MFiX - Multiphase Flow with Interphase Exchanges

Software tools and expertise to address multiphase flow challenges in research, design, and optimization

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Project Description and Objectives

CARD: CFD for Advanced Reactor Design

- Develop, enhance, and apply NETL's suite of MFiX software tools that are used for design and analysis of novel reactors and devices for fossil energy (FE) applications.
- Enable science-based models as viable tools to reduce the risk, cost, and time required for development of novel FE reactors.
- Open source codes are developed, validated, and supported in-house by NETL's software development and application specialists.
- Support the following FE pillars of research:
  - Modernization of existing coal fleet.
  - Development of coal plants of the future.
  - Reduction of the cost of carbon capture, utilization, and storage (CCUS).
- **Unique NETL competencies:**
  - Multiphase flow modeling expertise
  - Joule 2.0 Supercomputer
  - MFAL: high fidelity data that measures key performance parameters across a broad range of flow conditions-including fixed bed, bubbling, turbulent, entrained flow, and CFBs

Project Description and Objectives

CARD Tasks

- **Task 2:** Develop, validate, apply, publicly distribute, and support MFiX
  - Large-scale, reactor systems
  - Complex chemical reactions
  - Realistic geometry
- **Task 3:** Collaborate with industry partners
  - Apply computational tools and FE/NETL supercomputing resources
  - Understand and optimize circulating fluidized bed (CFB) boiler performance.
- **Task 4:** Accelerate time to solution (see Dr. Dirk Van Essendelft's update)
  - Google's TensorFlow™, will be linked to NETL's MFiX and the solvers will be written in TensorFlow to achieve significant code acceleration on the latest hardware.

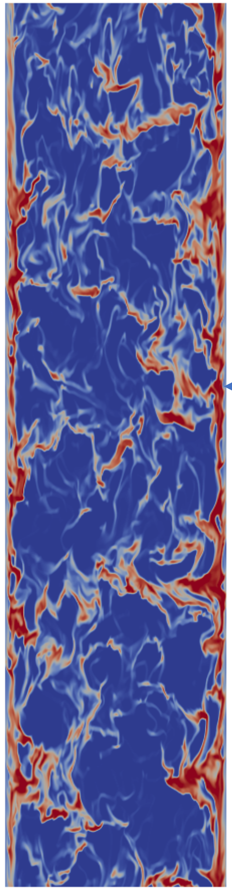
Project Update

Task 2: MFiX Development, Validation, and Enhancements

- Graphical user interface (GUI)
  - Increase usability of the code
  - Minimize error in setup, execution, and post processing.
- Additional Models/ physics required for challenging FE applications:
  - Particle in Cell
  - Coarse Grain Discrete Element Method
  - Non-spherical particles
  - Polydispersity
- Quality Assurance (QA) Program
  - Validation
  - Verification
  - Improved documentation, user guides, and validation experiments.
- Outreach capabilities through the MFiX web portal to better serve FE and NETL stakeholders.

MFiX Suite of Multiphase CFD Software

Managing the tradeoff between accuracy and time to solution



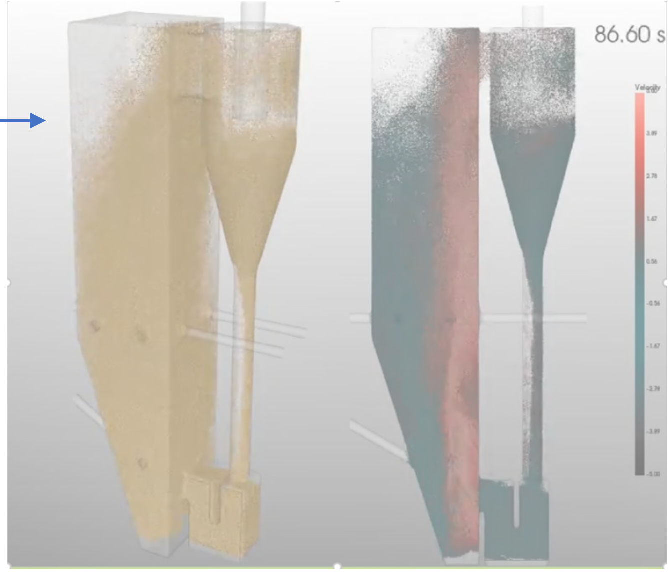
Time to Solution

DNS
Direct Numerical Simulation: fine scale, accurate simulations for limited size domain

MFiX DEM — *Discrete Element Method: Track individual particles and resolve collisions*

MFiX TFM — *Two-Fluid Model: Gas and solids form an interpenetrating continuum*

MFiX PIC — *Particle-in-Cell: Track parcels of particles and approximate collisions*



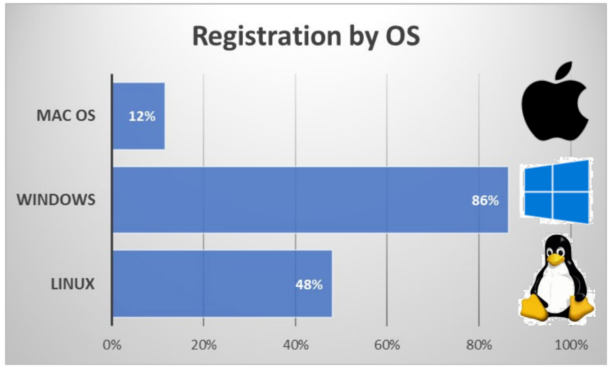
MFiX Exa — *Exascale: New code for new generation of computers*

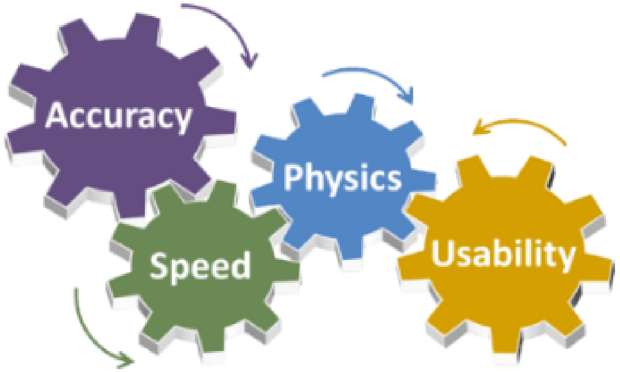
ROM
Reduced Order Models: Simplified models with limited application

Model Uncertainty

Graphical User Interface (GUI)

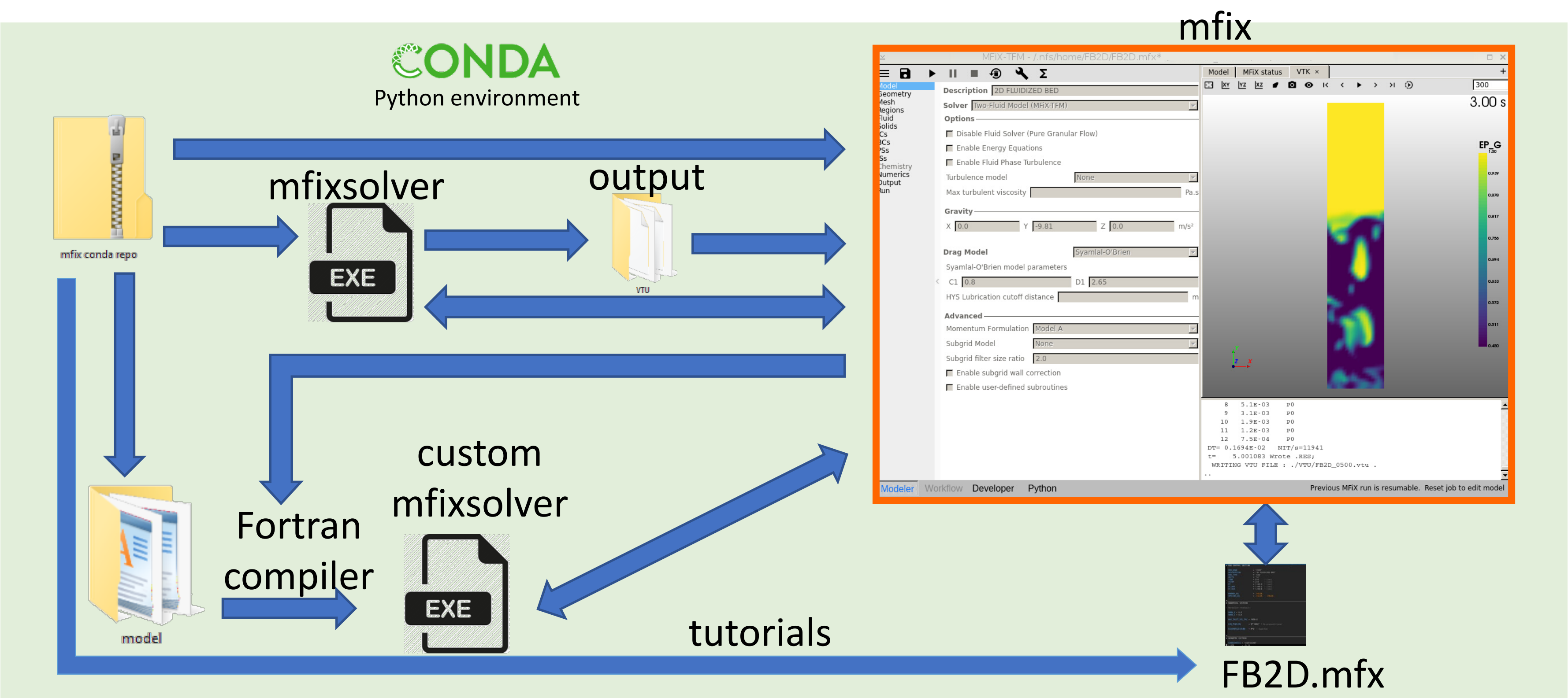
- **Open-source (https://mfix.netl.doe.gov)**
- **Motivation: Better serve MFiX community**
  – Improve usability of MFiX
  – Support Linux, macOS and Windows OS
  – Decrease time to setup, reduce error
- **Solution: Graphical User Interface**
  - Released in 2017
  - Between 1 and 4 releases per year





MFiX usability improvement

NETL Multiphase Flow Science
Home of the MFiX Software Suite.
https://mfix.netl.doe.gov



User responsibility

Preprocessor development

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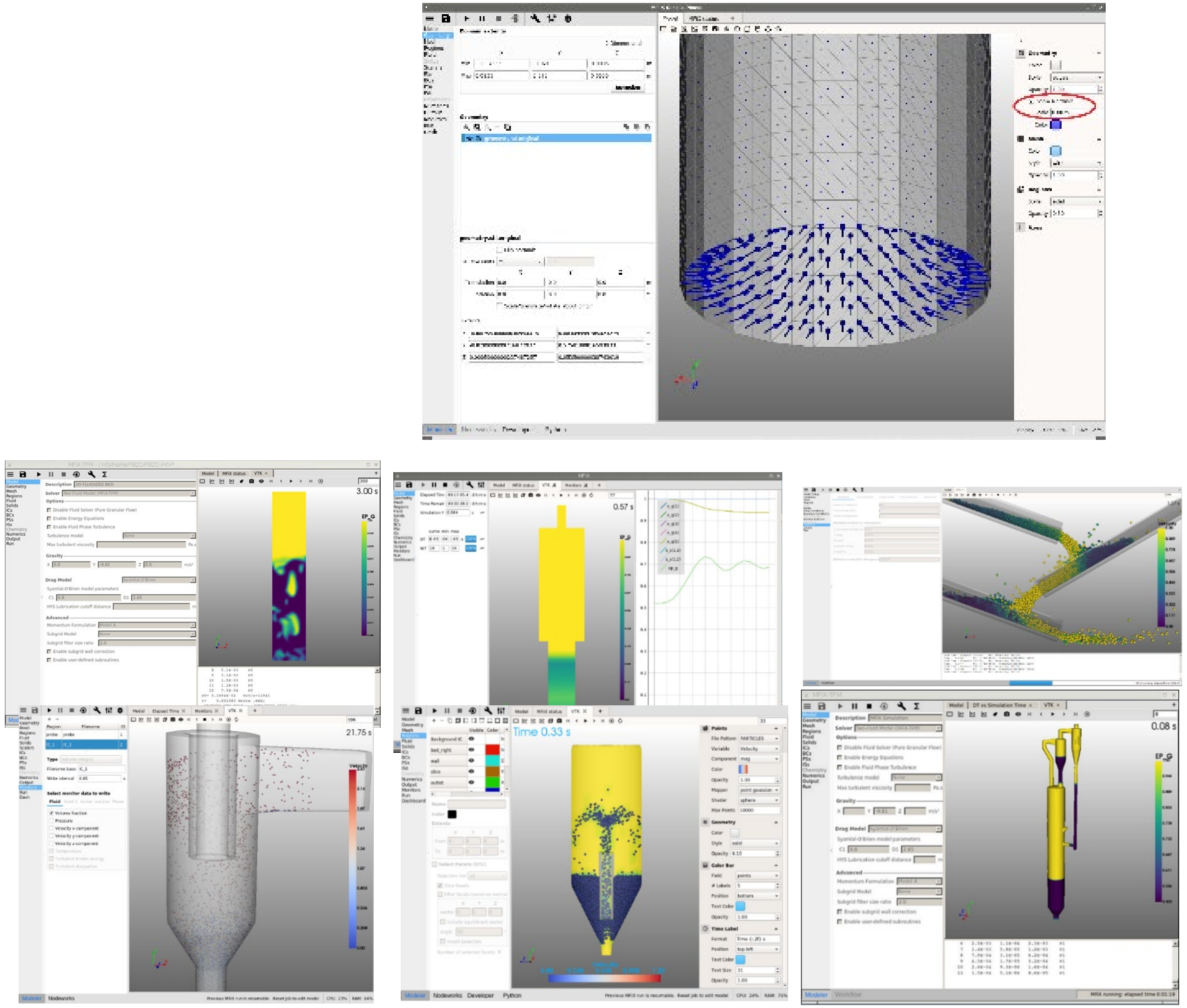
User setup (.mfx file) greatly improved by GUI

Increased demand for complex geometry

Mesh generation

- Workflow challenge
- Geometry input (STL file)
- Preprocessing (cut cells)
- Mesh quality
- Difficult to troubleshoot
- Specific constrains for TFM, DEM and PIC



U.S. DEPARTMENT OF ENERGY

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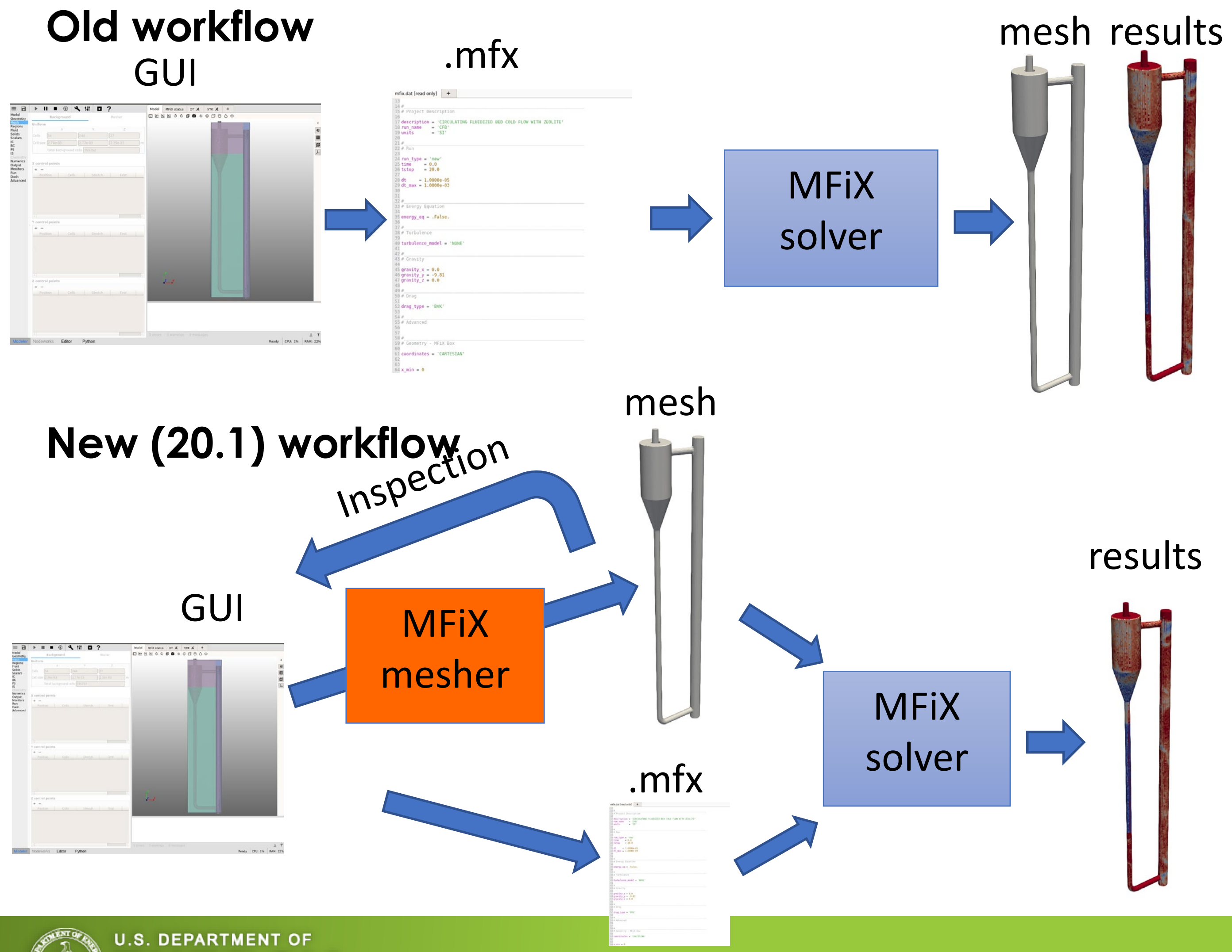
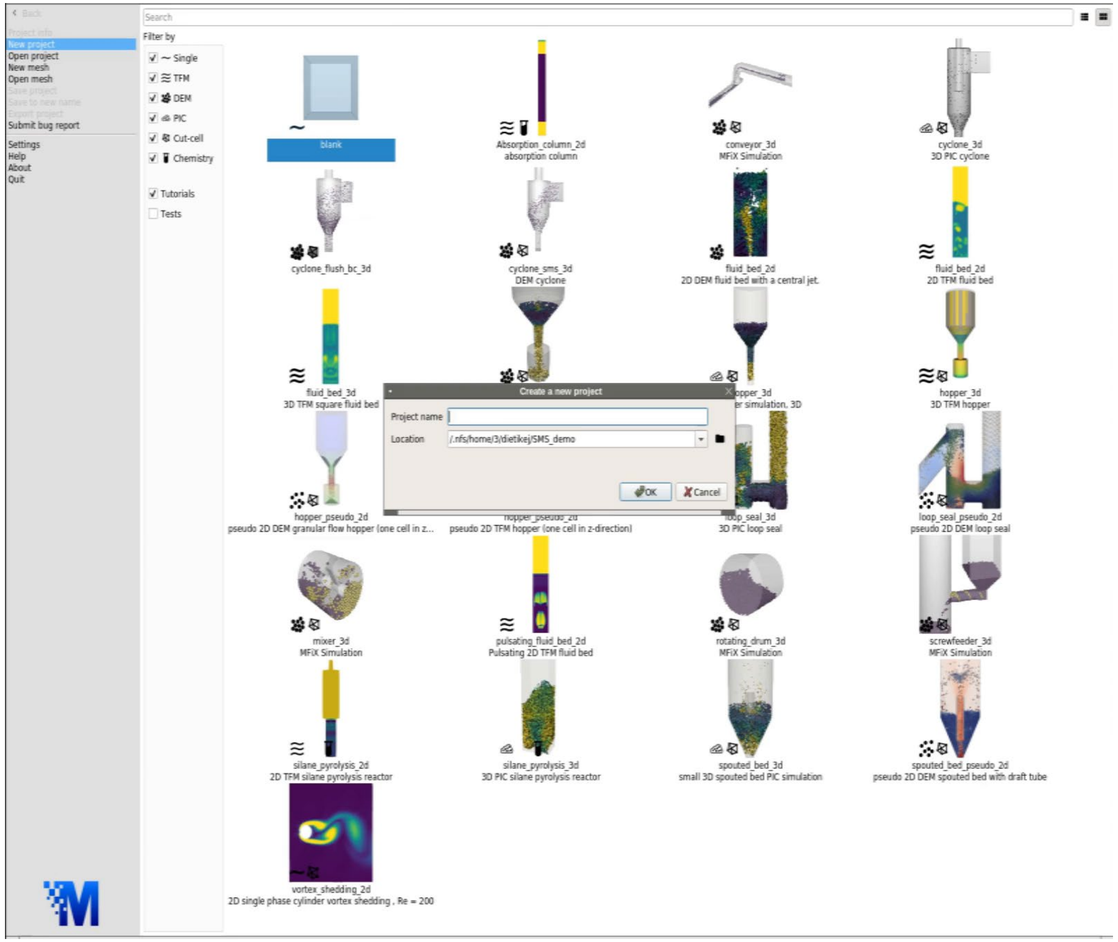
Preprocessor development





Enabling large Scale simulations

DEM example

Height = 0.68 m

Particle diameter = 800 microns

Particle count = 500,000 particles

Enabling large Scale simulations

Height = 4.0 m (x6)
Particle count = 650 Millions (x1,300)
☒ **DEM**
☑ **PIC,** Parcel counts = 13 Millions

Height = 0.68 m
Particle count = 500,000
☑ **DEM**

Multiphase Particle In Cell (MP-PIC)

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Use MP-PIC for computational speed and averaged accuracy

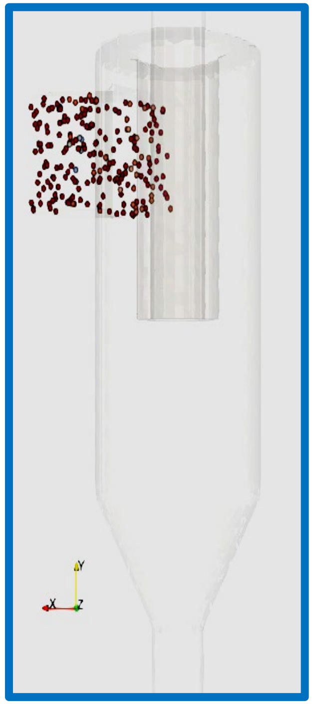
REDUCED ACCURACY ↑ SOLIDS REPRESENTATION

SOLIDS REPRESENTATION	Collision Resolved	Momentum Conservation	Solid Stress Gradient
Parcel	**CGPM** Coarse Grained Particle Method **Masaaki et al. 2000** **Sakai and Koshizuka,2009**	**CGHS** Coarse Grained Hard Sphere **Lu et al., 2017**	**MP-PIC** Multi Phase Particle In Cell **Andrews and O’Rourke, 1996**
Particle	**CFD-DEM** Computation Fluid Dynamic-Discrete Element Method **Tsuji et al., 1993**	**ED/TD HS** Event Driven/ Time Driven Hard Sphere **Hoomans et al., 1996** **Ouyang and Li, 1999**	

GENERALIZED IDEA FOR PARTICLE INTERACTIONS → INCREASED COMPUTATIONAL SPEED

Particle Flow in Cyclone

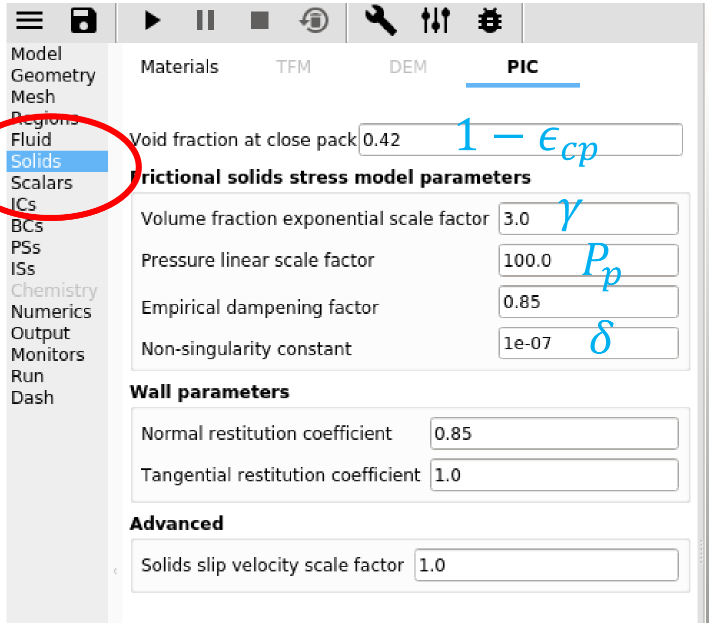
MP-PIC can significantly reduce computational effort, and in the right type of application, maintain accuracy.



Multiphase Particle In Cell (MP-PIC)

Basic Set-Up Information

The PIC model parameters are clustered under the Solids tab.



