MFiX - Multiphase Flow with Interphase Exchanges

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

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LRST

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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 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
    - 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

Capabilities and Benefits

MFiX

NETL flagship (CFD) code

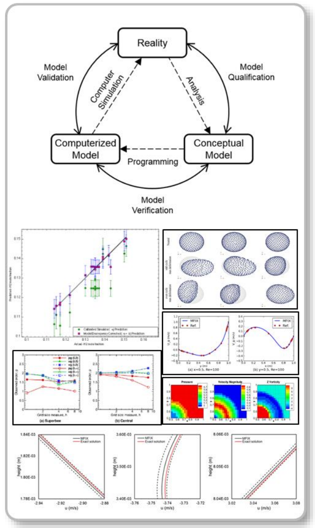
3 Decades of development history

300+ downloads per month

7,000 registered users

400 citations per year

- **Versatile toolset** (hydrodynamics, heat transfer, chemical reactions)
- **Gas/solids flows**
  - Gas: transport equations (continuity, momentum energy species)
  - Solids: transport equations or particle tracking
- **Open source**
  - Developed at NETL, in-house expertise
  - Runs on large HPC systems
- **Accelerate development and reduce cost**
- **Optimizes performance**
- **Reduces design risks**

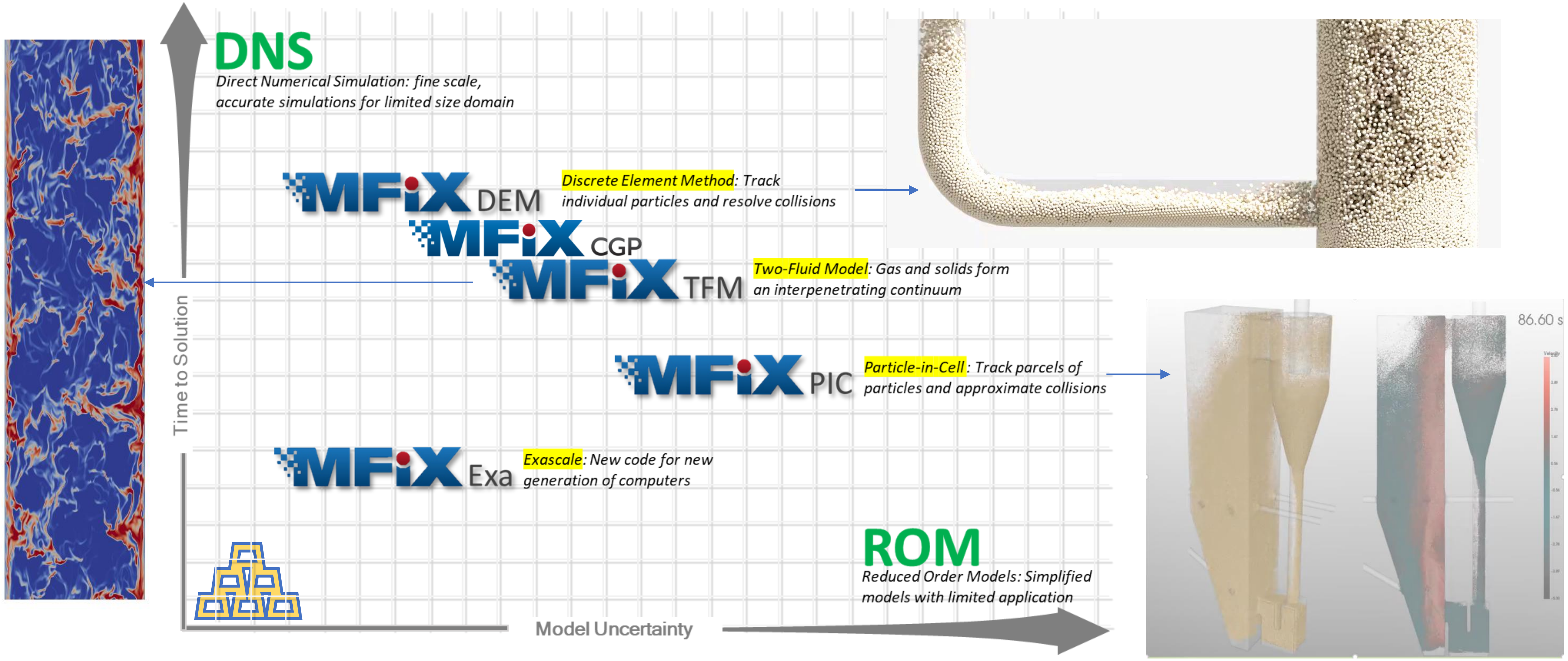


- MFiX-TFM (Two-Fluid Model)
- MFiX-DEM (Discrete Element Model)
- MFiX-PIC (Multiphase Particle-In-Cell)
- MFiX-CGDEM (Coarse Grain DEM)
- MFiX Exa (Exascale) – under development
- C3M multiphase chemistry management software
- Nodeworks: Optimization and UQ Toolsets
- Tracker: Object tracking in videos/image stack

MFS Software Portfolio

MFiX Suite of Multiphase CFD Software

Managing the tradeoff between accuracy and time to solution



MFiX-TFM : Two Fluid Model

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Continuous and disperse phases (e.g., gas and solids) are treated as coexisting continua.

