MFiX - Multiphase Flow with Interphase Exchanges

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

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Disclaimer

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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, including decarbonization of the energy sector.

- **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) 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

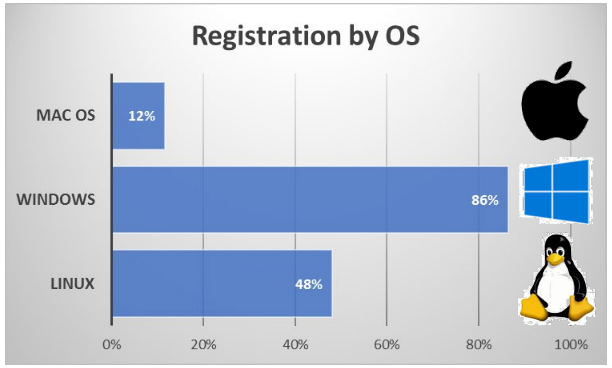
Project Update

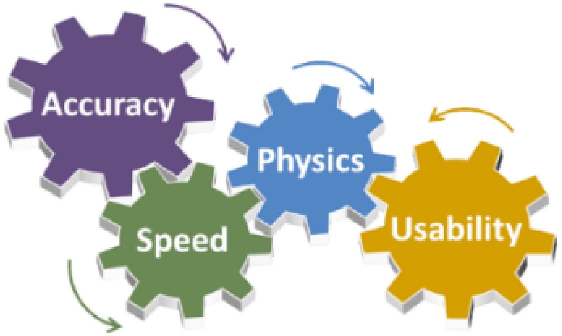
Task 2: MFiX Development, Validation, and Enhancements

- 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
  - Acceleration of the flow solver
- Quality Assurance (QA) Program
  - Verification
  - Validation
  - Improved documentation, user guides, and validation experiments.
- Outreach capabilities through the MFiX web portal to better serve FE and NETL stakeholders.

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 one and four releases per year





- **User support through online forum**

MFiX Suite of Multiphase CFD Software

Managing the tradeoff between accuracy and time to solution

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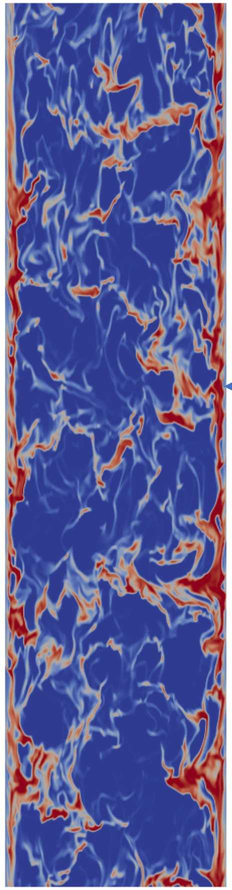


Time to Solution

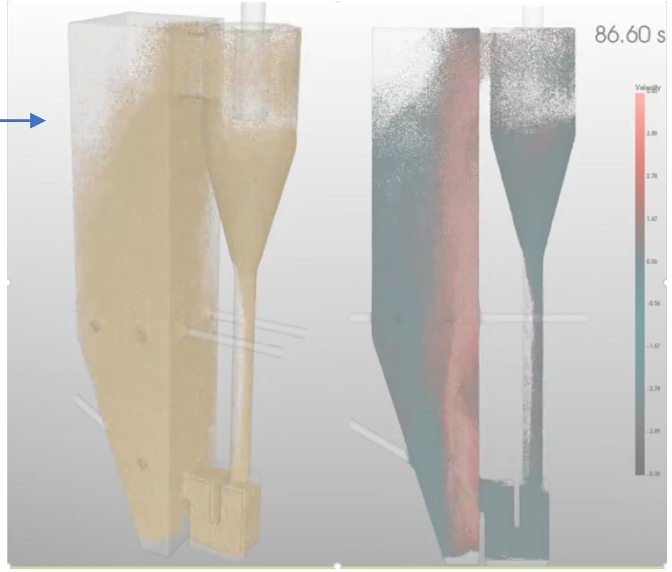
DNS
Direct Numerical Simulation: fine scale, accurate simulations for limited size domain

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

MFiX CGP

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

Eulerian-Lagrangian modeling

Use MP-PIC for computational speed and averaged accuracy

REDUCED ACCURACY

SOLIDS REPRESENTATION

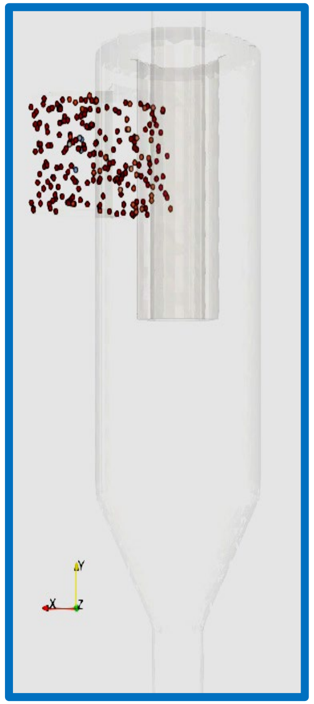
	Collision Resolved	Momentum Conservation	Solid Stress Gradient
Parcel	MFiX CGP **CGPM** Coarse Grained Particle Method **Masaaki et al. 2000** **Sakai and Koshizuka,2009**	**CGHS** Coarse Grained Hard Sphere **Lu et al., 2017**	MFiX PIC **MP-PIC** Multi Phase Particle In Cell **Andrews and O'Rourke, 1996**
Particle	MFiX DEM **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**	

INCREASED COMPUTATIONAL SPEED

GENERALIZED IDEA FOR PARTICLE INTERACTIONS

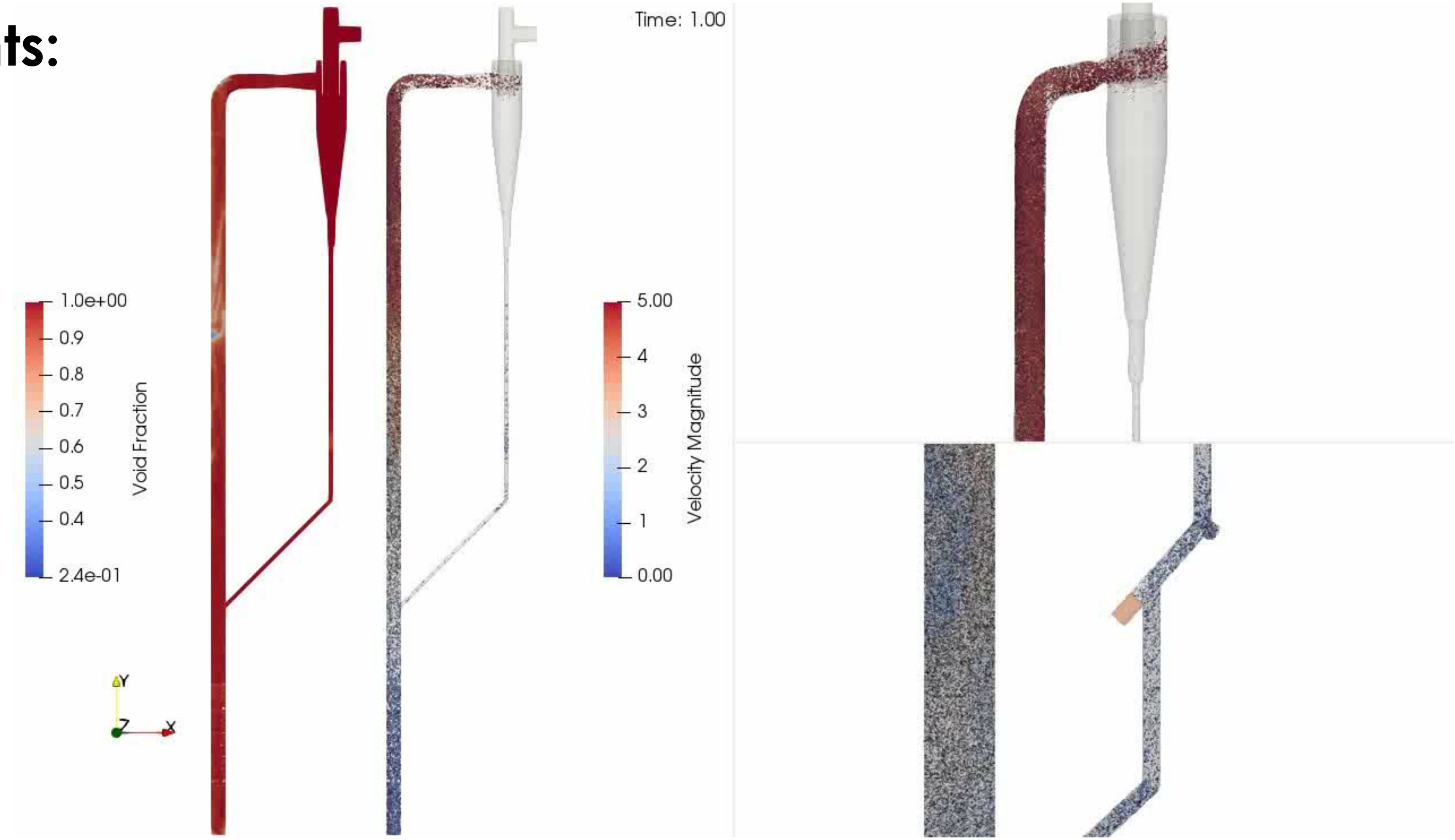
Particle Flow in Cyclone

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



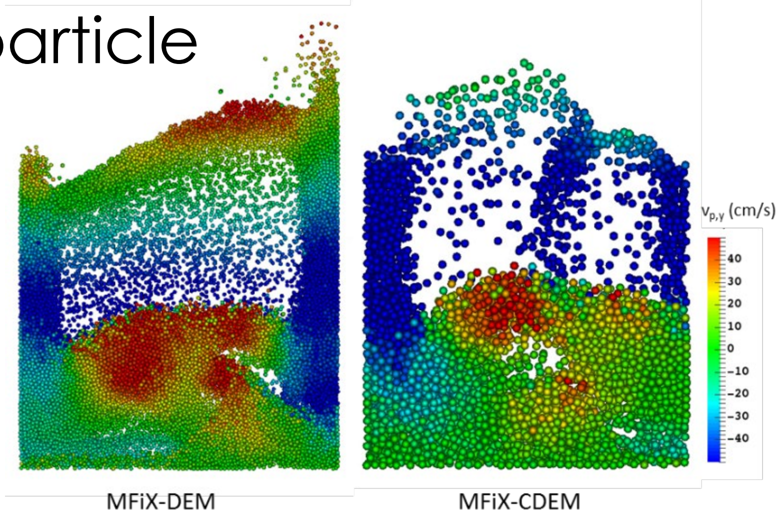
Multiphase Particle In Cell (MP-PIC)

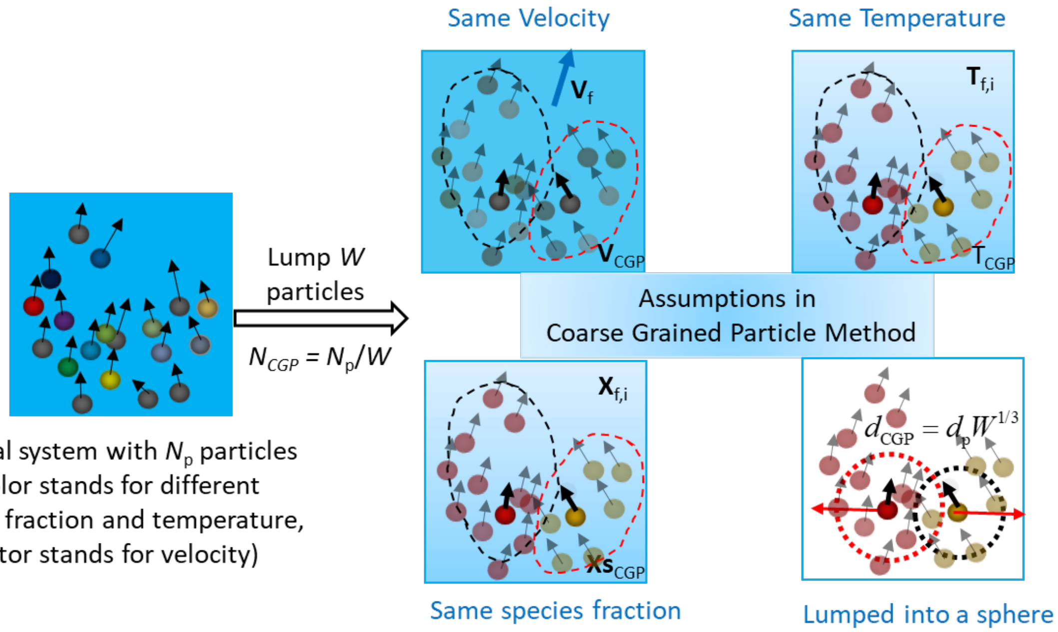
- **Recent PIC developments:**
  - CFL time step control
  - Collision damping model
- **Ongoing effort:**
  - Polydispersity
  - V&V
  - PIC parameter sensitivity analysis
  - PIC parameter calibration