Some parameters that a user defines directly influence the momentum equation through solids stress calculation.

$$\tau_p = \frac{P_p \epsilon_p^{\gamma}}{\max\left(\epsilon_{cp} - \epsilon_p, \delta(1-\epsilon_p)\right)}$$

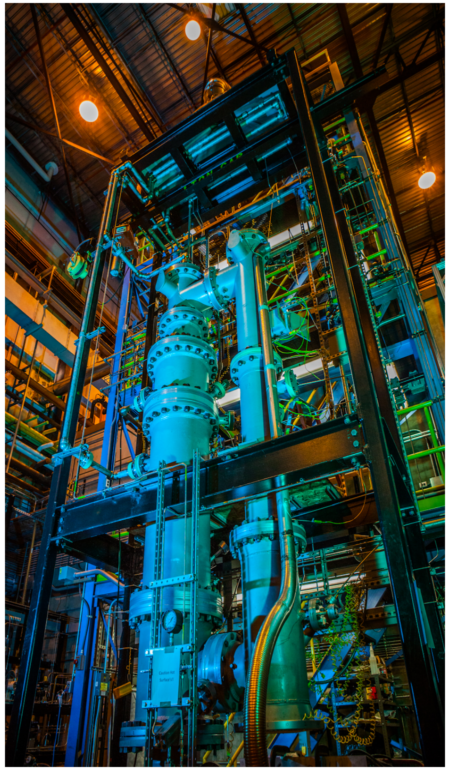
$$\frac{d\vec{V_p}}{dt} = \beta\left(\vec{U_g} - \vec{V_p}\right) - \frac{1}{\rho_p}\nabla p - \frac{1}{\epsilon_p \rho_p}\nabla \tau_p + \vec{g}$$

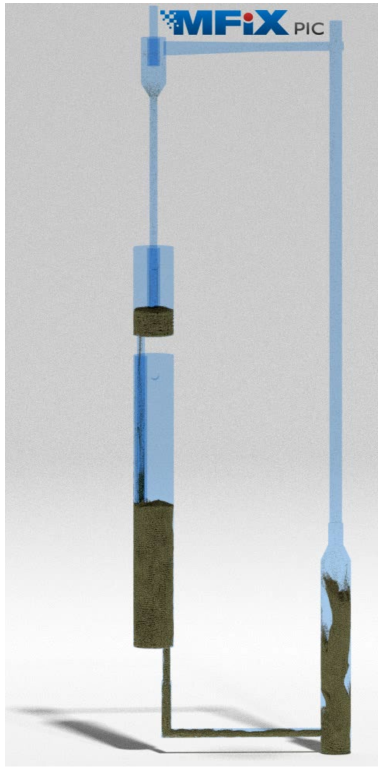
New in 20.2: PIC CFL setting

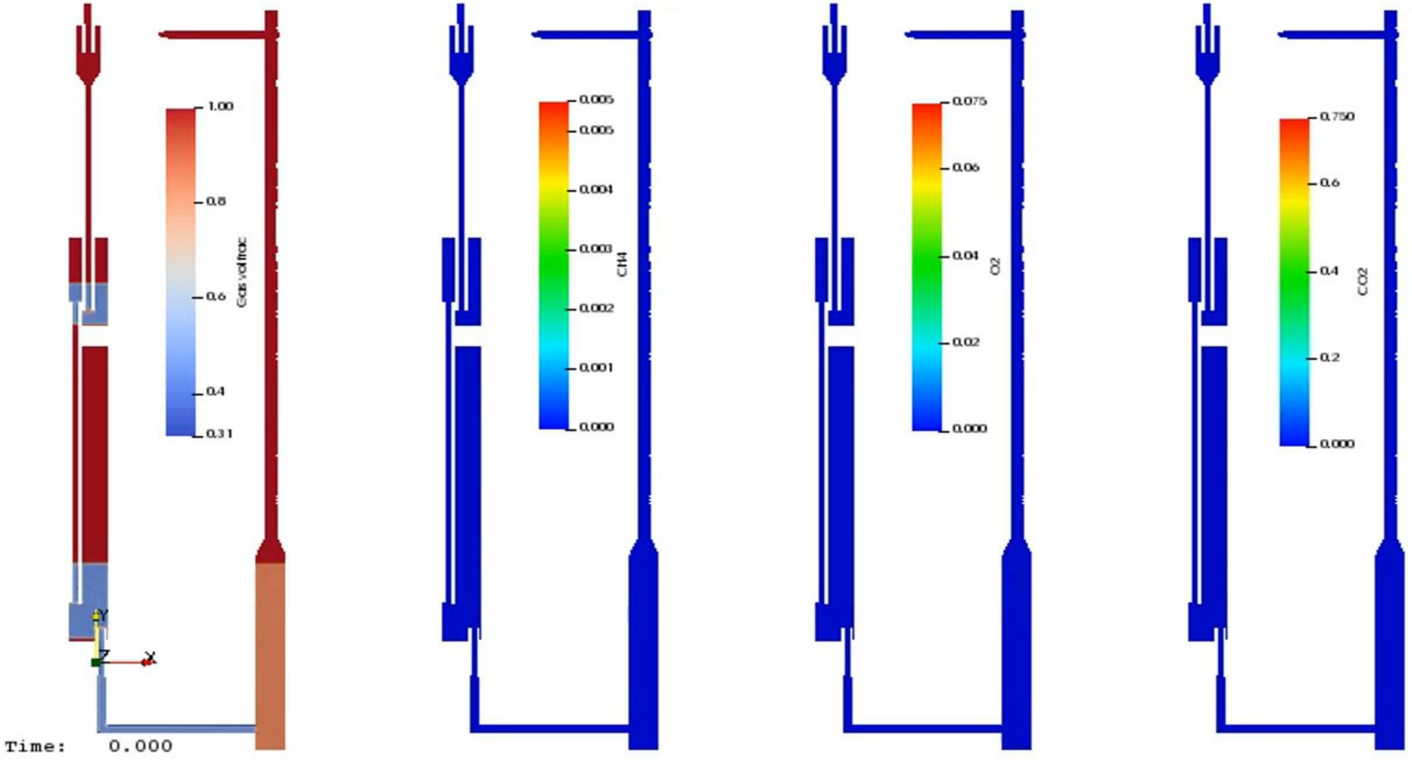
- Need for CFL identified by QA program
- Allows consistent results with large Fluid time step
- Showed speed up of 3 for a cyclone simulation

Other parameters act as scale factors for energy exchange between parcels and their surroundings.

Multiphase Particle In Cell (MP-PIC)







Simulation of industrial scale multi-phase flow devices is within MFiX's grasp!

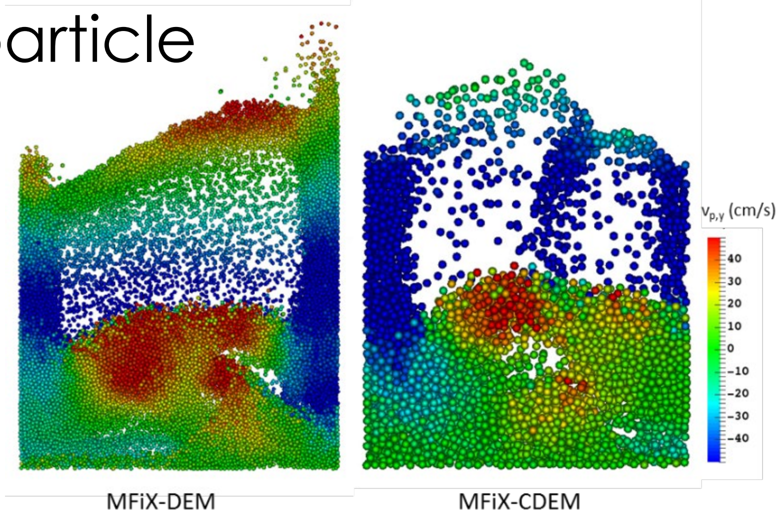
MFiX-PIC couples the MFiX Eulerian fluid solver with new Lagrangian solids stress model.

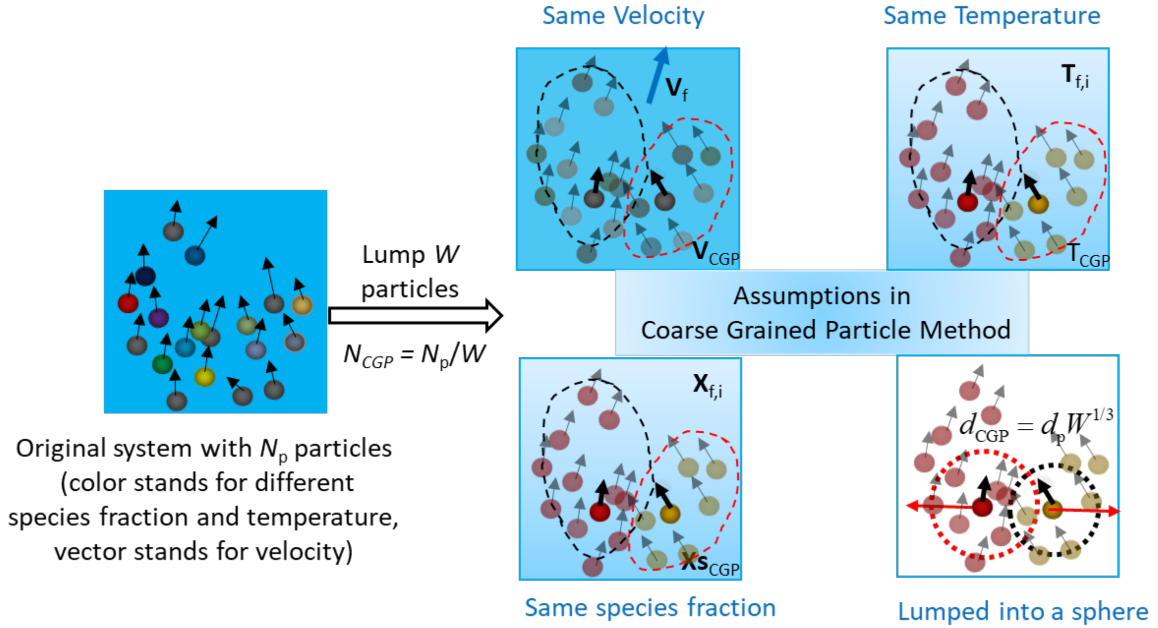
Excellent matching to pressure drop, temperature profiles and chemical species production at industrial scale.

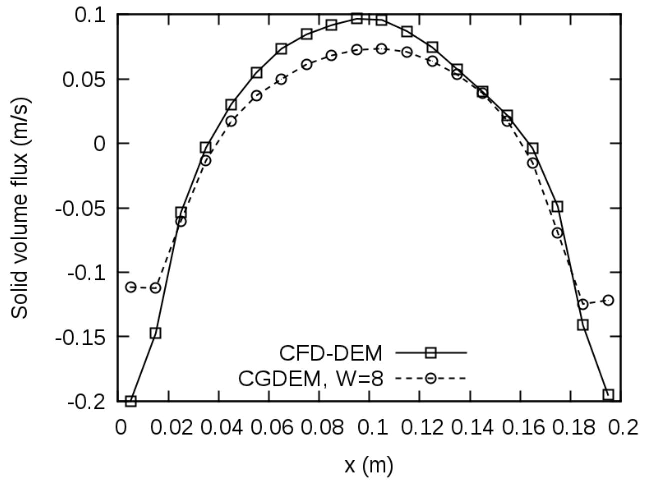
Tractable time to solution.

Coarse Grain DEM

- Particles are lumped together to create a CG particle
- CG particles collide with each other
- Heat transfer, chemical reactions
- MFiX-CGDEM formal release: 03/31/2021

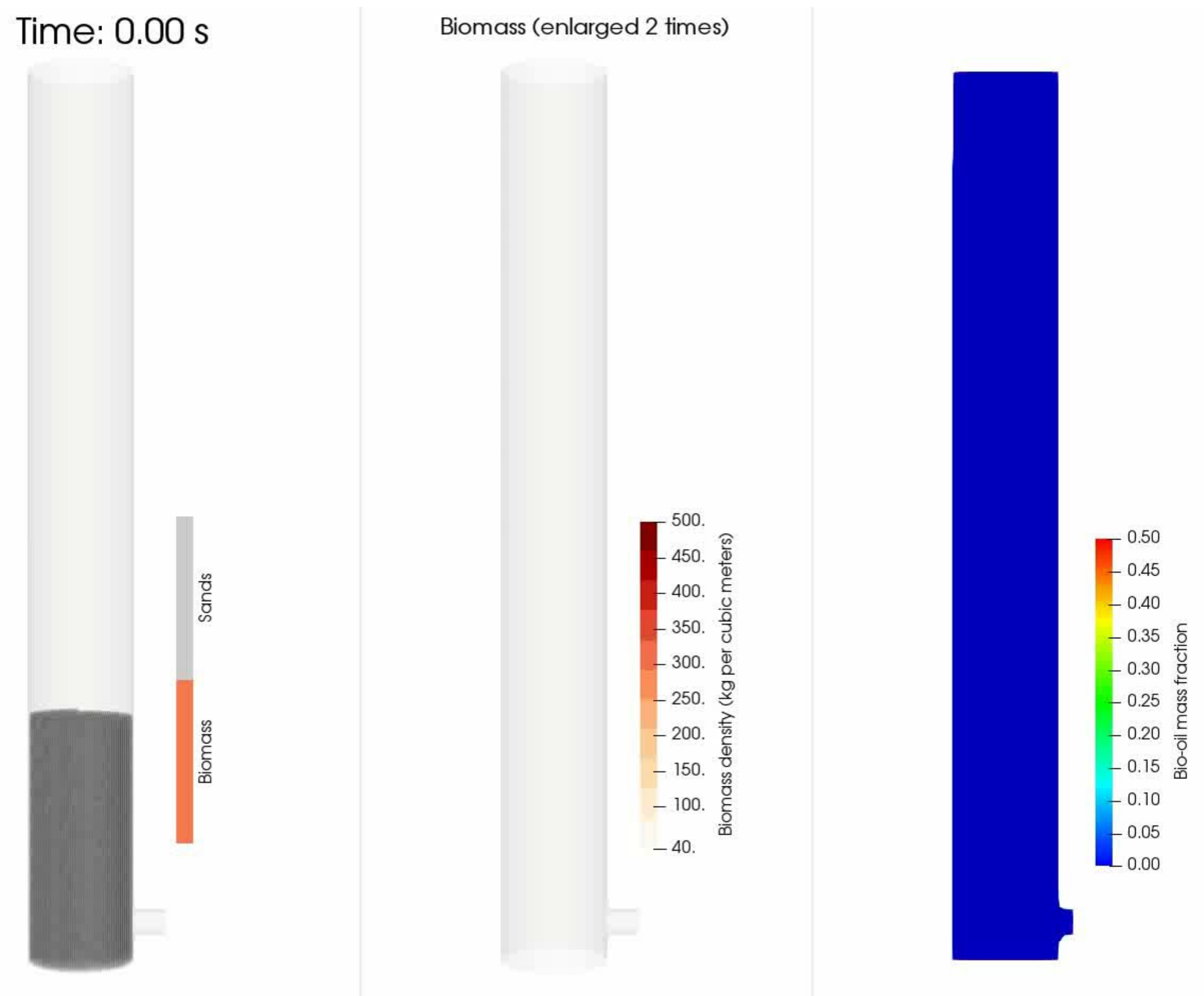




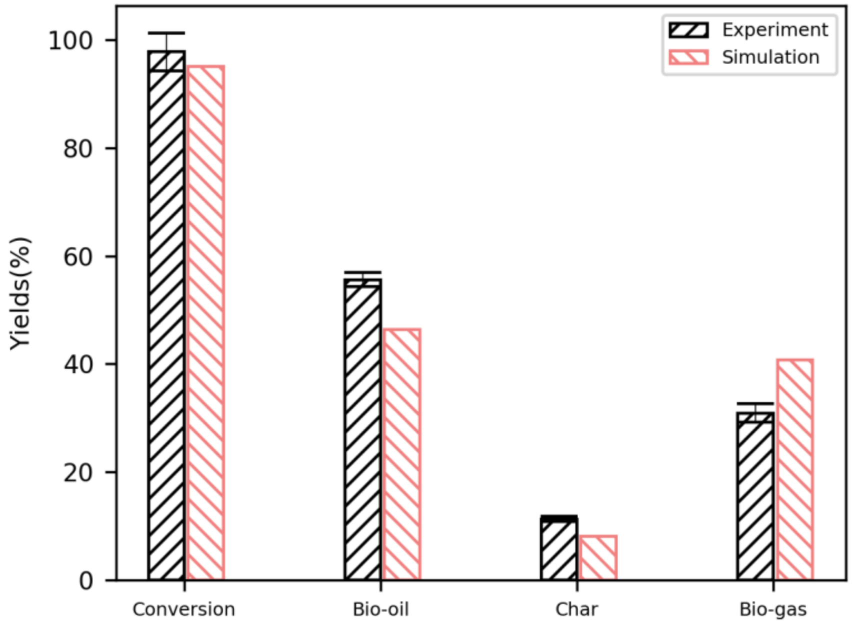


Coarse Grain DEM

CG-DEM Simulation of 2-inch Fluididzed Bed Pyrolysis Reactor



1. Sands & 130 micro Biomass
2. Coarse Grained DEM Simulation
3. Hybrid drag model
4. DNS calibrated heat transfer & reaction kinetics

