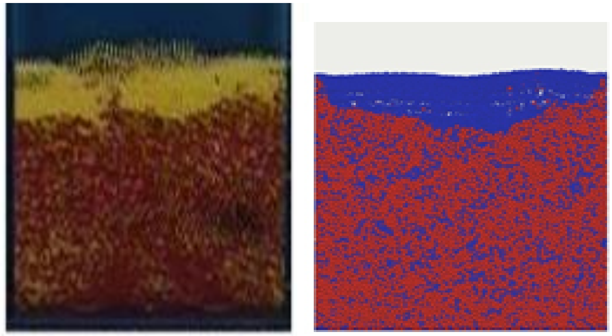
Terminal velocity



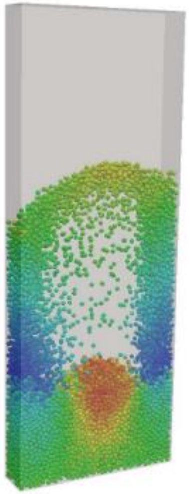
Granular shear flow



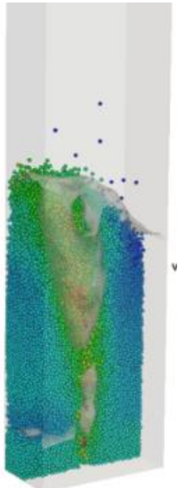
Particle segregation



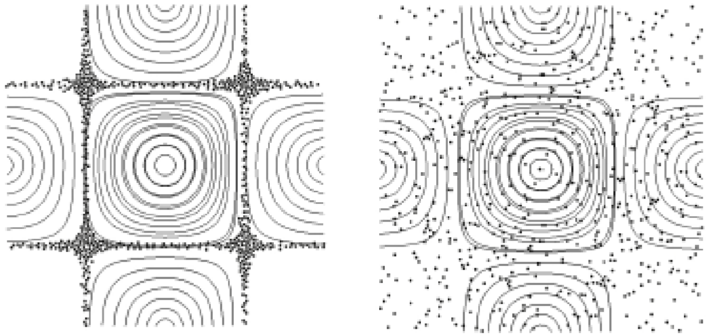
Bubbling bed



Spouted bed

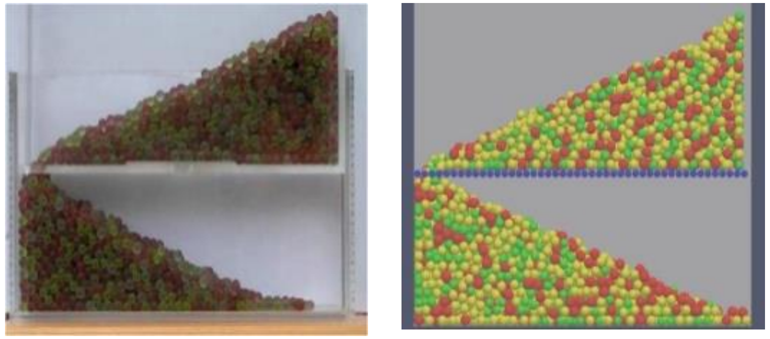


Motion in 2D Taylor-Green vortex



St = 2.0 St = 0.2

Sand pile repose angle



MFiX-PIC V&V

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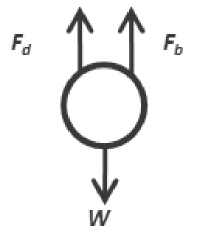
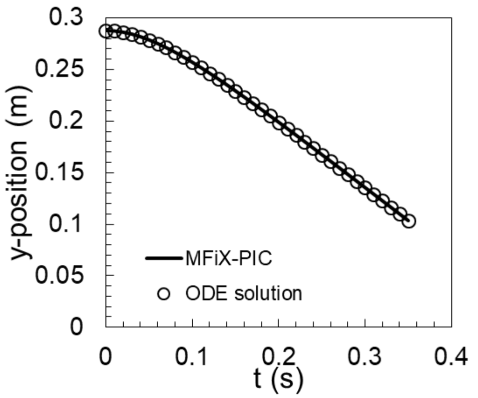
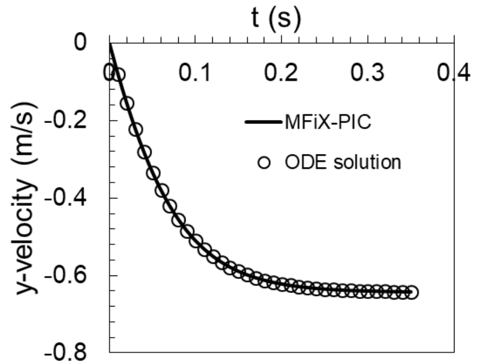
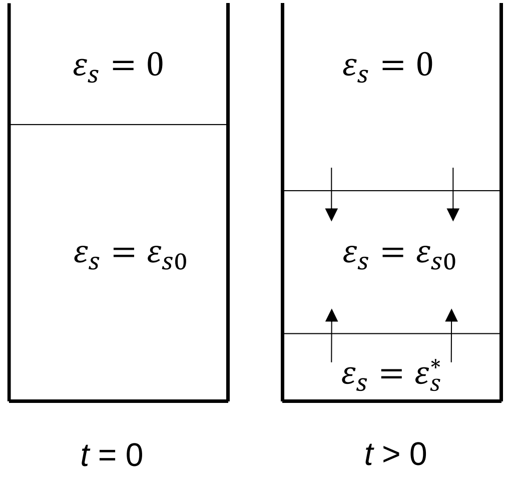
Terminal velocity







Particle Settling



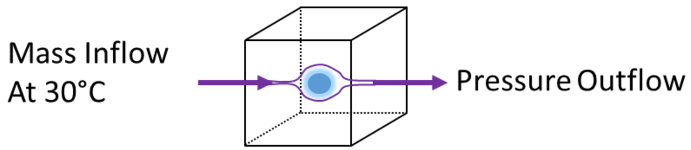
Settling shock velocity

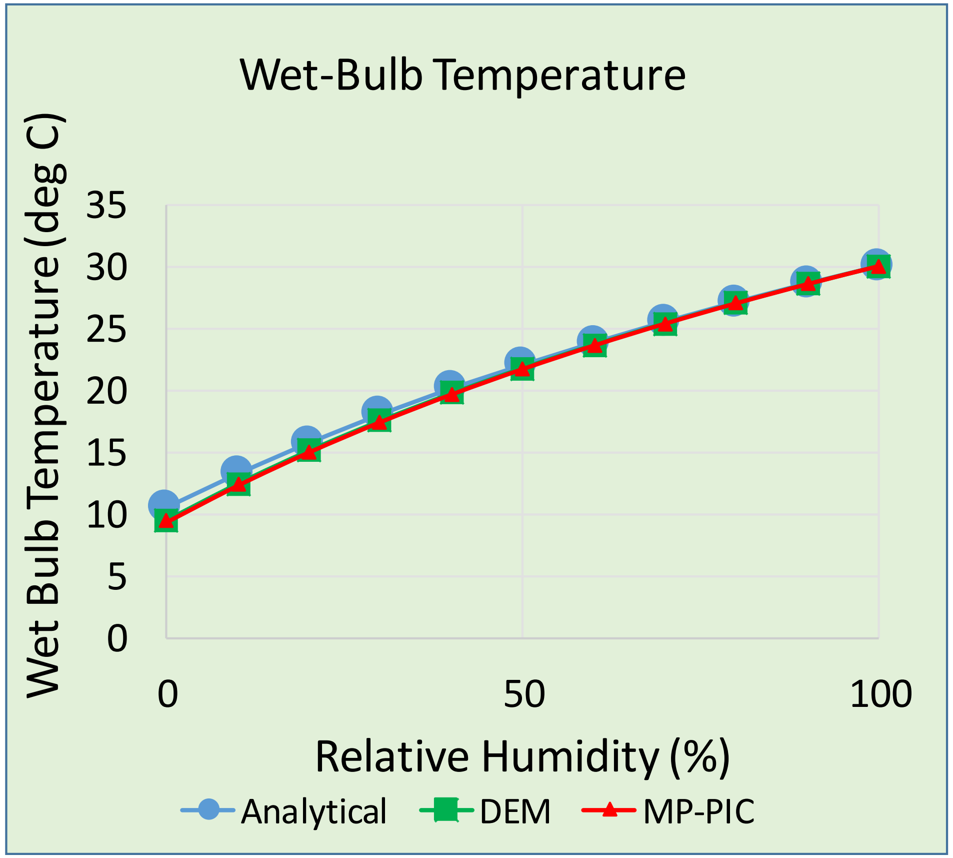
ε_{s0}	0.10	0.15	0.20
Analytical	0.334	0.256	0.193
PIC	0.34 ± 0.01	0.28 ± 0.01	0.22 ± 0.01
DEM	0.34 ± 0.01	0.28 ± 0.01	0.22 ± 0.01
TFM	0.32 ± 0.01	0.25 ± 0.01	0.19 ± 0.01