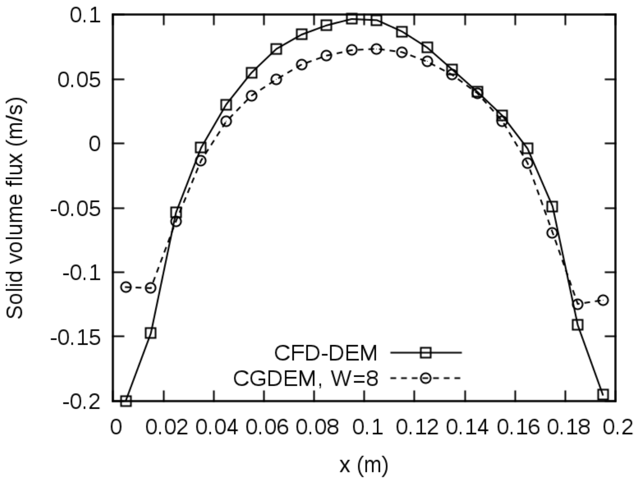


Coarse Grain DEM

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

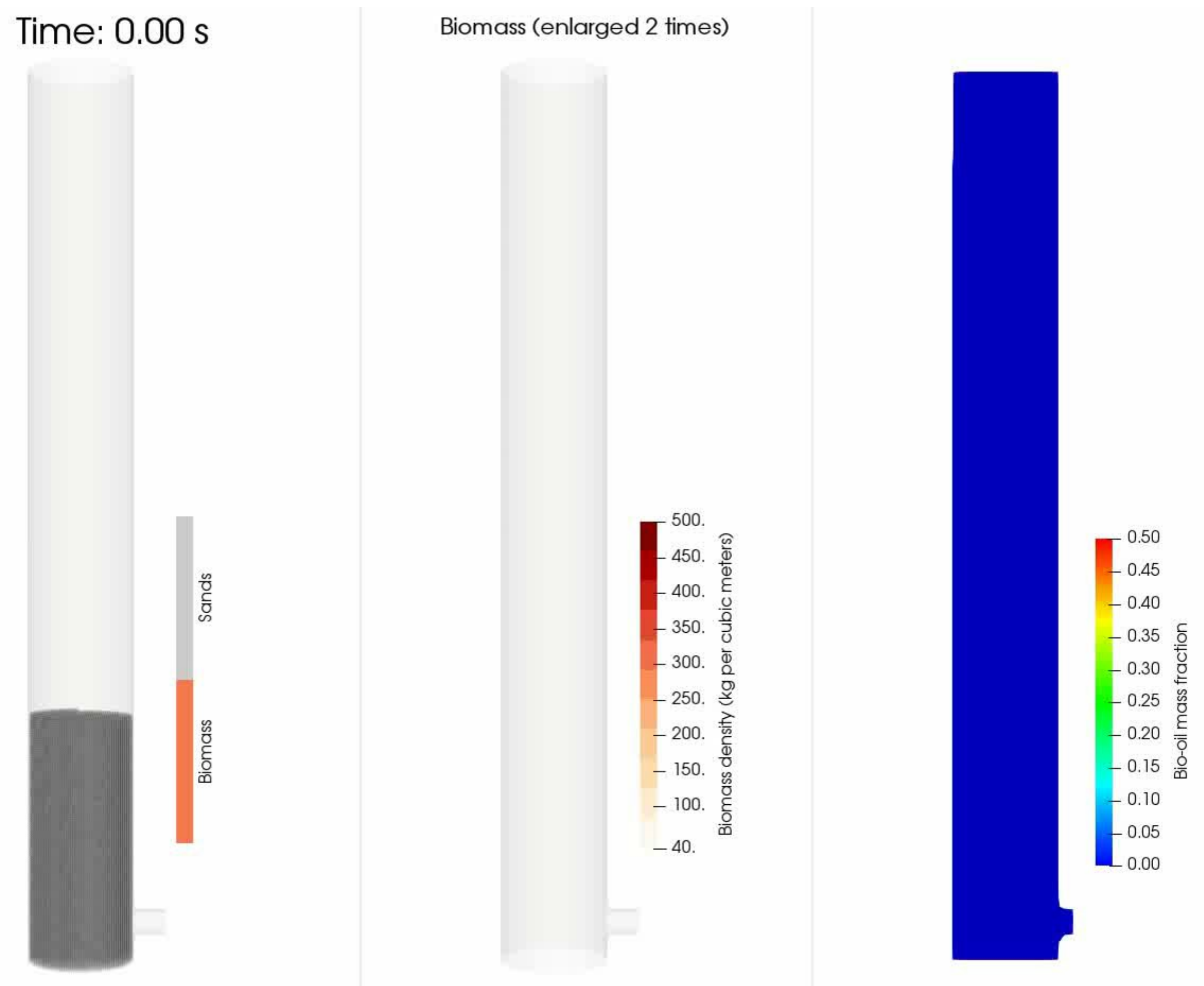




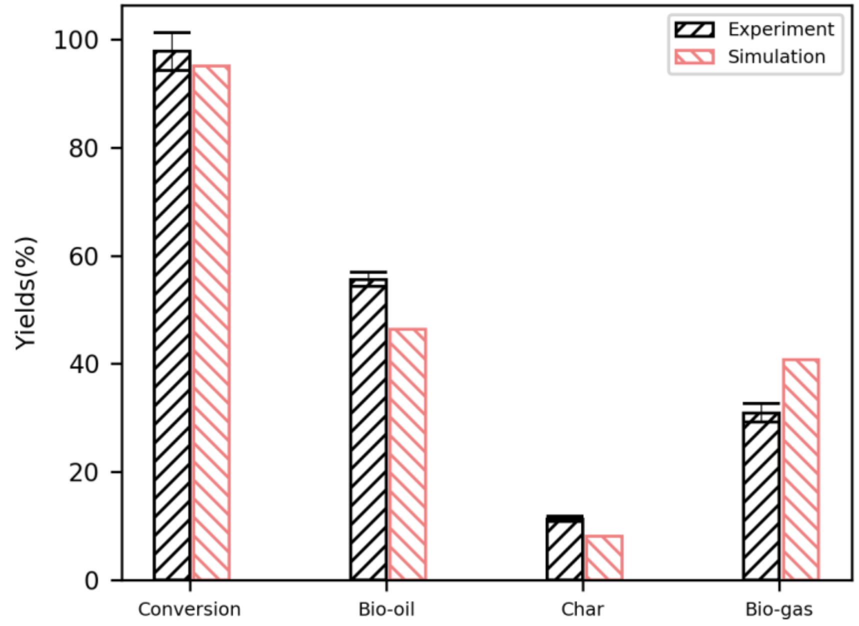


Coarse Grain DEM

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



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

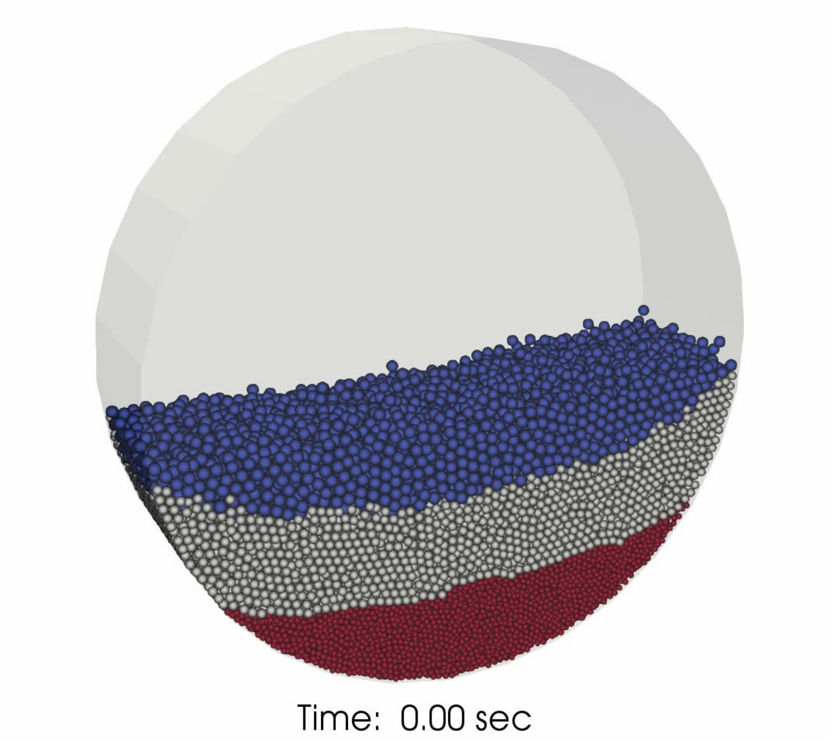


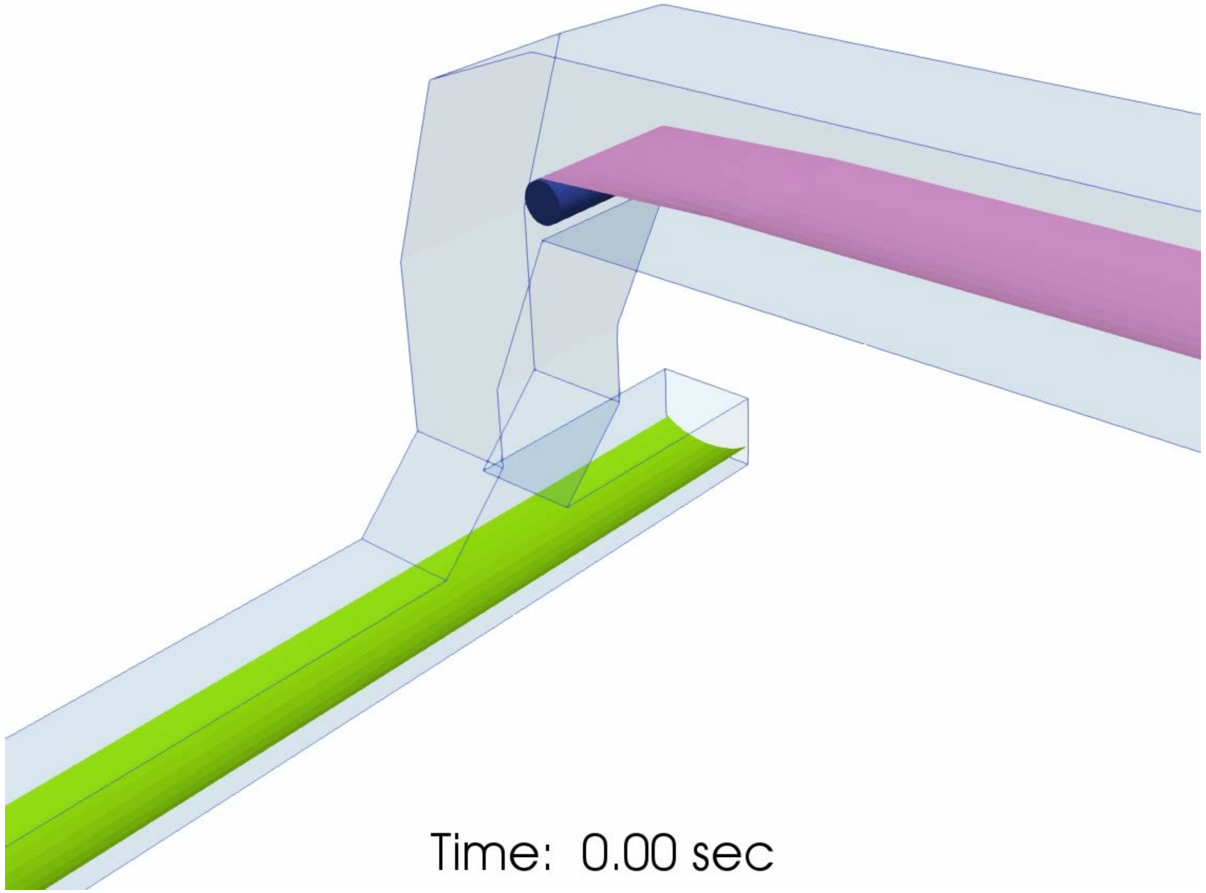
Moving Geometry

Several Options to Represent Moving Geometry

Moving STL walls through tangential velocity

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

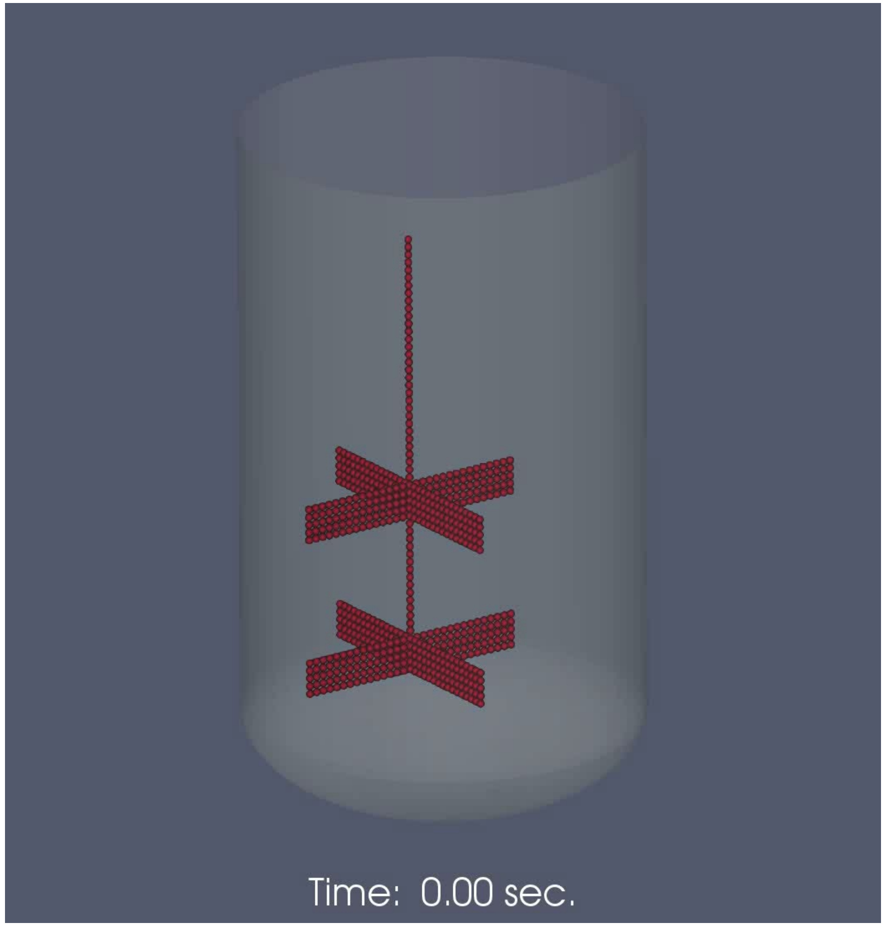




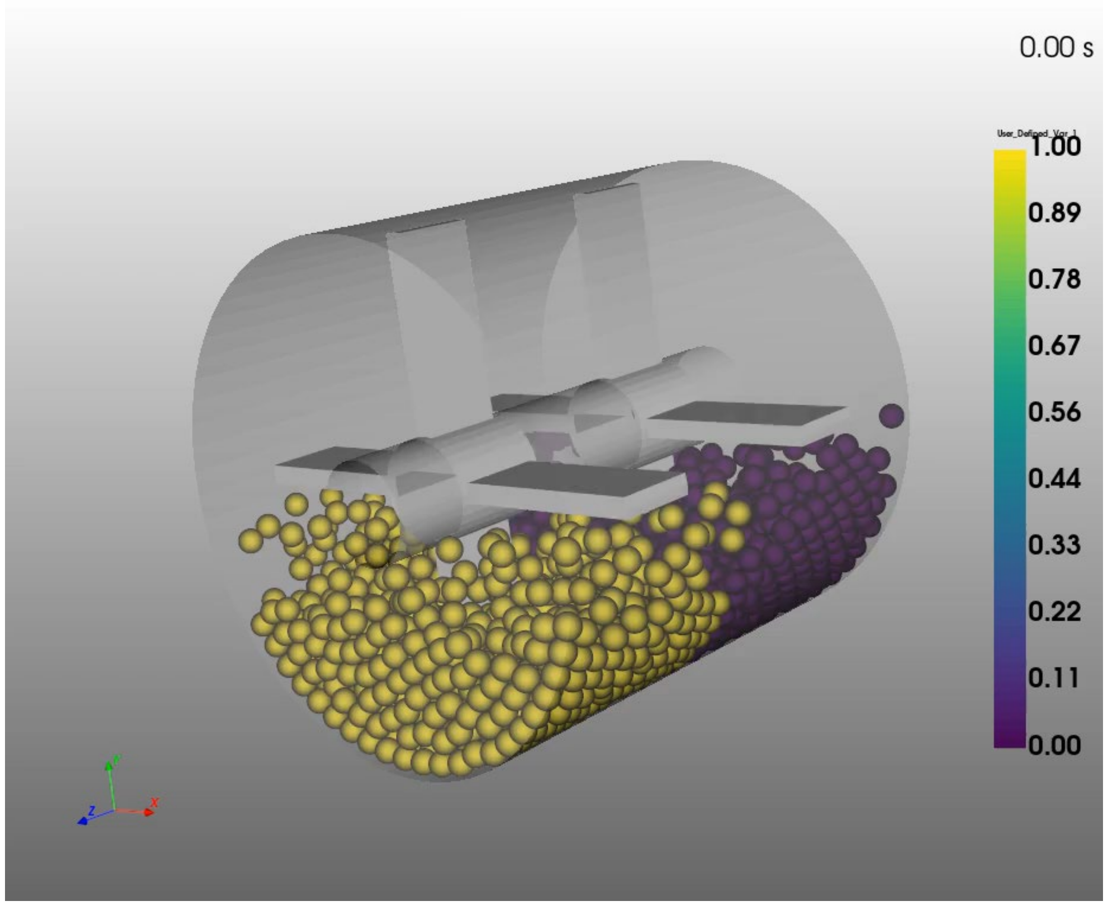
Moving Geometry

Several Options to Represent Moving Geometry

Freeze or set particle velocity

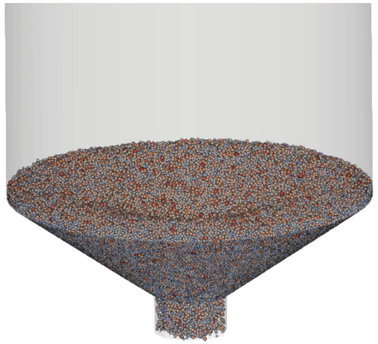


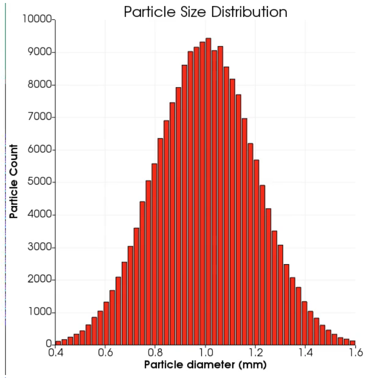
Move STL geometry (Granular DEM)

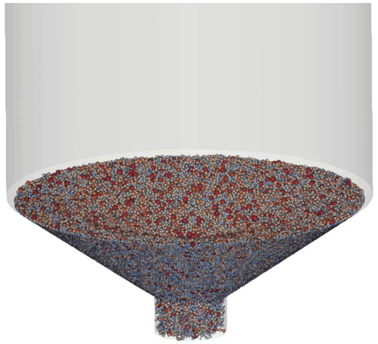


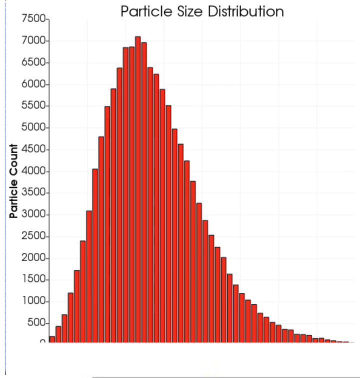
Polydispersity (DEM)

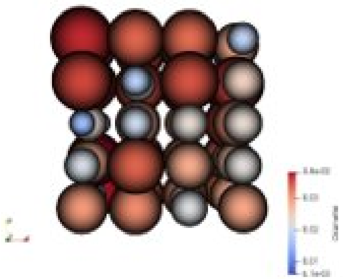
- Available in 20.3 Release (September 2020)
- Merge and complement ASU implementation
- Initial and Boundary (mass inflow) conditions
- DEM Particle size distribution
  - Normal
  - Log-normal
  - Custom (user-defined)
- Improvement in IC seeding
  - Robust
  - Lattice
  - Spacing
  - Flexibility in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



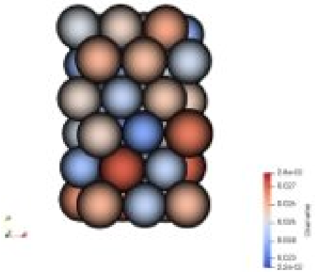




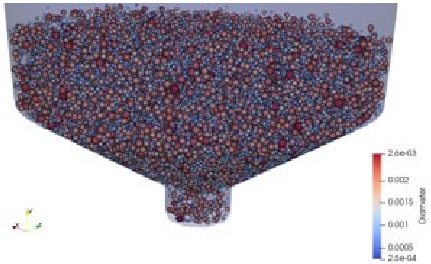


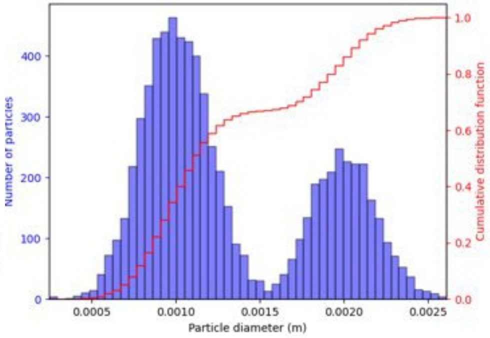


Cubic lattice



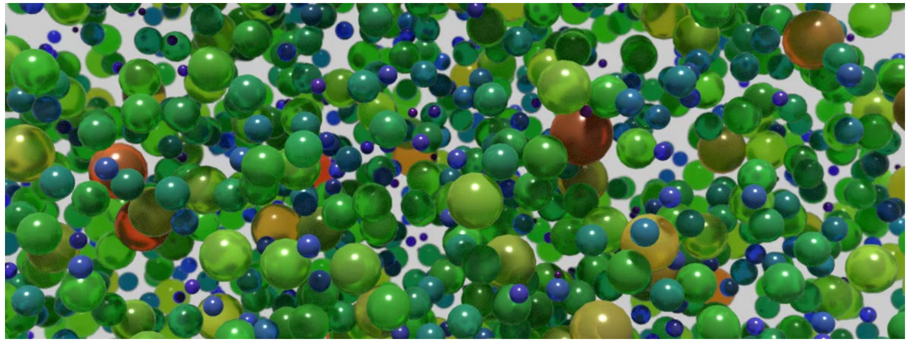
Hexagonal lattice



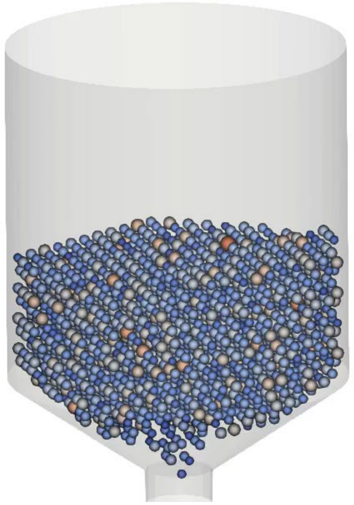


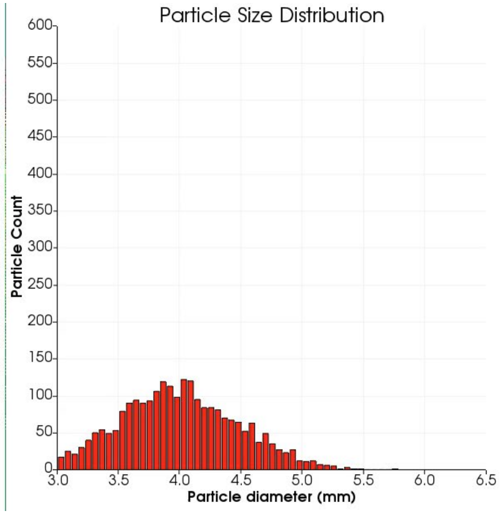
Polydispersity (DEM)