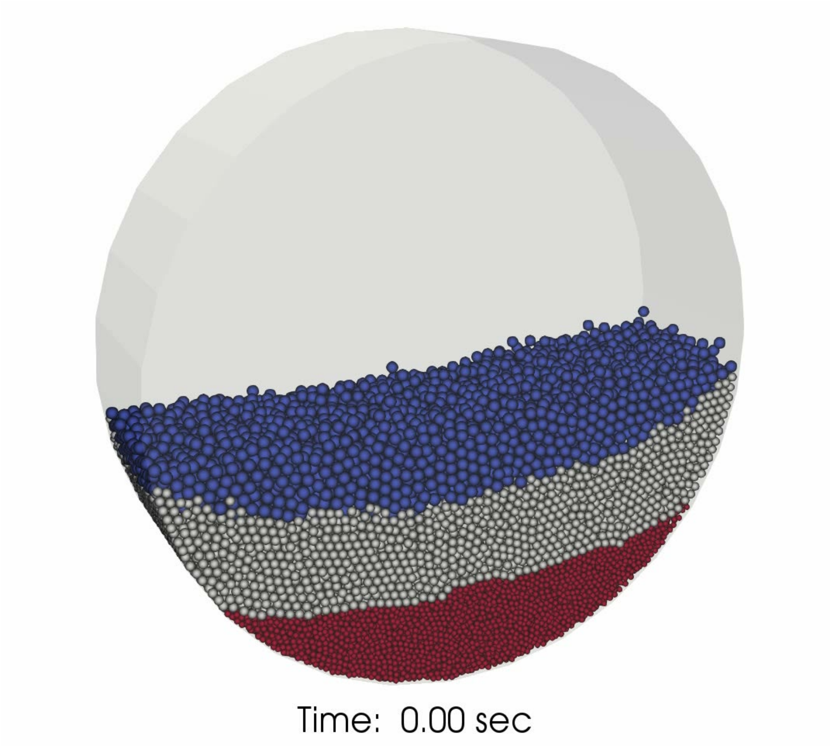


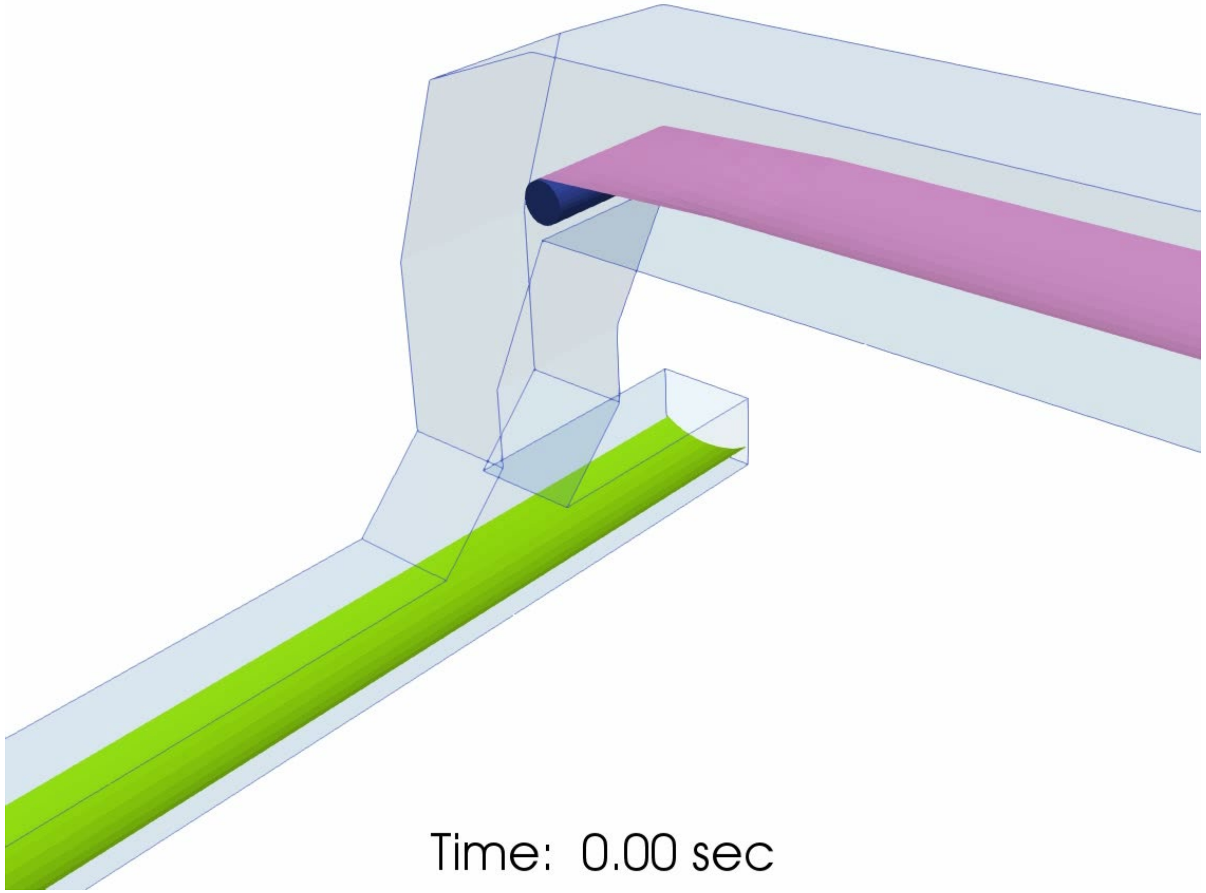
Moving geometry

Several options to represent moving geometry

Moving STL walls through tangential velocity

- Add Collection of UDFs and tutorials
- Rotating drum
- Conveyor belts

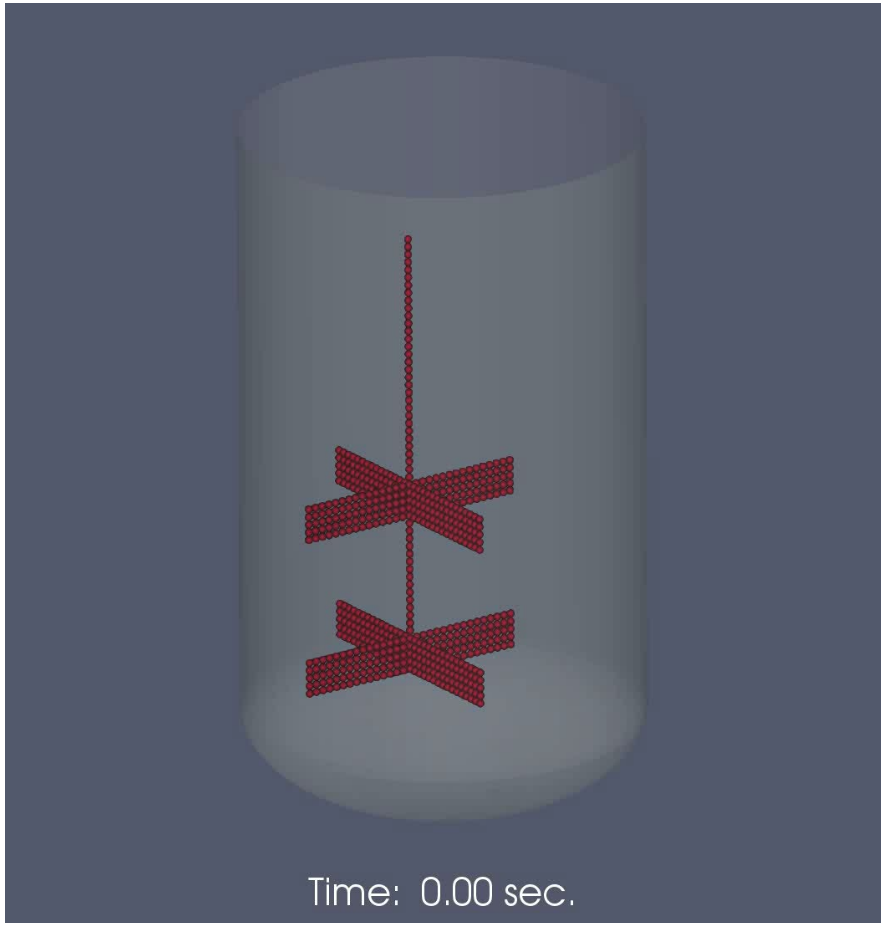




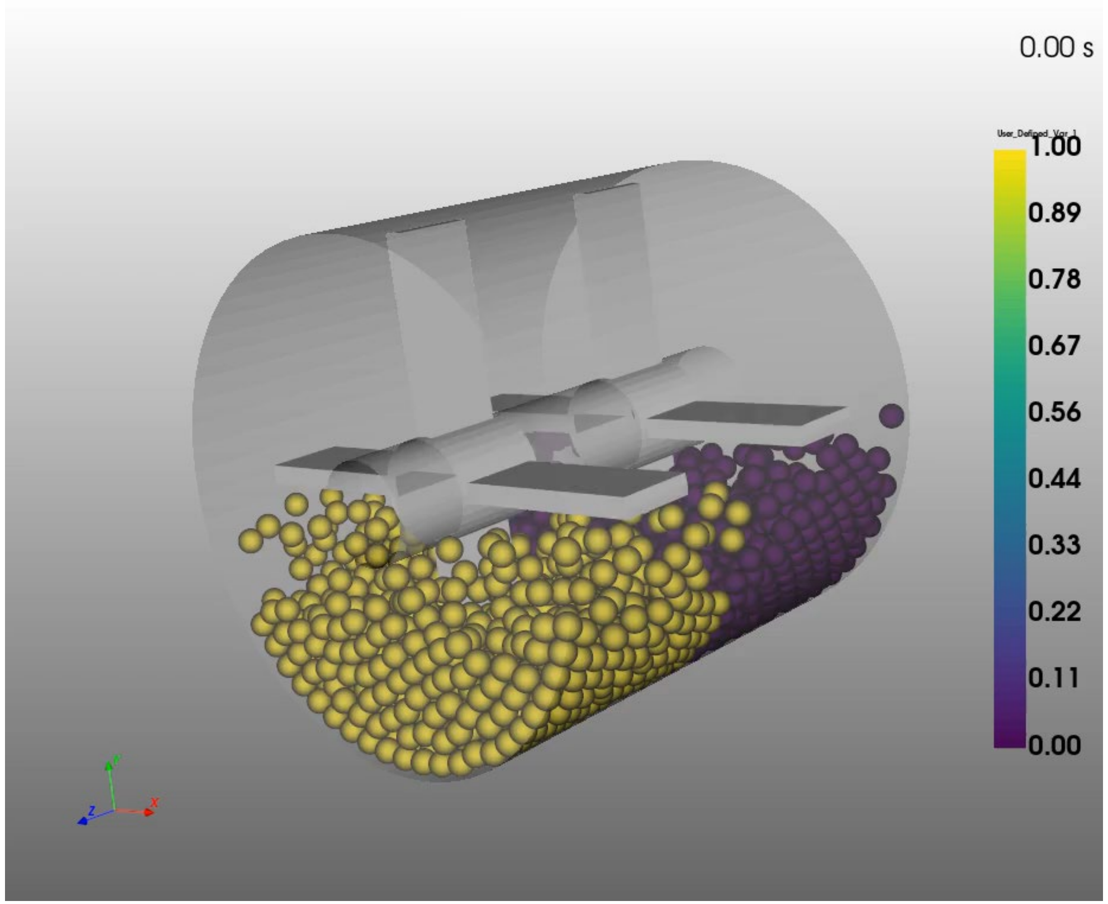
Moving geometry

Several options to represent moving geometry

Freeze or set particle velocity



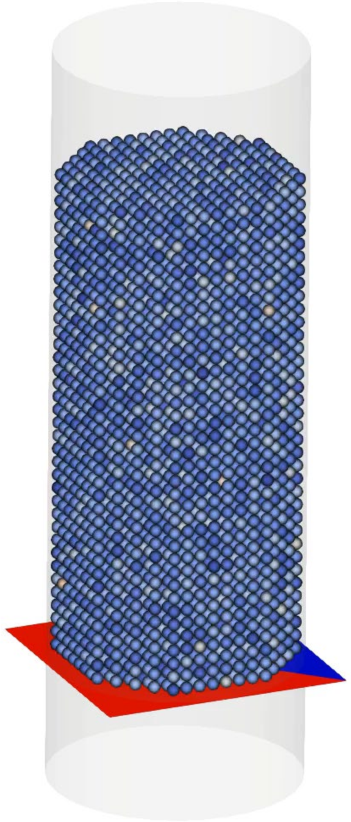
Move STL geometry (Granular DEM)

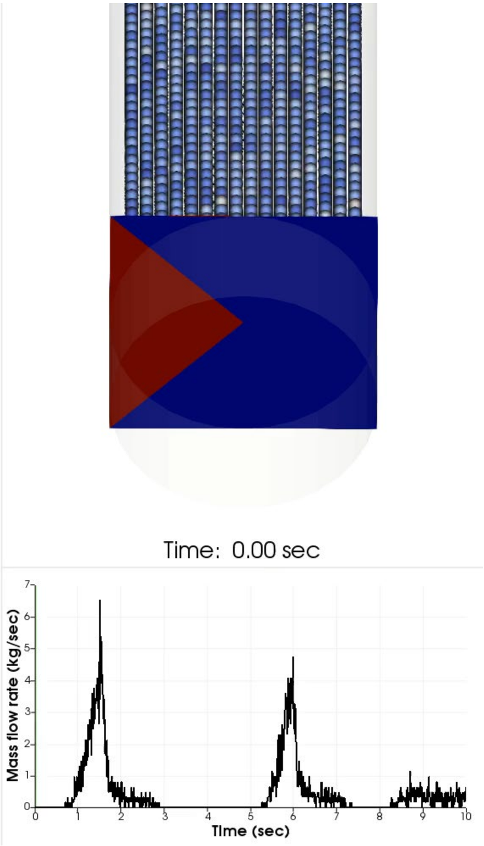


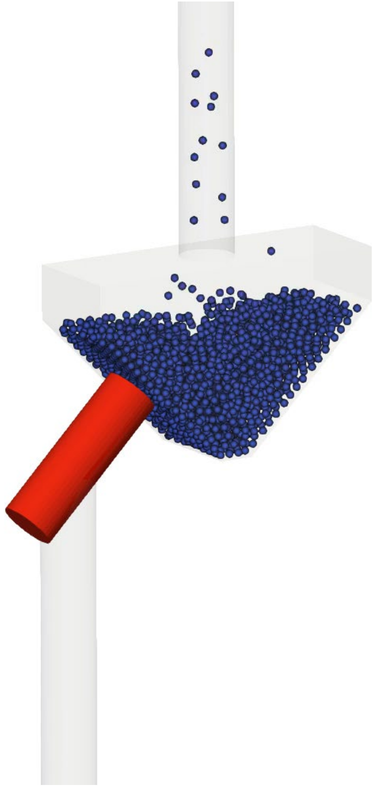
Moving geometry

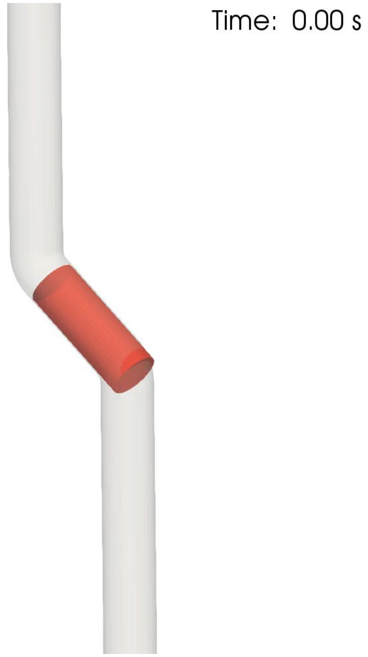
Several options to represent moving geometry

- Ability to control flow rate



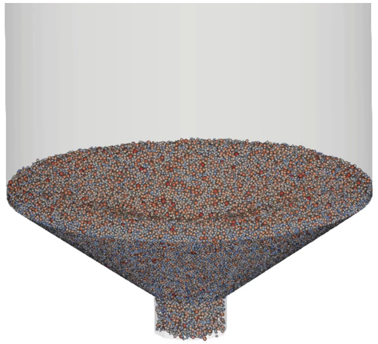


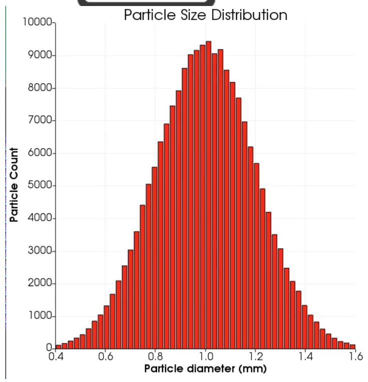


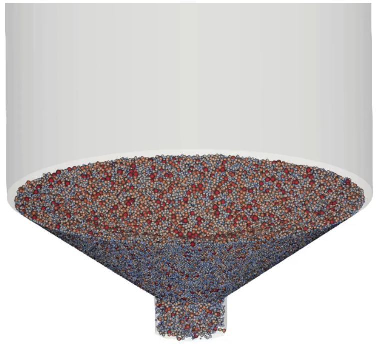


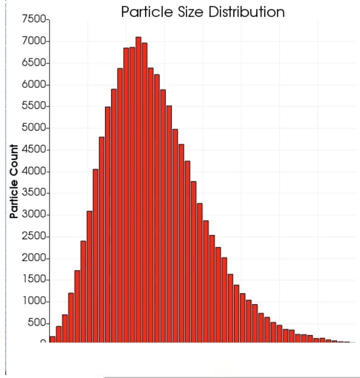
Polydispersity (DEM)

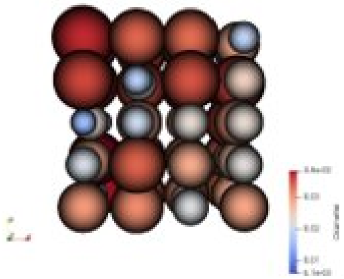
- Available in 20.3 Release (September 2020)
- Merge and complement ASU implementation
- Initial and Boundary (mass inflow) conditions
- DEM Particle size distribution
  - Normal
  - Log-normal
  - Custom (user-defined)
- Improvement in IC seeding
  - Robust
  - Lattice
  - Spacing
  - Flexibility in input
    - Volume fraction
    - Solid inventory
    - Particle count



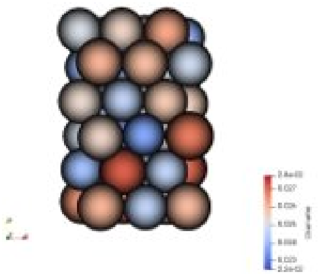




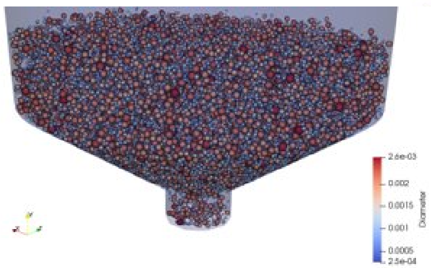


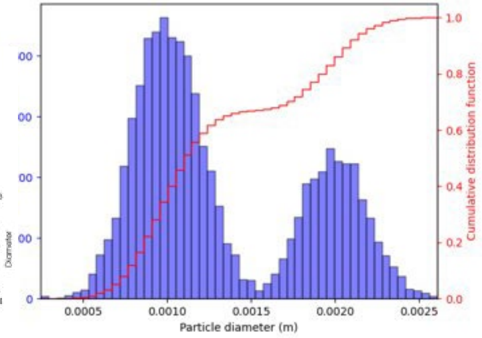


Cubic lattice



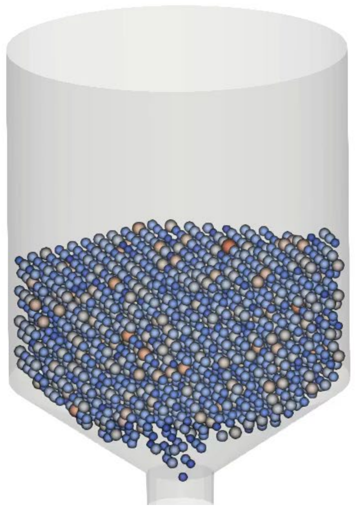
Hexagonal lattice

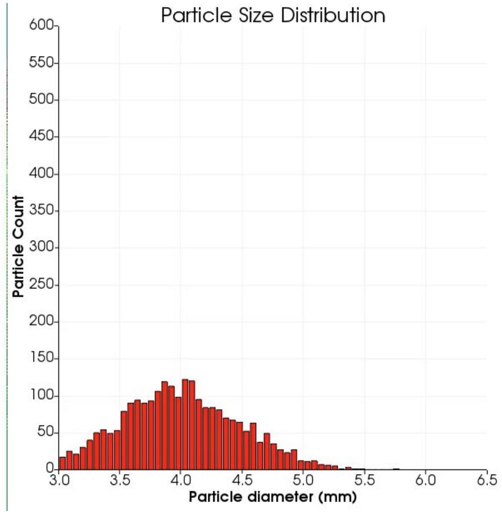




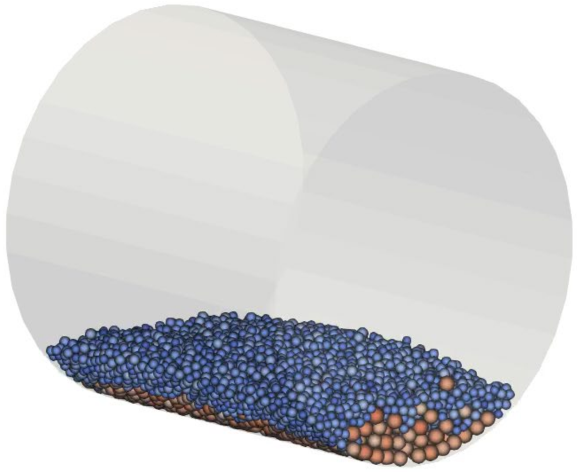
Polydispersity (DEM)

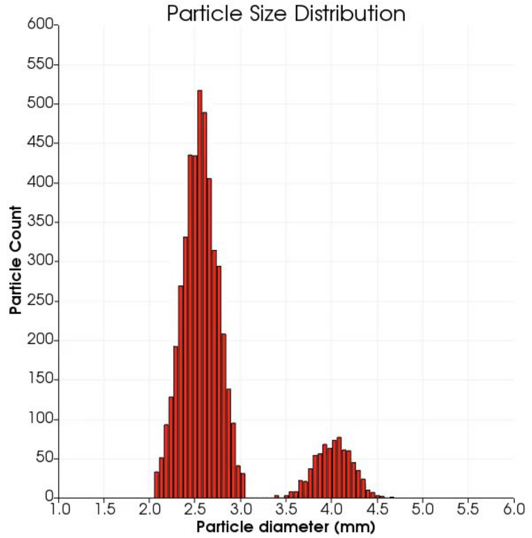
Polydispersity examples





Initial + Boundary Conditions





Particle coating

Non-spherical particles (SuperDEM)

- Superquadrics are a family of geometric shapes defined as

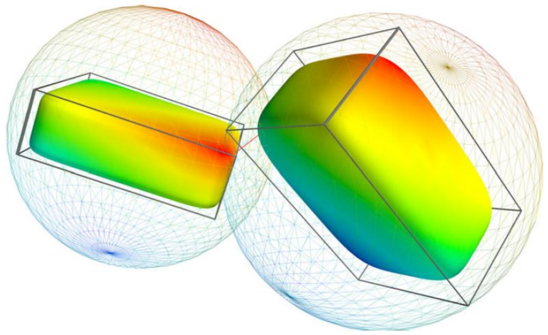
$$\left[\left(\frac{x}{a_1}\right)^{\frac{2}{\varepsilon_2}}+\left(\frac{y}{a_2}\right)^{\frac{2}{\varepsilon_2}}\right]^{\frac{\varepsilon_2}{\varepsilon_1}}+\left(\frac{z}{a_3}\right)^{\frac{2}{\varepsilon_1}}=1$$

- Can represent ~ 80% of all shapes by varying **five parameters**

$$[a_1, a_2, a_3, \varepsilon_1, \varepsilon_2]^T$$

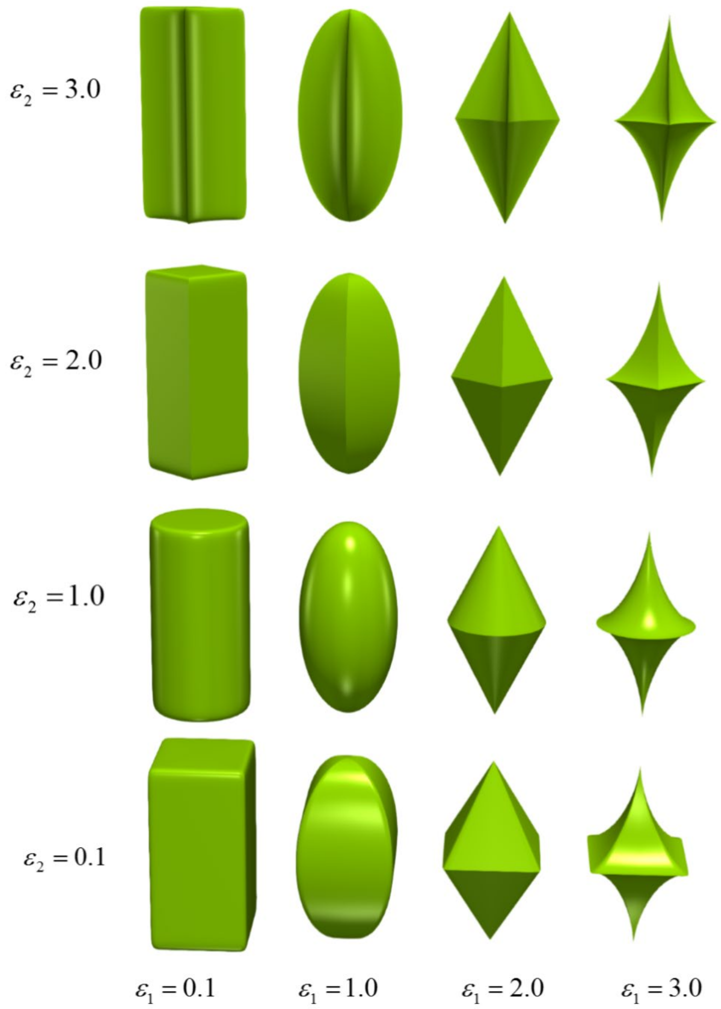
Semi-axis

roundness parameters



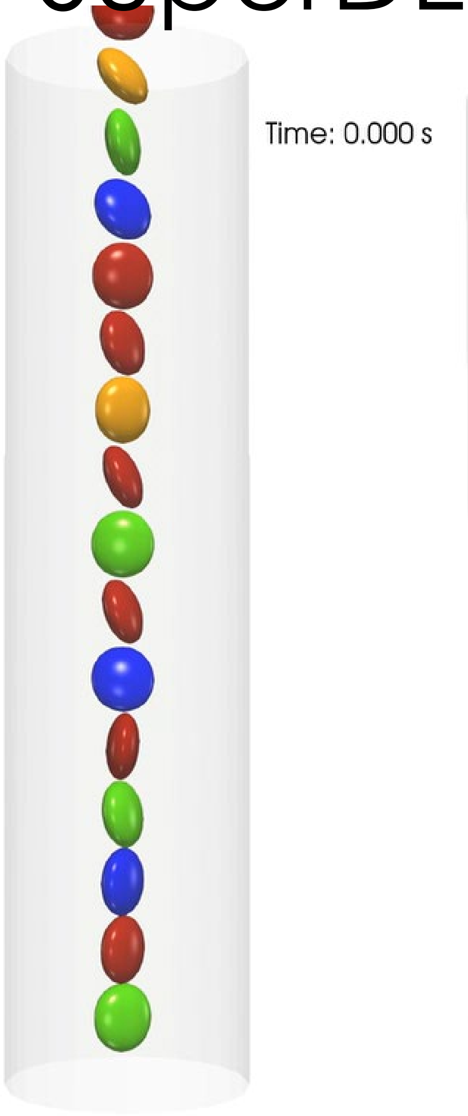
Bounding spheres and oriented bounding boxes