Filling shock velocity

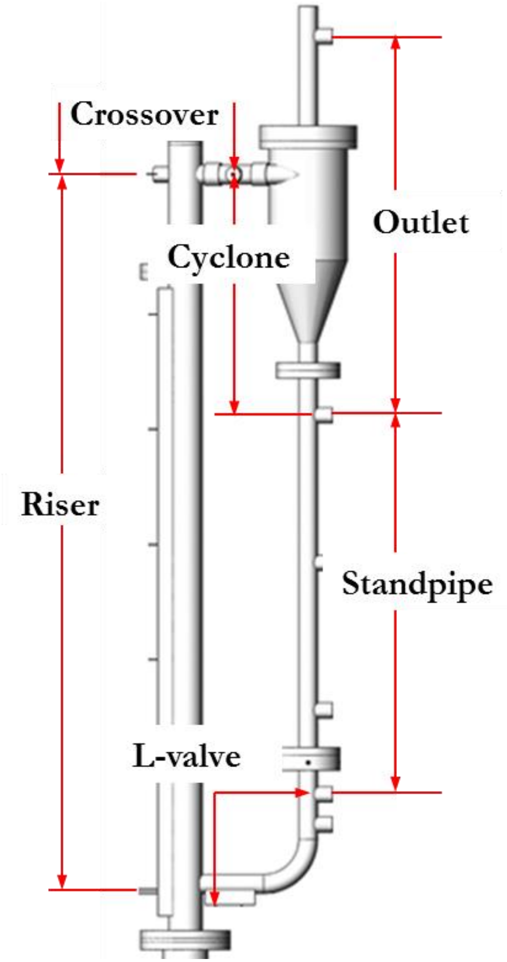
ε_{s0}	0.10	0.15	0.20
Analytical	0.058	0.075	0.085
PIC	0.06 ± 0.01	0.08 ± 0.01	0.10 ± 0.01
DEM	0.06 ± 0.01	0.08 ± 0.01	0.10 ± 0.01
TFM	0.06 ± 0.01	0.07 ± 0.01	0.09 ± 0.01

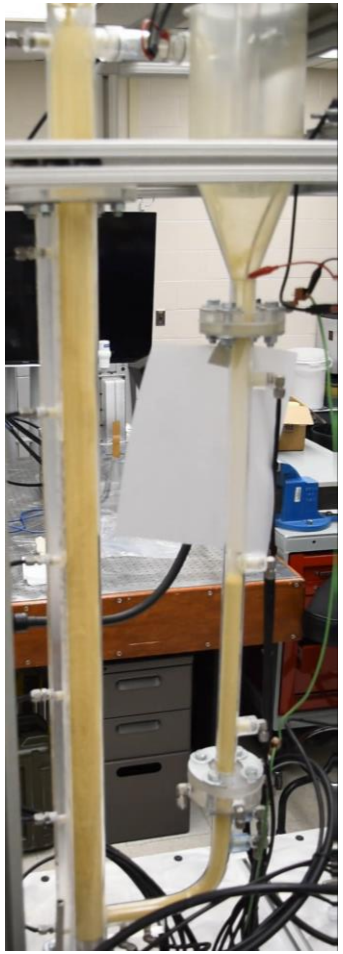
Evaporation





Circulating Fluidized Bed

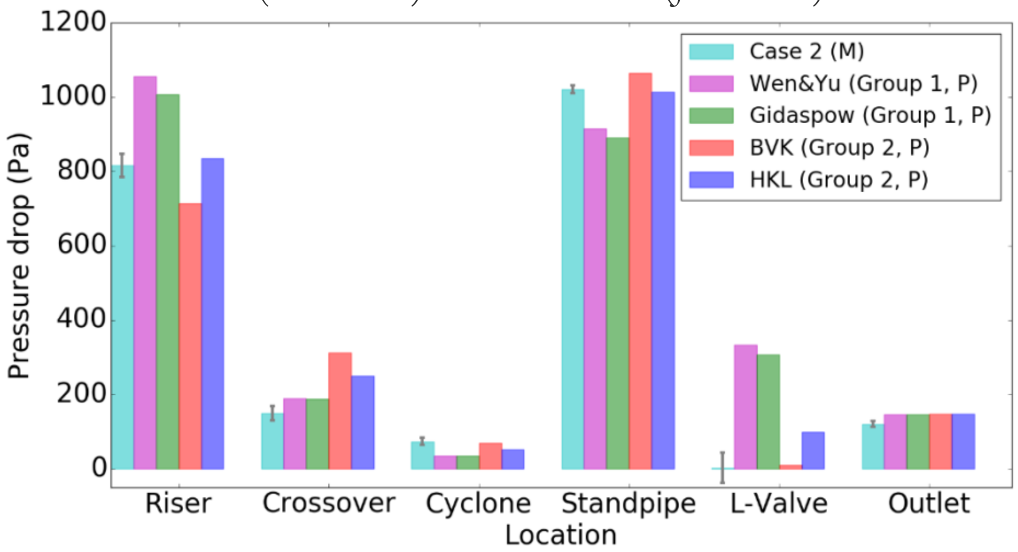




Material	High density polyethylene
Particle density	863 kg/m^3
Mean particle diameter	871 μm
Particle count	800,000

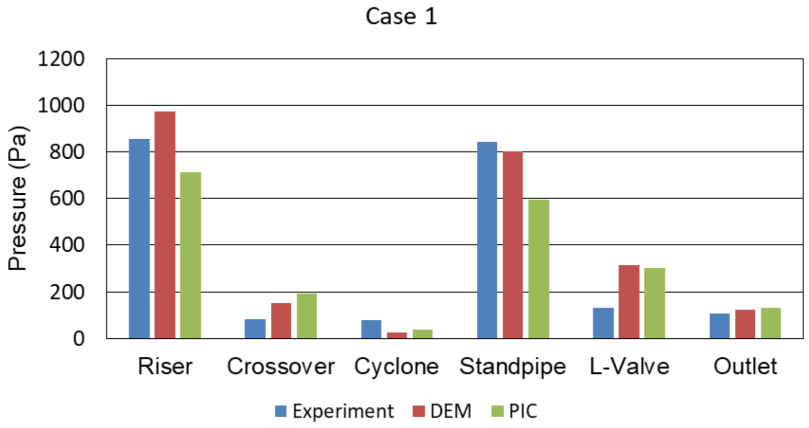
Wen & Yu (AIChE 1966) Gidaspow (AIChE 1990)

BVK (CES 2007) HKL (JFM 2001)

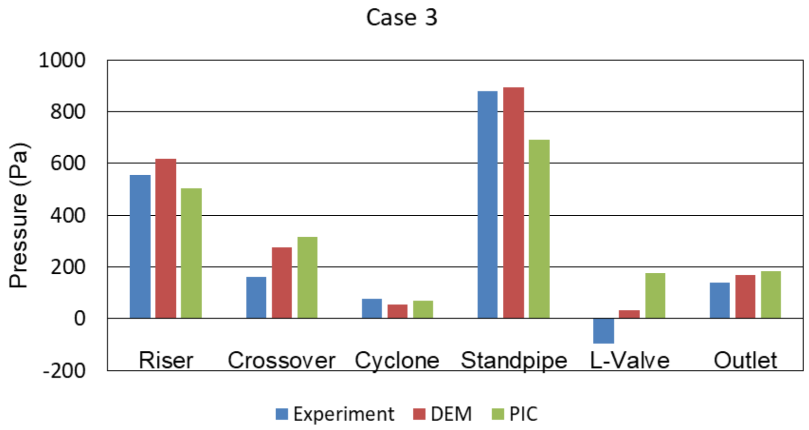


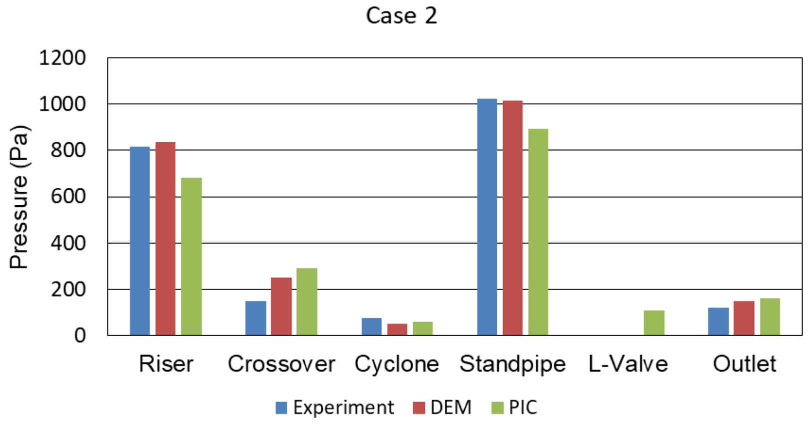
Circulating Fluidized Bed – MFiX PIC

- Simulations with PIC using BVK drag law
- Maximum deviation in pressure drop across riser and standpipe about 20%
- Time to solution reduced to 1 day with PIC (~8X DEM)
- Maximum deviation for Case 1 (lower flow rates)