To address the polydispersity nature of feedstock

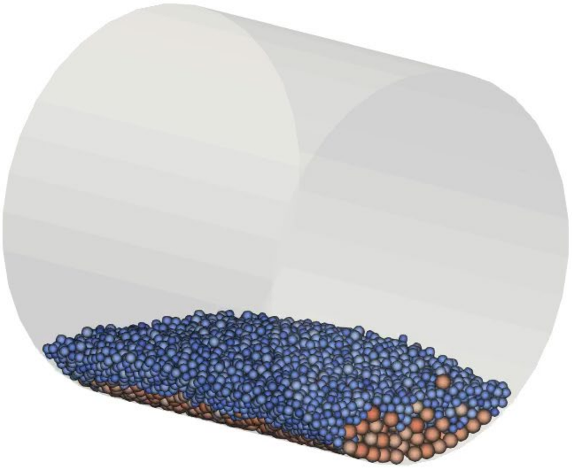


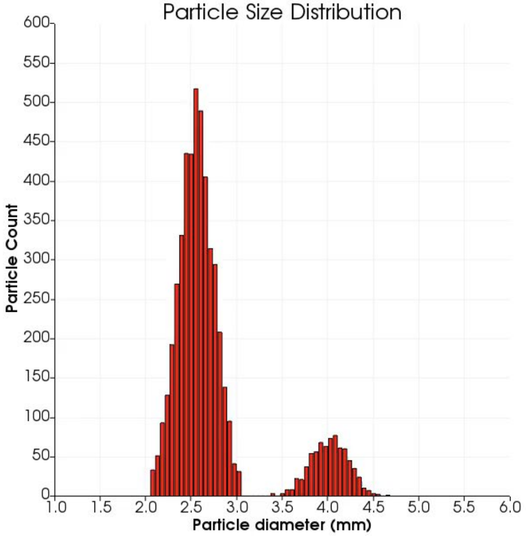
- DEM Particle size distribution
  - Normal
  - Log-normal
  - Custom (user-defined)





Initial + Boundary Conditions





Particle coating

Non-spherical Particles (SuperDEM)

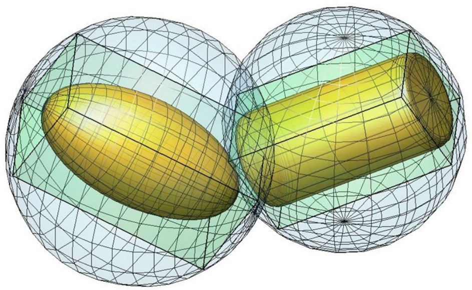
- Superquadrics are a family of geometric shapes defined as

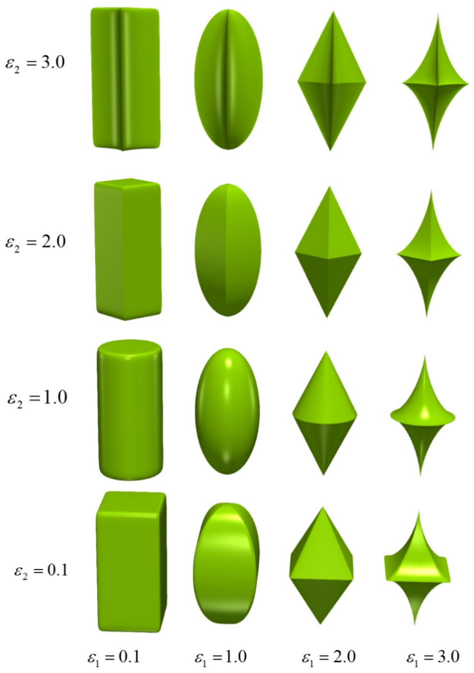
$$\left[\left(\frac{x}{a_1}\right)^{\frac{2}{\varepsilon_2}} + \left(\frac{y}{a_2}\right)^{\frac{2}{\varepsilon_2}}\right]^{\frac{\varepsilon_2}{\varepsilon_1}} + \left(\frac{z}{a_3}\right)^{\frac{2}{\varepsilon_1}} = 1$$

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

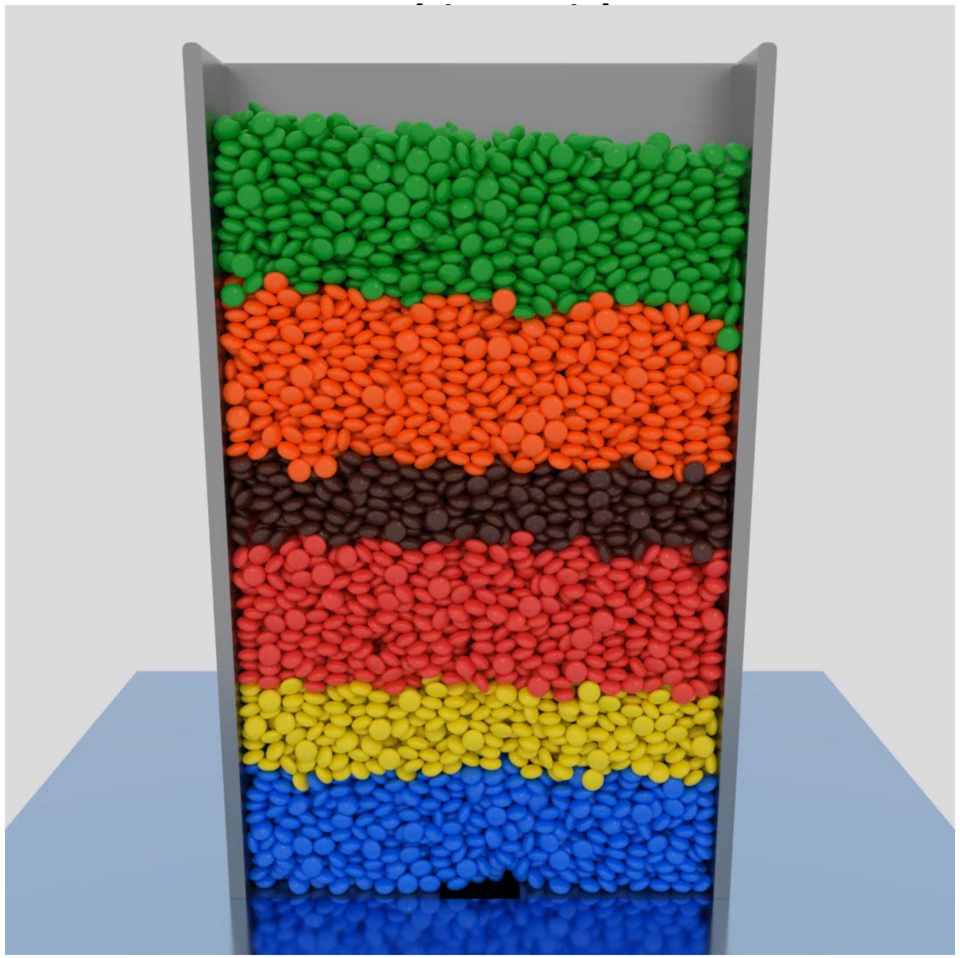
$[a_1, a_2, a_3, \varepsilon_1, \varepsilon_2]^T$

Semi-axis roundness parameters

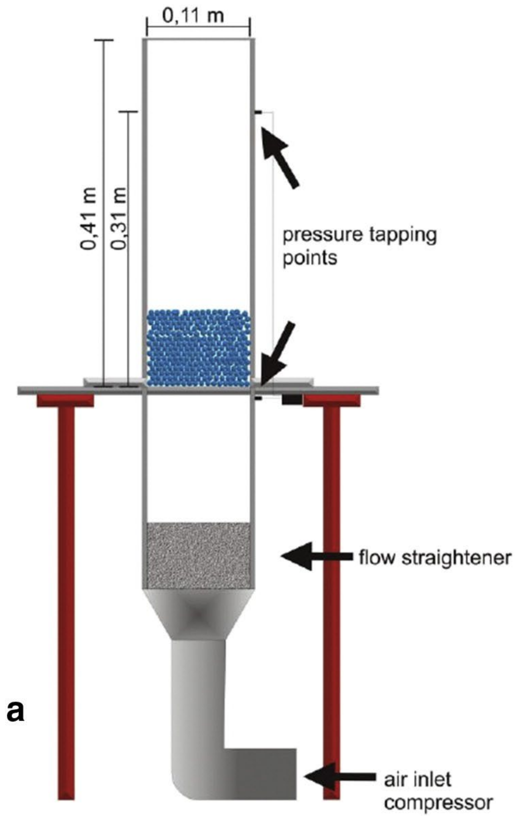


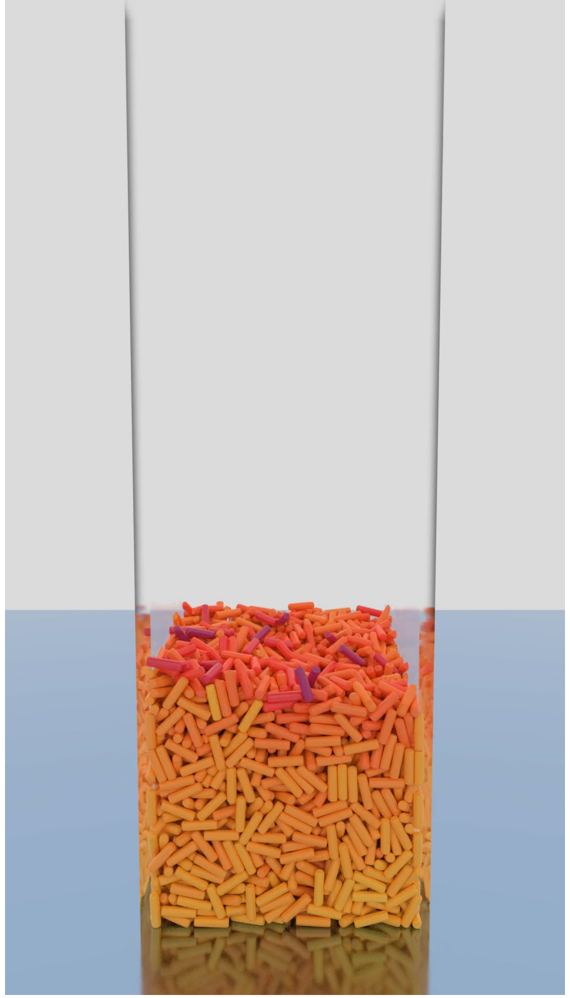


a1=2
a2=2
a3=4



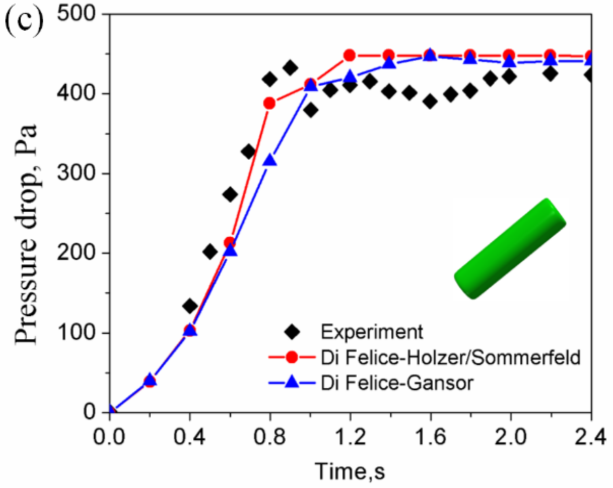
Validation Experiment





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 $\bar{\varepsilon}$ 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**			
d_e–class [mm]	5	7			
Size [mm]	2.0 3.0 11.0	2.2 9.0 9.8			
ϕ [–]	0.64	0.63			
ρ_p [kg/m³]	728.1	672.8			
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	117 0.48	121 0.46			



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.

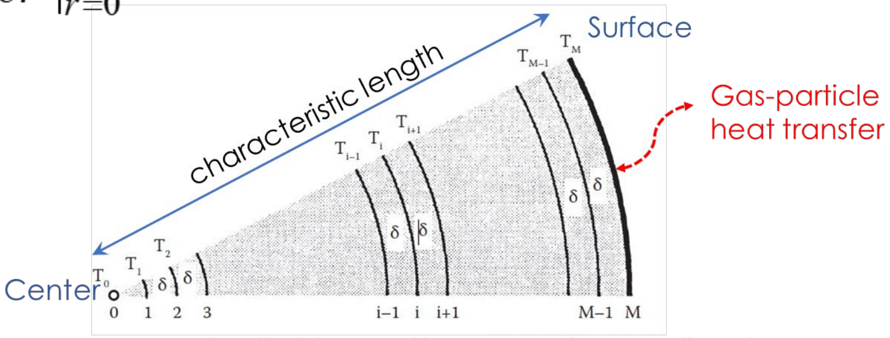
Single-particle Pyrolysis

$$\frac{\partial}{\partial t}\left(\rho_s c_{p,s} T_s\right) = \frac{1}{r^b}\frac{\partial}{\partial r}\left(k_{s,eff} r^b \frac{\partial T_s}{\partial r}\right) + \sum\left(-\Delta H_i R_i\right)$$

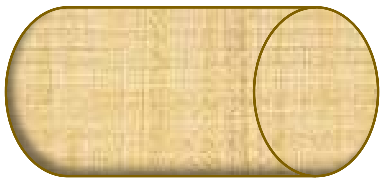
Boundary conditions:

$$k_{s,eff}\left.\frac{\partial T_s}{\partial r}\right|_{r=r_0} = f_c h_{conv}(T_f - T_s) + \sum Q_{i,j,cond} / A_p + Q_{i,wall} / A_p$$

$$\left.\frac{\partial T_s}{\partial r}\right|_{r=0} = 0$$

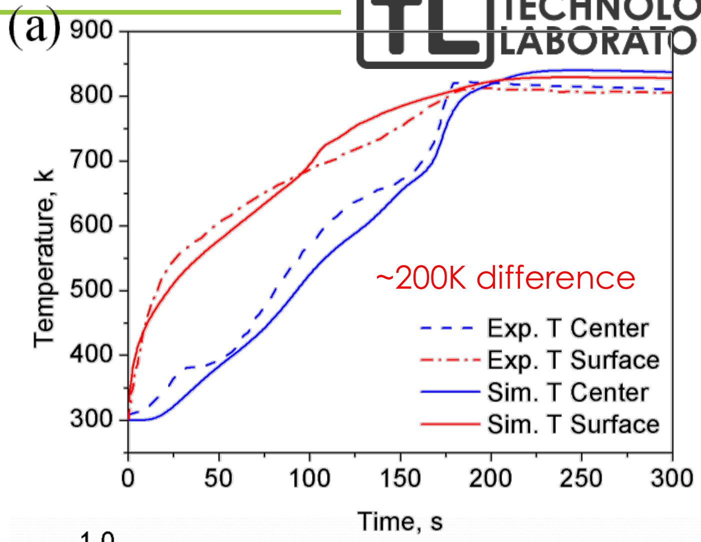


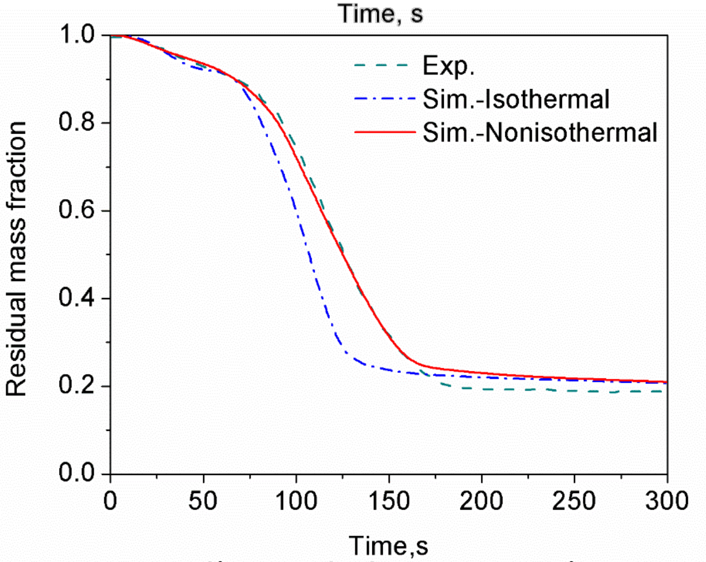
Discretize into several layers (T, species, properties, rates, etc)



biomass spruce pellet

44% CELL, 26% HCE, 17.5% LIG-C, 9.5% LIG-H, 3% LIG-O



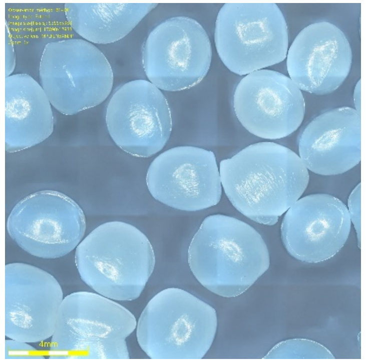


Isothermal model overpredicted the reaction rate!