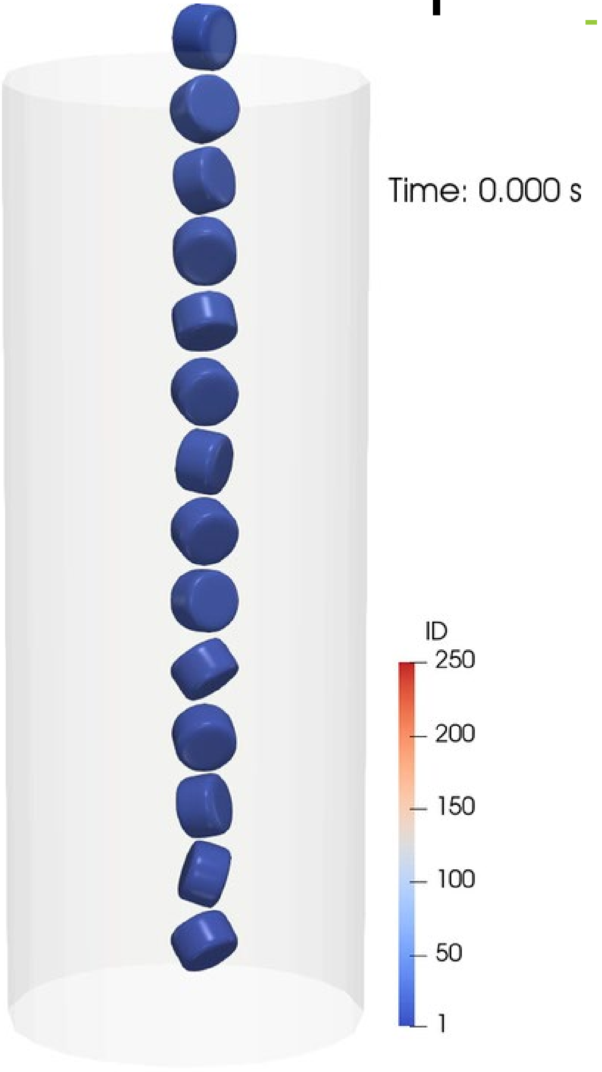
Superquadric particles

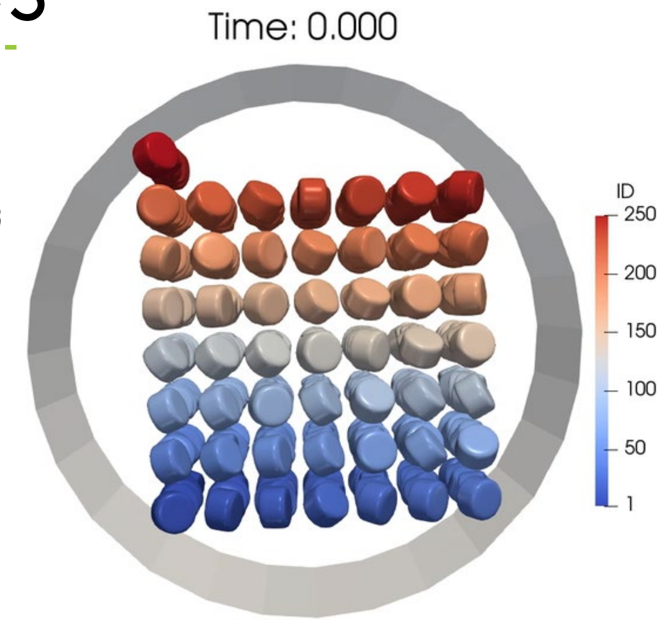


a1=2
a2=2
a3=4

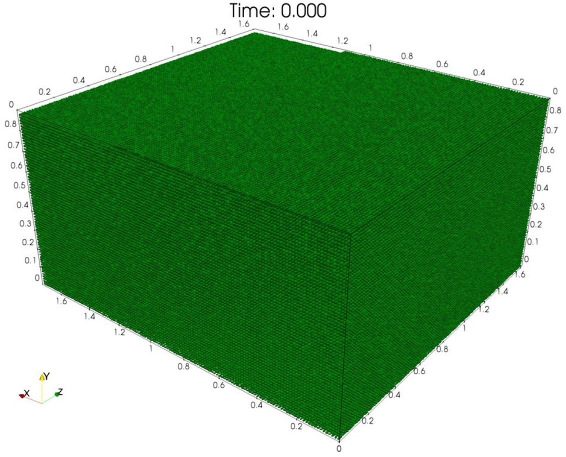
SuperDEM examples

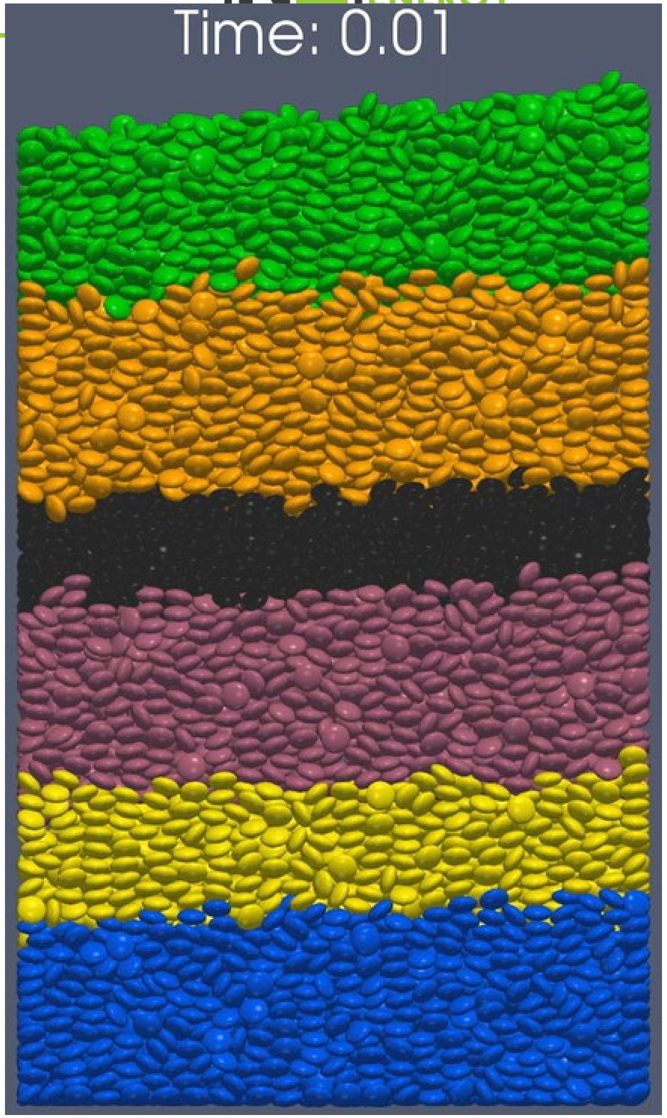






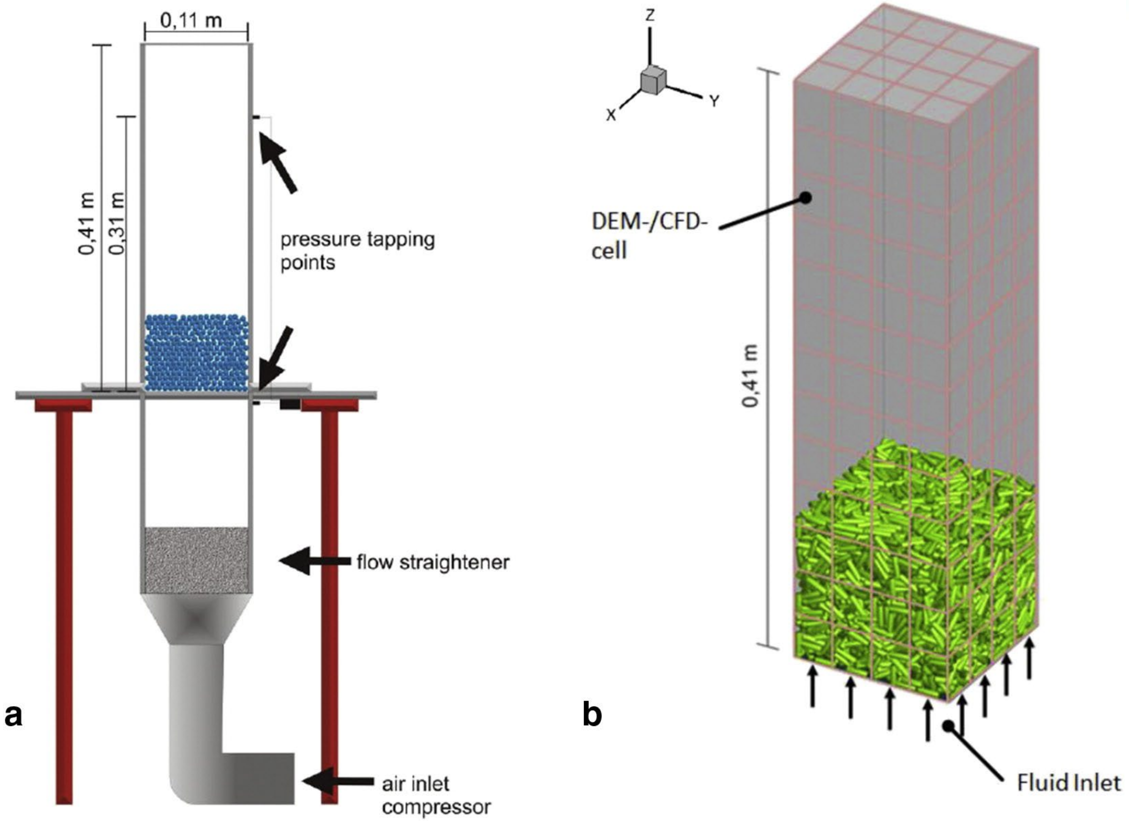
Cylinder rotating drum





M&M candy static packing **Cylinder candy static packing** **1 million non-spherical particles** **M&M candy discharging from a hopper**

Validation experiment



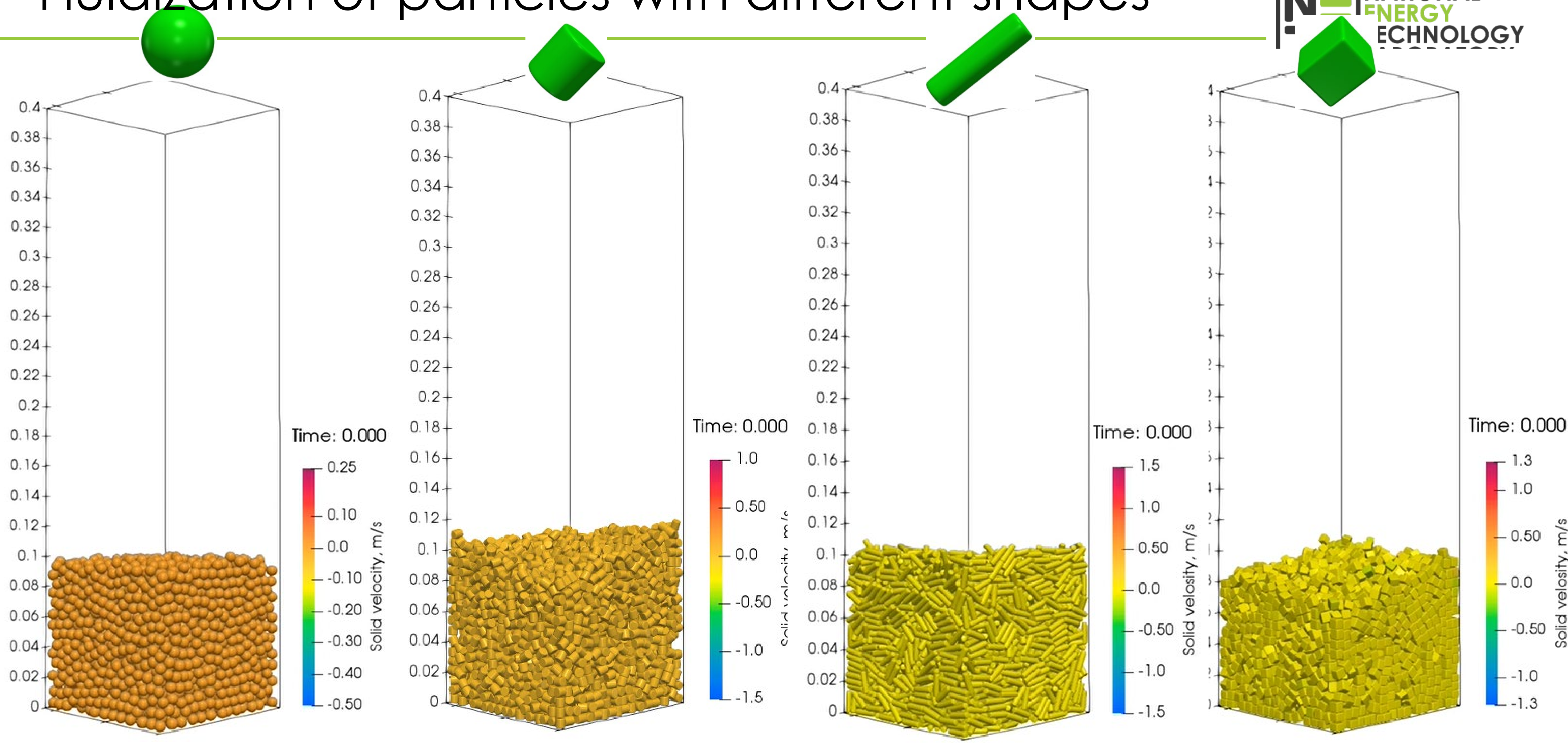
Particle properties including the volume equivalent diameter d_e-class, the particle dimensions, the sphericity ϕ, the particle density ρ_p, the bed height L and the averaged porosity ε for the initial, unfluidized setup.

Shape	Sphere	Sphere	Ideal Cylinder	Cube	Cube
d_e–class [mm]	7	5	7	5	7
Size [mm]	7.2	5	6.1 6.2	4.2 4.3 4.5	5.2 6.3 6.3
ϕ [–]	1.00	1.00	0.87	0.81	0.80
ρ_p [kg/m³]	772.5	823.0	708.5	639.7	746.9
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	95 0.40	88 0.40	98 0.36	98 0.37	103 0.43
Shape	**Elongated Cylinder**	**Elongated Cuboid**	**Elongated Cuboid**	**Plate**	**Elongated Plate**
d_e–class [mm]	7	5	7	5	5
Size [mm]	3.9 14.0	3.0 3.0 7.1	4.2 4.2 11.4	2.0 4.9 6.0	2.0 4.0 8.0
ϕ [–]	0.75	0.75	0.73	0.71	0.69
ρ_p [kg/m³]	764.4	745.6	639.7	754.1	756.6
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	103 0.44	103 0.42	115 0.40	102 0.43	108 0.46
Shape	**Elongated Cuboid**	**Plate**	**Elongated Plate**		
d_e–class [mm]	5	7	7		
Size [mm]	2.0 3.0 11.0	2.2 9.0 9.8	2.0 6.0 14.9		
ϕ [–]	0.64	0.63	0.58		
ρ_p [kg/m³]	728.1	672.8	721.7		
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	117 0.48	121 0.46	124 0.51		

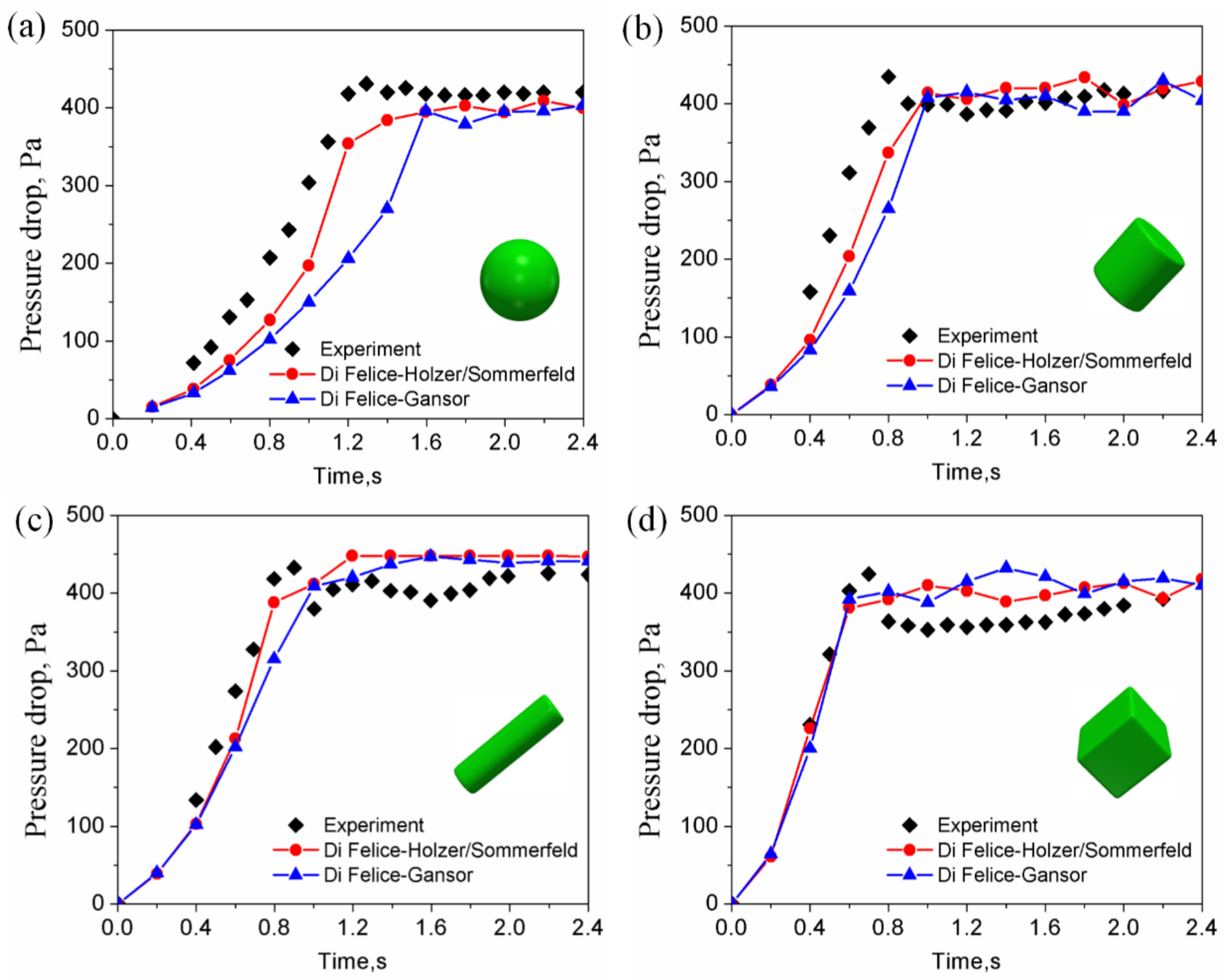
Experiment: Vollmari K, Jasevičius R, Kruggel-Emden H. Experimental and numerical study of fluidization and pressure drop of spherical and non-spherical particles in a model scale fluidized bed. Powder Technology. 2016;291:506-521.

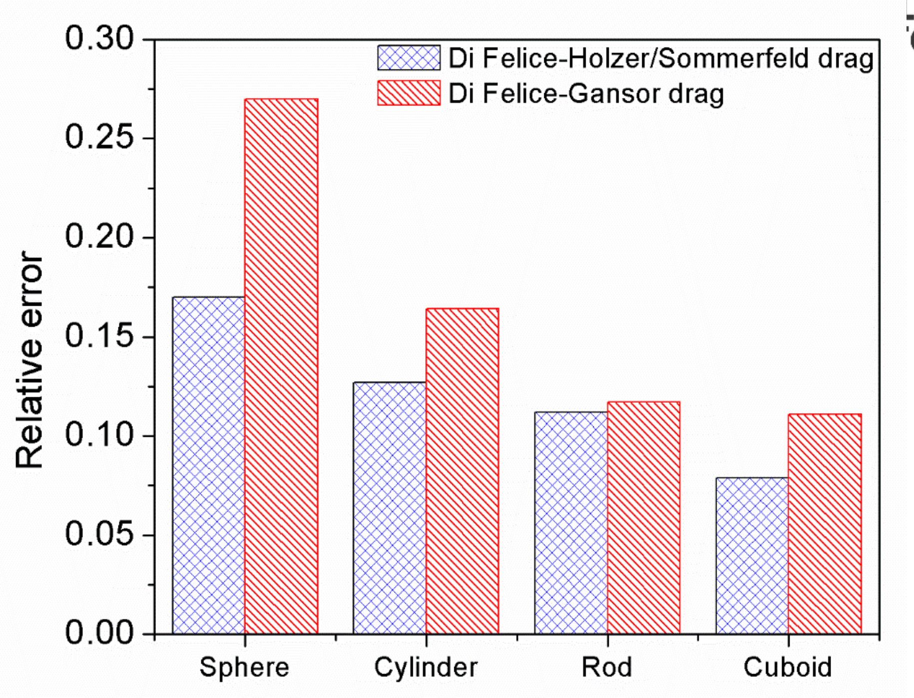
Fluidization of particles with different shapes

Ug=1.6 m/s



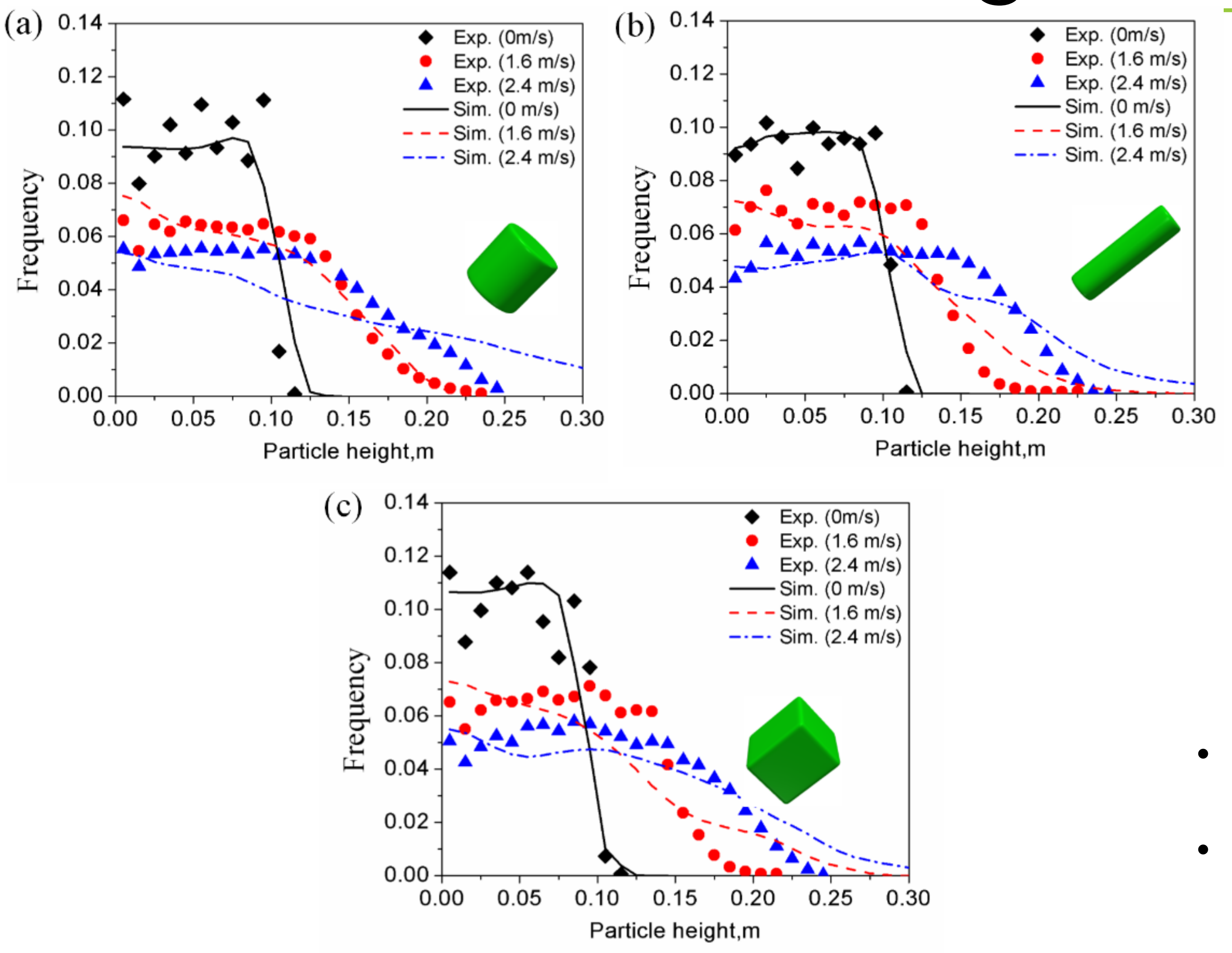
Validation-Pressure drop





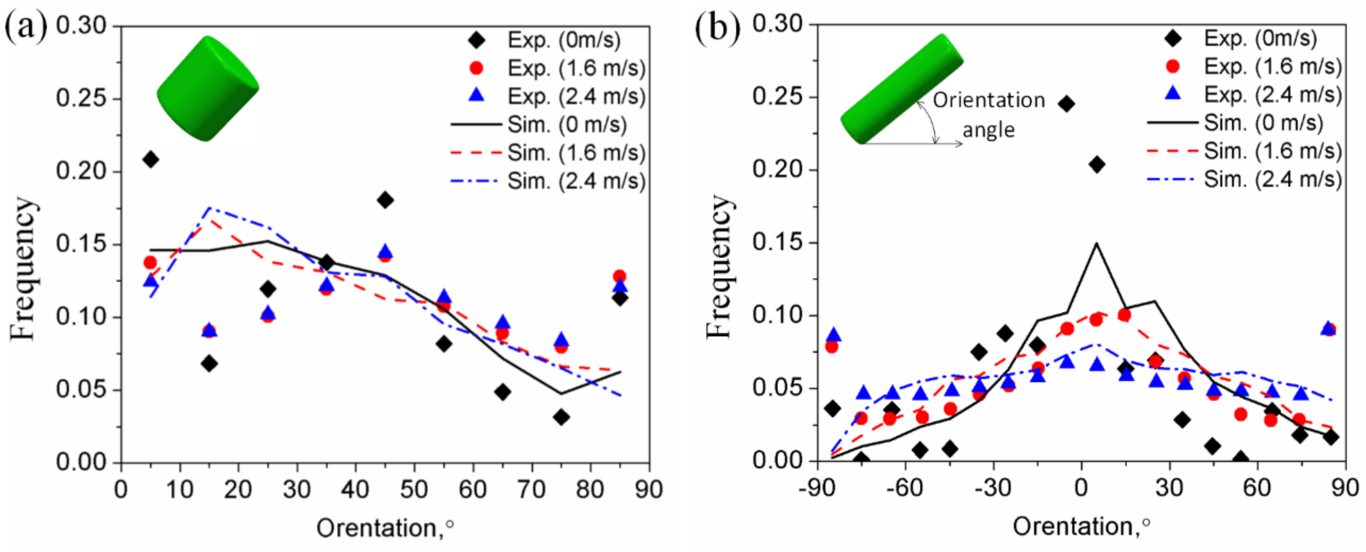
- Both drag models consider the effects of particle orientation and cell voidage
- Di Felice-Holzer/Sommerfeld drag correctly capture the pressure in both fixed bed and fluidized bed regimes for each shape particles.
- Unresolved SuperDEM-CFD can not capture the channeling flow. Particle-resolved DEM-CFD may be tested in the future.

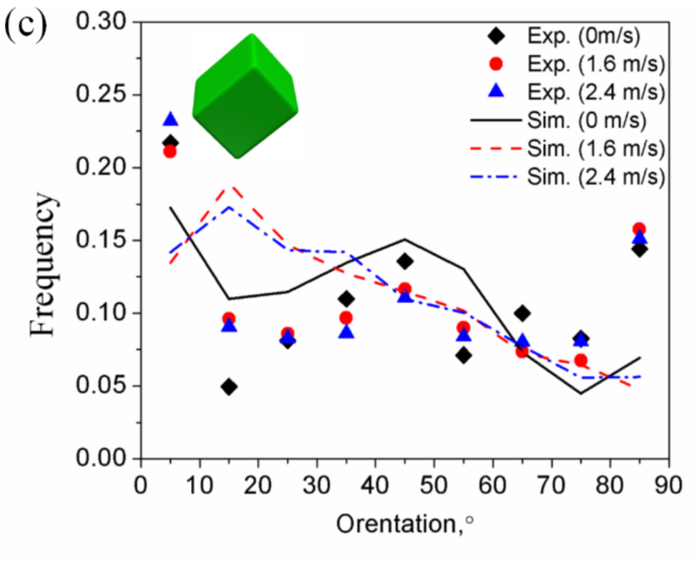
Validation-Particle height distribution



- SuperDEM-CFD correctly predict the particle height distribution at different gas velocities.
- Slight over predicted the expansion bed height as higher gas velocity.