	FTC180	FTC135	FTC115
Case 1	275	6	1.5
Case 2	300	7.5	2.5
Case 3	325	6	1.5





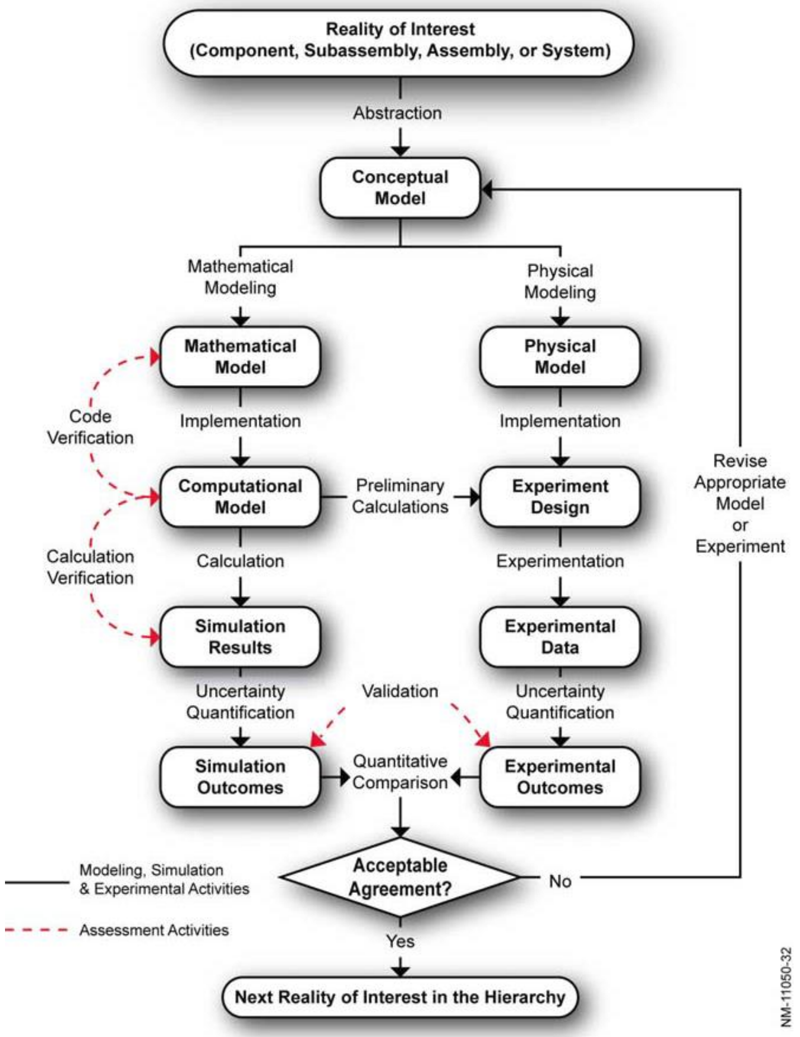
VV&UQ Challenges

- Complex hydrodynamics and inter-phase interactions
- Numerous physical and modeling parameters
- Need for objectively-assessed experimental uncertainty

- **ASME V&V 20**

"Ideally as a V&V program is initiated, those responsible for the simulations and those responsible for the experiments should be involved cooperatively in designing the V&V effort."

"The scope of this standard is the quantification of the degree of accuracy of simulation of specified validation variables at a specified validation point for cases in which the conditions of the actual experiment are simulated. Consideration of solution accuracy at points within a domain other than the validation points (e.g., interpolation/extrapolation in a domain of validation) is a matter of engineering judgment specific to each family of problems and is beyond the scope of this standard."



VV&UQ Roadmap

Verification

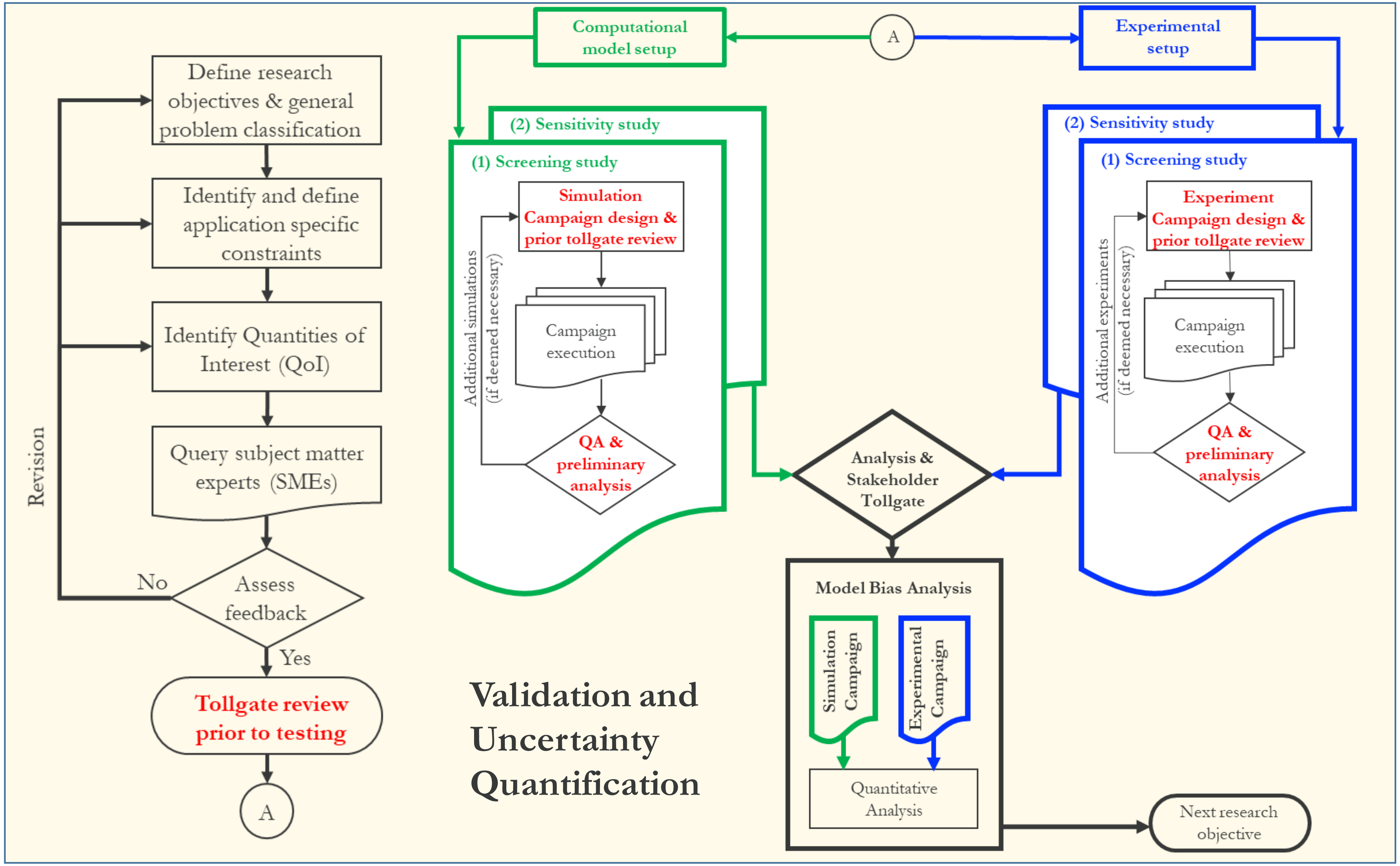
- Code Verification
- Solution Verification

Features

Survey of subject matter experts

Systematic design of experiments and simulation campaign

Tollgates for reviews, analysis and discussions with stakeholders



Hopper discharge

Survey of Subject Matter Experts

8. Subject Matter Expert (SME) Feedback Summary	
Computational model - Response Variables	
Accepted - Ranked by overall score 1. Discharge rate (kg/s) 2. Angle of repose (degree)	Rejected • Particle Size Distribution (PSD) of discharged particles • Flow pattern - lowest point in hopper • Flow pattern - Highest point in hopper • particle-wall friction coefficient • Particle-particle restitution coefficient • Young's Modules • Particle-particle dynamic friction coefficient • Particle-particle static friction coefficient
Computational model - Control Variables	
Accepted - Ranked by overall score 1. PP coefficient of friction (sliding) 2. PW coefficient of friction (sliding) 3. PP restitution coefficient 4. PP LSD normal spring stiffness coefficient 5. PW restitution coefficient 6. PW LSD normal spring stiffness coefficient 7. PP LSD tangential spring stiffness coefficient 8. PW LSD tangential spring stiffness coefficient 9. PP LSD tangential damping factor 10. PW LSD tangential damping factor	Rejected • Coefficient of friction (rolling) • Initial voidage • Initial bed height • Particle density • Initial particle size distribution (PSD) • Wall asperities • Orifice diameter • Apex angle • Height above collection plate
Computational model - Held Constant Variables	
Accepted - Ranked by overall score 1. Particle density (kg/m^3) 2. Particle diameter (m) 3. Particle sphericity	Rejected • Normal spring stiffness • Time step

Computational model - Rejected Response Variables

SME	Rejected response variable	Justification of rejected response variable
1	PSD of discharged particles	Computational simulations will be conducted with mono-disperse particles so there is no PSD will be generated of discharged particles
3	Flow pattern - highest and lowest points in hopper	These are connected to model input parameters, specifically the total number of particles.
4	Particle-wall friction coefficient	This is a model input parameter.
4	Particle-particle restitution coefficient	This is a model input parameter.
4	Particle-particle friction coefficients	This is a model input parameter.