Experiment reference: Andrés Anca-Couce, Peter Sommersacher, Robert Scharler, Journal of Analytical and Applied Pyrolysis, 127, 2017, 411-425

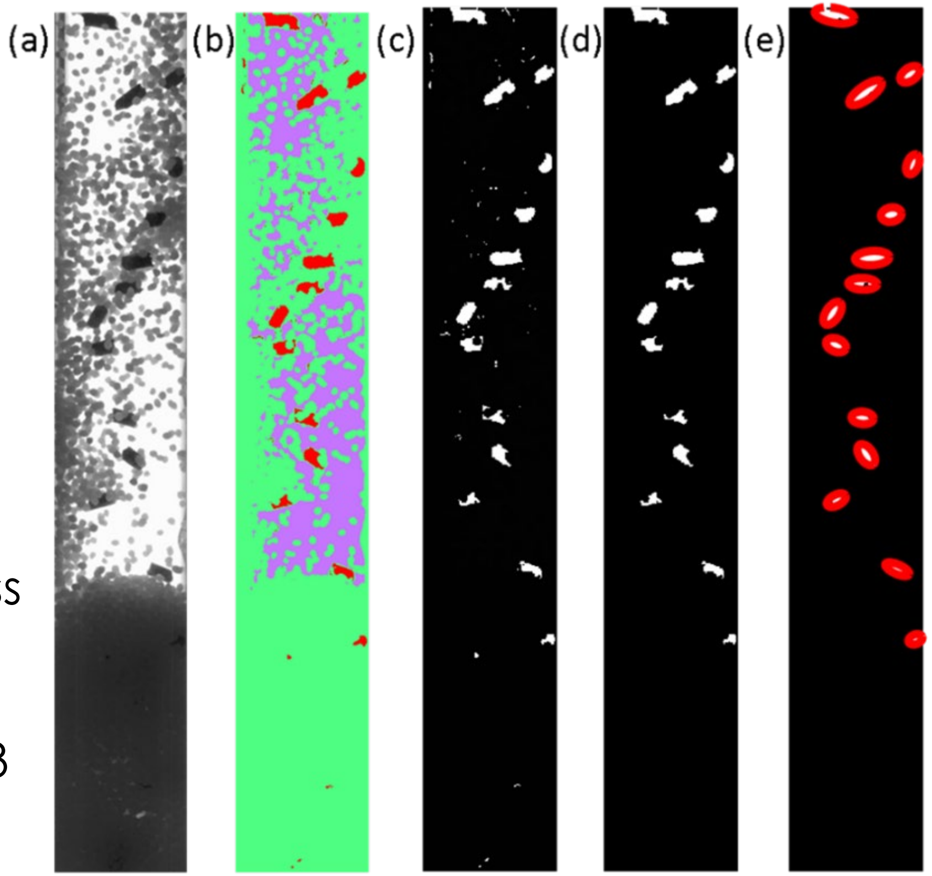
Hydrogen Production by Co-firing of Biomass & Plastics

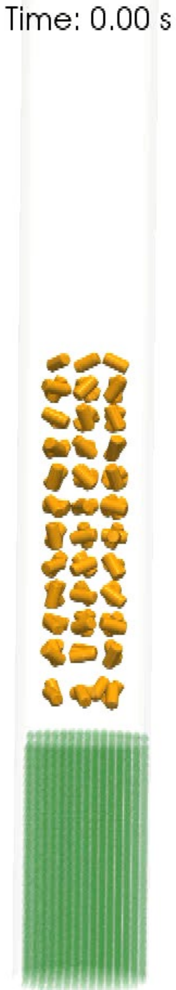
Challenge to address: Fluidization and mixing of feedstock



LDPE particles
Dp = 3.755 mm
ρ = 930 kg/m3
N=5788

Woody biomass
Dp = 6mm
Length=12mm
ρ = 1158 kg/m3
N=100

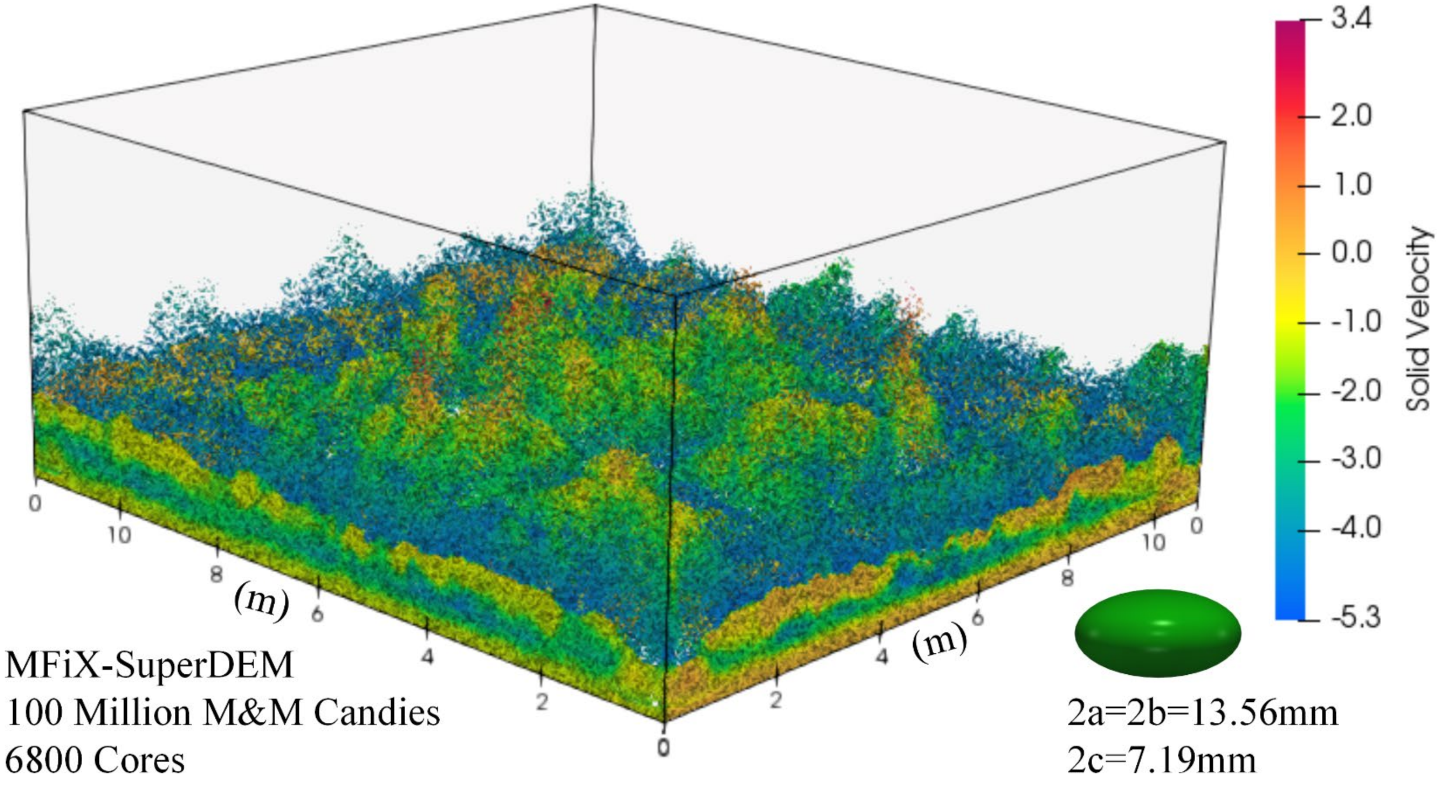


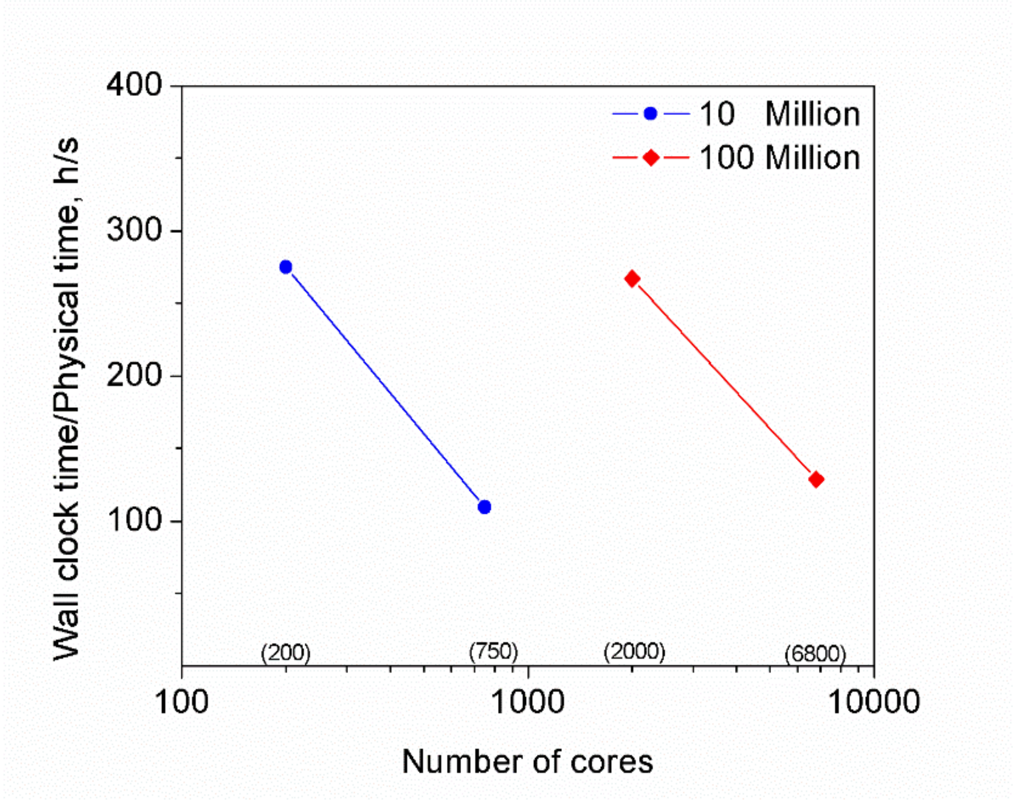


Bed diameter: 2.5inch
Initial bed height: 3.0 inch
Ug=3.0Umf
Umf=74.42cm/s

Extension of SuperDEM for polydisperse particulate flows and validation with experimental data obtained in fluidization of HDPE and cylindrical biomass particles.

Massively Parallel SuperDEM Simulation





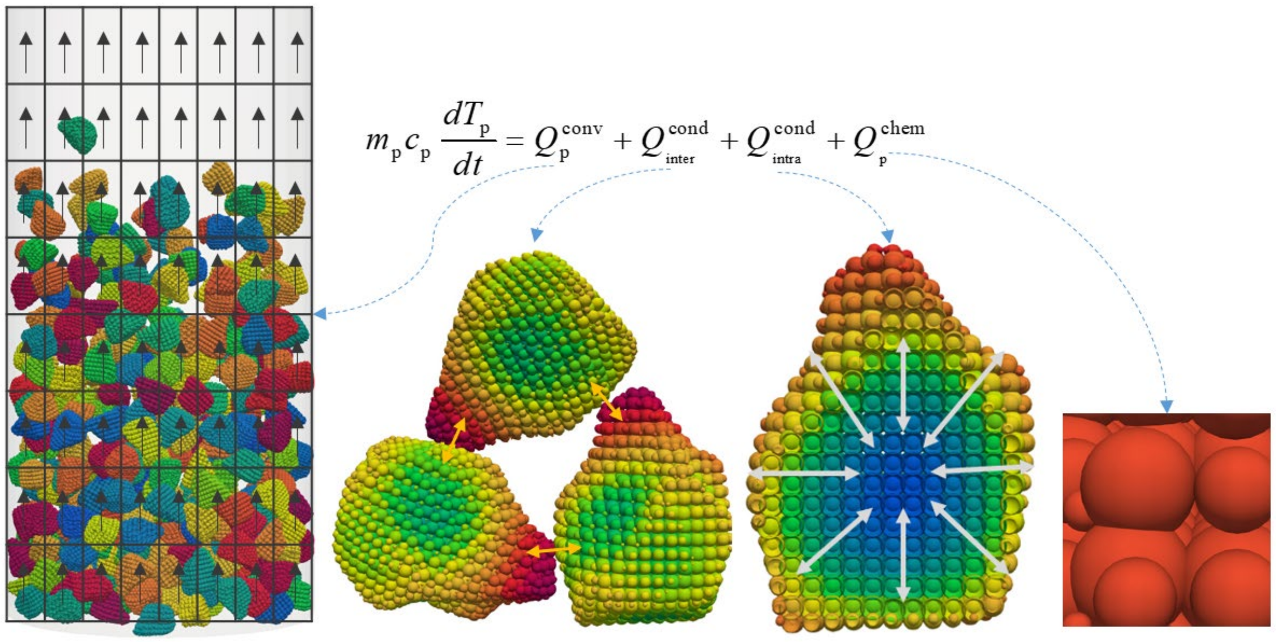
- The solver was parallelized using MPI.
- Simulation on NETL supercomputer Joule 2 (80K cores) , World Top 60, 2020
- Non-spherical particles fluidization simulation, 100 million (6800 cores)

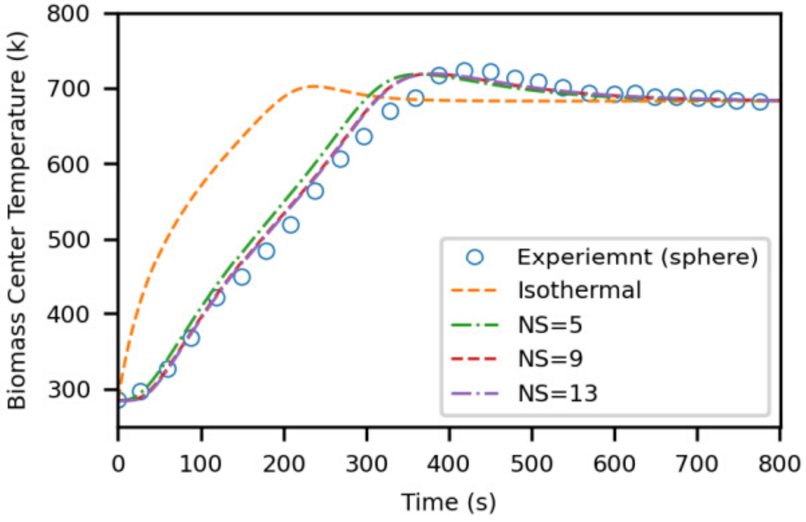
Glued-Sphere Approach

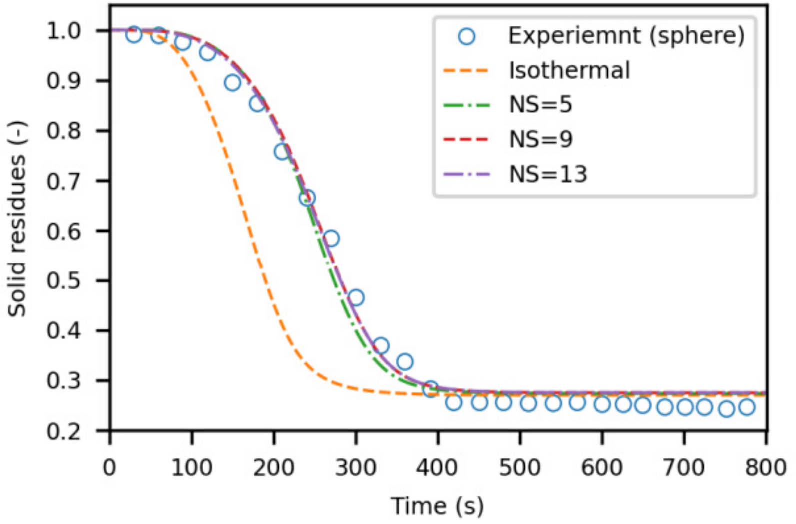
To account for Irregular Shape of Particles

- Composite spheres
- Intra-particle temperature distribution

$$m_p c_p \frac{dT_p}{dt} = Q_p^{conv} + Q_{inter}^{cond} + Q_{intra}^{cond} + Q_p^{chem}$$