Validation-Particle orientation distribution

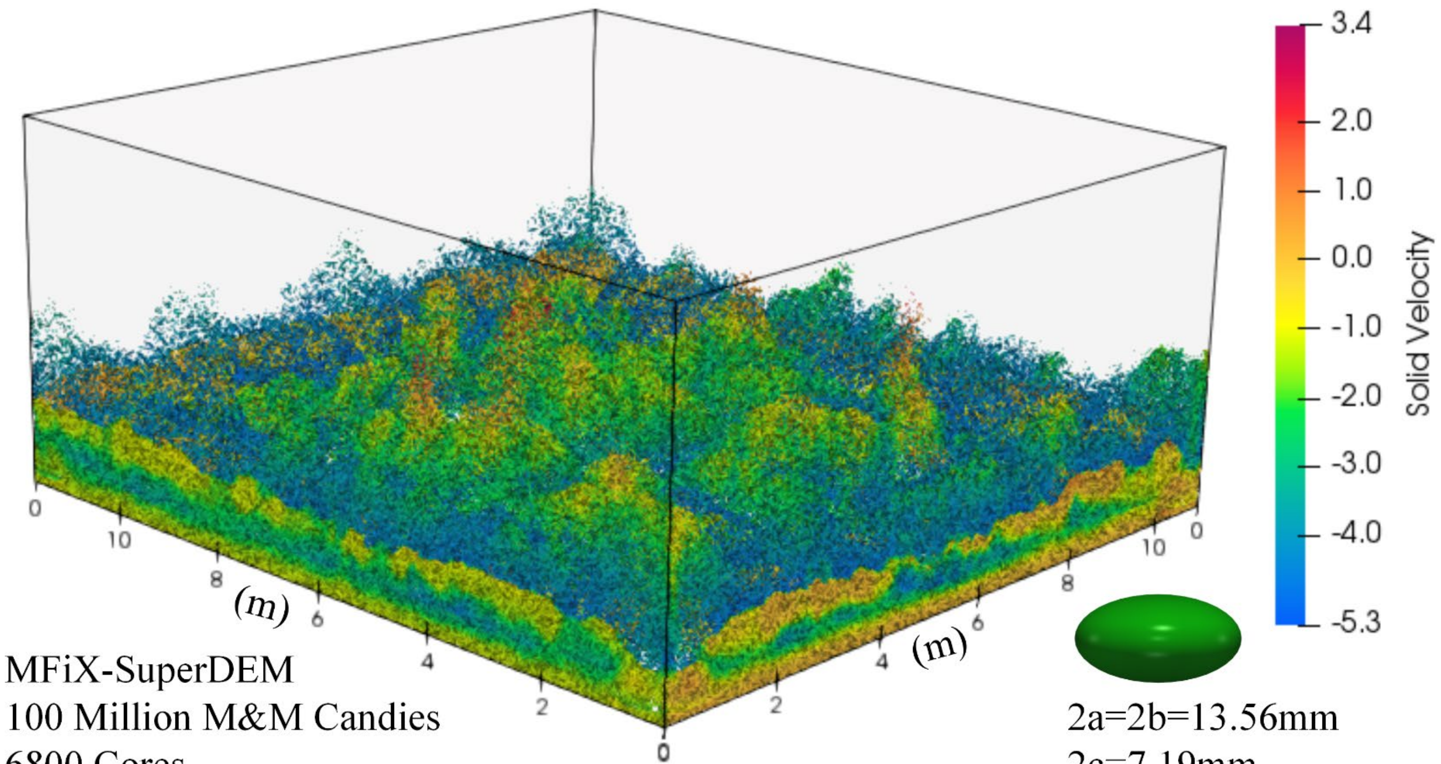




- For rod, with an increase of superficial gas velocity, the fraction of sanding up particles increase, and the fraction of laying down particles decreases

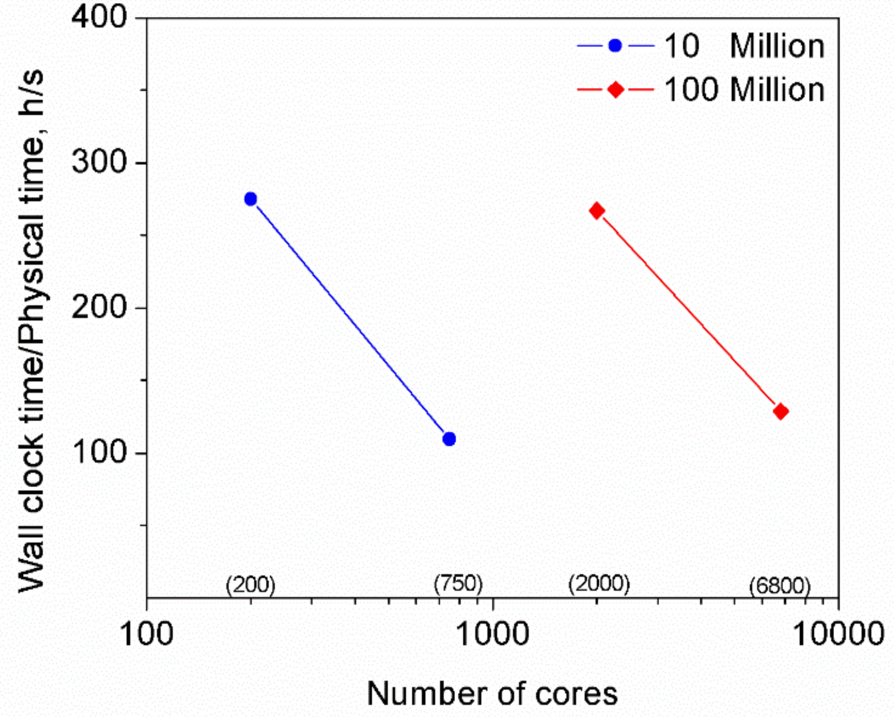
- The ideal cylinder and cuboid do not show a decrease of the fraction of laying down particles with the increasing of gas velocity.
- The SuperDEM-CFD correctly reproduced the behavior.

Massively Parallel SuperDEM Simulation



MFiX-SuperDEM
100 Million M&M Candies
6800 Cores

2a=2b=13.56mm
2c=7.19mm



- The solver was parallelized using MPI.
- Simulation on NETL supercomputer Joule 2 (80K cores) , World Top 60, 2020
- Non-spherical particles fluidization simulation, 100 million (6800 cores)

SuperDEM development progress

- **Summary**
  - Oriented bounding box (OBB) algorithm has been implemented and verified
  - Superquadric contact algorithm has been implemented and verified
  - Quaternion theory for object orientation (rotation between local and global) has been implemented and verified
  - VTP (xml) was modified to output tensor for superquadric particle visualization
  - Superquadric particle collision with wall (plane, STL)
  - Non-linear forces between superquadric particles
  - Parallelization (MPI)
  - 100 million non-spherical particles large scale simulation on 6800 cores
  - A new interpolation scheme (DPVM-Satellites) was developed.
  - Non-spherical drag models (Di Felice-Gansor and Di Felice Holzter/SommerFeld) considering particle orientation and cell voidage were implemented
  - A new general scheme to calculate the projection area of non-spherical particle perpendicular to the flow was developed.
  - 100 million non-spherical particles fluidization simulation on 6800 cores

- **Future work**
  - Heat transfer, mass transfer, chemical reaction
  - Coupling with other sub-models
  - Multi-superquadric particles to model moving internals, such as baffle, moving wall, etc.
  - Advanced superquadric contact algorithm

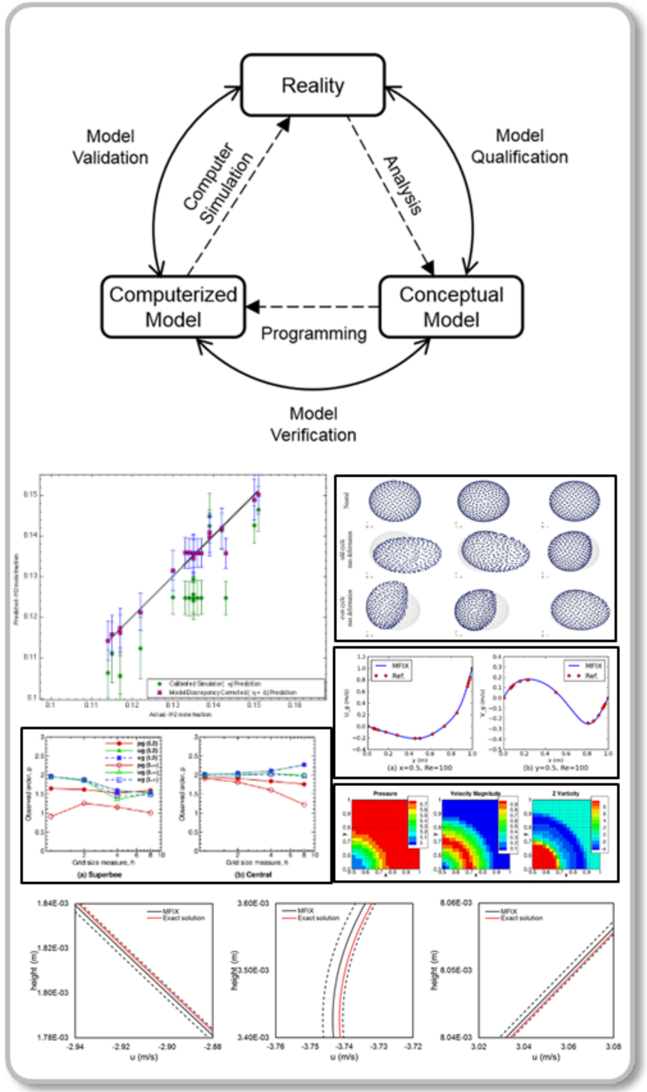
MFiX Quality Assurance

Building Confidence in Simulation Results

- **Verification**
  - Code verification – Does the code do what we expect?
  - Solution verification – Is the answer any good?
- **Validation -** How does the answer compare to the real world?
- **Uncertainty Quantification**
  - Where is the error in my solution coming from?
  - What happens to my answer when I change an input to my model?

Accomplishments

- MFiX Verification and Validation Manual 2nd Ed. (PDF & html)
- PIC theory guide (May 2020)



MFiX Quality Assurance

Building Confidence in Simulation Results

- **PIC parameter sensitivity and calibration**
  - How sensitive are PIC simulations to PIC model parameters?
  - Recommend parameter values for a given type of application

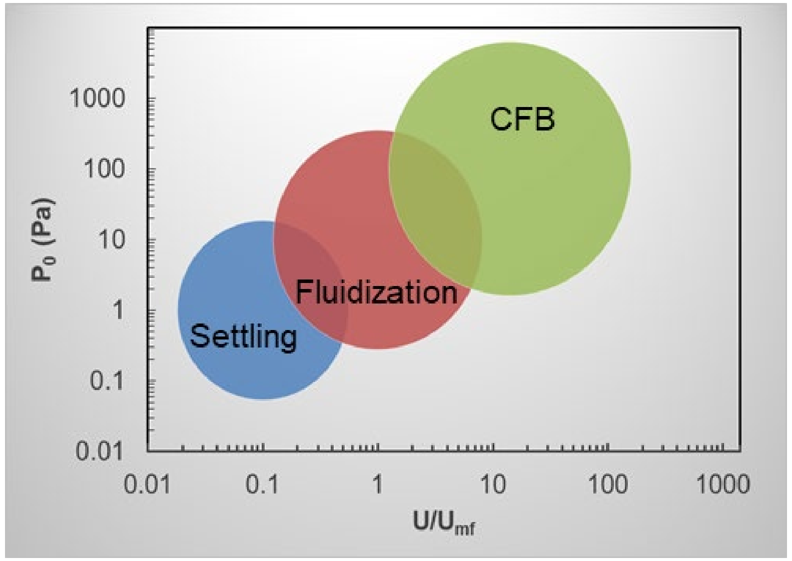
Parcel momentum equation

$$\frac{d\vec{V_p}}{dt} = \beta\left(\vec{U_g} - \vec{V_p}\right) - \frac{1}{\rho_p}\nabla p - \frac{1}{\varepsilon_p \rho_p}\nabla \tau_p + \vec{g}$$

$$\tau_p = \frac{\boldsymbol{P_0}\varepsilon_p^{\beta}}{\max\left(\varepsilon_{cp} - \varepsilon_p, \delta\left(1 - \varepsilon_p\right)\right)}$$

Cases selected to cover a broad range of flow conditions

- Particle Settling: $U/U_{mf} < 1.0$ ($\boldsymbol{P_0} \sim 1$) (Analytical solution)
- Bubbling Fluidized bed: $U/U_{mf} \sim 1$ ($\boldsymbol{P_0} \sim 10$)
- Circulating Fluidized bed: $U/U_{mf} >> 1.0$ ($\boldsymbol{P_0} \sim 100$)



Summary of model parameters used:

	t1 Pressure linear scale factor	t2 Volume fraction exponential scale factor	t3 Statistical weight	t4 Volume fraction at maximum packing	t5 Solid slip velocity factor
C1: Particle Settling	[1,20]	[2,5]	[3,20]	[0.35,0.5]	[0.5,1.0]
C2: Fluidization	[1,100]	[2,5]	[10,100]	[0.4,0.5]	[0.85,0.98]
C3: Circulating Fluidized Bed	[1,250]	[2,5]	[4]	[0.4,0.5]	[0.85,0.98]

*Parameters selected based on prior sensitivity study

C1: Particle settling

Problem setup

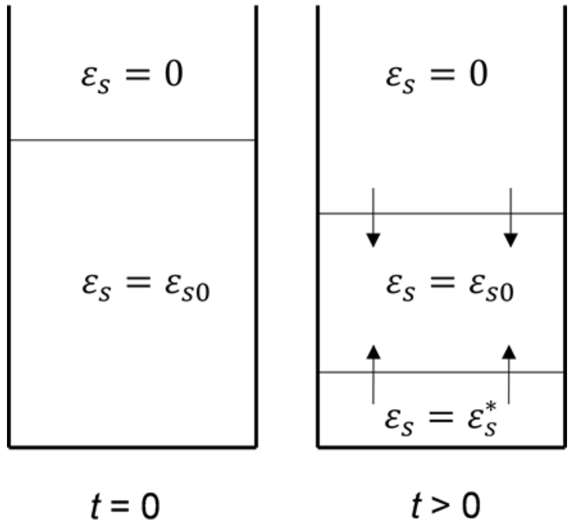
Control variable: Initial solids concentration
Range: [0.05,0.25]

	x1 Initial solids concentration
C1: Particle Settling	[0.05,0.25]

Response variable: Location of filling shock (y2)
CFD results are compared with analytical solutions

Control variables: CFD (PIC parameters)

	t1 Pressure linear scale factor	t2 Vol. fraction exponential scale factor	t3 Statistical weight	t4 Vol. fraction at maximum packing	t5 Solid slip velocity factor
C1: Particle Settling	[1,20]	[2,5]	[3,20]	[0.35,0.5]	[0.5,1.0]



Analytical Solution:

Location of shock $x(t) = -t\left(\frac{\varepsilon_s^*\varepsilon_g^*u_r^* - \varepsilon_{s0}\varepsilon_{g0}u_{r0}}{\varepsilon_s^* - \varepsilon_{s0}}\right)$

Rel. velocity (Stokes' drag) $u_r = \frac{g\Delta\rho d_p^2}{18\mu_g}\varepsilon_g^{3.65}$

C1: Particle settling

Sensitivity analysis and Deterministic calibration

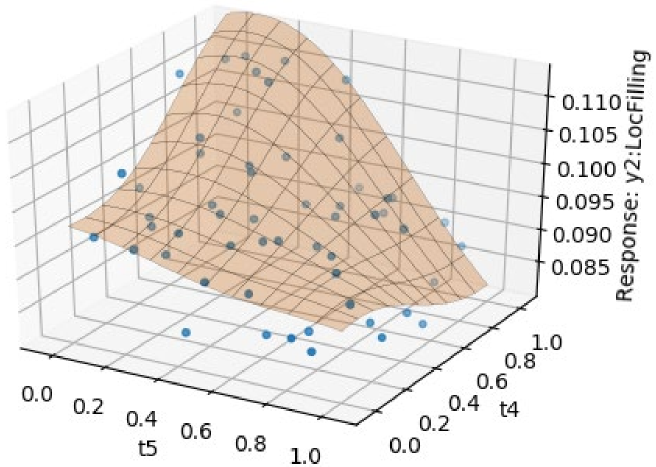
Response surface constructed from 55 samples

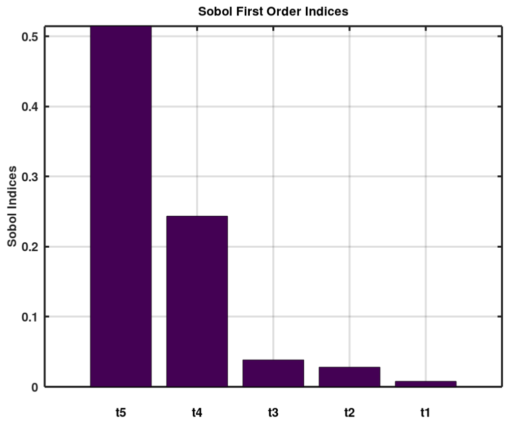
Sobol indices show the following:

- main effects (first oder)
- interactive effects (second order)

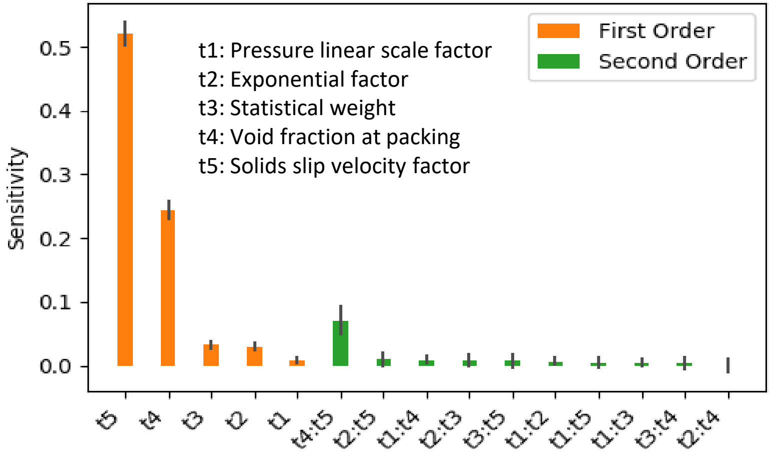
Code-to-Code comparison with PSUADE

3D plot of the data-fitted surrogate model





Sensitivity Analysis using Sobol Indices



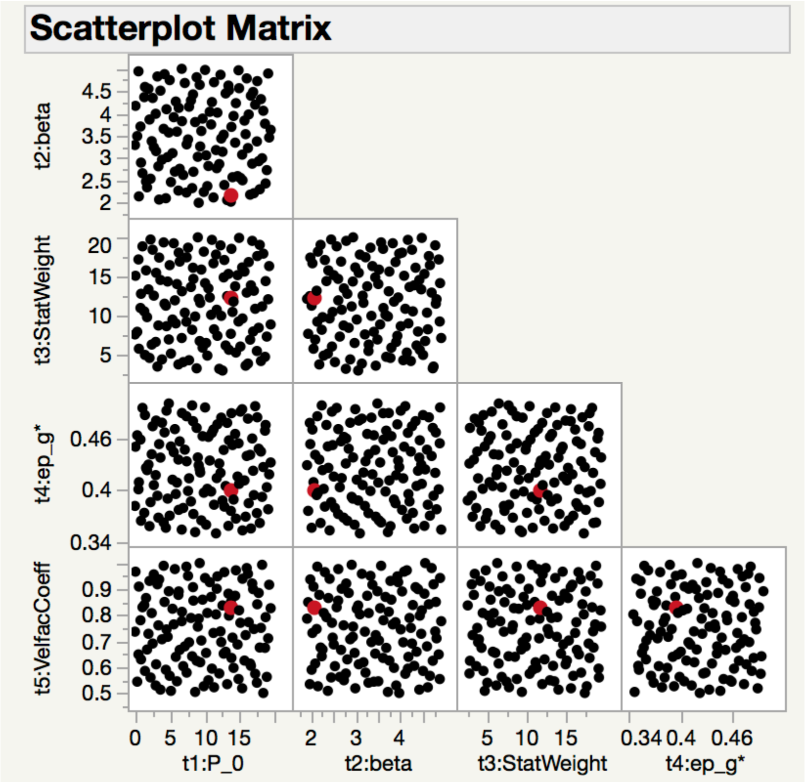
Parameters obtained through deterministic calibration

Parameter	Default	Range	Calibrated
t1 Pressure linear scale factor	100	[1,20]	14.309
t2 Vol. fraction exponential scale factor	3.0	[2,5]	2.165
t3 Statistical weight	5.0	[3,20]	12.241
t4 Vol. fraction at maximum packing	0.42	[0.35,0.5]	0.399
t5 Solid slip velocity factor	1.0	[0.5,1.0]	0.828

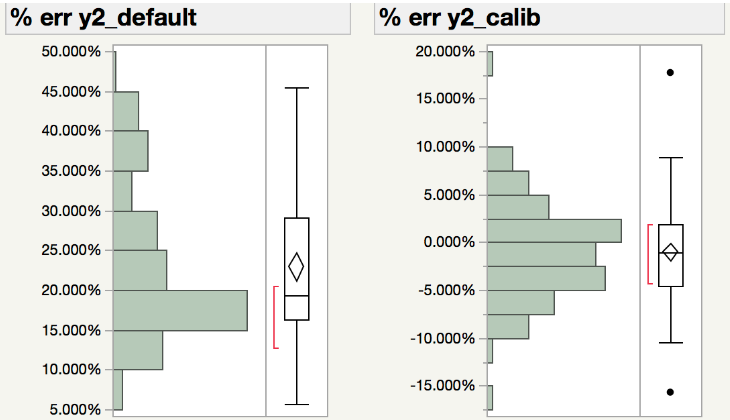
C1: Particle settling

Deterministic calibration (using 120 samples and PSUADE)

Testing calibrated parameters at "unseen" settings



Comparing Distribution of % Error (Default vs Calibrated Settings)



% err y2_default

Quantiles

100.0%	maximum	45.450%
99.5%		45.450%
97.5%		44.450%
90.0%		38.590%
75.0%	quartile	29.090%
50.0%	median	19.390%
25.0%	quartile	16.340%
10.0%		13.190%
2.5%		9.080%
0.5%		5.620%
0.0%	minimum	5.620%

Summary Statistics

Mean	0.2299454
Std Dev	0.0950501
Std Err Mean	0.0087132
Upper 95% Mean	0.2471999
Lower 95% Mean	0.2126908
N	119

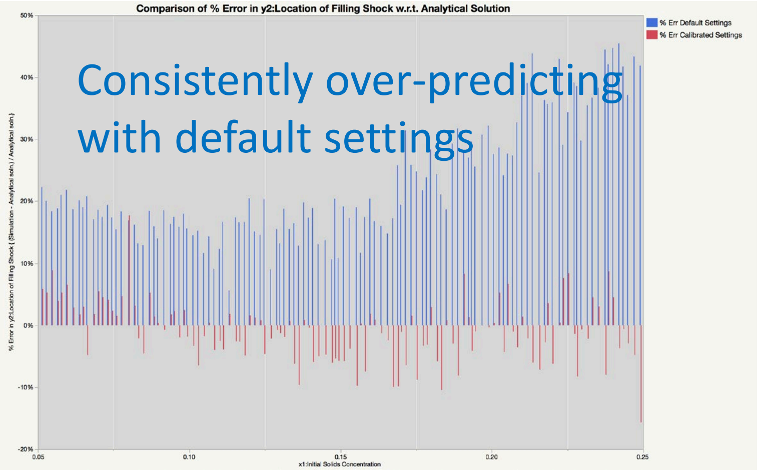
% err y2_calib

Quantiles

100.0%	maximum	17.730%
99.5%		17.730%
97.5%		8.670%
90.0%		5.250%
75.0%	quartile	1.850%
50.0%	median	-1.030%
25.0%	quartile	-4.530%
10.0%		-7.180%
2.5%		-9.960%
0.5%		-15.690%
0.0%	minimum	-15.690%

Summary Statistics

Mean	-0.009611
Std Dev	0.0500527
Std Err Mean	0.0045883
Upper 95% Mean	-0.000525
Lower 95% Mean	-0.018697
N	119