Computational model - Accepted Control Variables

Particle-particle coefficient of friction (sliding) — **Rank: 1 of 10**

SME	Proposed control variable value range: Rank	Normal	Low	High	Justification
1	1	0.5	0.0	1.0	I have seen the friction coefficient can be very sensitive to things like humidity. It would be best to measure the friction coefficient in house if possible.
2	2	0.3	0.0	1.0	[It is] unclear whether distinction should be made between dynamic/static value but MFIX doesn't have this fine control.
3	7	0.5	N/R	N/R	N/R
4	4	N/R	N/R	N/R	*JM: Rank assumed from list order and inputs of dynamic and static friction.*
5	1	N/R	N/R	N/R	N/R
6	TBD (5)	0.35	0.31	0.39	*JM: Not specific on pp or pw*

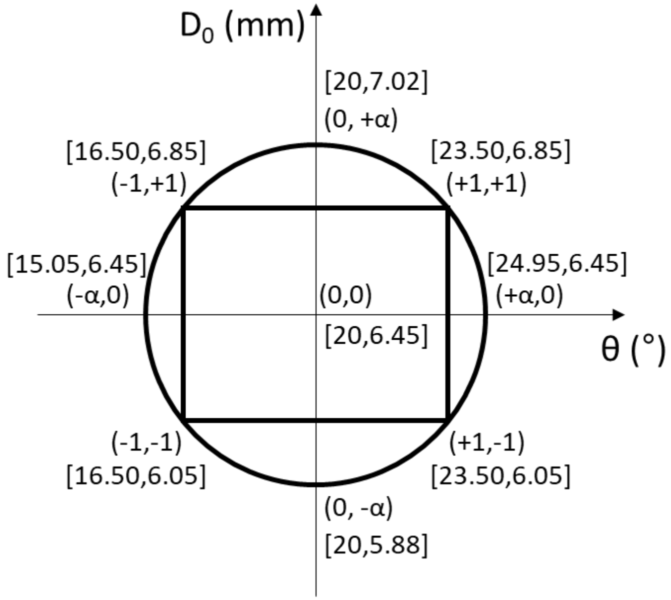
Particle-wall coefficient of friction (sliding) — **Rank: 2 of 10**

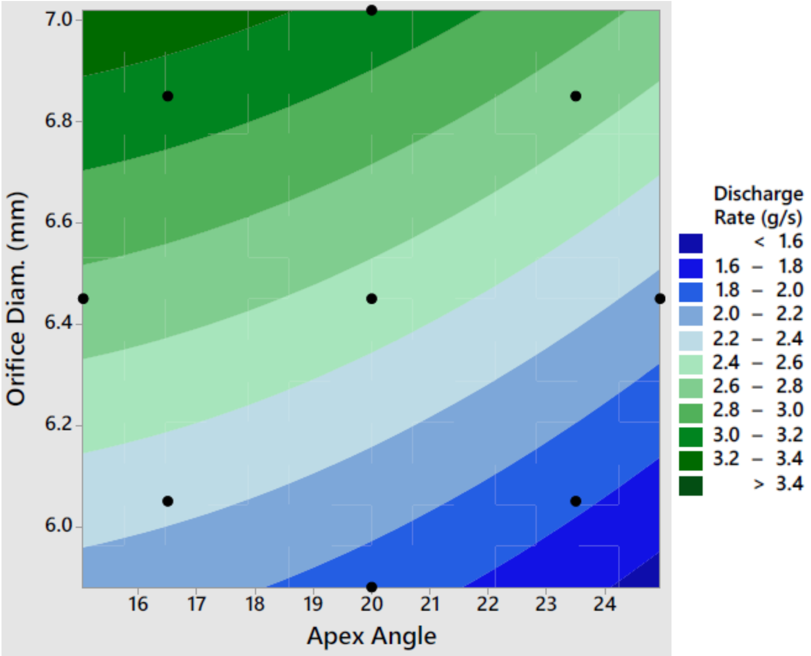
SME	Proposed control variable value range: Rank	Normal	Low	High	Justification
1	2	0.68	0.45	0.90	I have seen the friction coefficient can be very sensitive to things like humidity. It would be best to measure the friction coefficient in house if possible.
2	4	N/R	N/R	N/R	N/R
3	8	0.5	N/R	N/R	N/R
4	1	N/R	N/R	N/R	*JM: Rank assumed from list order.*
5	2	N/R	N/R	N/R	N/R
6	TBD (5)	0.35	0.31	0.39	*JM: Not specific on pp or pw*

Hopper discharge

Experiments

- Design of experiments - Central composite
- Replicates to assess uncertainty
- Control variables from the survey of SMEs
  - Apex angle
  - Orifice diameter





Index	Apex angle (deg)	Orifice diameter (mm)	Discharge rate (g/s)	Index	Apex angle (deg)	Orifice diameter (mm)	Discharge rate (g/s)
6	20	5.88	1.90	1	20	7.02	3.09
1	20	7.02	3.15	3	20	6.45	2.53
6	20	5.88	1.92	5	23.5	6.05	1.91
4	16.5	6.05	2.21	3	20	6.45	2.53
3	20	6.45	2.49	9	15.05	6.45	2.80
8	16.5	6.85	3.09	5	23.5	6.05	1.94
3	20	6.45	2.51	3	20	6.45	2.53
3	20	6.45	2.52	3	20	6.45	2.49
7	23.5	6.85	2.78	8	16.5	6.85	3.09
1	20	7.02	3.12	3	20	6.45	2.47
2	24.95	6.45	2.01	3	20	6.45	2.46
4	16.5	6.05	2.19	3	20	6.45	2.48
6	20	5.88	1.91	2	24.95	6.45	2.00
2	24.95	6.45	2.05	5	23.5	6.05	1.93
9	15.05	6.45	2.78	3	20	6.45	2.49
3	20	6.45	2.53	9	15.05	6.45	2.80
7	23.5	6.85	2.78	3	20	6.45	2.52
3	20	6.45	2.50	4	16.5	6.05	2.20
7	23.5	6.85	2.78	8	16.5	6.85	3.07
3	20	6.45	2.50				