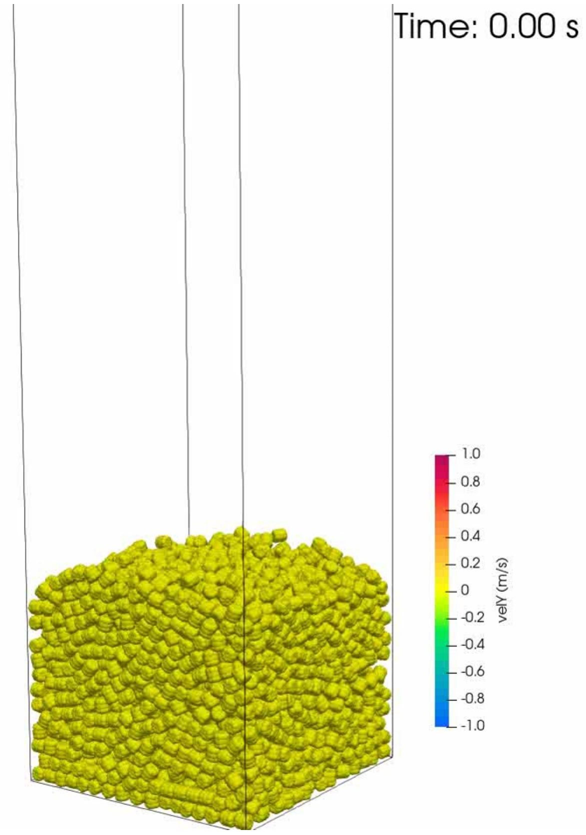


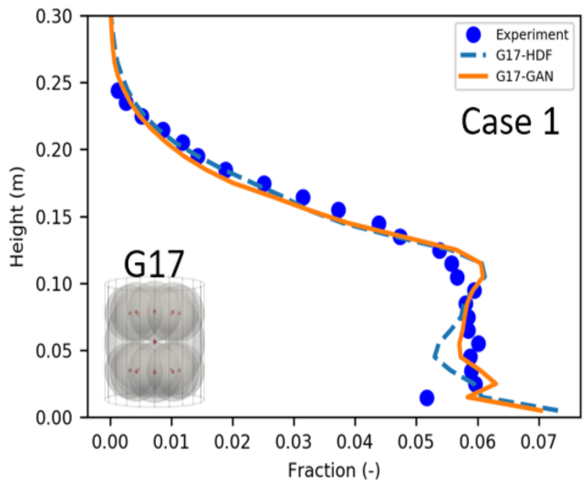




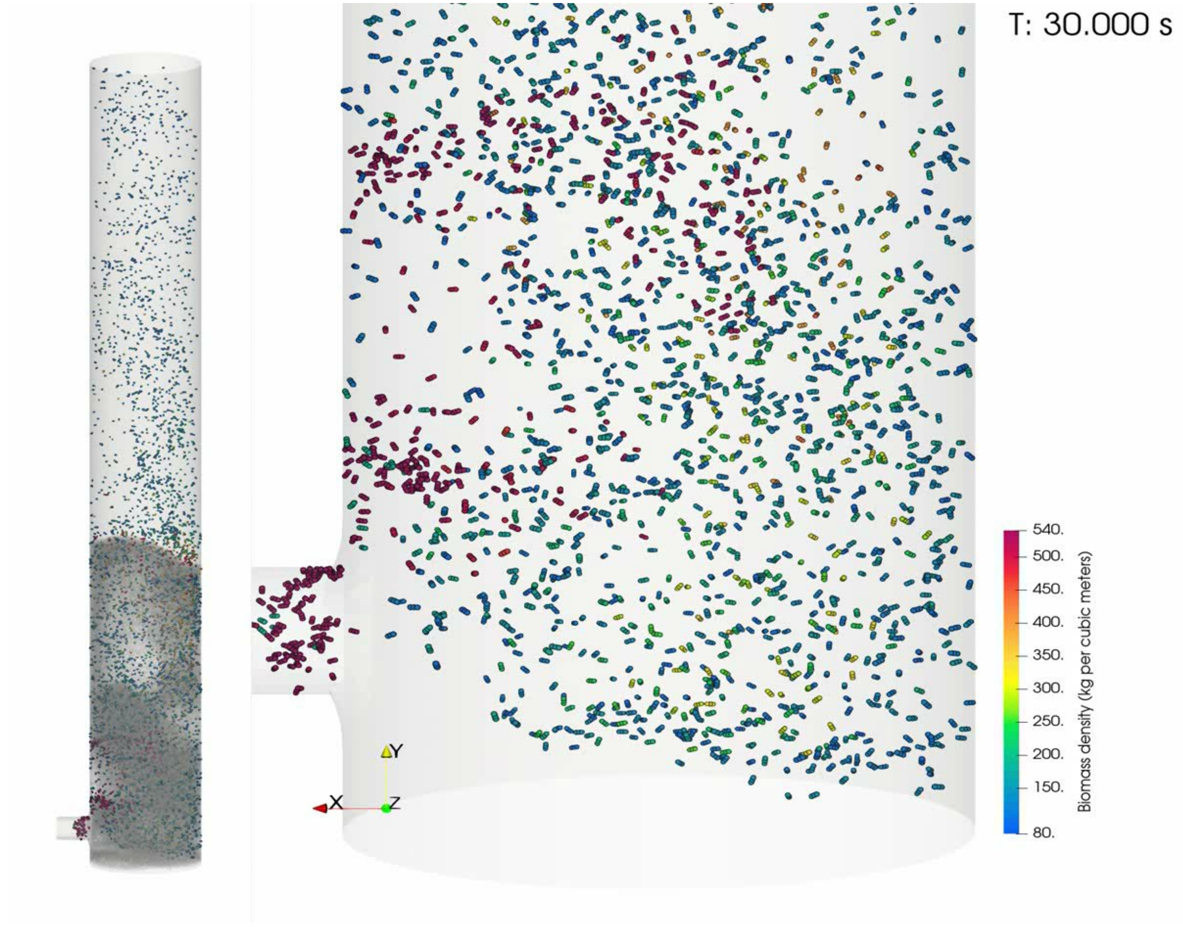
Glued-Sphere Approach

To account for Irregular Shape of Particles



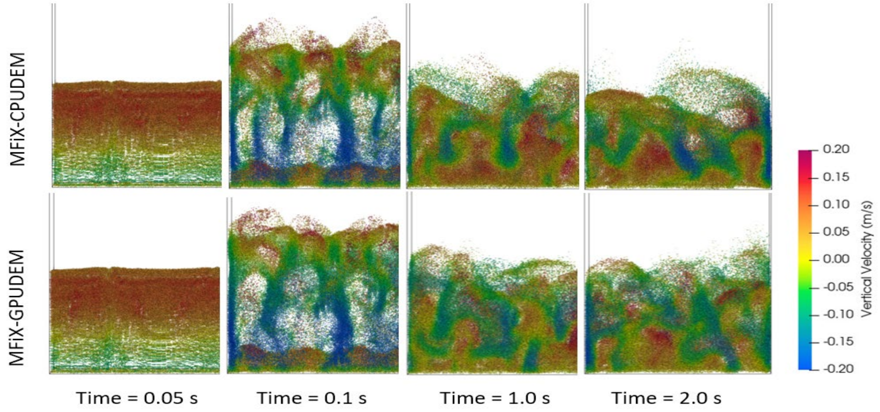


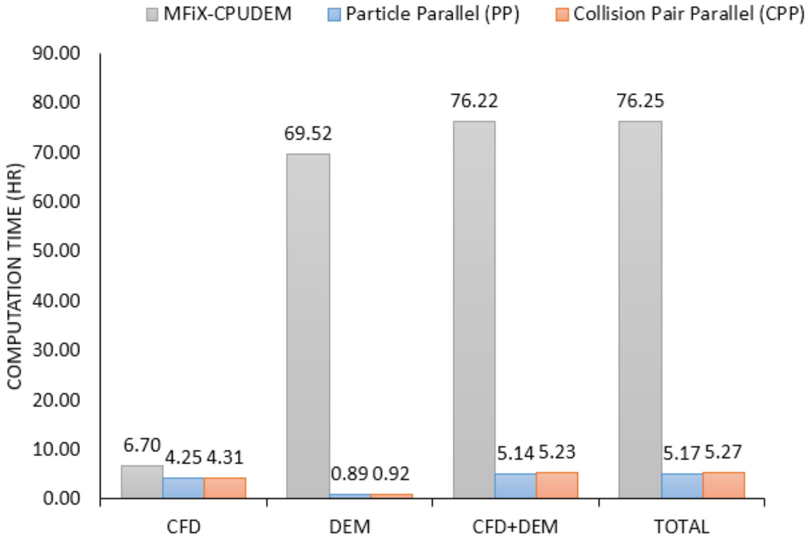
Time averaged solids vertical distribution across the bed compare well with experiment.



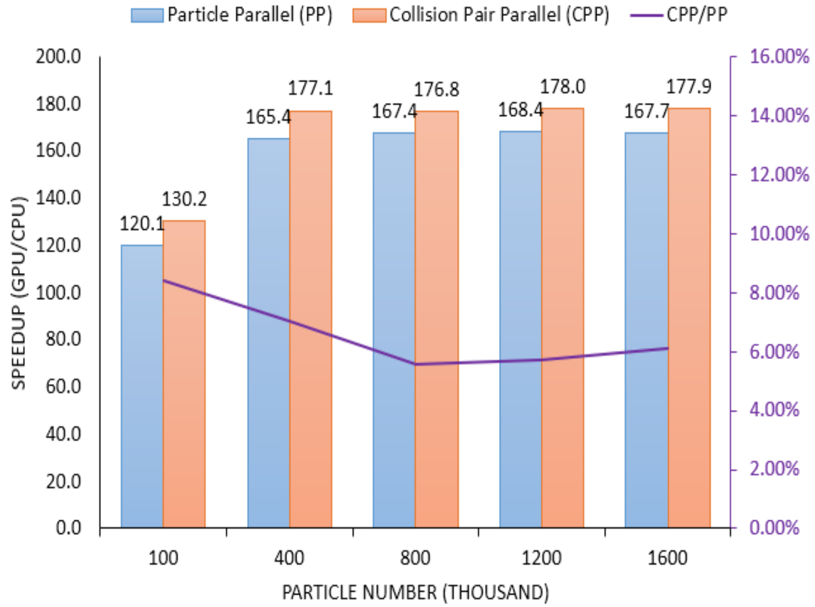
Hundredfold Speedup of MFiX-DEM using GPU

- DEM solver was ported to GPU (prototype)
- 170-fold speedup with double precision, 243-fold with single precision
- Re-use CFD, interphase coupling, and chemical reaction modules in MFiX

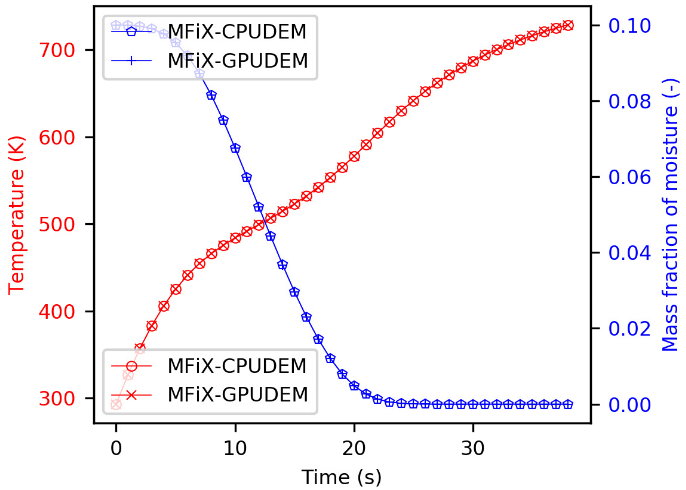




Fluidized bed Speedup



Particle packing Speedup



Heat transfer & chemical reactions (biomass drying)

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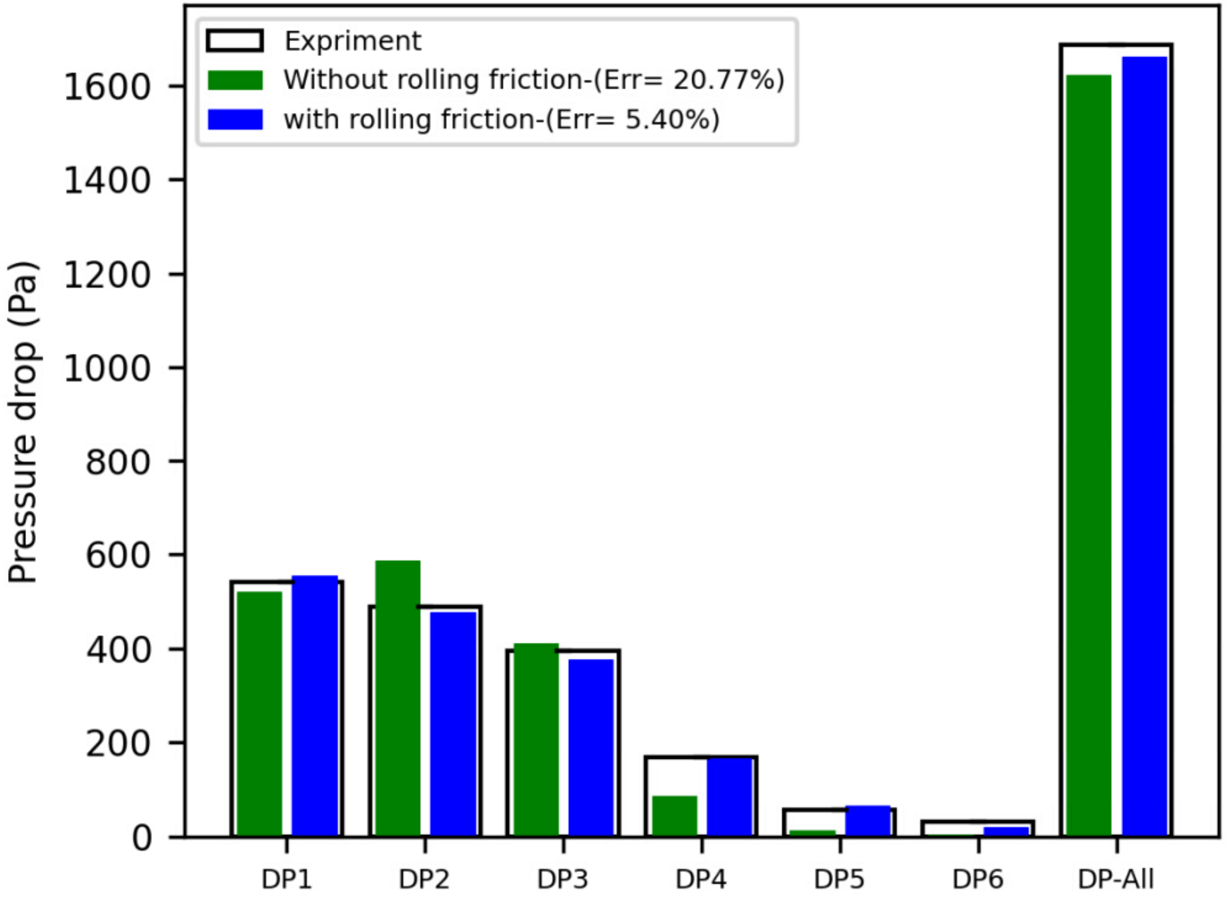
DEM Rolling Friction

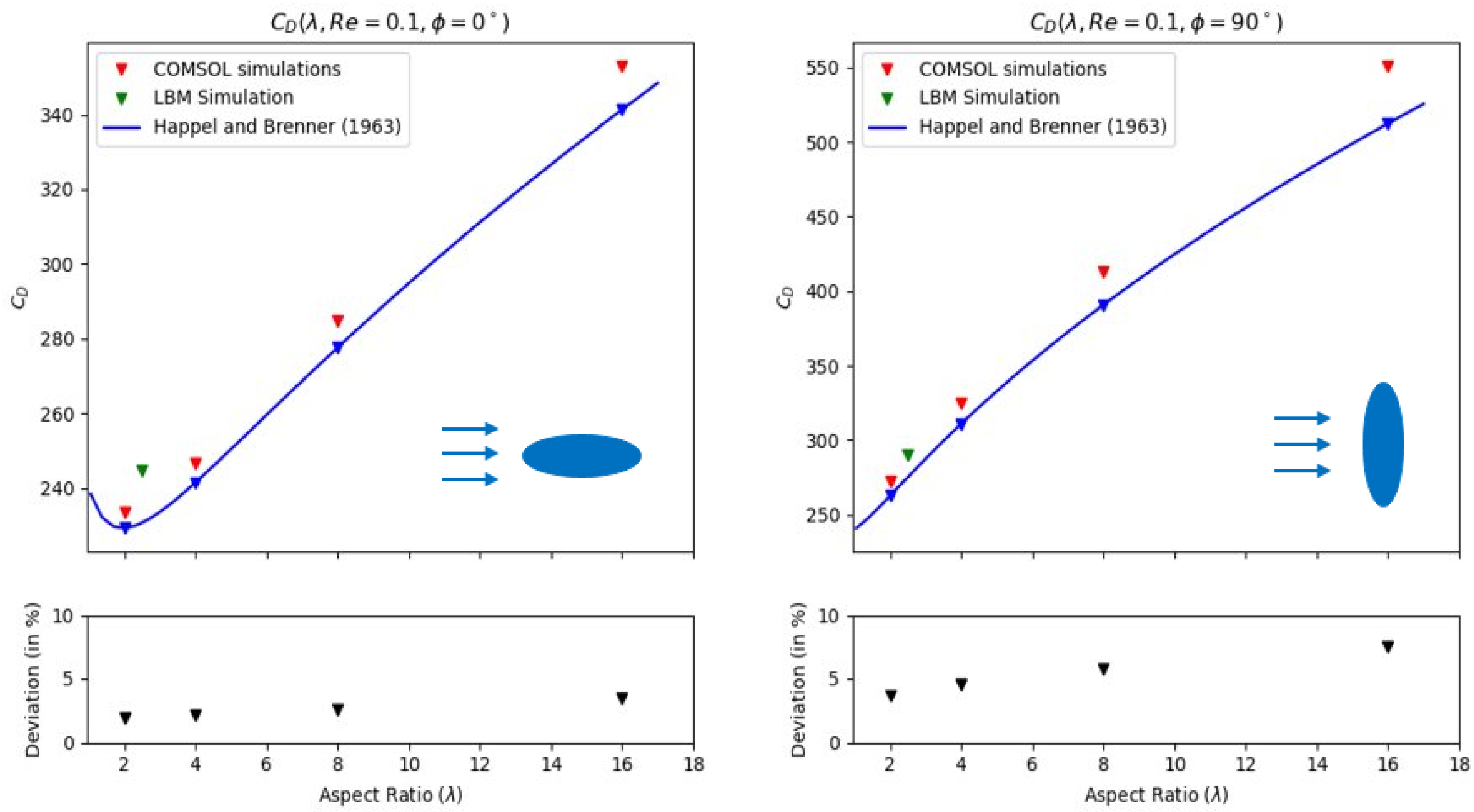
- Implementation of rolling friction in DEM
- Beta release in 21.2
- Ongoing V&V



Pressure drops at different locations of fluidized bed with sand and biomass mixtures measured in experiment and simulations

Drag Model for Non-Spherical Particles

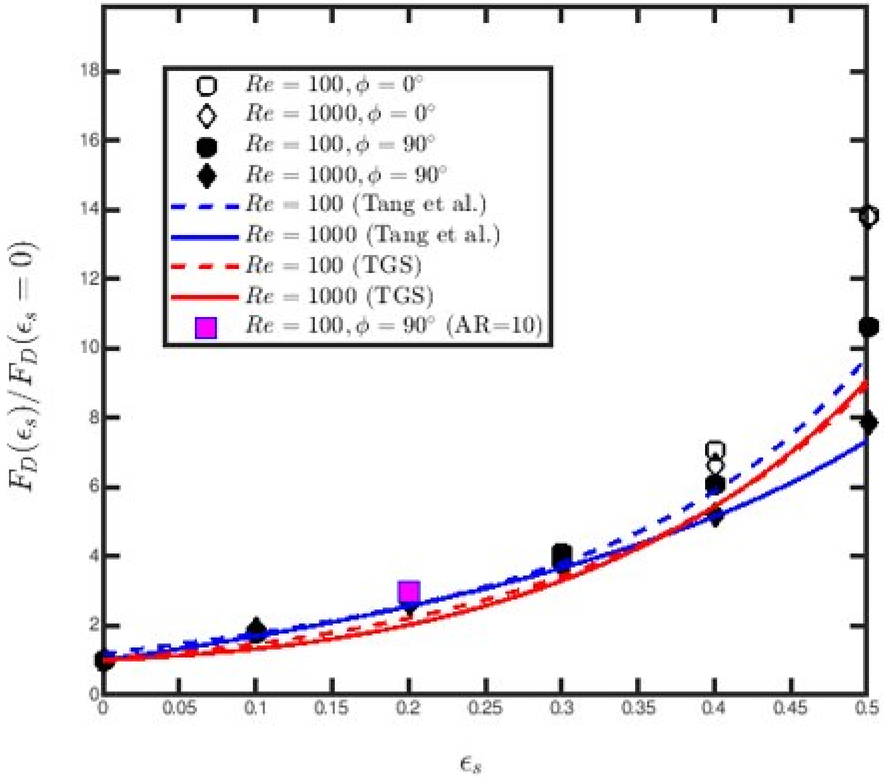
- Drag, lift, and torque correlations for a family of prolate spheroids from Stokes flow regime to high Reynolds number (Re=2000).