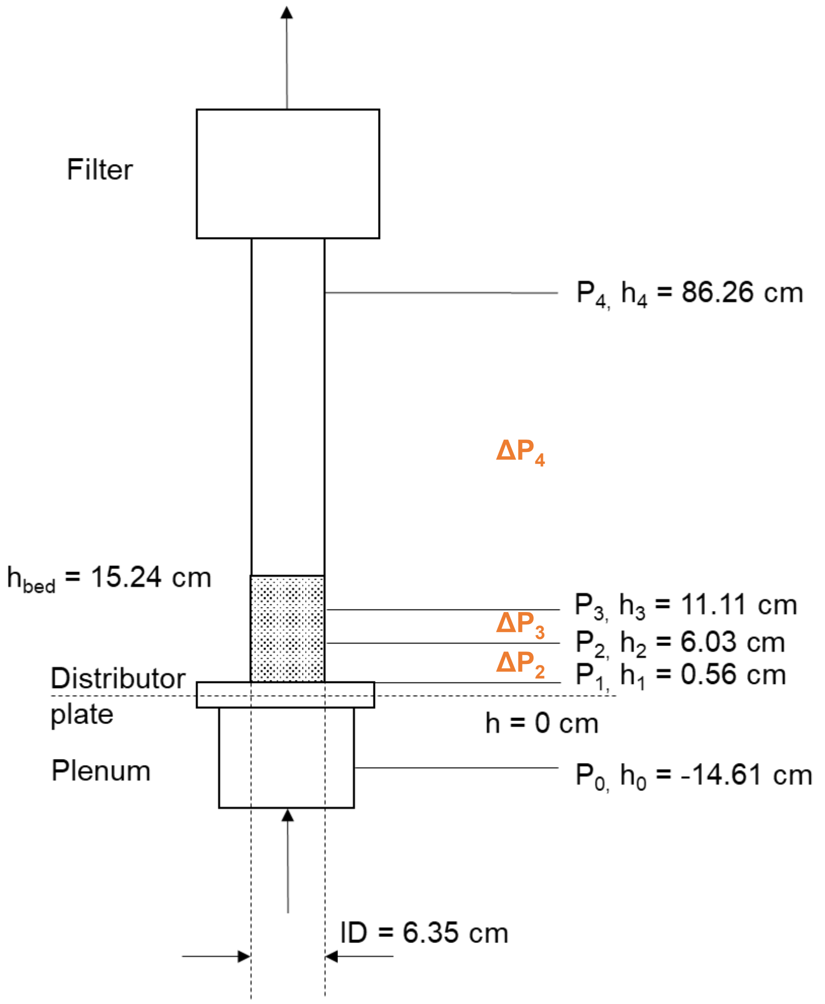
Consistently over-predicting with default settings

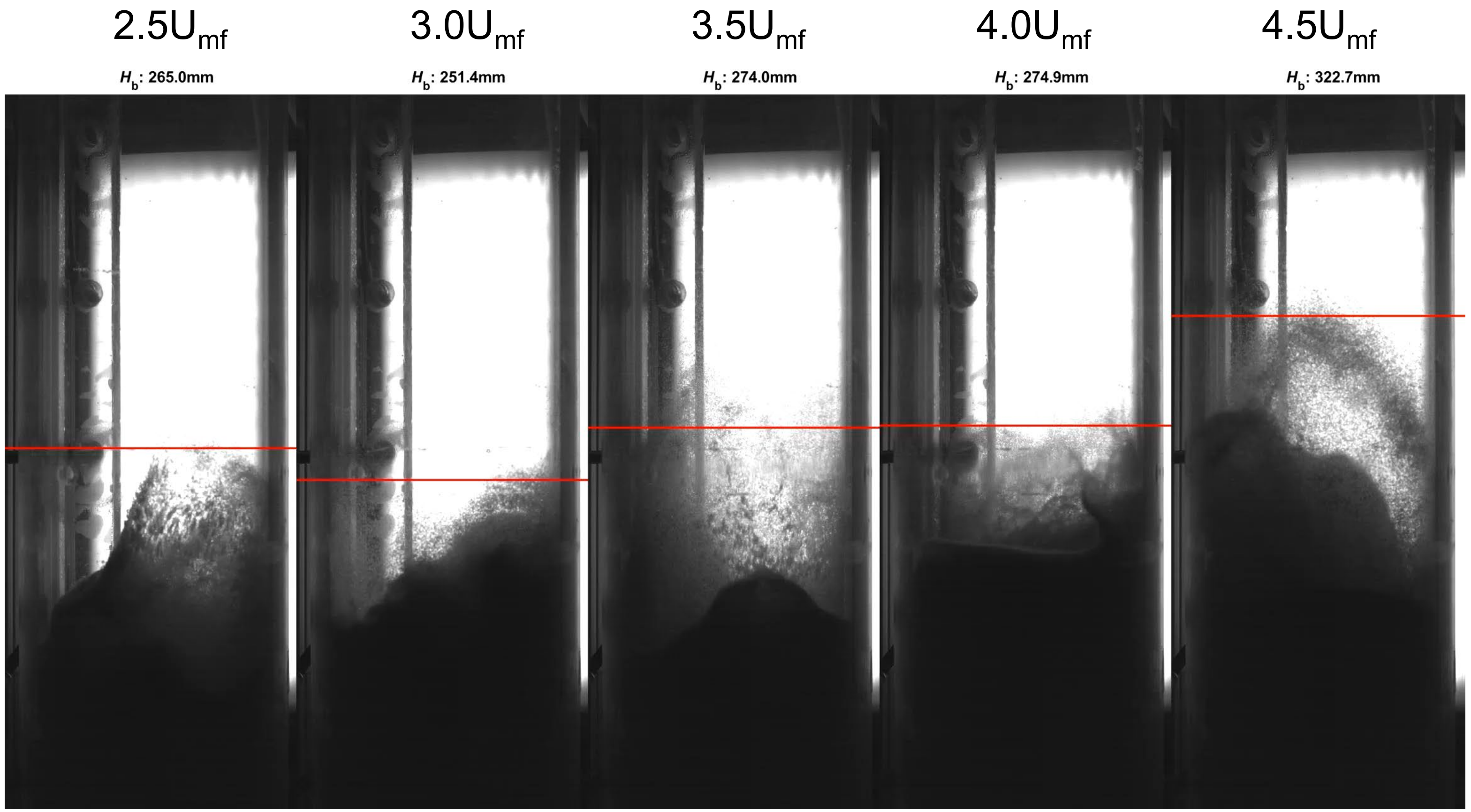
22.99% vs -0.96%

With calibrated settings for all 5 parameters both over-predicting with default settings

C2: Bubbling Fluidization

Experiments





C2 identified the need to implement a PIC CFL time step control

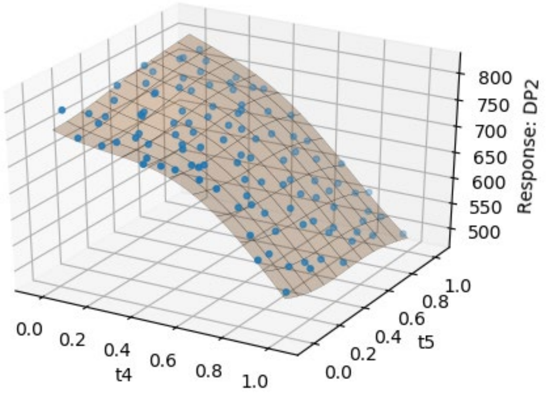
C2: Bubbling Fluidization

Sensitivity Analysis

3D plot of the data-fitted surrogate model (Radial Basis Function)

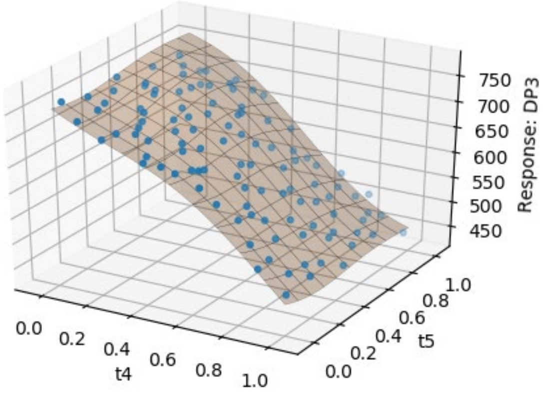
ΔP_2

*t1,t2,t3 set at nominal values



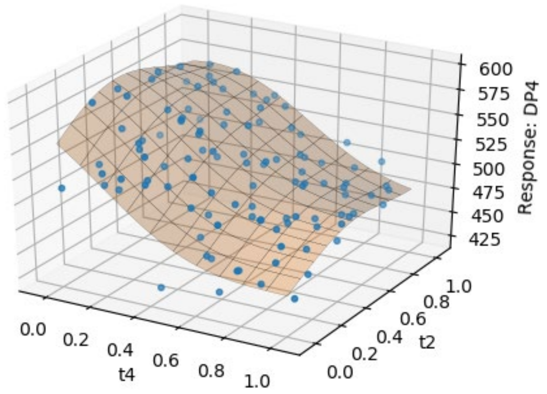
ΔP_3

*t1,t2,t3 set at nominal values

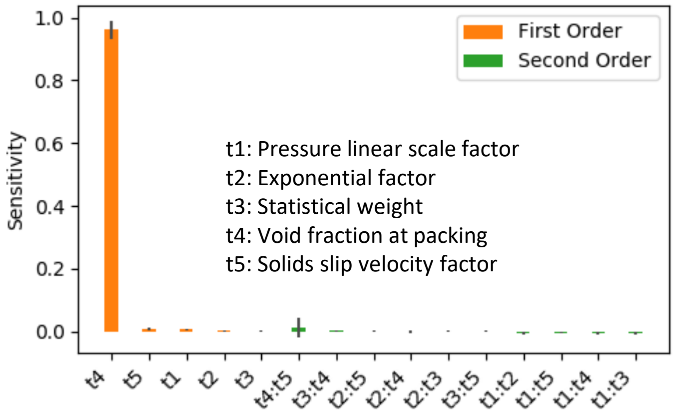


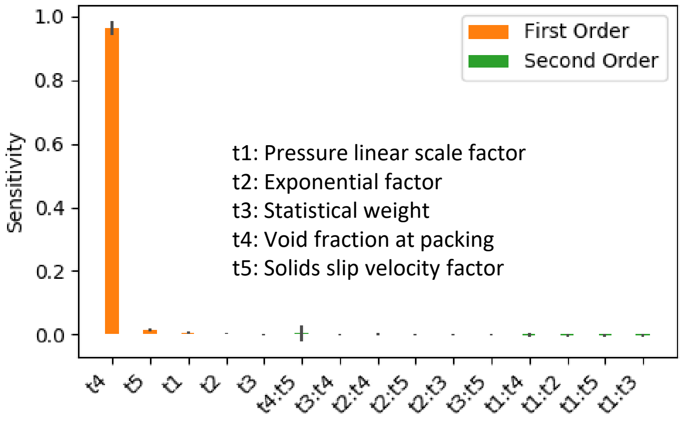
ΔP_4

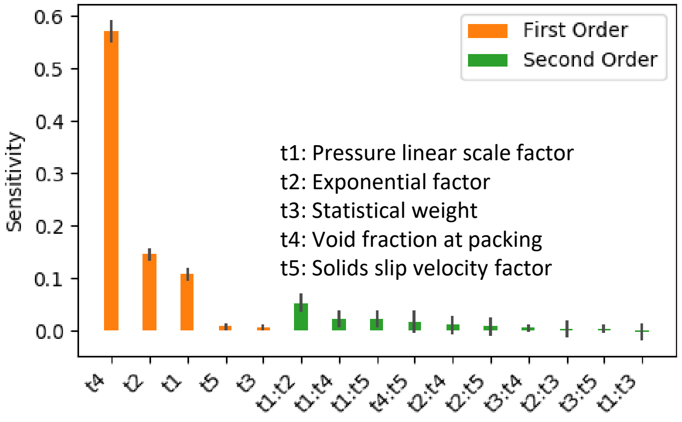
*t1,t2,t5 set at nominal values



Sensitivity Analysis using Sobol Indices

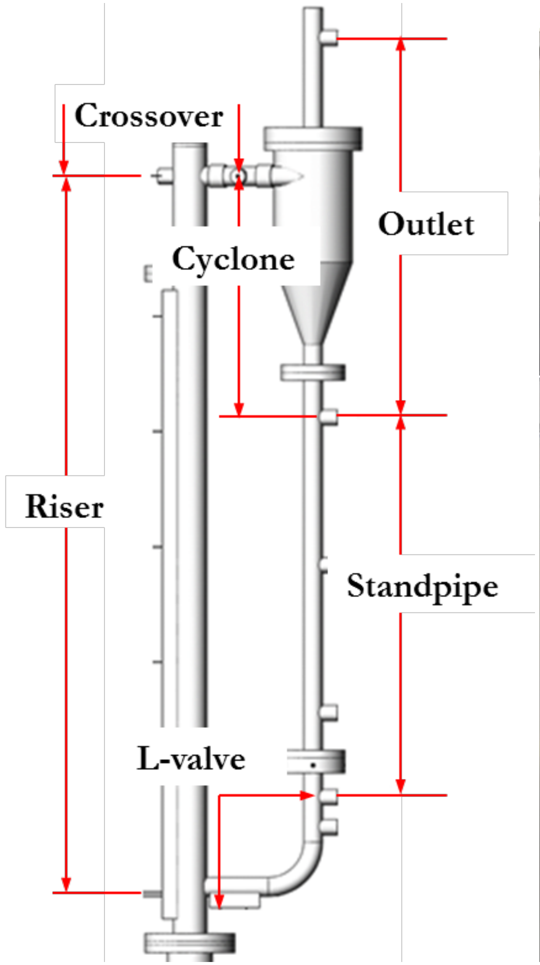


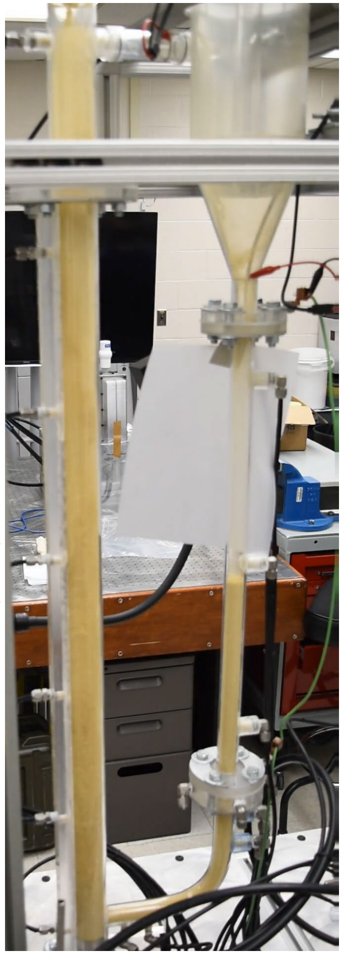




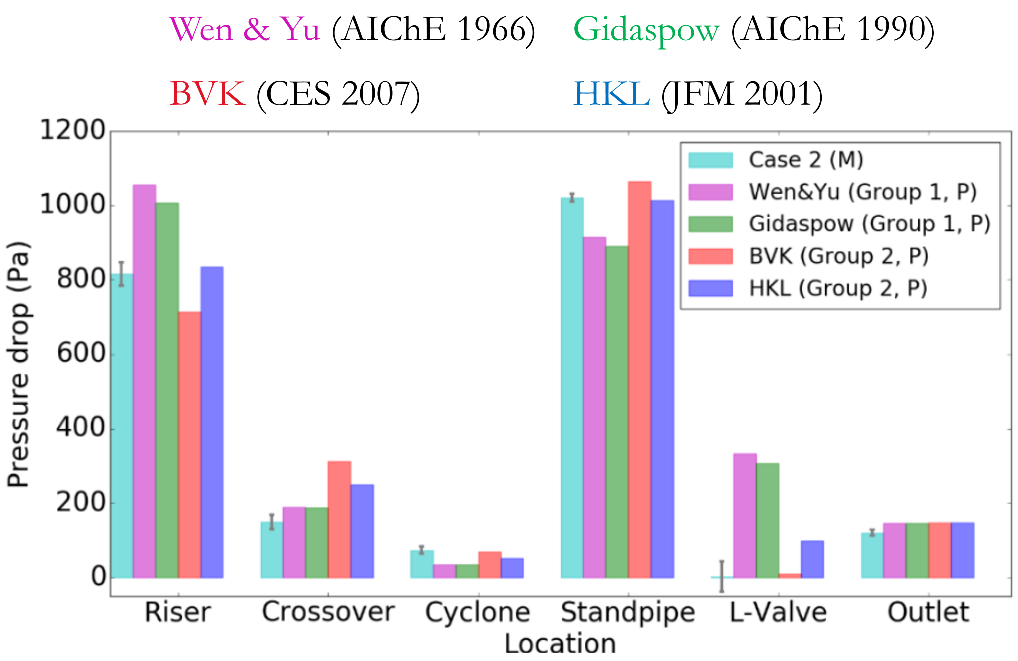
C3: Circulating Fluidized Bed

Experiments





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



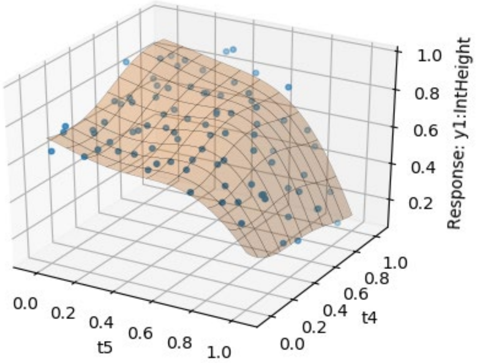
C3: Circulating Fluidized Bed

Sensitivity Analysis

3D plot of the data-fitted surrogate model (Radial Basis Function)

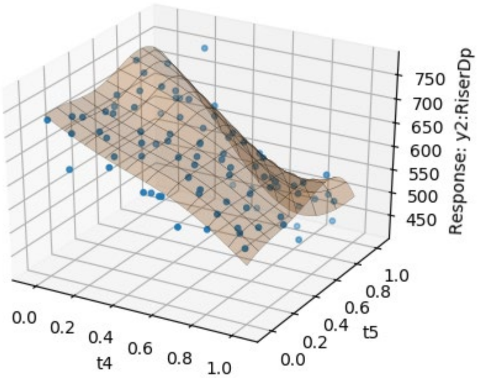
Interface height

*t1,t2 set at nominal values



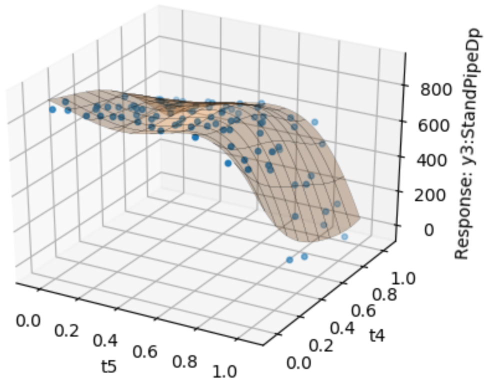
ΔP - Riser

*t1,t2 set at nominal values

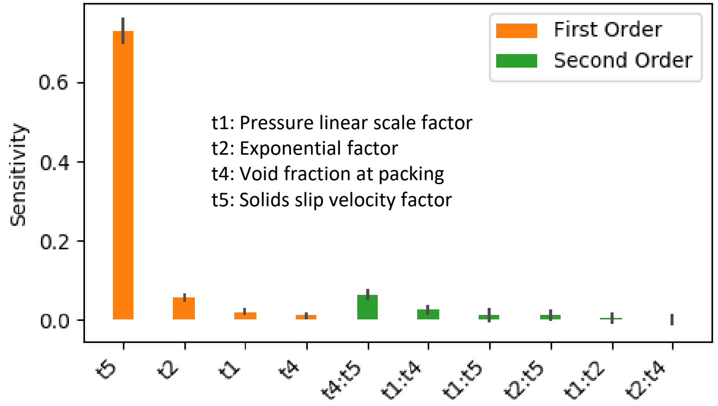


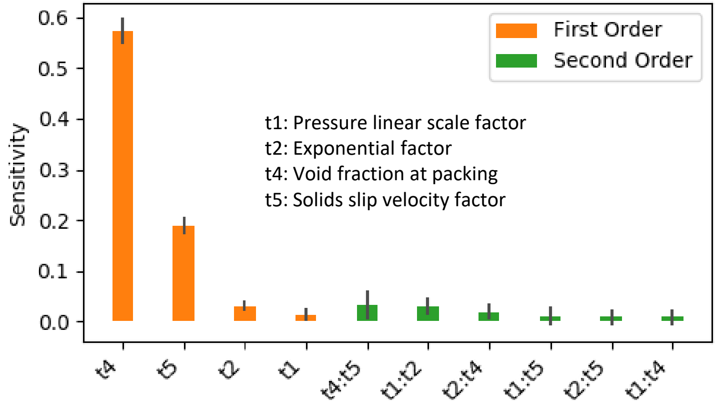
ΔP - Standpipe

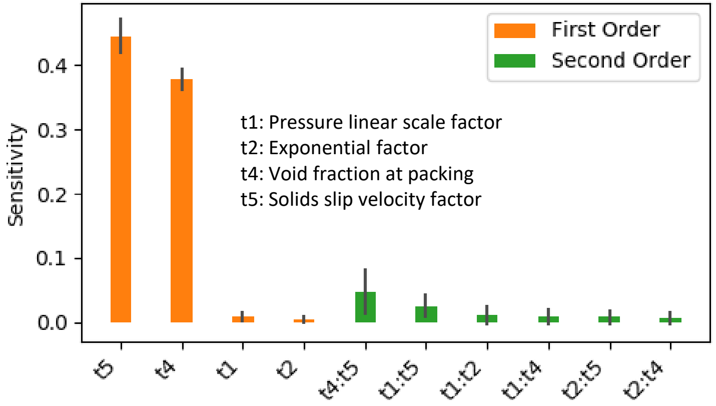
*t1,t2 set at nominal values



Sensitivity Analysis using Sobol Indices







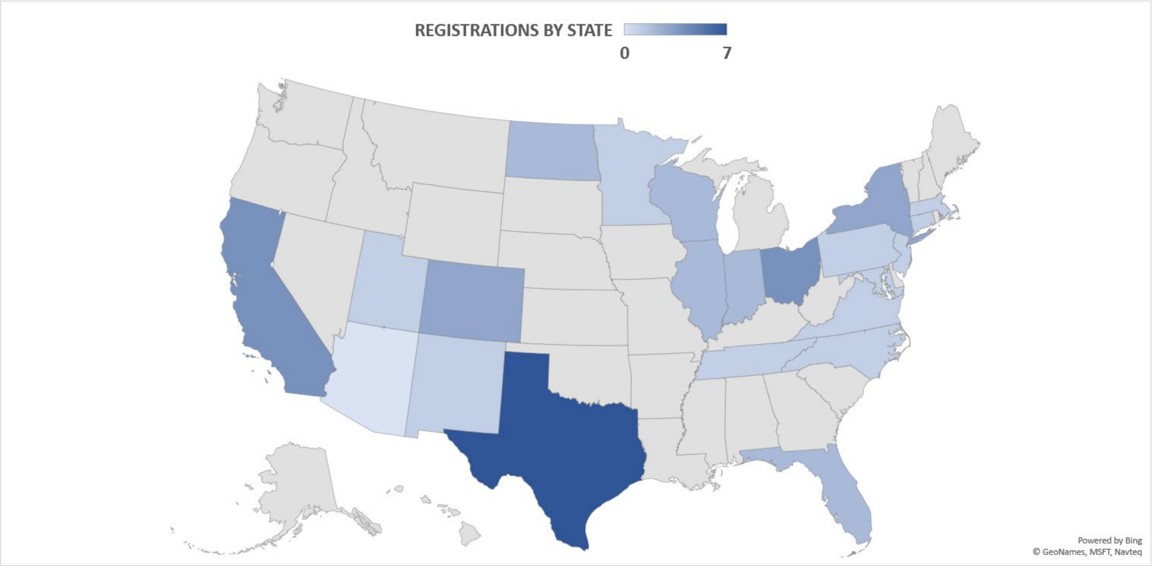
Outreach: User base

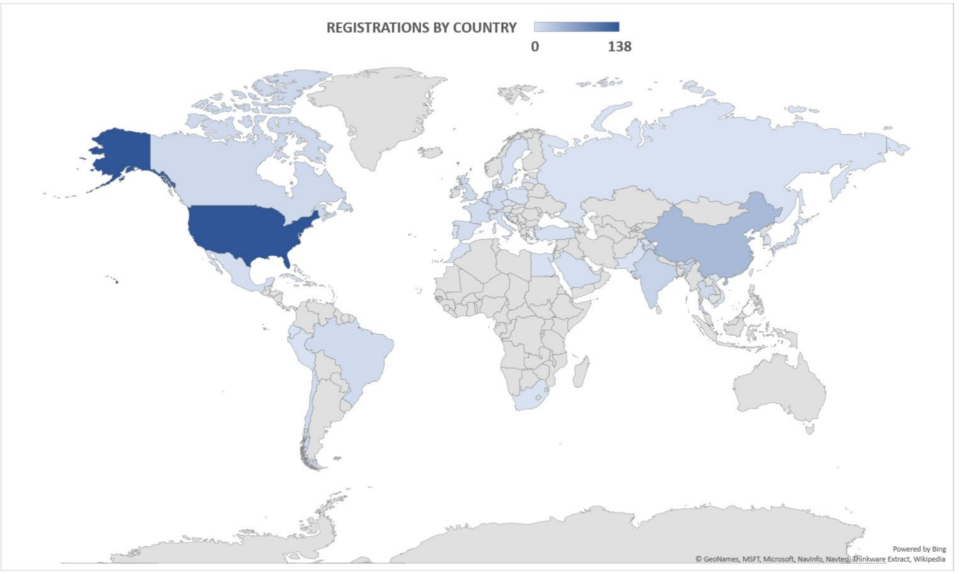
Still going strong amid pandemic crisis

Q2FY20 (Jan-March 2020) : 158 registrations, 831 MFiX Downloads

Q3FY20 (April-June 2020) : 161 registrations, 815 MFiX Downloads

All-time registrations = **6,264** (June 30th 2020)