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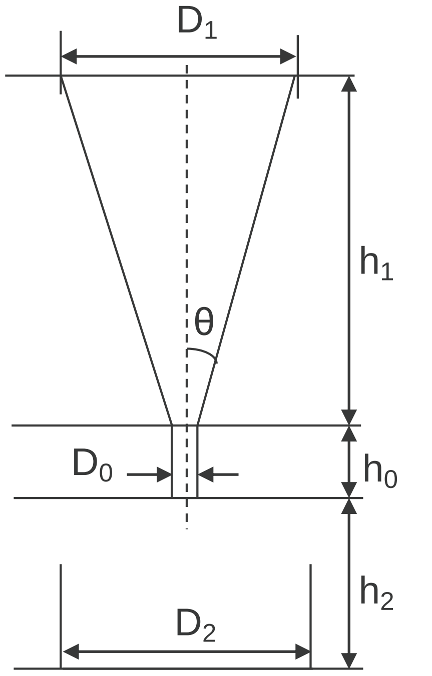
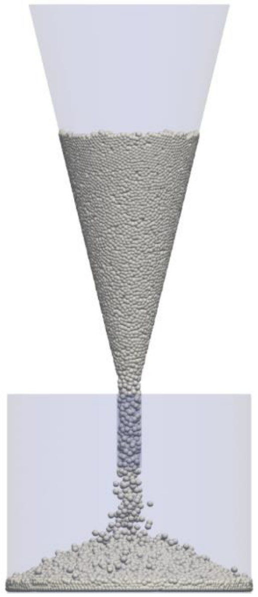
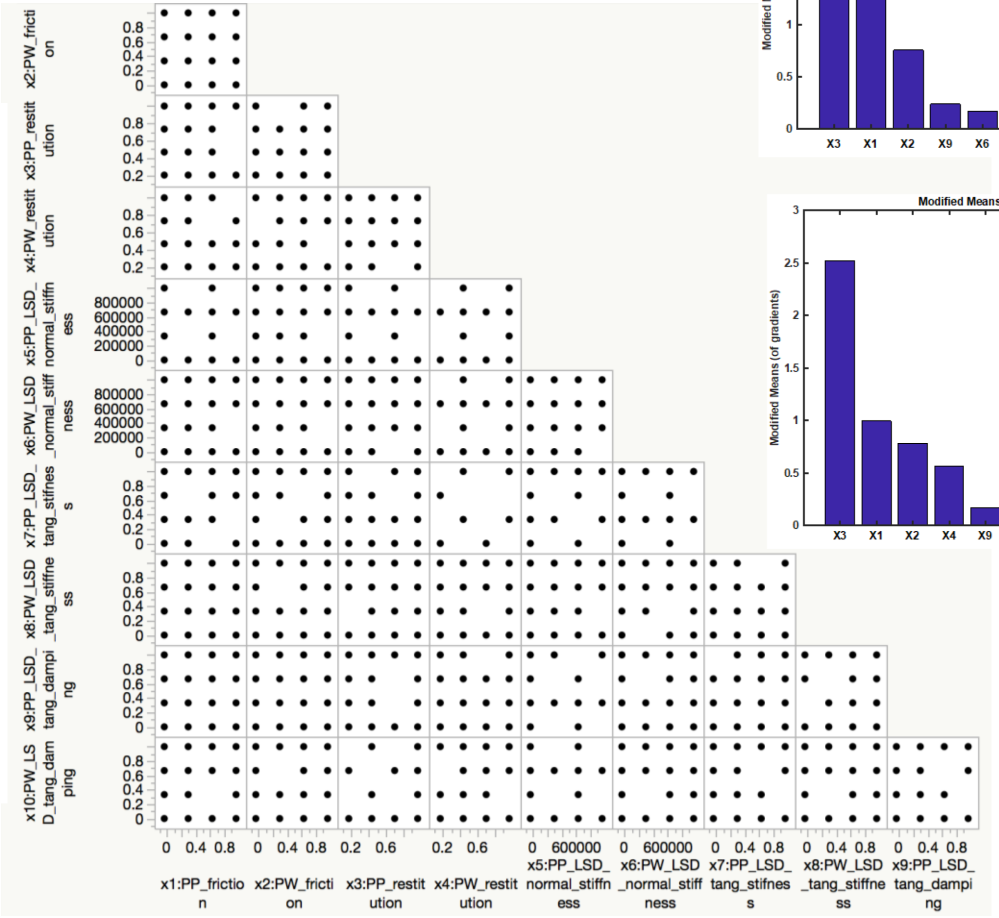
Hopper discharge

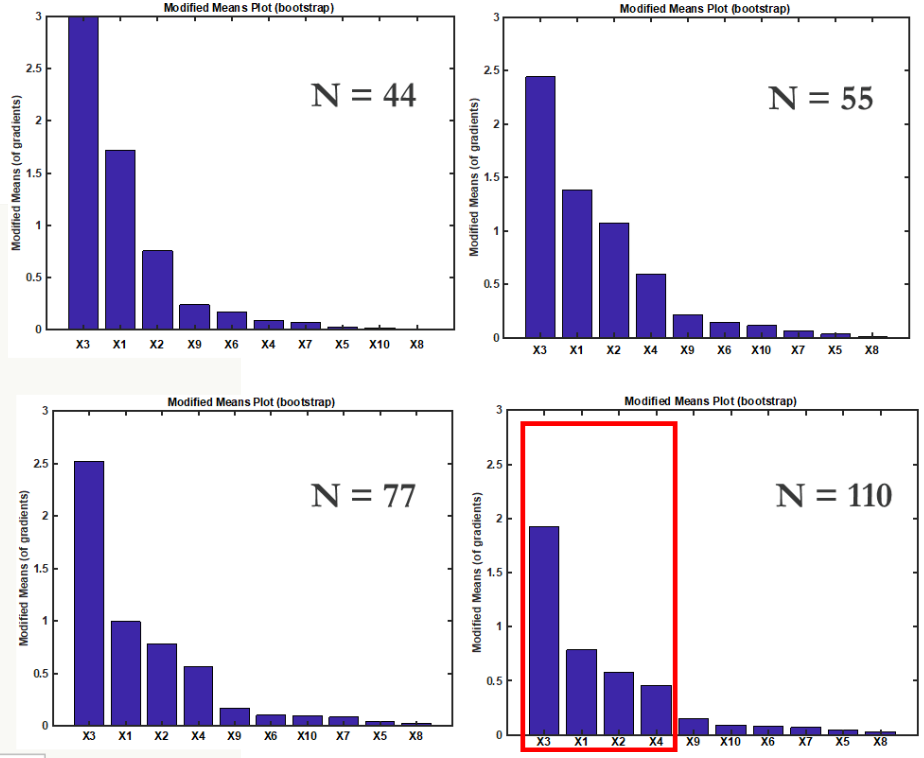
Screening study

- Granular discharge through a conical hopper
- “Mass-flow” operation mode









Rank	N=44	N=55	N=77	N=110
1	x3	x3	x3	x3
2	x1	x1	x1	x1
3	x2	x2	x2	x2
4	x9	x4	x4	x4
5	x6	x9	x9	x9
6	x4	x6	x6	x10

Hopper discharge

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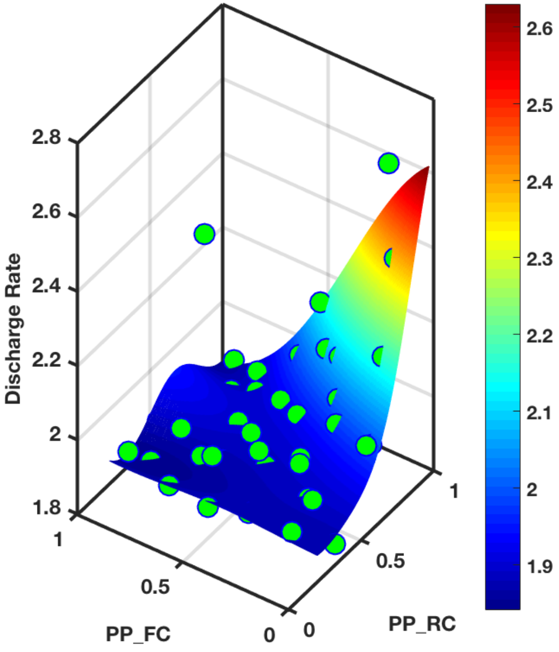
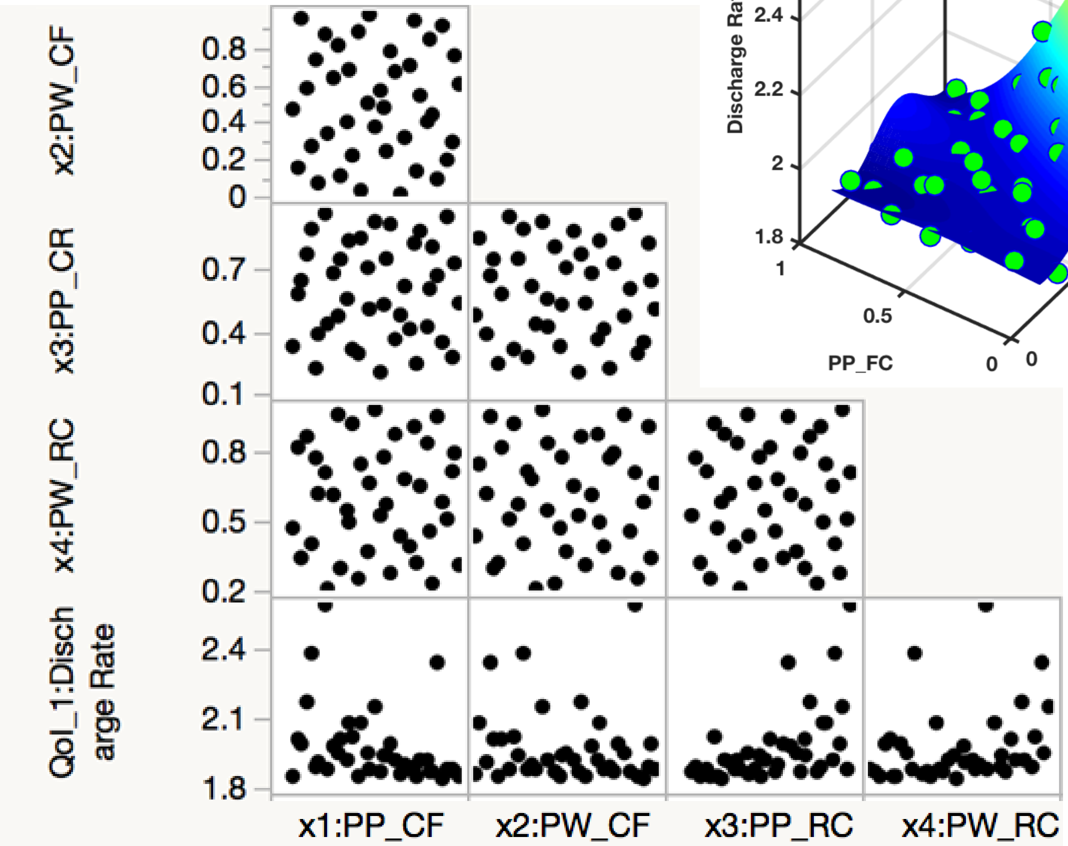
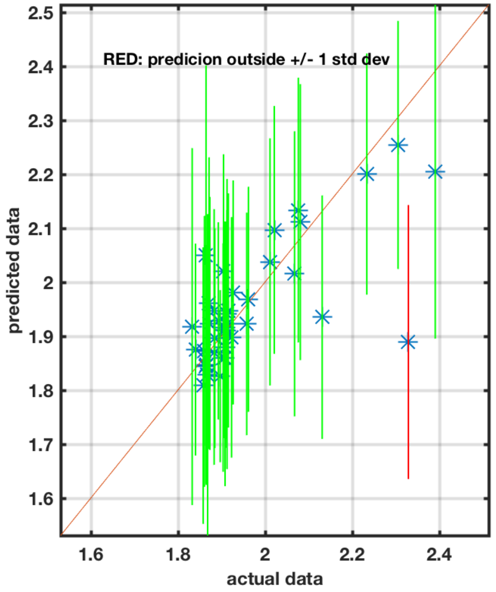
Global Sensitivity Analysis