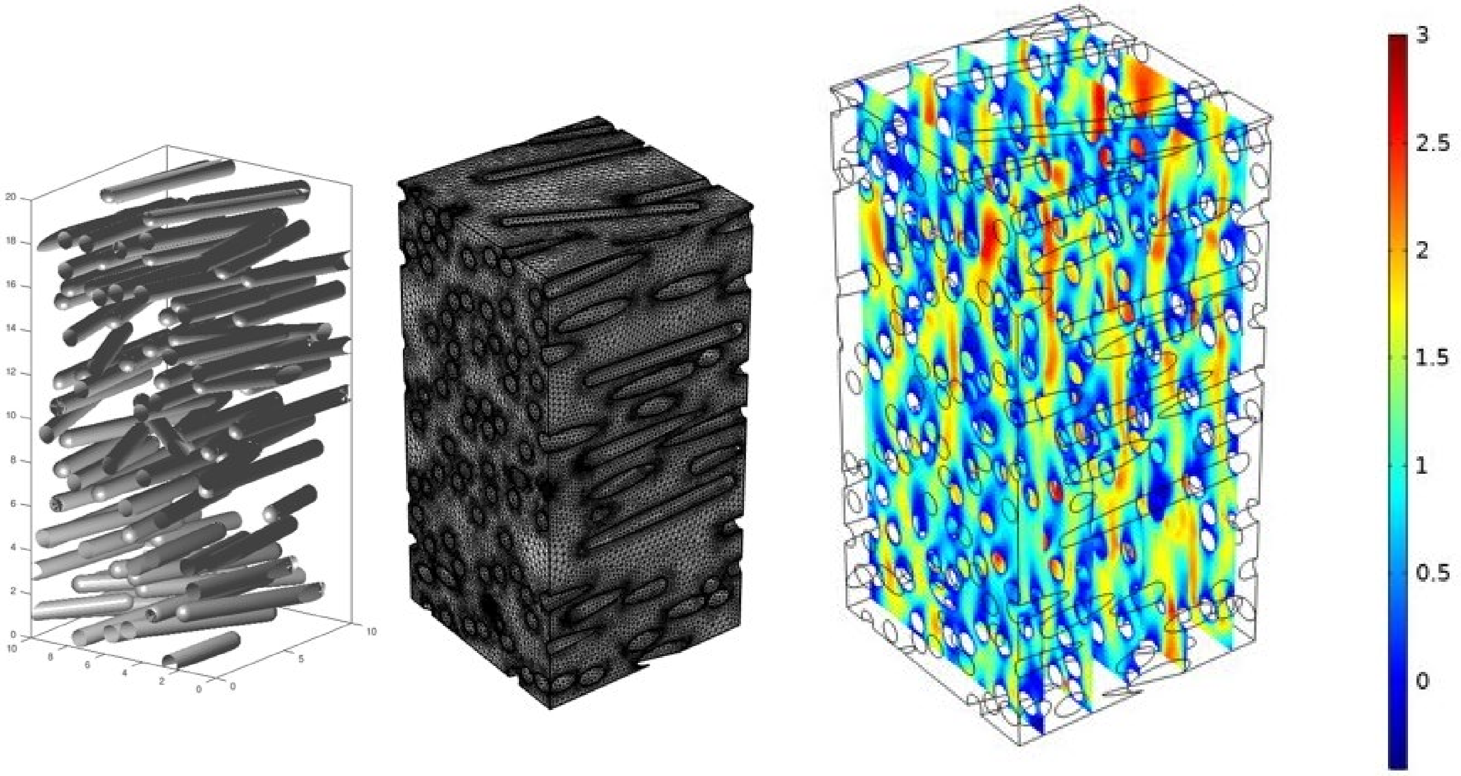


The variation of drag coefficient for Stokes flow (Re=0.1) for different aspect ratios at angle of attack 0 and 90 degrees respectively.

Drag Model for Non-Spherical Particle Assemblies

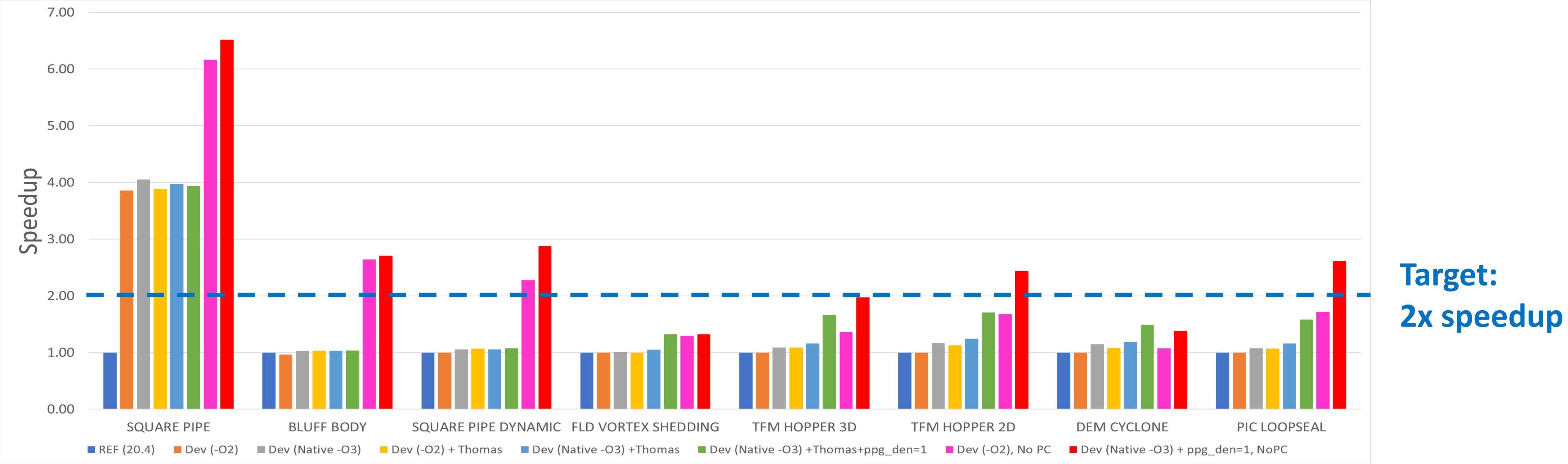
- Drag of a nonspherical, multiparticle system





Fluid Solver Acceleration

- New convergence criteria for Steady State: ~ 4x speedup
- "march=native –O3": 3 to 14% faster
- Optimized Thomas algorithm: 3 to 11% faster
- Lowering ppg_den from 10 to 1: up to 25% faster (helps when ppg is dominant residual)
- Turning off the PC: ~ 2x speedup (fluid solver)
    - May fail to converge if DT=cst with bad initial conditions (need to set adaptive DT)
- Best combination: No PC, "march=native –O3" flag, ppg_den=1



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

Cases selected to cover a broad range of flow conditions

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

Summary of model parameters used:

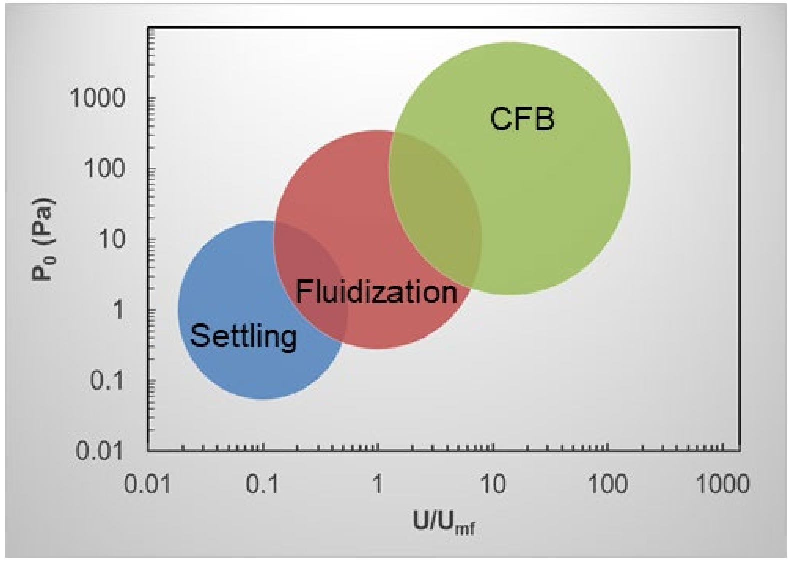
	t1 Pressure linear scale factor	t2 Volume fraction exponential scale factor	t3 Statistical weight	t4 Volume fraction at maximum packing	t5 Solid slip velocity factor
C1: Particle Settling	[1,20]	[2,5]	[3,20]	[0.35,0.5]	[0.5,1.0]
C2: Fluidization	[1,100]	[2,5]	[10,100]	[0.4,0.5]	[0.85,0.98]
C3: Circulating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

*Parameters selected based on prior sensitivity study

Parcel momentum equation

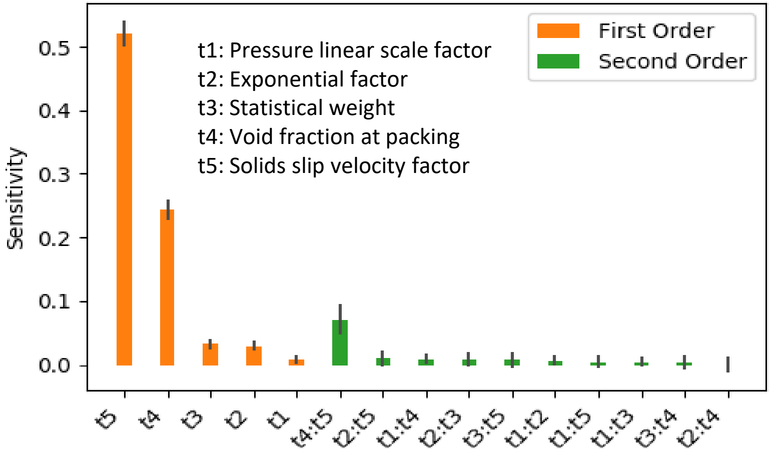
$$\frac{d\vec{V_p}}{dt} = \beta(\vec{U_g} - \vec{V_p}) - \frac{1}{\rho_p}\nabla p - \frac{1}{\varepsilon_p \rho_p}\nabla \tau_p + \vec{g}$$

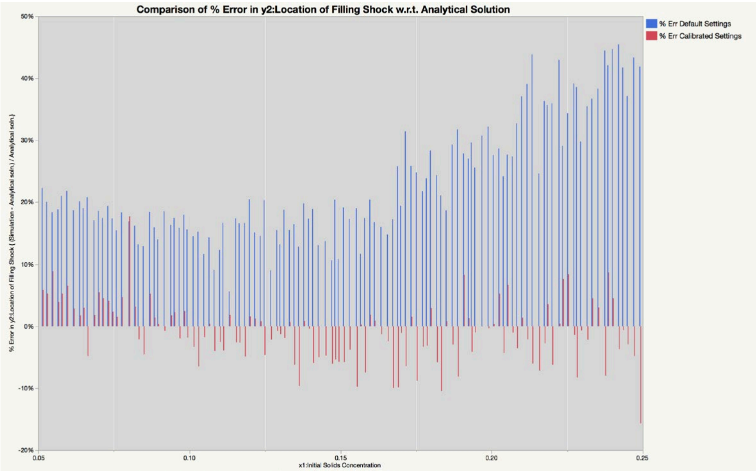
$$\tau_p = \frac{P_0 \varepsilon_p^{\beta}}{\max\left(\varepsilon_{cp} - \varepsilon_p, \delta(1-\varepsilon_p)\right)}$$



C1: Particle settling

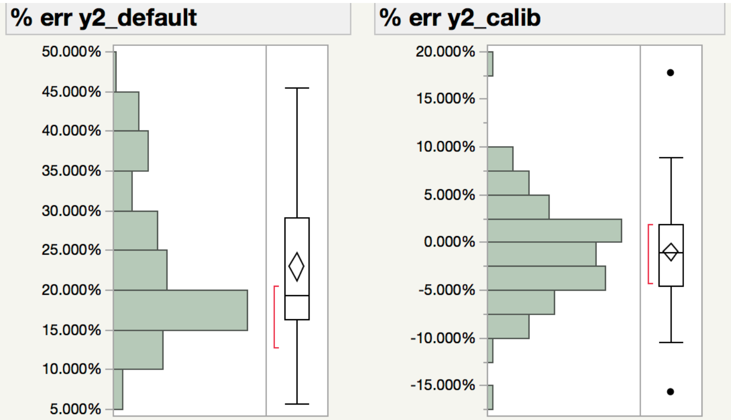
Sensitivity analysis and Deterministic calibration





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**



Quantiles (% err y2_default)

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

Quantiles (% err y2_calib)

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%

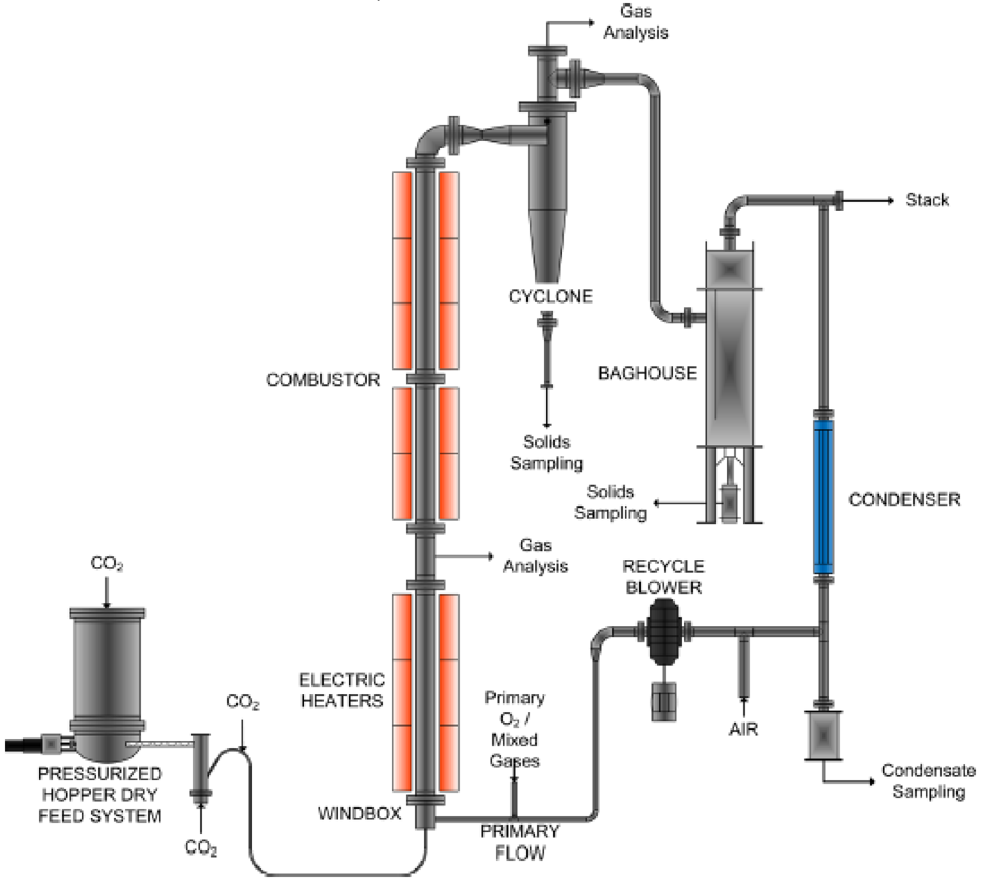
Summary Statistics

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

23%
vs
-1%

50kWth CFB Combustor Experiment

Bench-scale experimental facility designed, built, and operated at CanmetENERGY, Natural Resources Canada[1] (NRCan)



Operating Conditions	
Inert material	Olivine sand, 273 µm, 3063 kg/m³
Biomass	Torrefied hardwood, 375 µm, 520 kg/m³
Initial mass of inert	9.0 kg
$\dot{m}$ **of fluidizing gas (air)**	15.6 kg/h
$\dot{m}$ **of fuel feed gas (air)**	3.06 kg/h
$\dot{m}$ **of biomass**	2.65 kg/h
Sidewall temperature	850°C
Fluidizing gas inlet temperature	120°C
Fuel feed gas inlet temperature	20°C

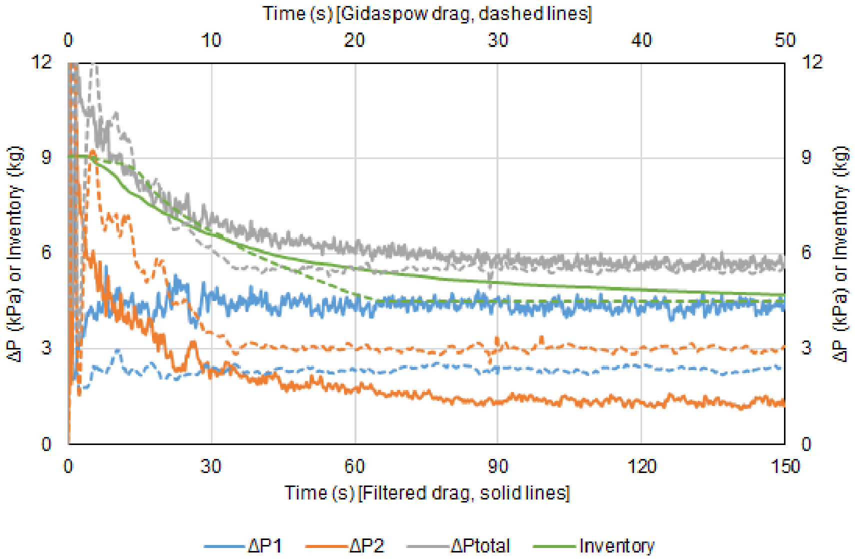
[1] Hughes, R.W. et al., 2015. Oxy-fluidized bed combustion using under bed fines fuel injection. In 22nd International Conference on Fluidized Bed Conversion. Turku, Finland, 2015.