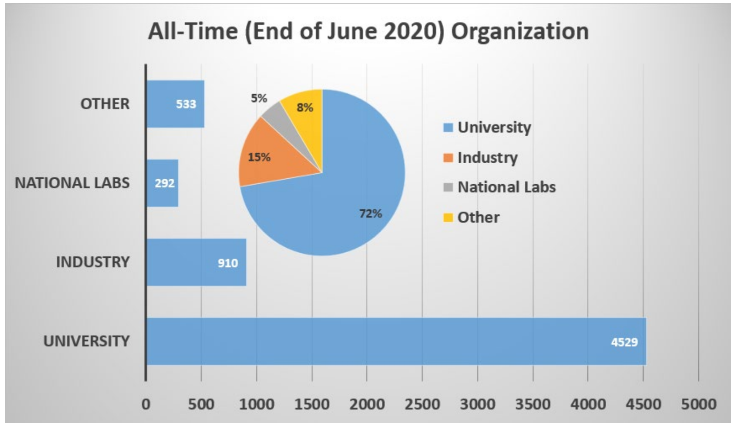
Registrations location (Q2FY20 + Q3FY20)

Outreach: All-time MFiX Stats

Stakeholders and Technology Transfer

- All-time MFiX registrations = **6,264**

  - University = 4,529
  - Industry = 910
  - Nat. Labs = 392
  - Other = 533



  - **81 countries, Top 5:**

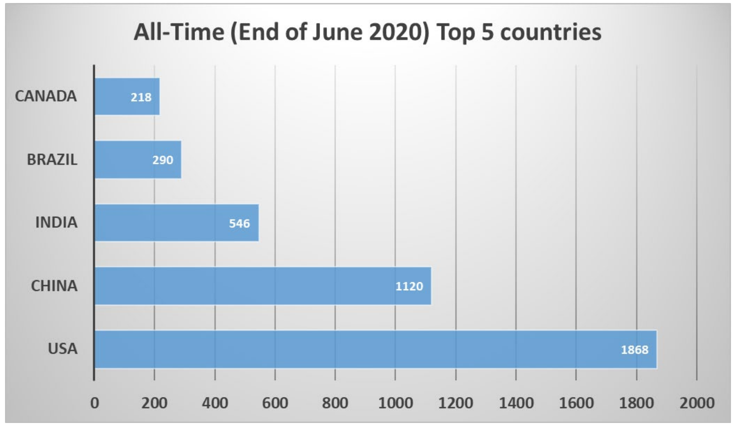
USA : 1,632

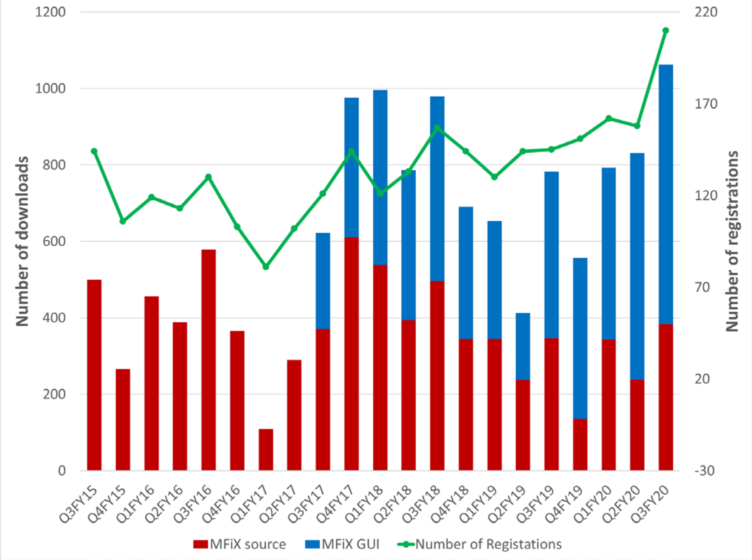
China : 1,020

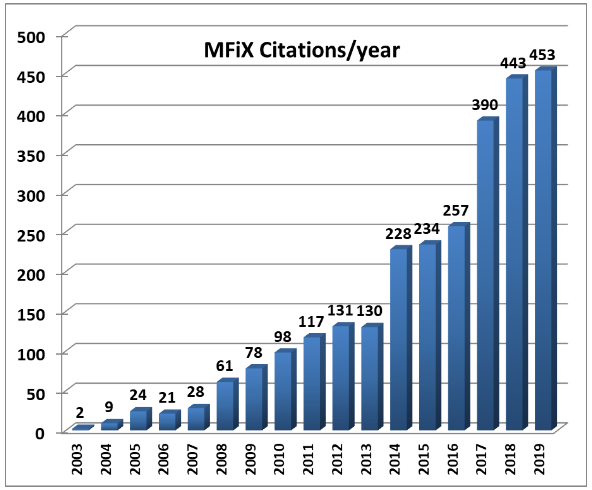
India : 509

Brazil : 268

Canada : 196







MFiX Forum

https://mfix.netl.doe.gov/forum

User support

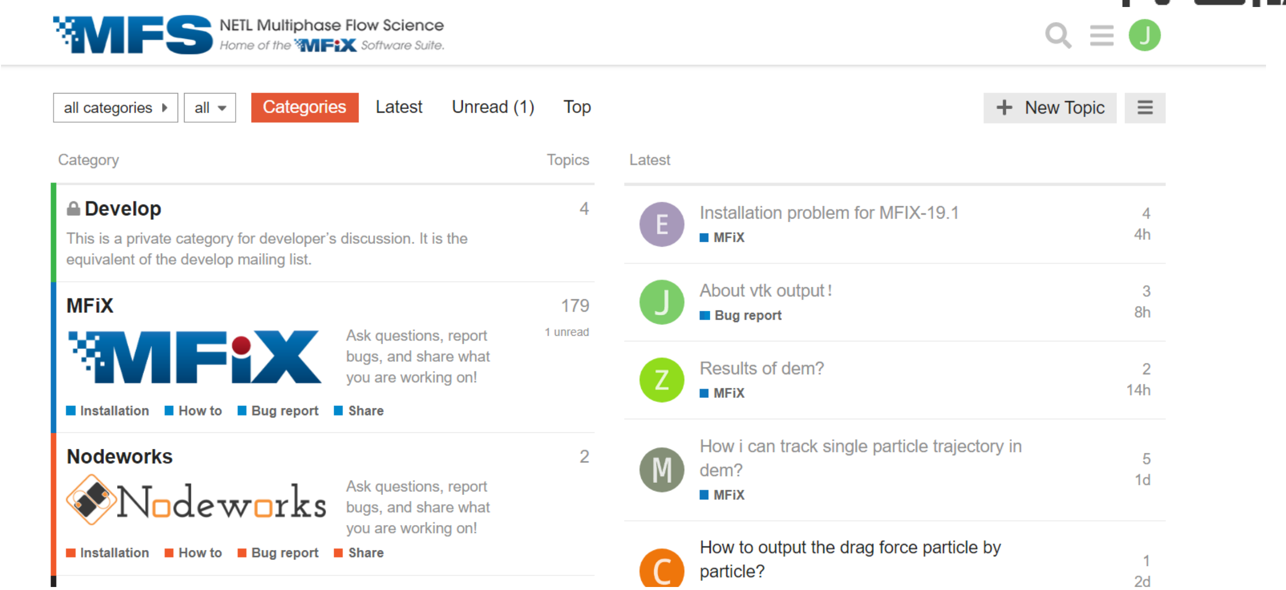
Categories

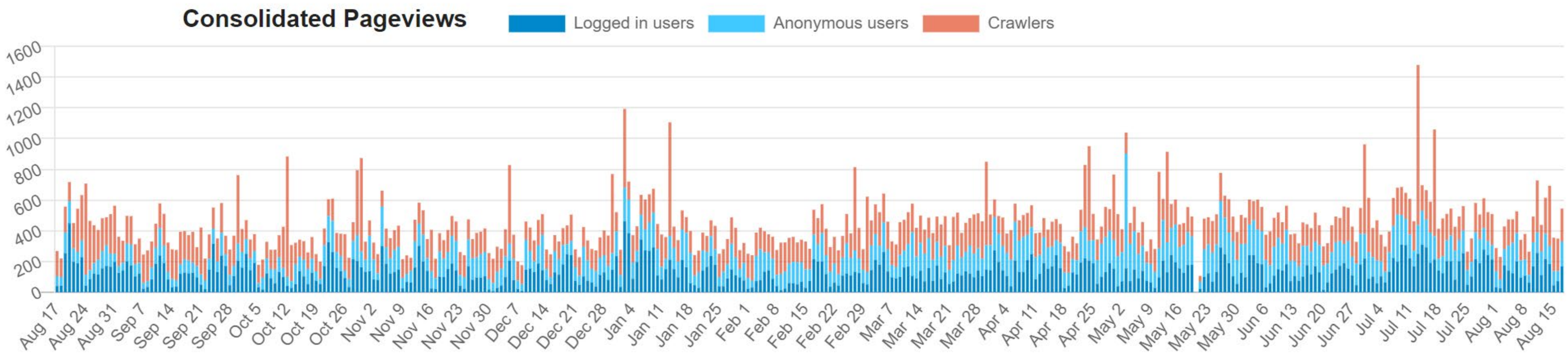
- Installation
- How to
- Bug report
- Share

Topics (threads)

File attachment

Searchable





MFiX Documentation

NETL Multiphase Flow Science
Home of the MFiX Software Suite.

https://mfix.netl.doe.gov/doc/mfix/19.2.0

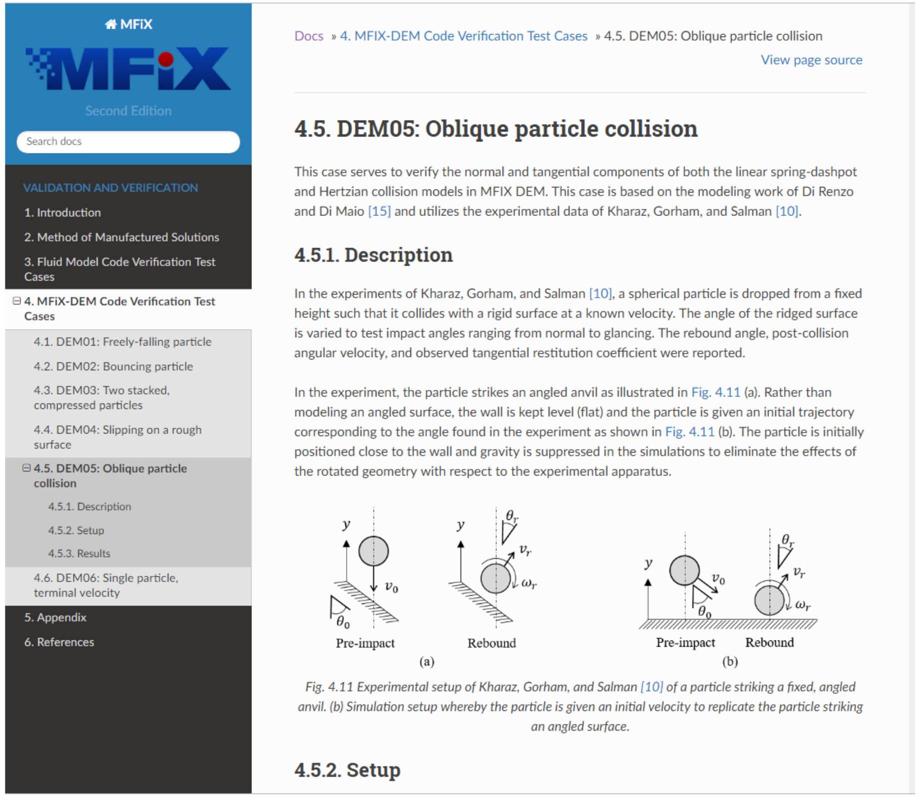
NATIONAL ENERGY TECHNOLOGY LABORATORY

User manual

V&V manual

Html and pdf

Text and video tutorials



MFiX

Second Edition

Search docs

VALIDATION AND VERIFICATION

1. Introduction
2. Method of Manufactured Solutions
3. Fluid Model Code Verification Test Cases
4. MFiX-DEM Code Verification Test Cases
   - 4.1. DEM01: Freely-falling particle
   - 4.2. DEM02: Bouncing particle
   - 4.3. DEM03: Two stacked, compressed particles
   - 4.4. DEM04: Slipping on a rough surface
   - 4.5. DEM05: Oblique particle collision
     - 4.5.1. Description
     - 4.5.2. Setup
     - 4.5.3. Results
   - 4.6. DEM06: Single particle, terminal velocity
5. Appendix
6. References

Docs » 4. MFIX-DEM Code Verification Test Cases » 4.5. DEM05: Oblique particle collision

View page source

4.5. DEM05: Oblique particle collision

This case serves to verify the normal and tangential components of both the linear spring-dashpot and Hertzian collision models in MFIX DEM. This case is based on the modeling work of Di Renzo and Di Maio [15] and utilizes the experimental data of Kharaz, Gorham, and Salman [10].

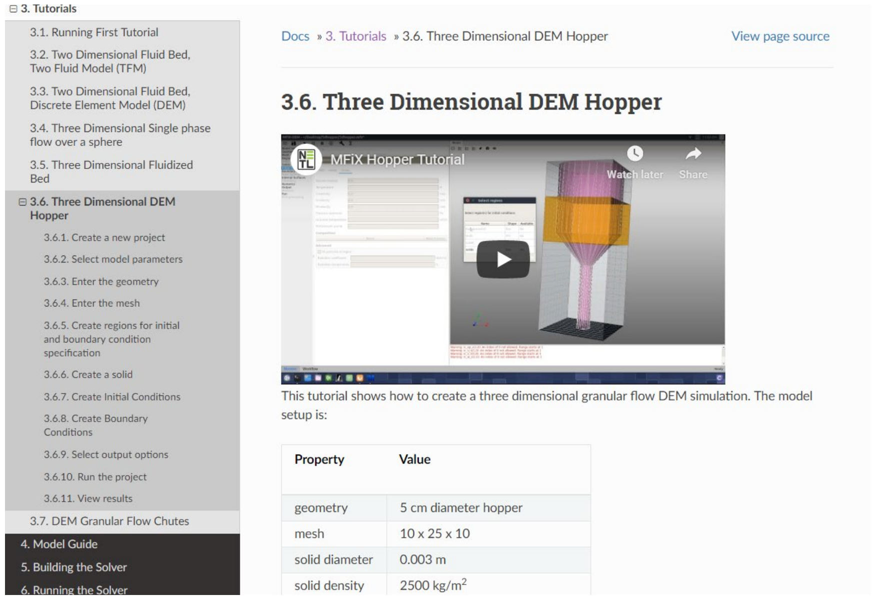
4.5.1. Description

In the experiments of Kharaz, Gorham, and Salman [10], a spherical particle is dropped from a fixed height such that it collides with a rigid surface at a known velocity. The angle of the ridged surface is varied to test impact angles ranging from normal to glancing. The rebound angle, post-collision angular velocity, and observed tangential restitution coefficient were reported.

In the experiment, the particle strikes an angled anvil as illustrated in Fig. 4.11 (a). Rather than modeling an angled surface, the wall is kept level (flat) and the particle is given an initial trajectory corresponding to the angle found in the experiment as shown in Fig. 4.11 (b). The particle is initially positioned close to the wall and gravity is suppressed in the simulations to eliminate the effects of the rotated geometry with respect to the experimental apparatus.

Fig. 4.11 Experimental setup of Kharaz, Gorham, and Salman [10] of a particle striking a fixed, angled anvil. (b) Simulation setup whereby the particle is given an initial velocity to replicate the particle striking an angled surface.

4.5.2. Setup



3. Tutorials
- 3.1. Running First Tutorial
- 3.2. Two Dimensional Fluid Bed, Two Fluid Model (TFM)
- 3.3. Two Dimensional Fluid Bed, Discrete Element Model (DEM)
- 3.4. Three Dimensional Single phase flow over a sphere
- 3.5. Three Dimensional Fluidized Bed
- 3.6. Three Dimensional DEM Hopper
  - 3.6.1. Create a new project
  - 3.6.2. Select model parameters
  - 3.6.3. Enter the geometry
  - 3.6.4. Enter the mesh
  - 3.6.5. Create regions for initial and boundary condition specification
  - 3.6.6. Create a solid
  - 3.6.7. Create Initial Conditions
  - 3.6.8. Create Boundary Conditions
  - 3.6.9. Select output options
  - 3.6.10. Run the project
  - 3.6.11. View results
- 3.7. DEM Granular Flow Chutes

4. Model Guide
5. Building the Solver
6. Running the Solver

Docs » 3. Tutorials » 3.6. Three Dimensional DEM Hopper

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3.6. Three Dimensional DEM Hopper

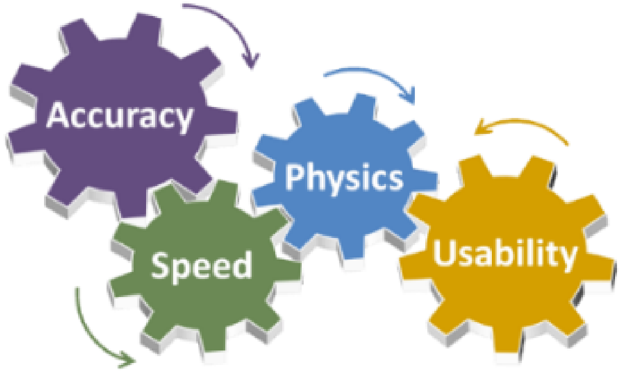
This tutorial shows how to create a three dimensional granular flow DEM simulation. The model setup is:

Property	Value
geometry	5 cm diameter hopper
mesh	10 x 25 x 10
solid diameter	0.003 m
solid density	2500 kg/m^2

Task 2: Summary

- MFiX releases
  - 19.3: Moving geometry (tangential velocity)
  - 20.1: New meshing workflow
  - 20.2: Moving geometry (STL), PIC CFL

- MFiX development
  - GUI continuous development
  - Polydispersity (20.3 release, Sept. 2020)
  - Coarse grain DEM
  - Non-spherical DEM particles
  - PIC parameter sensitivity/calibration



Task 3: Device scale modeling

Problem Statement

- Design and optimization of reactors for FE applications is a challenging and expensive process
- CFBC systems: Important to existing power generation fleet and next generation (Coal FIRST Program)
- CFBC advantages: fuel flexibility, lower operating temperatures, high efficiencies
- Challenges for existing plant in designing and operating multiphase flow systems fluctuating load conditions

Benefits

- Science-based models: reduce the risk, cost, and time required for development of novel FE reactors.
- NETL is providing an advanced suite of multiphase flow CFD models that enable this capability.

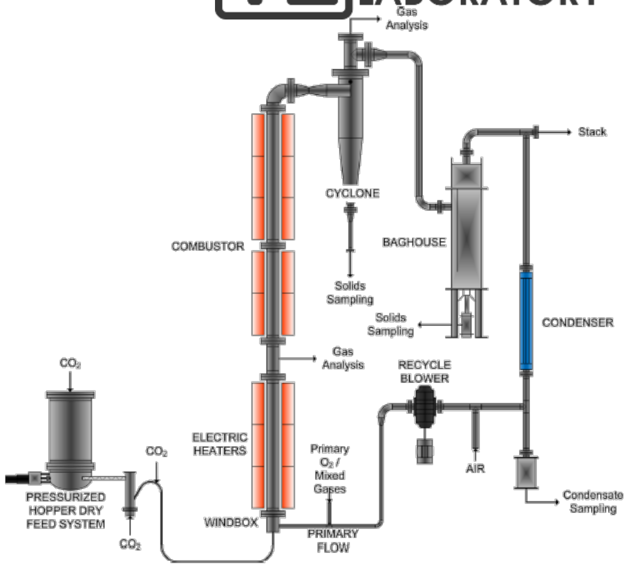
R&D Challenges

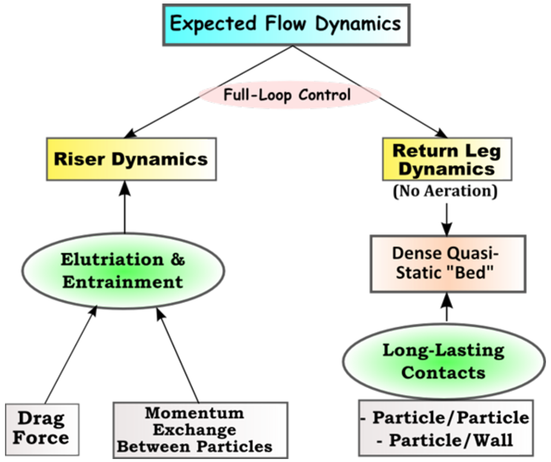
- Large physical size of the reactor, high particle count, and the complex physics
- Study several scales of CFB combustor ranging from small pilot scale through commercial scale
- Requires High Performance Computing systems
- Complex modeling effort: broad range of fluidization conditions, high temperature reacting flow, complex geometry (heat transfer surfaces), gas/solids coupling

Task 3: Device scale modeling

50kW$_{th}$ CFB Combustor Experiment

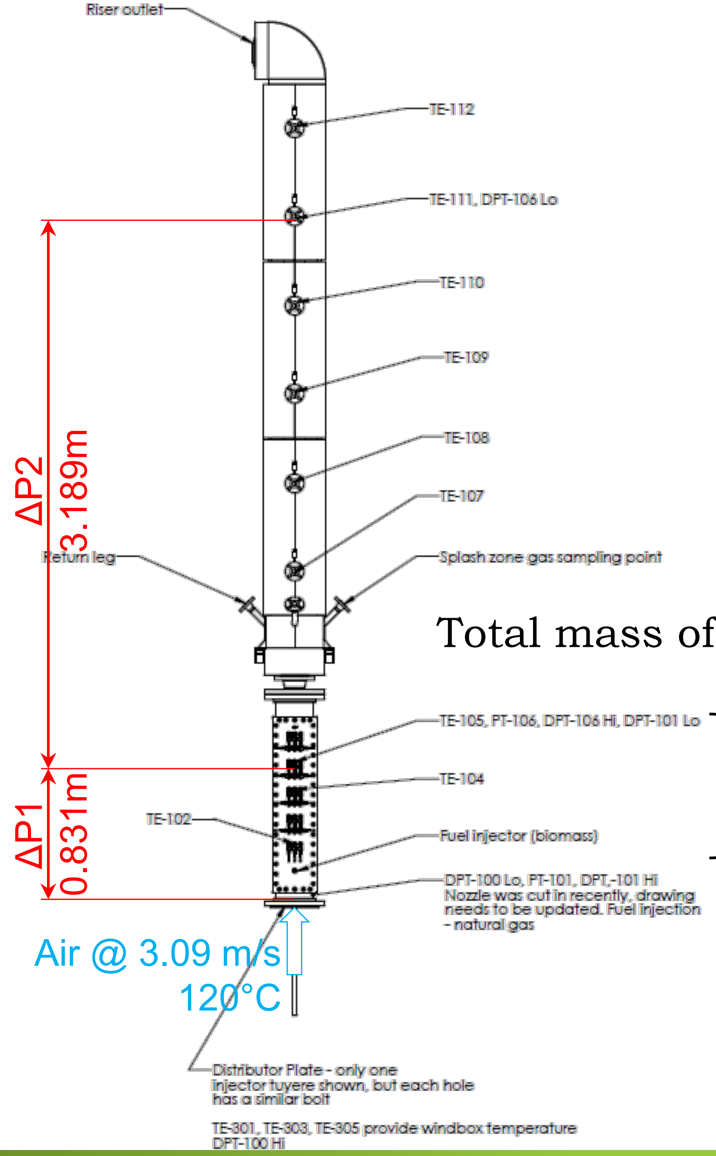
- Objectives:
  - ***Detailed analysis of industrial scale CFBC systems to advance both existing fleet and coal plants of the future needs***
  - ***Study existing CFBC boilers over a range of operating conditions to optimize fuel-air mixing and plant flexibility***
- Collaborative effort between NRCan and NETL in the study of CFB combustion of coal and biomass over a range of oxyfuel conditions
- Experimental facility designed, built, and operated at Natural Resources Canada, CanmetENERGY1 (NRCan)
- Apply computational tools and FE/NETL supercomputing resources to aid in understanding and optimizing CFB boiler performance
- Hydrodynamics study with PIC model (MFiX and OpenFOAM)
- Identify modeling challenges
- Riser and full-loop simulations
- Benchmarking





[1] Hughes, R.W. et al., 2015. Oxy-fluidized bed combustion using under bed fines fuel injection. In 22nd International Conference on Fluidized Bed Conversion. Turku, Finland, 2015.