Response surface

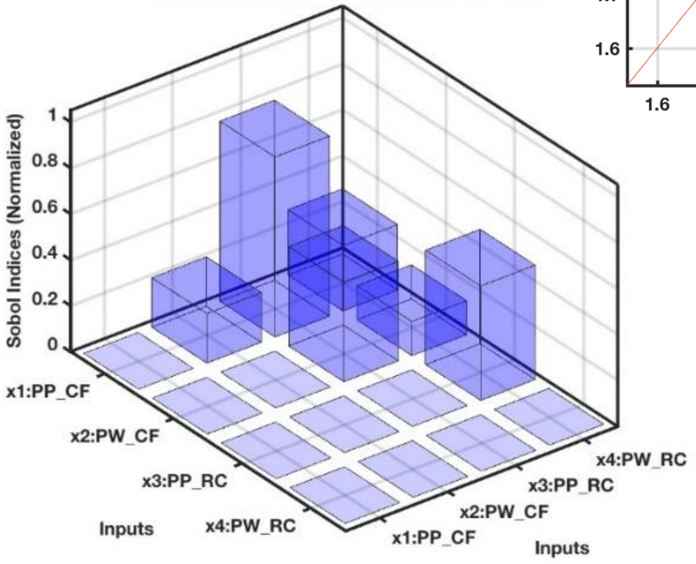




Parity plot



Sobol indices



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Pulsed Fluidized Bed

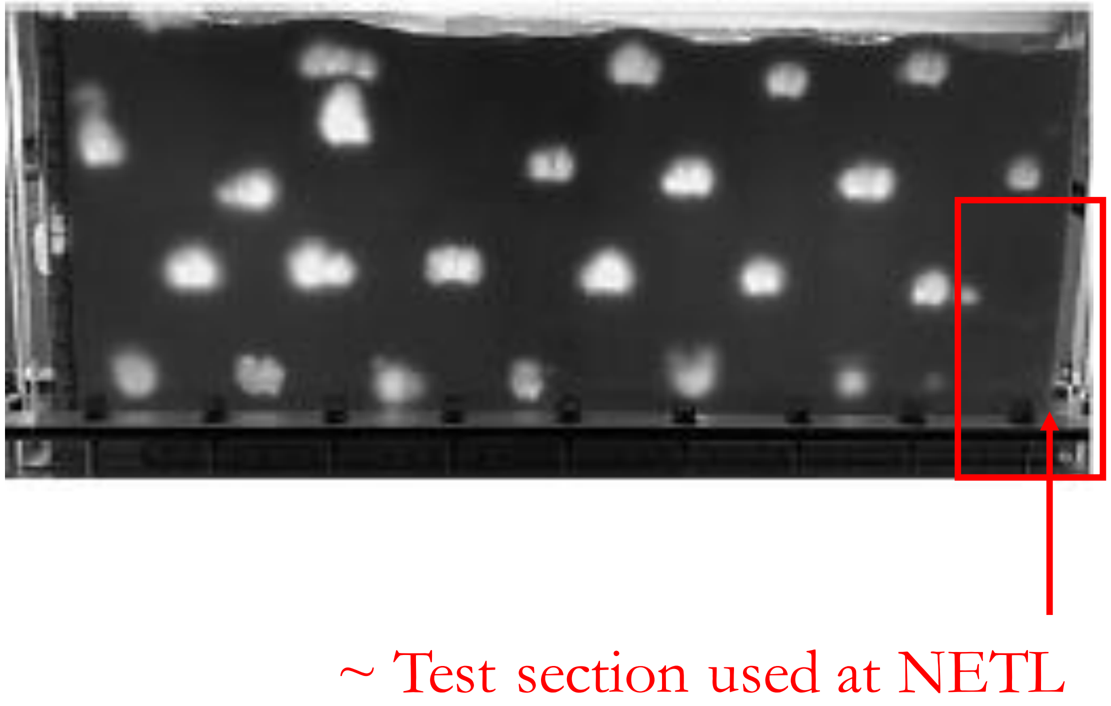
Experiments

- **Periodic fluidization leads to structured bubbling pattern depending on material properties and operating conditions**

- **Bench-scale system to facilitate UQ study**

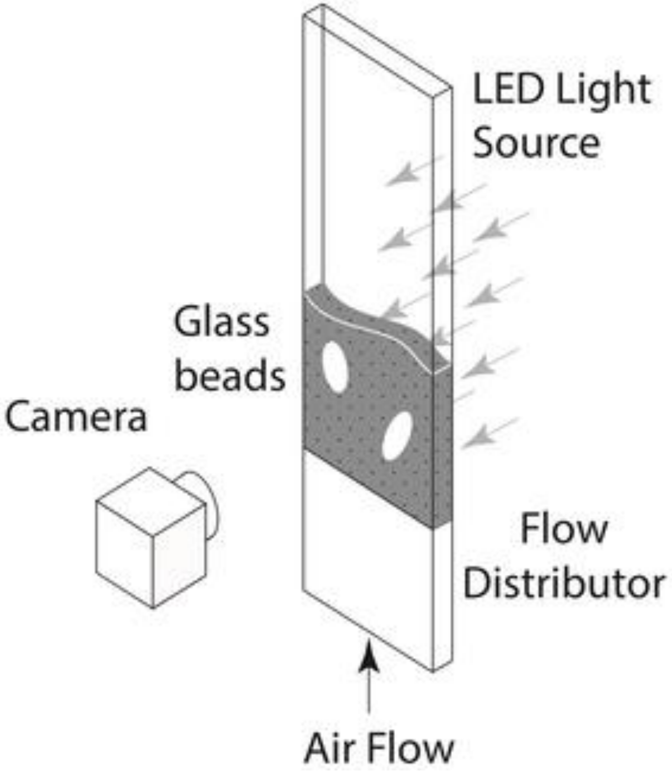
Material	Glass
Particle density	2500 kg/m^3
Mean particle diameter	394 µm
Particle count	188,496
Dimensions of the bed	50 mm X 5 mm
Pulsing frequency	4 Hz, 5 Hz, 6 Hz
Particle count	188k

Coppens and co-workers (University College London)