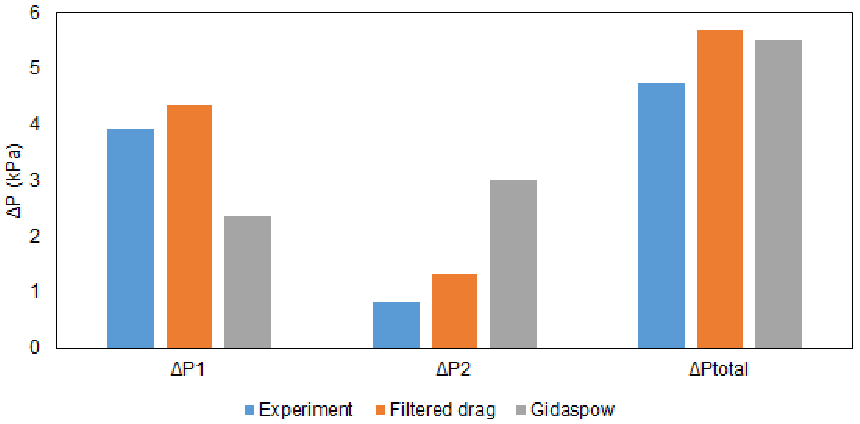
Hydrodynamics Benchmarking – Effect of Drag Model

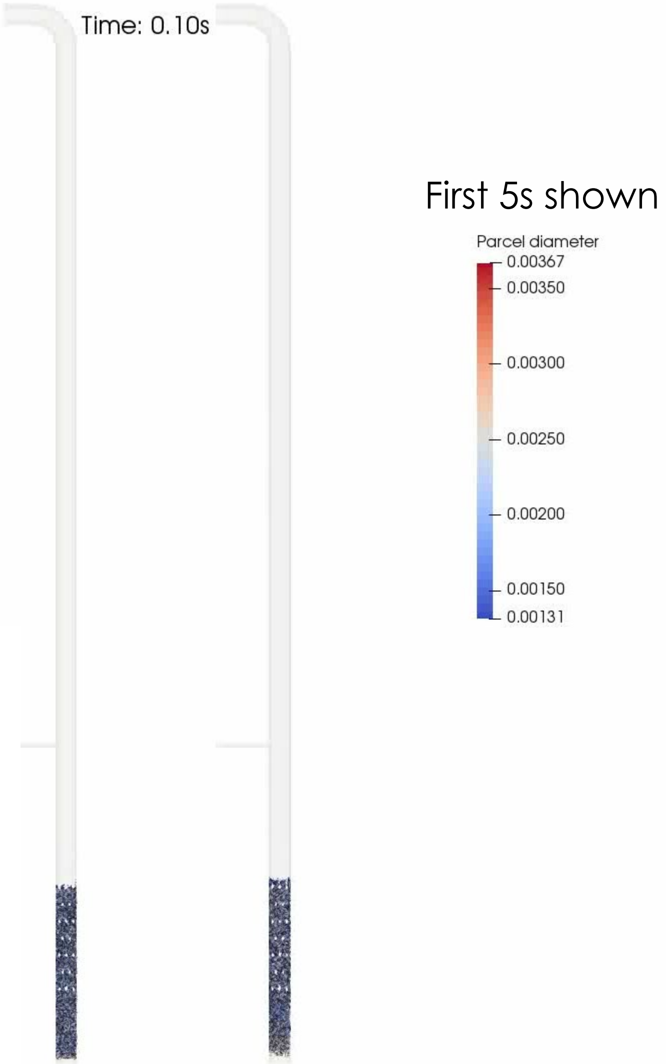
Fluidization is impeded by applying the filtered drag model, so more particles are retained in the lower riser

Circulation rate is reduced, reflected in the average mass of recirculated particles in the side inlet

Pressure drop distribution and overall pressure drop using the filtered drag model show better agreement with the experimental results ($P_p = 10, \gamma = 3$)

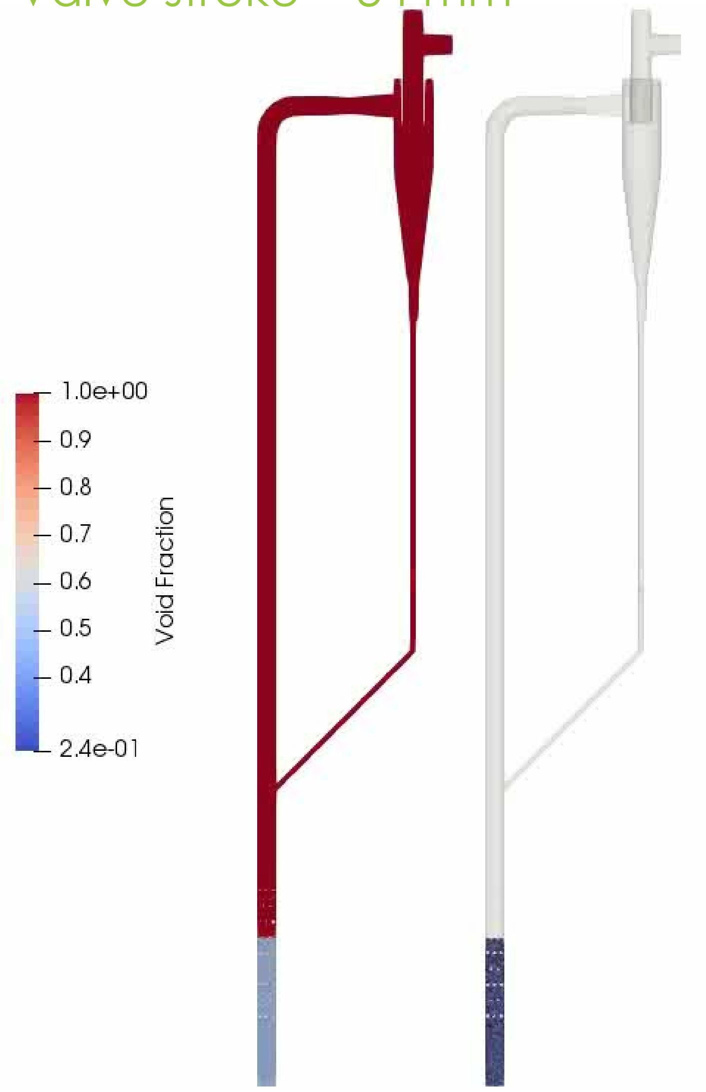


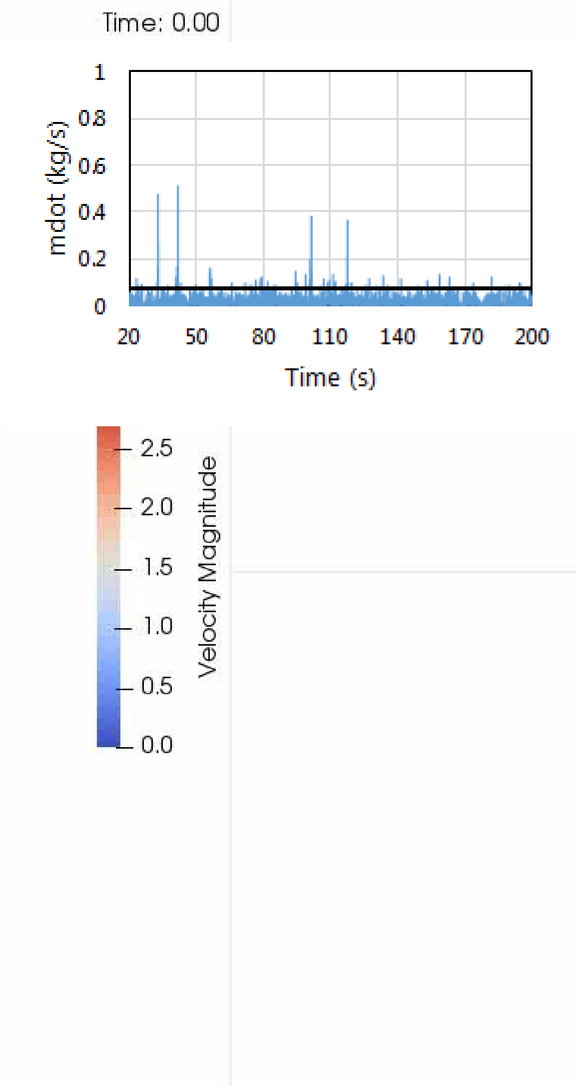


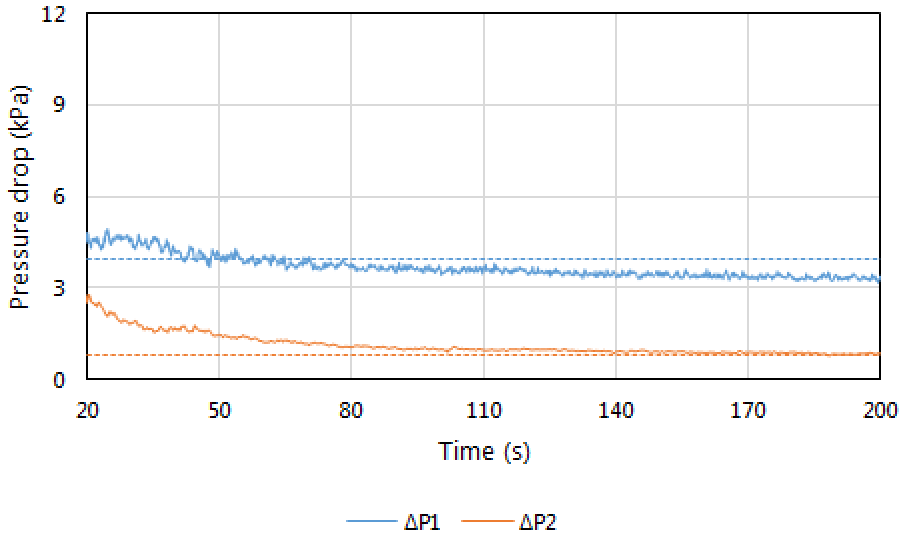


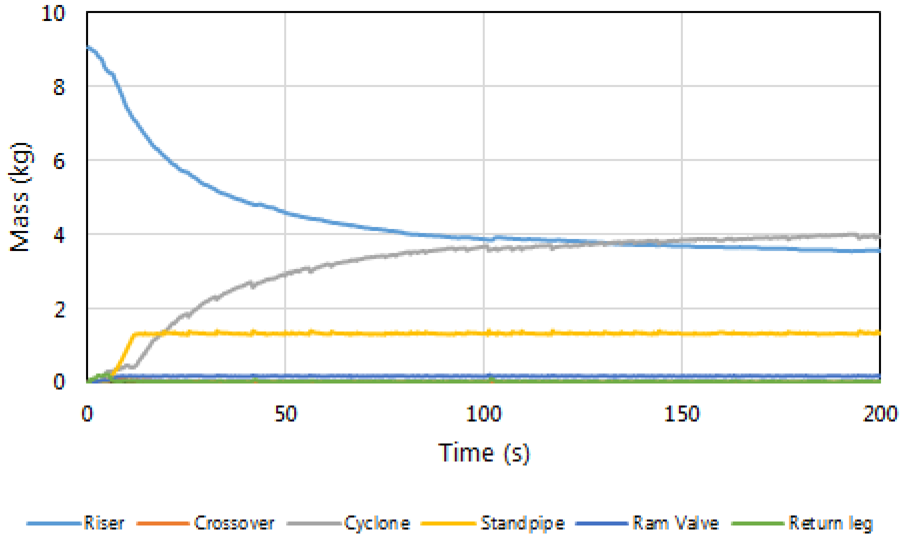
Full Loop Simulation with Valve Partially Closed

Valve stroke = 34 mm

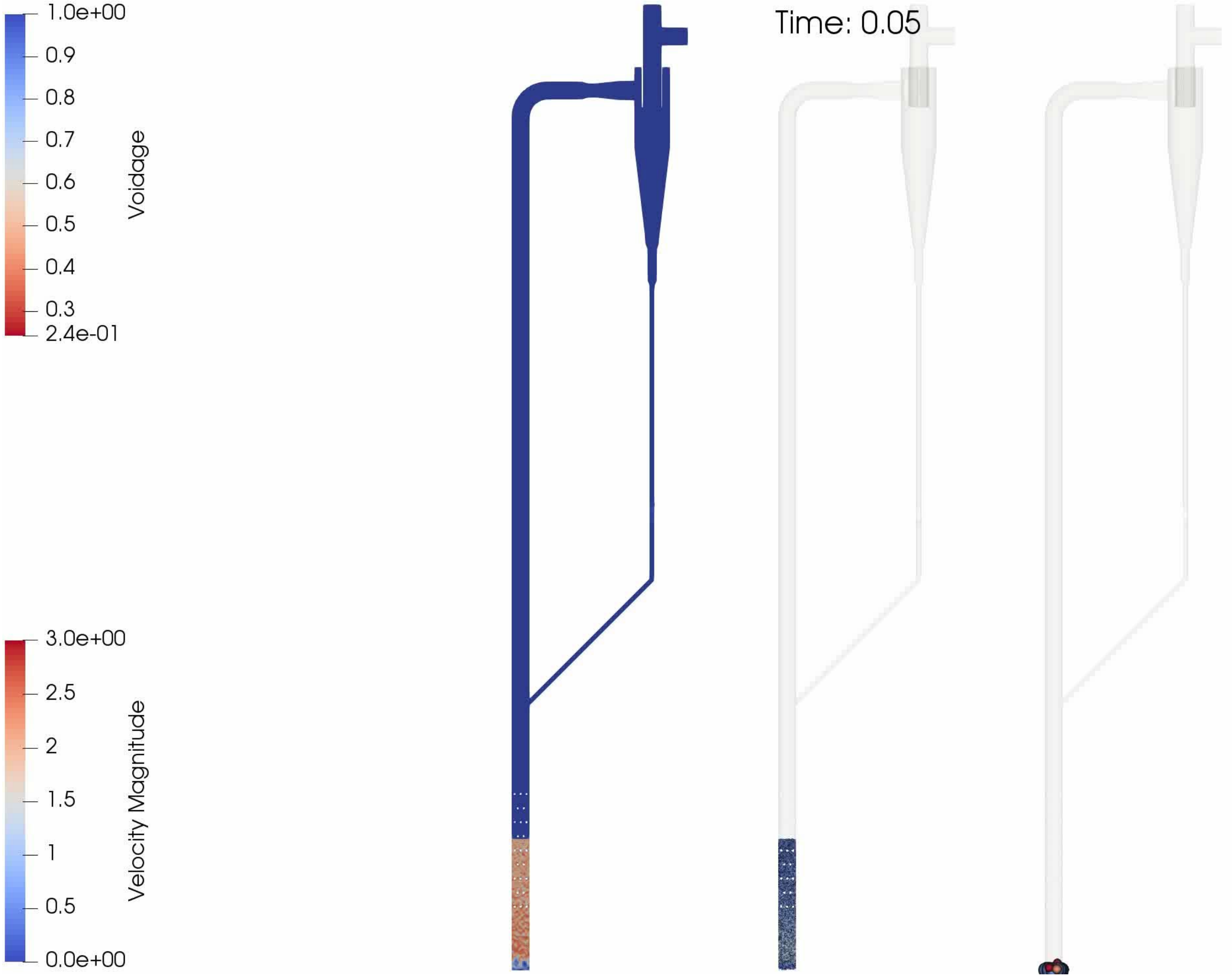




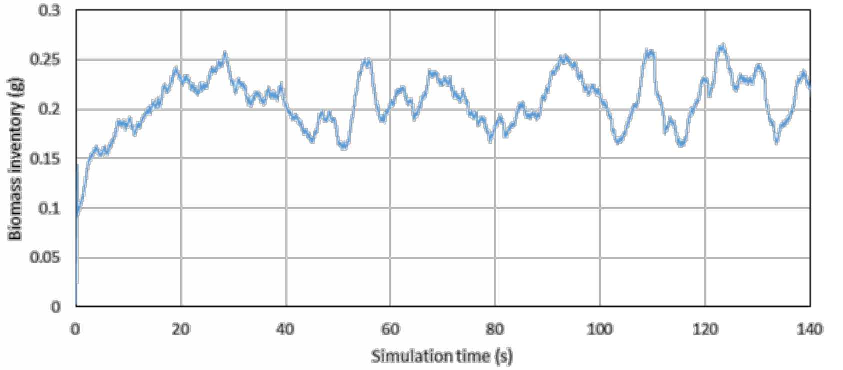




Simplified Chemical Reaction Scheme Results

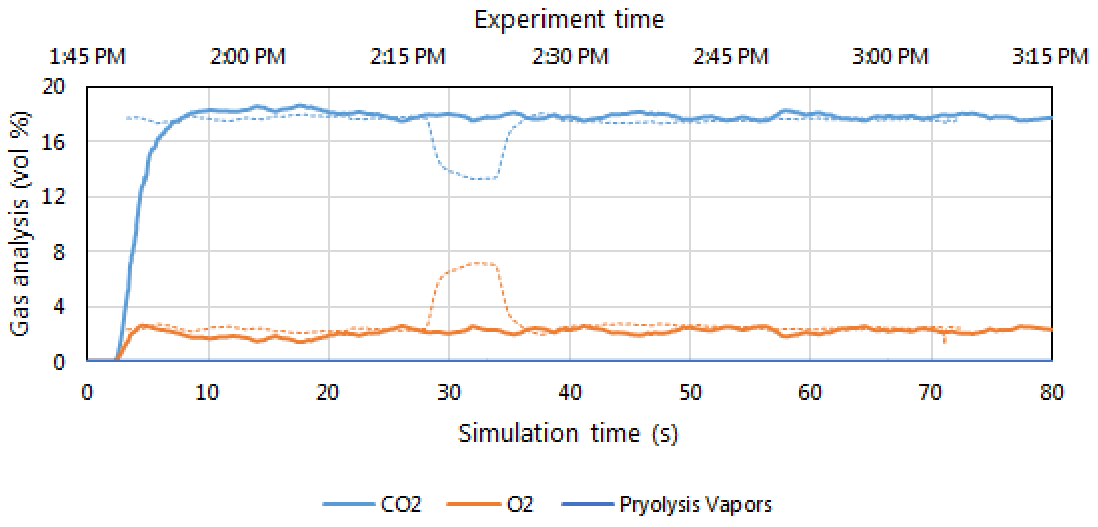


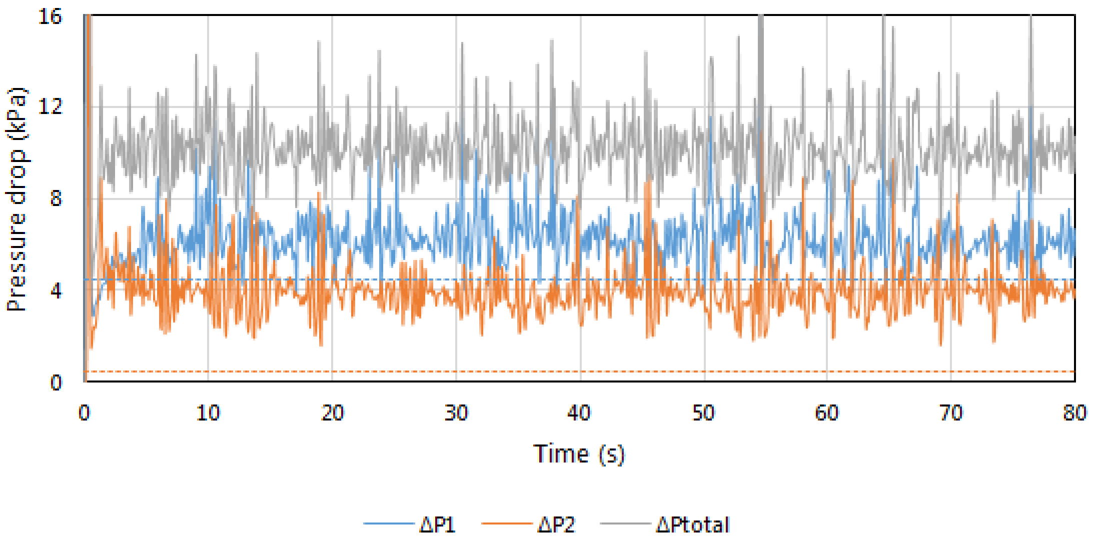
Total biomass inventory in the riser is negligible compared to sand inventory