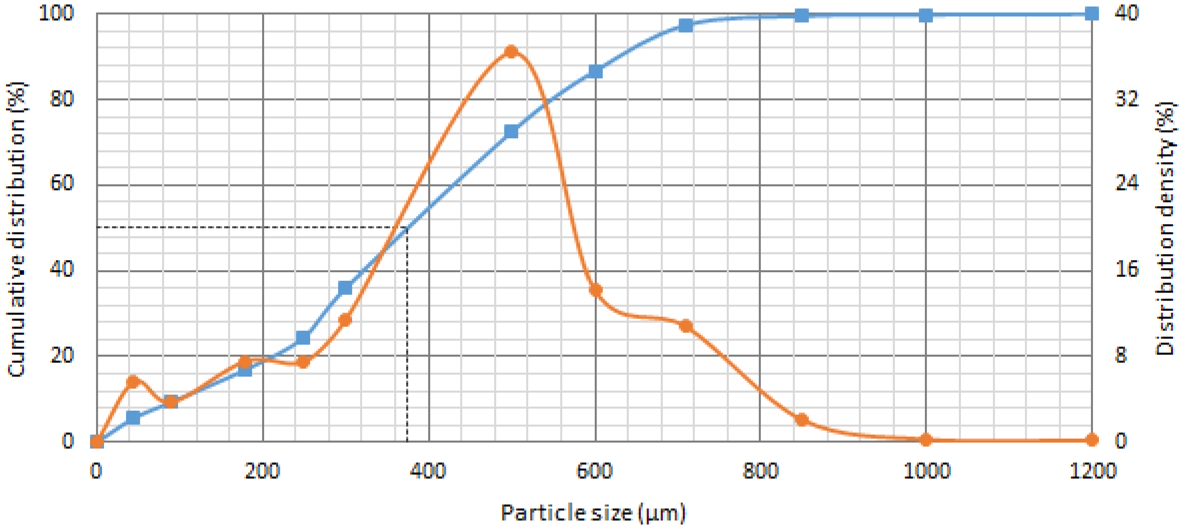
Cold Flow Experiment



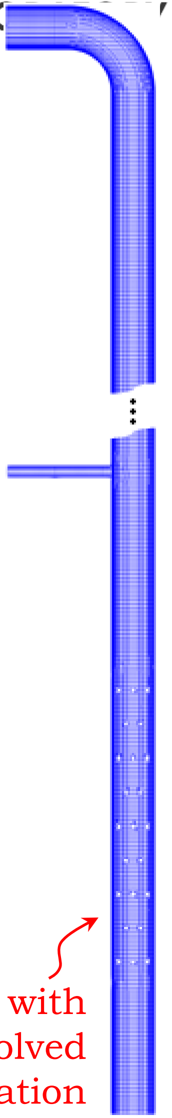
Total mass of inert = 9 kg

23 heat exchanger tubes modeled as adiabatic walls

Inert material: Olivine sand, ρ_p = 3,063 kg/m³



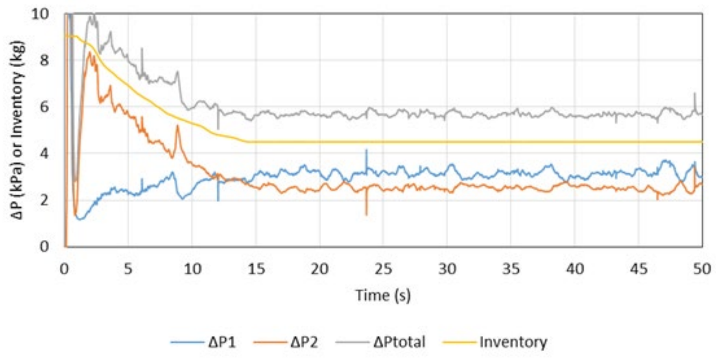
MFiX-PIC Parameters	
Stat. weight	500
Drag model	Gidaspow
$\alpha_{p,max}$	0.34
e_c	0.85
e_w	0.85
μ'_w	1.0
P_s, β	Varies

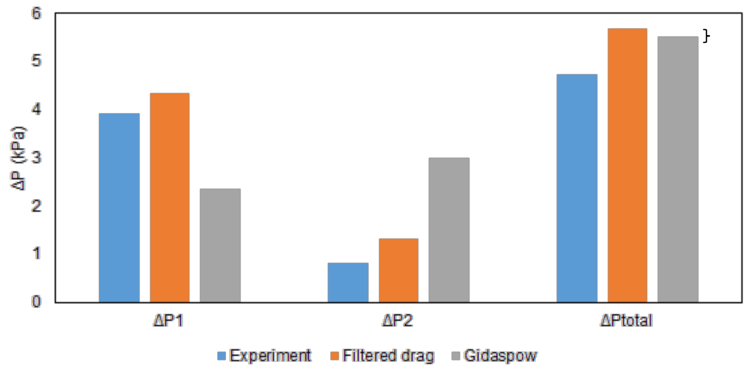


Computational grid with tube bank resolved for riser-only simulation

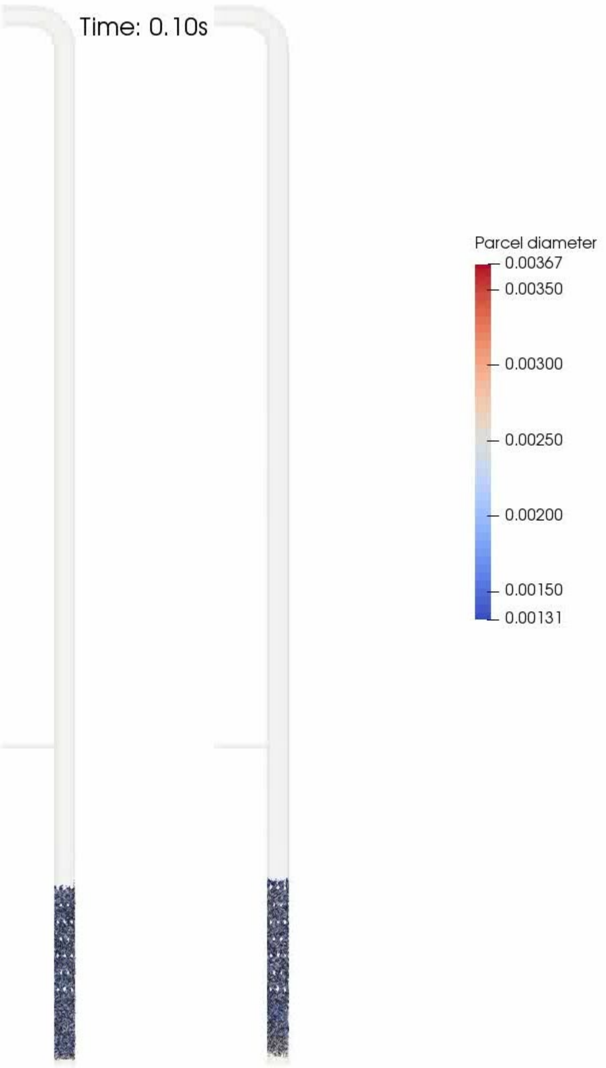
Riser Hydrodynamics

- Challenge: For U_g = 3.09 m/s, sand particles are elutriated out of the riser and the recirculation must be considered to maintain accurate inventory for comparison with experiment
- Fluidization is impeded by the filtered drag model so more particles are retained in the lower riser
- Circulation rate is reduced, reflected in the average mass of recirculated particles in the side inlet
- Pressure drop distribution and overall pressure drop are both in agreement with experimental results



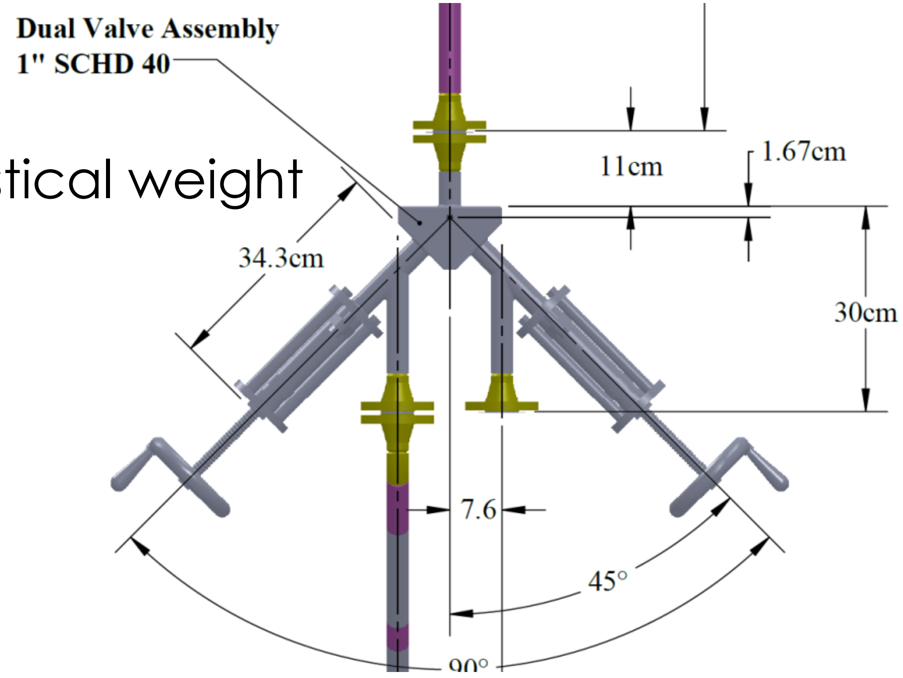


Overall ΔP is lower for Gidaspow drag because at each time step, more particles stay in the side inlet due to the higher recirculation



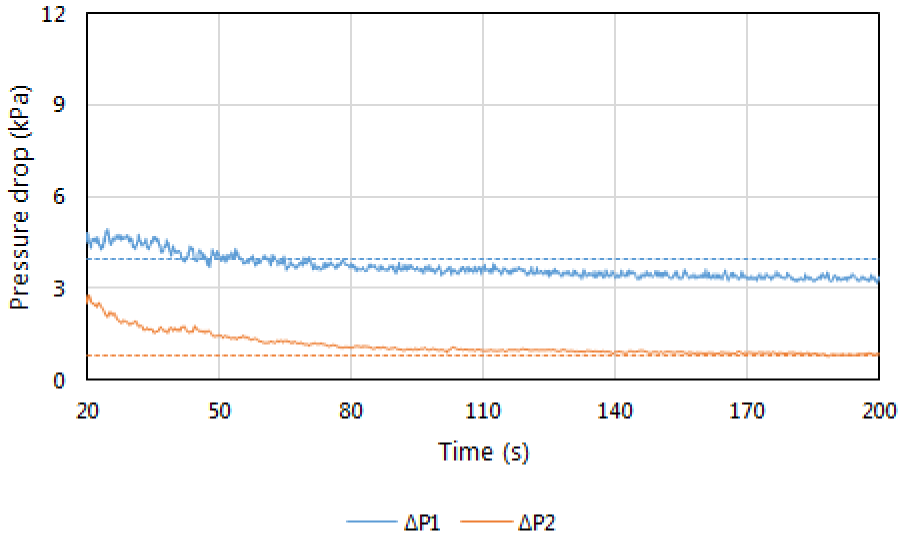
Full Loop Simulation of Cold Flow

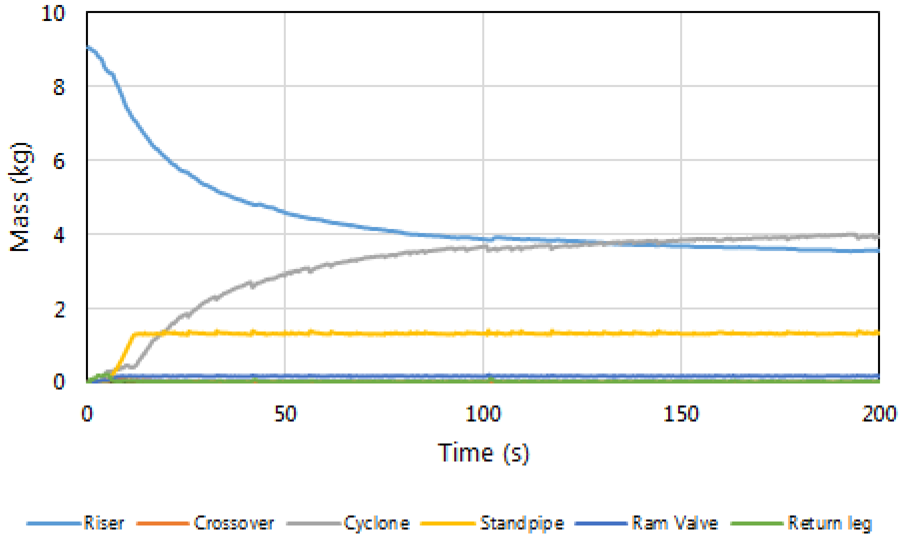
- From the riser-only simulations, the experimental pressure drop distribution in the riser can be matched *as long as* the riser holdup matches the experiment
- It is desirable to model the full loop so that the riser holdup can be allowed to evolve as a function of the operating parameters instead of being fixed at a prescribed value
- Challenge: Ram valve operation
- Filtered drag performs better than homogeneous drag
- Results are independent of parcellation (constant statistical weight or constant parcel size)
- Need to tune Ram valve position to match DP (fully open, 31.1, 32.5, and 34.0mm)



Particle recirculation mechanism is via a ram valve

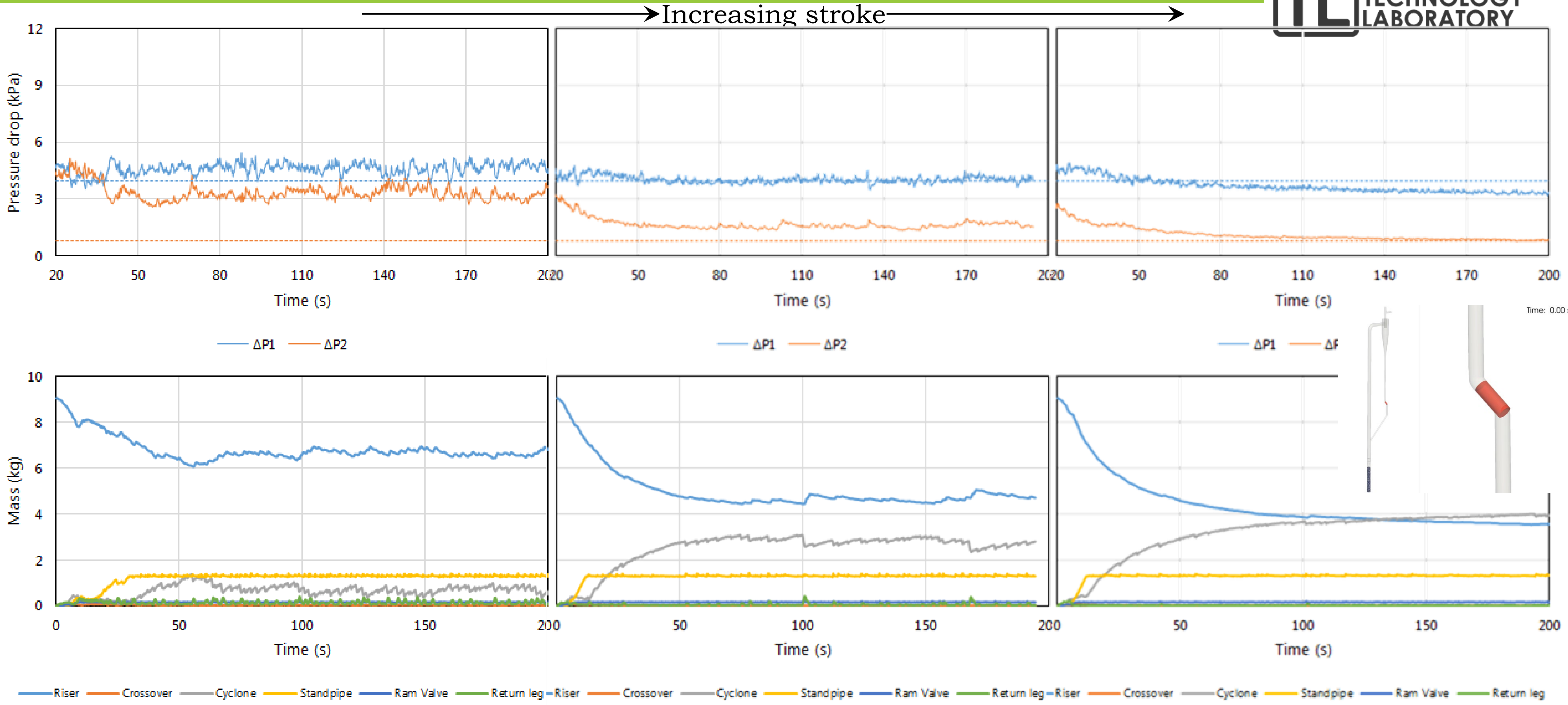
Full Loop Simulation of Cold Flow



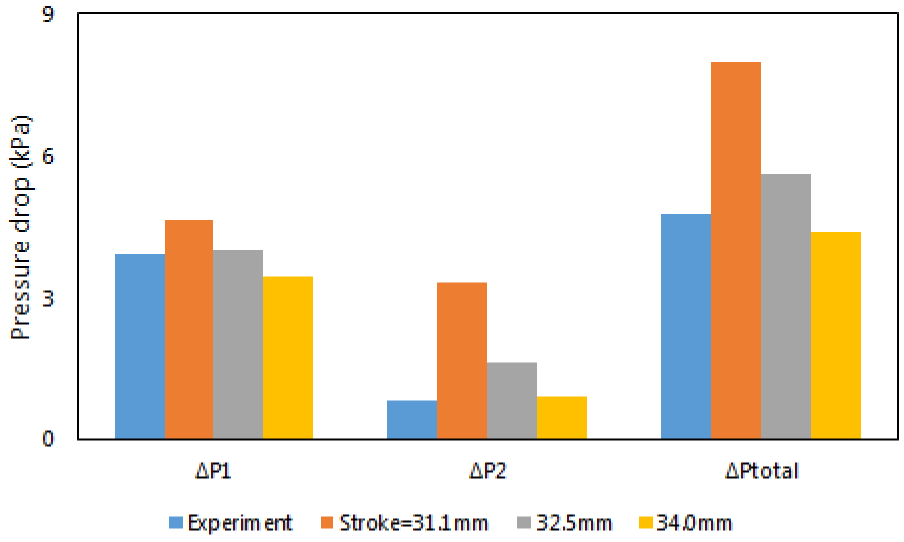


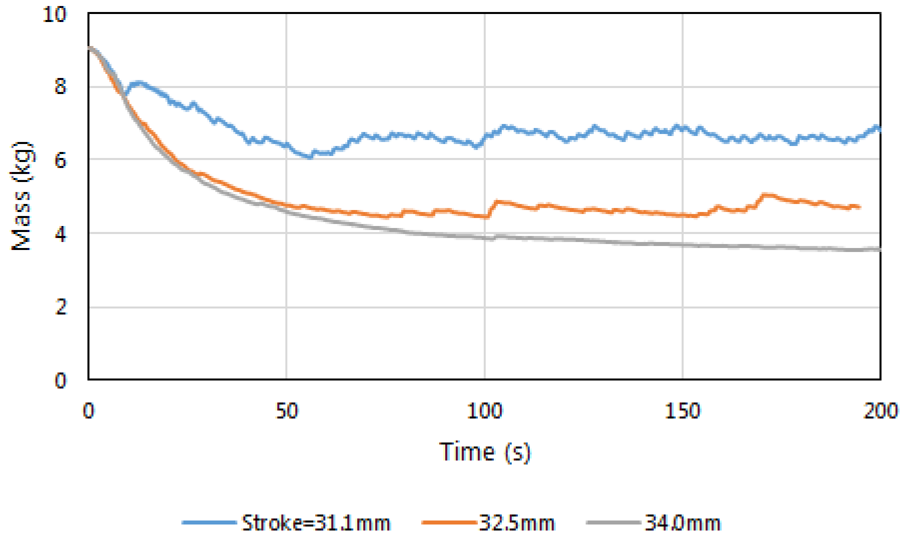
Valve stroke = 34.0 cm

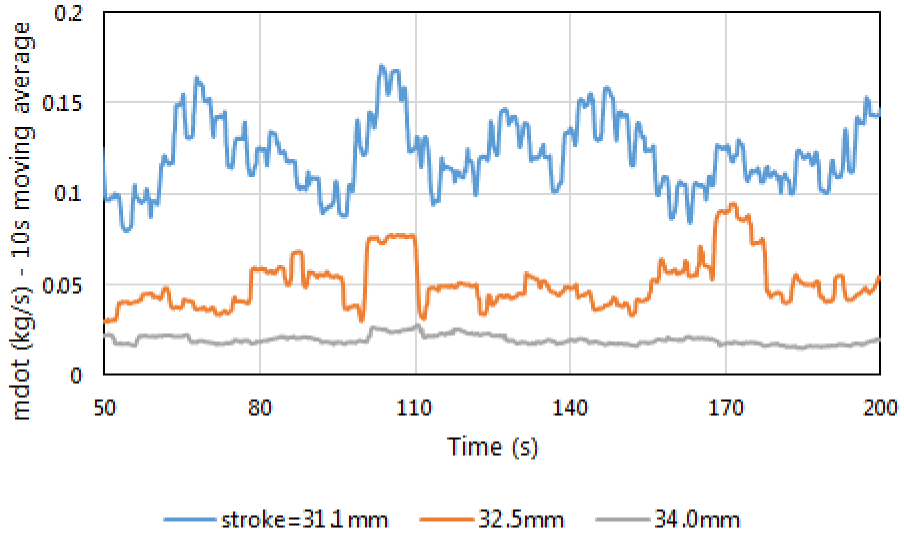
Tuning Riser Inventory w/ Ram Valve



Effect of Valve Stroke







	Exp.	Open	31.1mm	32.5mm	**34.0mm**
ΔP_1 (kPa)	**3.92**	3.96	4.64	4.01	**3.45**
ΔP_2 (kPa)	**0.82**	5.53	3.33	1.61	**0.92**
ΔP_T (kPa)	**4.74**	9.49	7.97	5.62	**4.37**
m_{riser} (kg)	–	8.18	6.69	4.69	3.70
$\dot{m}$ (kg/s)	–	0.21	0.12	0.054	0.020

Values averaged over final 100s of simulation

Comparison MFiX-OpenFOAM

Tetrahedra Grid

Mesh

- Grid density (Coarse): 363,286 cells
  - Δ_{min}= 0.6mm ($\Delta_{min}/d_{p,max}$ = 1.4)
  - Δ_{max}= 14.9mm ($\Delta_{max}/d_{p,max}$ = 35.1)
- Time step: 1e-3s

Laplacian Filter (of gas volume fraction)

$$\begin{cases} \nabla \cdot \left(D_f \nabla \alpha_g\right) = 0 \\ \textbf{Grid–based diffusion } \boldsymbol{D_f} \\ D_f = \dfrac{2|\Omega|}{|\partial\Omega|\delta}\epsilon \end{cases}$$

Grid-based diffusion length-scale: $\sqrt{\boldsymbol{D_f}} \approx \mathbf{3.98}\boldsymbol{d_{parcel}}$

	Exp.	MFiX-Filtered	OF-Filtered
ΔP_1 (kPa)	3.92	4.24	3.63
ΔP_2 (kPa)	0.82	5.11	5.76
ΔP_{total} (kPa)	4.74	9.36	9.39
m_{riser} (kg)	-	7.98	8.36
$\dot{m}$ (kg/s)	-	0.22	0.0087

Data	MFiX	OpenFoam
Grid size (fluid cells)	347K	363K
Number of Parcels	1.467M	1.460M
Cores	160	160
Simulated time/day (s)	26	53

Task 3: Summary

- Riser and full loop simulations of the CANMET 50 kW reactor were conducted
- A good match with experimental data was achieved for lower bed pressure drop
- Filtered drag performs better than homogeneous drag
- Circulation rates and pressure drop in upper section of riser are sensitive to valve opening setting
- MFiX and OpenFOAM provide comparable results
- Future work:
  - Full loop reacting flow (50 kW)
  - Develop cold flow 12 MWth CFB Boiler Model
  - Develop reacting flow 12 MWth CFB Boiler Model

Concluding Remarks

- Advancing Multiphase flow modeling capabilities to address FE strategic goals of modernizing existing coal fleet, developing coal plants of the future, and reduce the cost of carbon capture, utilization, and storage
- Improvement in science-based models confidence, accuracy, speed, usability will make them viable tools to reduce the risk, cost, and time required for development of novel FE reactors.
- Open source

Concluding Remarks

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Publications/ presentations

- Clarke, M.A., and Musser, J.M.H., "Particle in Cell Method (MFiX-PIC) Theory Guide," DOE/NETL-2020/2115, April 2020.
- Clarke, M.A., Gel, A., Rogers, W.A., and Vaidheeswaran, A., "Sensitivity Analysis of Particle-in-Cell Modeling Parameters in MFiX-PIC," ASME Verification and Validation Symposium, Baltimore, MD, May 20–22, 2020.
- Ashfaq, H., Clarke, M.A., Pandey, R., Rogers, W.A., and Vaidheeswaran, A., "Fluidization of Group A Glass Particles: Experiments and Preliminary Validation," DOE/NETL-2020/2135, NETL Technical Report Series (2020), p. 32, DOI: 10.2172/1632859.

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