Pulsed Fluidized Bed

Experiments



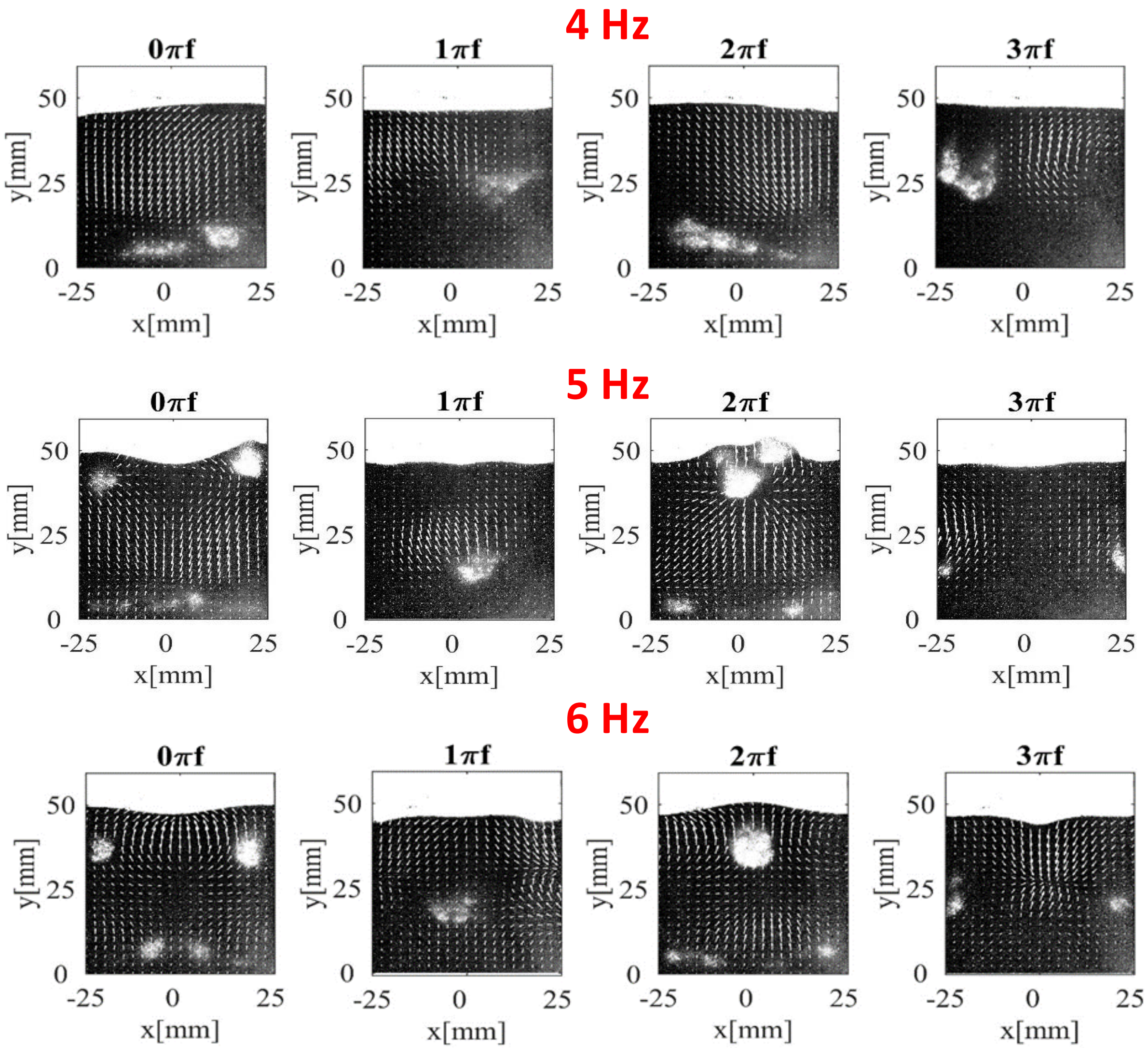
$$U = u_0 + u_A \sin(2\pi f t)$$

J. Higham, M. Shahnam, A. Vaidheeswaran, *arXiv.* 2018; 1809.05033

Pulsed Fluidized Bed

Experiments

- Controlled repeatable bubbling pattern every 2 cycles
- Change in the bubbling characteristics with pulsing frequency
- Larger bubbles at 4 Hz: bubbles migrate from one side to the other (1-1 pattern)
- The pattern changes to 1-2 at 5 Hz and 6 Hz and the average size of bubbles decreases

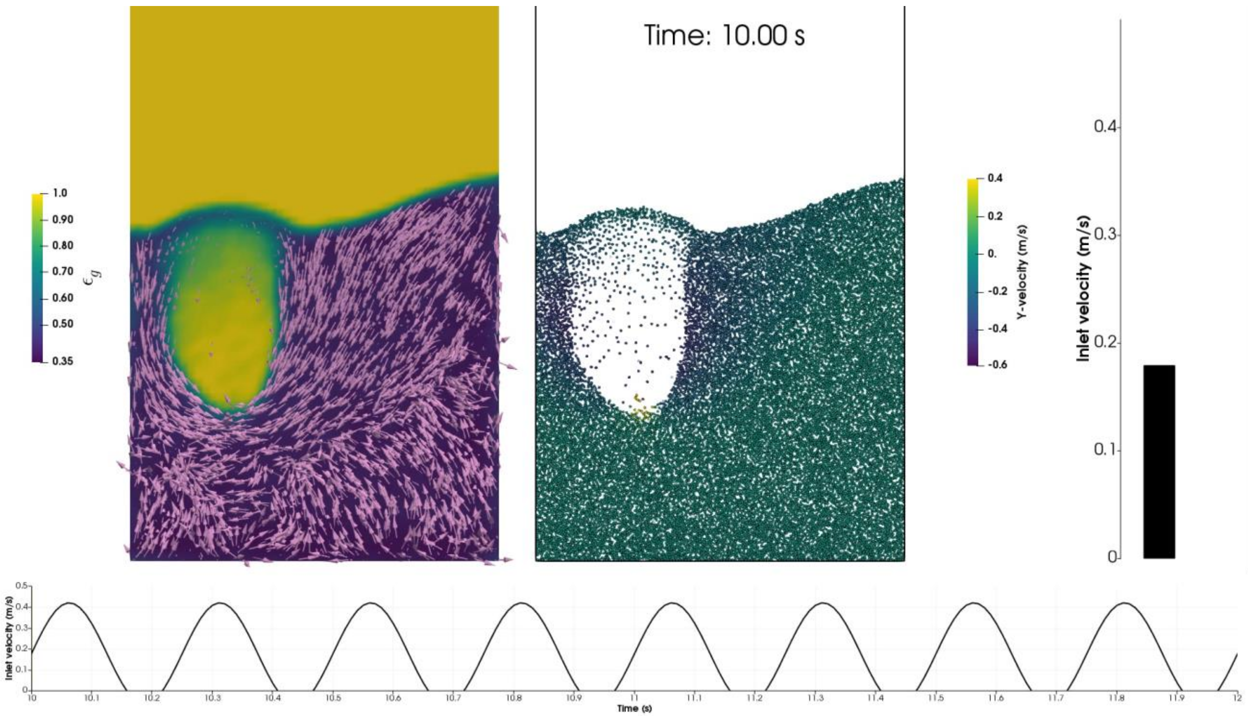


J. Higham, M. Shahnam, A. Vaidheeswaran, *arXiv.* 2018; 1809.05033

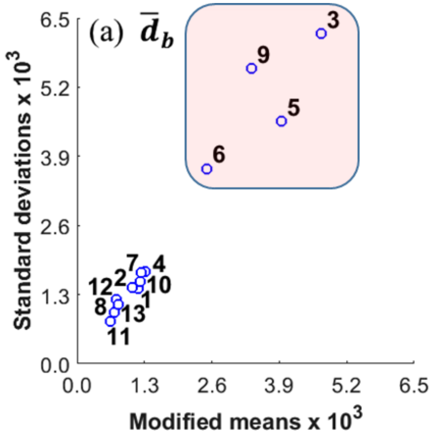
Pulsed Fluidized Bed

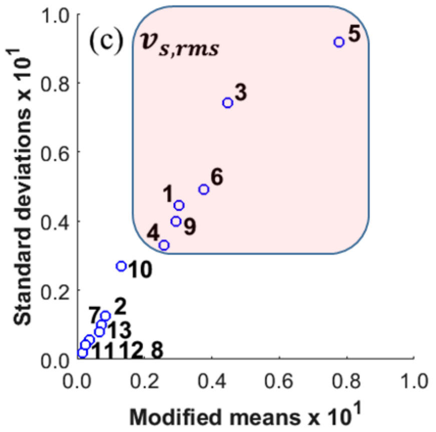
Simulations

- Sensitivity analysis of pulsed-fluidized bed system using MFiX DEM
- Parameters influencing mean diameter and root mean square velocity
- Coefficients of friction restitution and ratio of damping factors seen to be influential

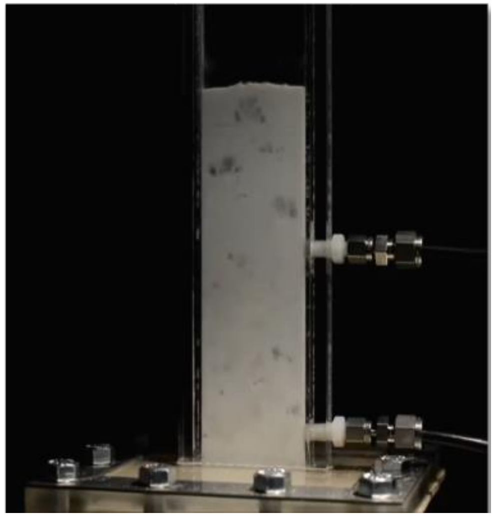


p1: k_n	p2: k_{nw}	p3: μ
p4: μ_w	p5: e_n	p6: e_{nw}
p7: k_t/k_n	p8: k_{tw}/k_{nw}	p9: η_t/η_n
p10: η_{tw}/η_{nw}	p11: t_{DEM}/t_c	p12: tol
p13: w_{DES}		