Simplified Chemical Reaction Scheme Results

The outlet compositions of CO_2 and O_2 show excellent match with experimental results (dashed lines)





Particle fluidization is reduced compared to cold flow simulations, leading to reduced circulation and higher particle holdup in riser, and hence higher pressure drops

- Air flow of 15.6 kg/h corresponds to an inlet air velocity of 0.67 m/s, lower than the 3.09 m/s used in the cold flow simulations
- Further investigation of hot flow hydrodynamics is required

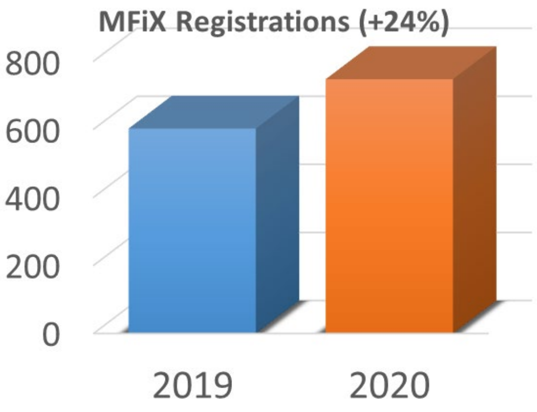
50kWth CFB Summary

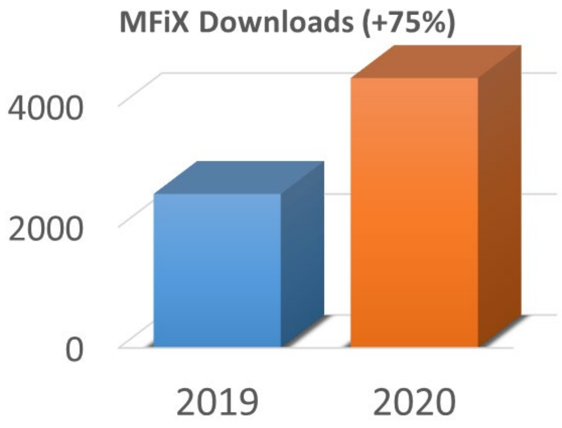
- Hydrodynamics of the 50kW$_{th}$ riser at CanmetENERGY, Natural Resources Canada are validated against experiment via inert simulations using olivine sand
- Filter size dependent corrections to the homogeneous drag laws are incorporated to take into account the mesoscale effects such as bubbles and clusters to ensure accuracy
- In the full loop simulation, once the lower bed pressure drop matches the experiment, the upper riser pressure drop can be tuned independently of the lower bed by modeling pseudo-packing in the return leg by adjusting the ram valve stroke
- The validated cold flow model is extended to model reacting flow with torrefied hardwood as the feedstock and validate a simplified global one-step mechanism for combustion
- Species concentrations at the riser outlet are compared against the experiment and show excellent agreement
- The simulations demonstrate the ability of MFiX-PIC to accurately capture the physics and chemistry of a circulating fluidized bed combustor at bench scales, which can be further extended to pilot- and industrial-scale systems

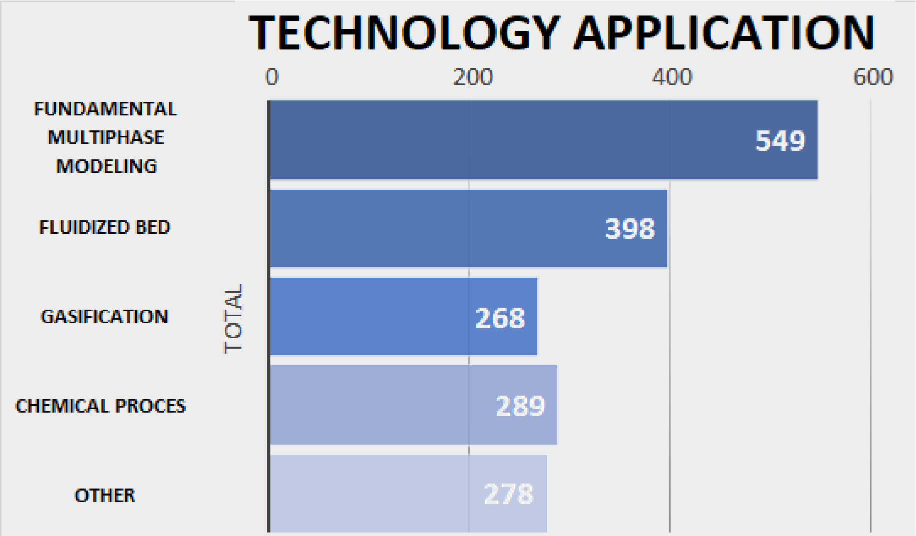
Outreach: All-time MFiX Stats (CY2020)

Stakeholders and Technology Transfer

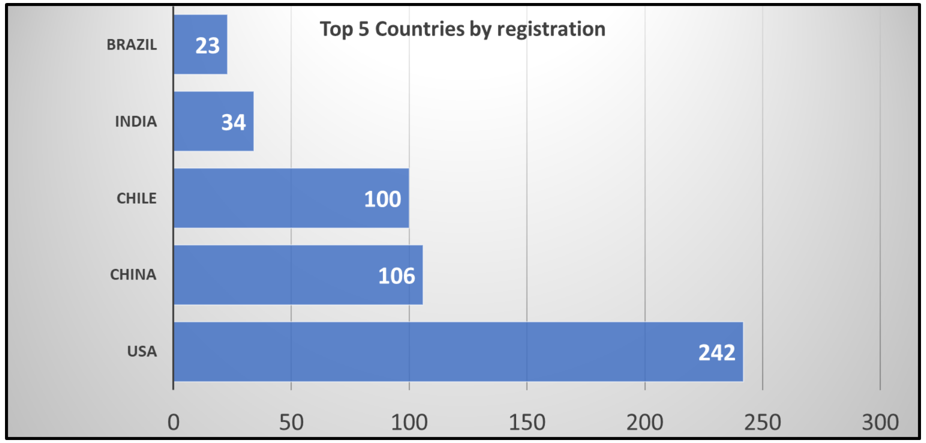
- All-time MFiX registrations = **6,643**

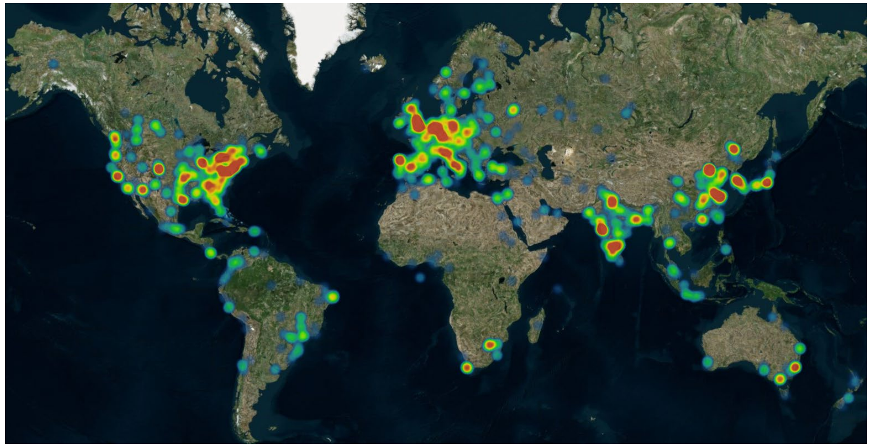






3 Universities using MFiX for course project:
- Arizona State University
- Ohio State University
- Universidad de la Serena, Chile



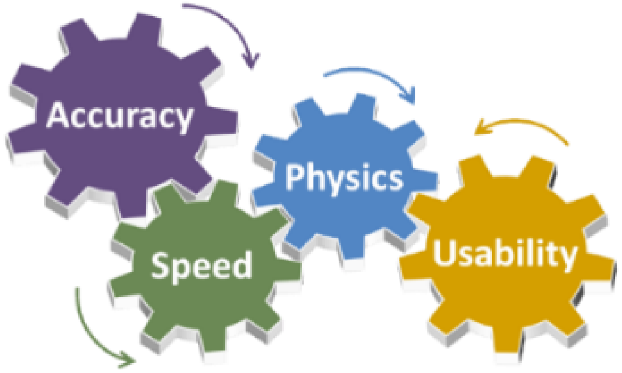


Publications

- Clarke, M.A. and Musser, J.M.H., "Particle in Cell Method (MFIX-PIC) Theory Guide," DOE/NETL-2020/2115, April 2020.
- A. Vaidheeswaran, A. Gel, M.A. Clarke, W.A. Rogers, "Sensitivity Analysis of Particle-in-Cell Modeling Parameters in MFIX-PIC", ASME Verification and Validation Symposium, Baltimore, MD, May 20-22, 2020.
- Vaidheeswaran, A.; Pandey, R.; Clarke, M. A.; Ashfaq, H.; Rogers, W. A. Fluidization of Group A Glass Particles: Experiments and Preliminary Validation; DOE/NETL-2020/2135; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2020; p 32. DOI: 10.2172/1632859.
- Gao, X., Yu, J., Lu, L., Li, C., Rogers, W. SuperDEM-CFD: Open Source Parallel Solver for Non-Spherical Particle-Fluid Fluidization Systems. *AIChE 2020 Annual Meeting*, San Francisco, Nov 2020.
- Vaidheeswaran, A.; Li, C.; Ashfaq, H.; Wu, X.; Rowan, S.; Rogers, W. Geometric Scale-up Experiments on Fluidization of Geldart B Glass Beads; DOE.NETL-2020.2146; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2020; pp. 40. DOI: 10.2172/1647458.
- Aytekin Gel, Justin Weber, Charles Tong, "Nodeworks: An Open-source Visual Workflow Toolset for Uncertainty Quantification, Optimization, Machine Learning", Workflow Workshop and Hackathon summer seminar series (https://wowoha.org), August 2020.
- Gao, X., Yu, J., Lu, L., Rogers, W. Coupling particle scale model, and SuperDEM CFD for multiscale simulation of biomass pyrolysis in a packed bed pyrolyzer. AIChE Journal, In press,2020.
- Gel, A. Vaidheeswaran, M.A. Clarke, "Deterministic Calibration of MFiX-PIC, Part 1: Settling Bed, NETL Technical Report Series, US Department of Energy, National Energy Technology Laboratory, Morgantown WV.
- Liqiang Lu, Xi Gao, Aytekin Gel, Gavin M. Wiggins, Meagan Crowley, Brennan Pecha, Mehrdad Shahnam, William A. Rogers, James Parks, Peter N. Ciesielski, Investigating biomass composition and size effects on fast pyrolysis using global sensitivity analysis and CFD simulations, Chemical Engineering Journal, 2020, 127789, ISSN 1385-8947, https://doi.org/10.1016/j.cej.2020.127789.
- Vaidheeswaran, Avinash, and Steven Rowan. "Chaos and recurrence analyses of pressure signals from bubbling fluidized beds." Chaos, Solitons & Fractals (2020): 110354.
- Aytekin Gel, Avinash Vaidheeswaran, MaryAnn Clarke; "Deterministic Calibration of MFiX-PIC, Part 1: Settling Bed," DOE/NETL-2021/2646; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2021; p. 72. DOI: 10.2172/1764832.
- Avinash Vaidheeswaran, Aytekin Gel, MaryAnn Clarke, William Rogers; "Sensitivity Analysis of Particle-In-Cell Modeling Parameters in Settling Bed, Bubbling Fluidized Bed and Circulating Fluidized Bed," DOE/NETL-2021/2642, NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2021; p. 40. DOI: 10.2172/1756845.
- Liqiang Lu, Xi Gao, Mehrdad Shahnam, William A. Rogers. 2021 Simulations of Biomass Pyrolysis using Glued-Sphere CFD-DEM with 3-D Intra-particle Models. Chem. Eng. Journal, Accepted.

Task 2&3: Summary

- MFiX releases
  - 20.1: New meshing workflow
  - 20.2: Moving geometry (STL), PIC CFL
  - 20.3: DEM Polydispersity
  - 20.4: Coarse Grain DEM, PIC collision damping
  - 21.1: New drag laws, New Nusselt number, fluid solver acceleration
- MFiX development
  - GUI continuous development
  - Polydispersity
  - Coarse grain DEM
  - Non-spherical DEM particles
  - DEM GPU porting
  - DEM Rolling friction
  - PIC parameter sensitivity/calibration
- 50kW$_{th}$ CFB simulation
  - Validated cold flow model
  - Validated a simplified global one-step mechanism for combustion
  - Ability of MFiX-PIC to accurately capture the physics and chemistry of a circulating fluidized bed combustor at bench scales, which can be further extended to pilot- and industrial-scale systems



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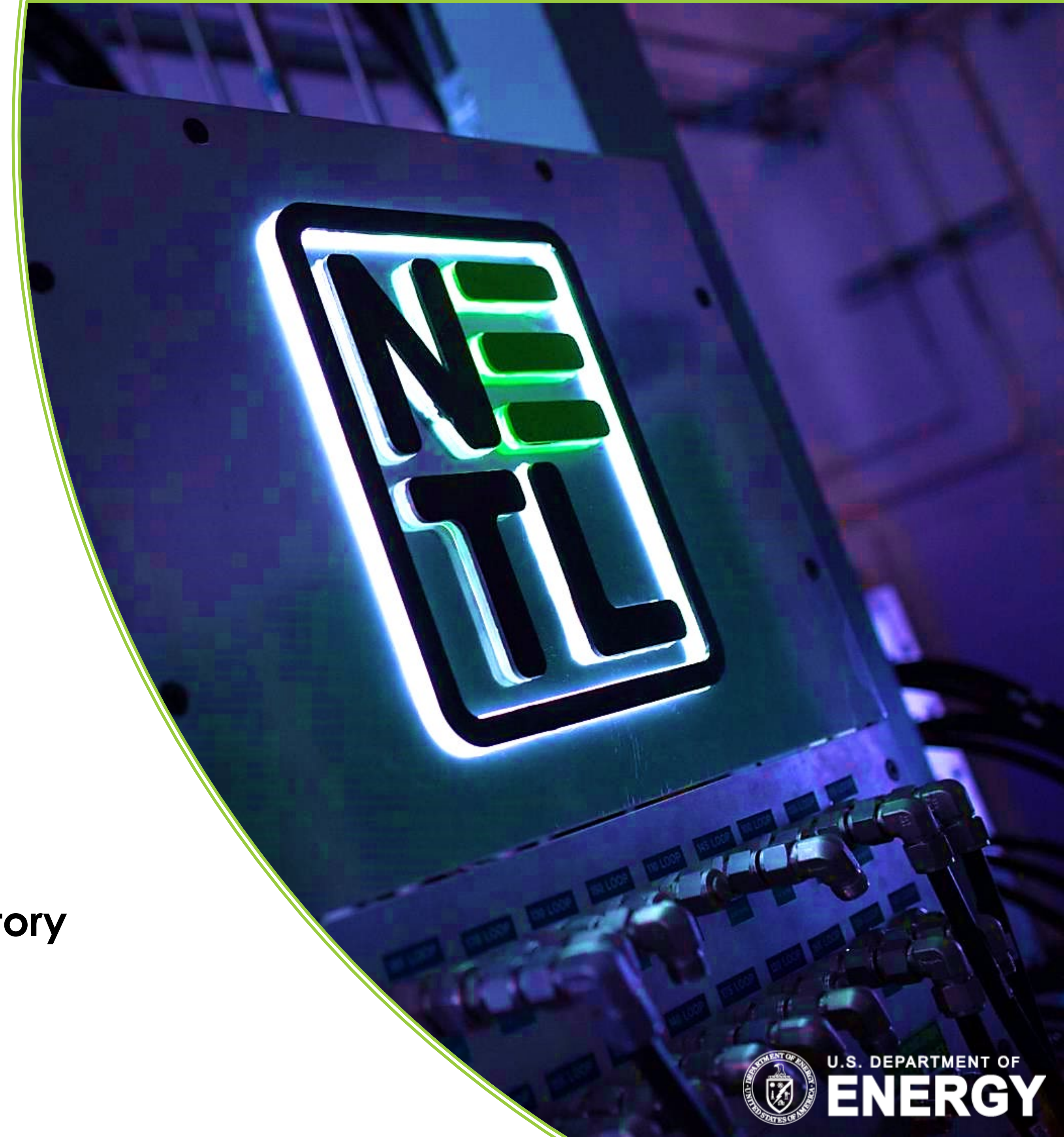

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