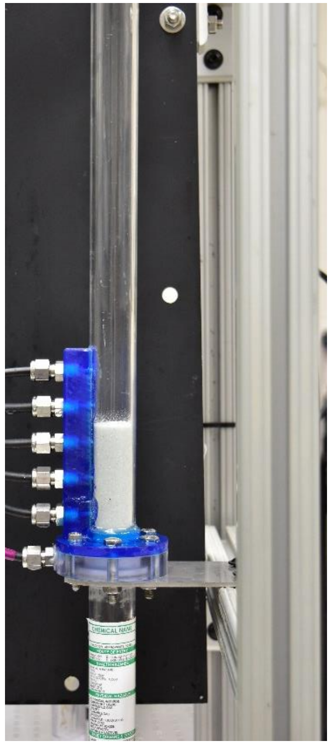




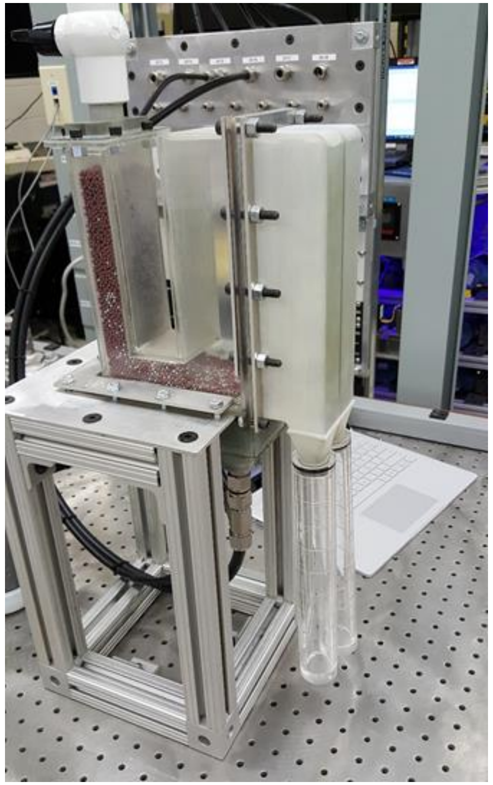
NETL Multiphase units - Cold flow



Pseudo-2D Fluid bed
2” X ¼”



Cylindrical Fluid beds 1”, 2.5”



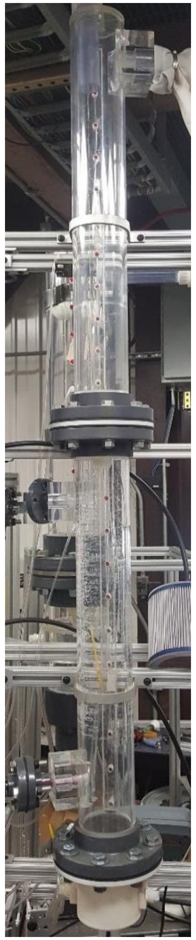
Continuous separator

Mini CFB

NETL Multiphase units - Cold flow

Fluid bed
4”

Spouted beds
1” x 4” & 3” x 12”



Moving bed
4”

Circulating fluid bed
4”

Circulating fluid bed
12”

Vortexing Circulating
fluid bed 8”

Courtesy: Justin Weber

NETL Multiphase units - Reacting flow

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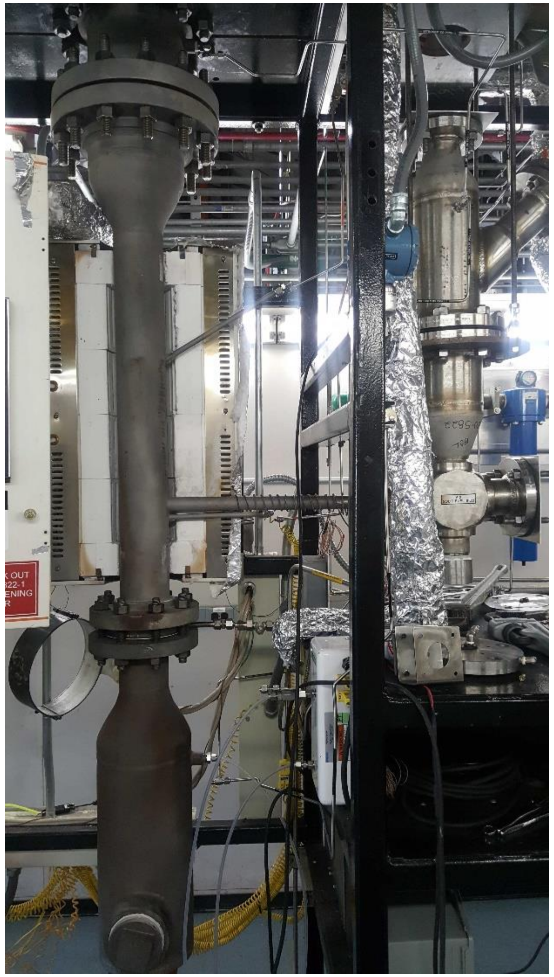
Chemical loop reactor
8" FR, 6" AR, 2" riser

Single fluid bed/jet cup 2"



Solid fuel fluid bed 4"

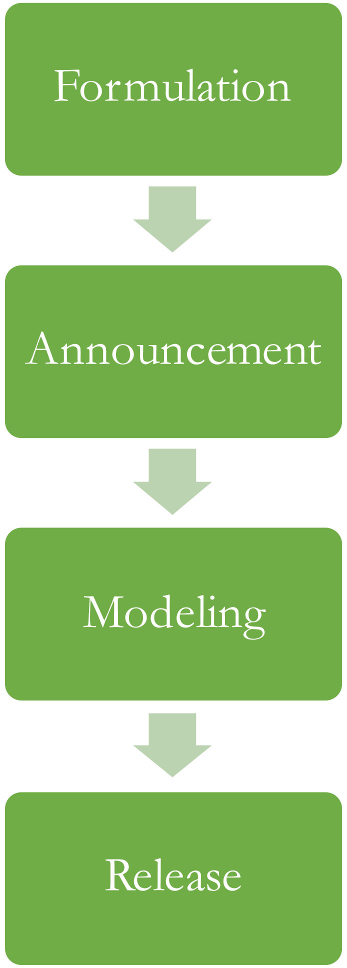
Spouted bed 2" x 8"

U.S. DEPARTMENT OF ENERGY

Courtesy: Justin Weber

Challenge Problems

- **Idea of CPs for particulate flows originated at Fluidization VII**
- **Accelerate the development of simulation-based engineering**
- **Test predictability, accuracy of numerical models and their implementations**
- **Identify existing modeling deficiencies**
- **Features**
  - Well-characterized operating conditions for accurate representation
  - Repeats or replicates for high-confidence measurements
- **CPs in the past**
  - CP III – Bubbling fluidized bed (NETL), Circulating fluidized bed (PSRI)
  - SSCP I – rectangular fluidized bed (NETL)



Small-Scale Challenge Problem II

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- **Fluidization in a bench-scale rectangular domain**
- **Smaller geometry for better control over operating conditions**
- **Data would include:**
  - Fluidization-defluidization characteristics
  - Particle size distribution
  - Properties including sphericity, coefficients of friction and restitution
- **Quantities of Interest:**
  - Pressure statistics
  - Particle velocity statistics
- **Possibly involve geometric scaling at 2X**
- **Long term data management**
- **Intended date of announcement – Spring/Summer 2020**

Potential operating conditions

	SSCP I	SSCP II
Geometry	9” X 3”	4.5” X 1.5”
Material	Nylon beads	Ceramic beads
Diameter	3 mm	1 mm
Particle count	100k	800k
Flow rates	$2U_{mf}$, $3U_{mf}$, $4U_{mf}$	Up to $3.5U_{mf}$

Feedback welcome !!

Ongoing efforts and plans for future

- Consistent development of MFiX-DEM & MFiX-PIC feeding in to MFiX-Exa
- Extension of VV&UQ methodologies for reactive flows – experiments and simulations
- Provide open-access data covering design of experiments and simulation campaign
- Larger-scale facility to support development of MFiX-PIC and coarse-grained modeling techniques
- Active collaboration with universities and research organizations, use external data for validation and cross-validation

MFiX Suite Quality Assurance

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Team

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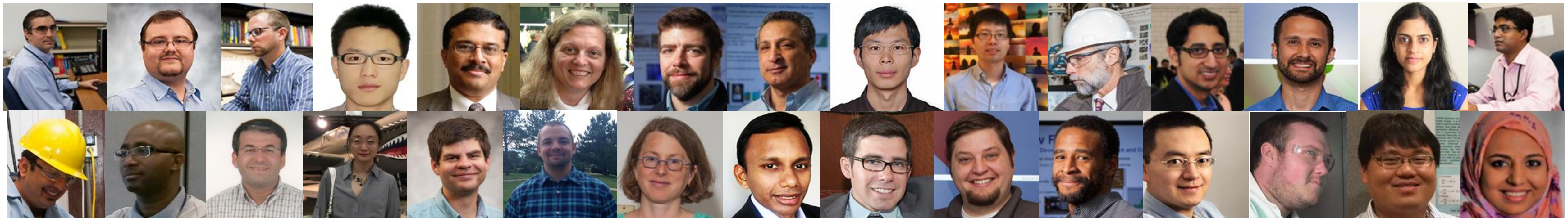

Thank you for your attention. Questions?