Highlights

- Long track record of successfully supporting DOE-FE priorities
- Computationally efficient
- Historical workhorse for large-scale FE applications

Technical limitations

- Unable to efficiently model phenomena like particle size distributions
- Relies on complex constitutive relations to approximate solid stresses
- Ad hoc extension to multiple solids phases

Fluid continuity equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) = \mathcal{S}_g$$

Fluid momentum equation:

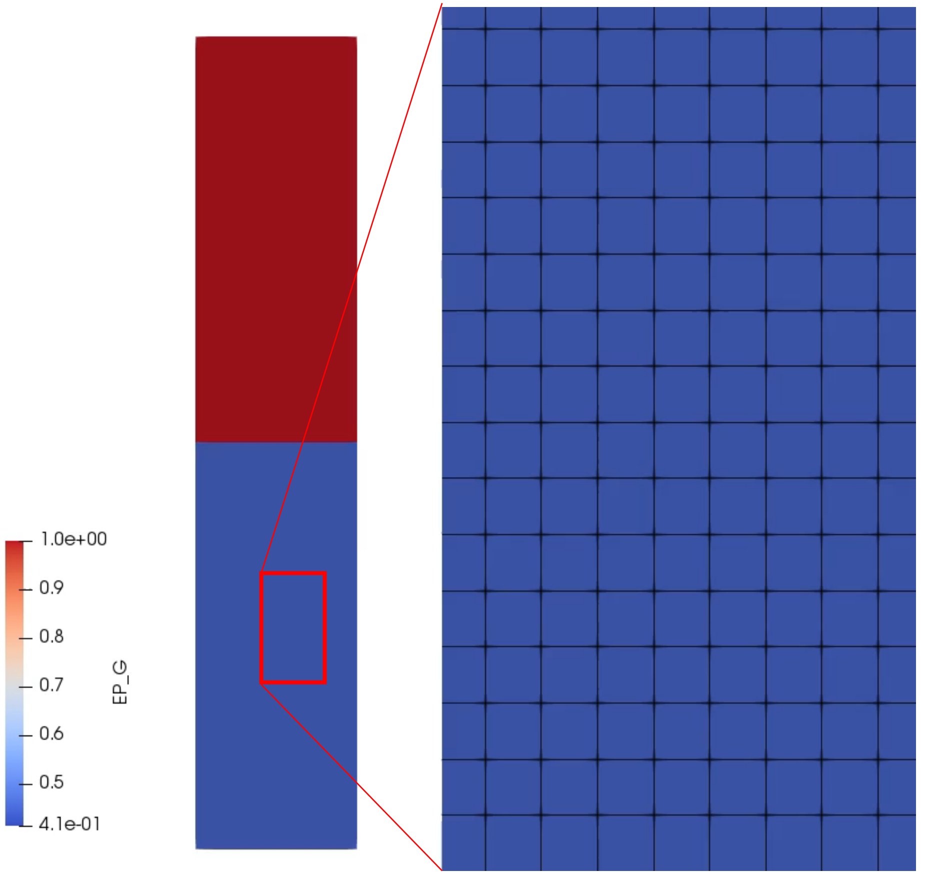
$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g\right) = -\varepsilon_g \nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \boldsymbol{g} + \sum_m \boldsymbol{\mathcal{I}}_{g,m}$$

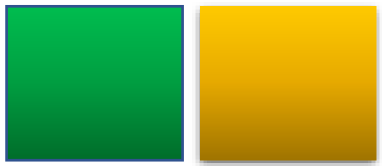
Solids continuity equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_m \rho_m\right) + \nabla \cdot \left(\varepsilon_m \rho_m \boldsymbol{u}_m\right) = \mathcal{S}_m$$

Solids momentum equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_m \rho_m \boldsymbol{u}_m\right) + \nabla \cdot \left(\varepsilon_m \rho_m \boldsymbol{u}_m \boldsymbol{u}_m\right) = -\nabla p_m + \nabla \cdot \boldsymbol{\tau}_m + \varepsilon_m \rho_m \boldsymbol{g} - \boldsymbol{\mathcal{I}}_{g,m}$$





Solver time: Fluid Solid (one solids phase)

MFiX-DEM : Discrete Element Model

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Fluid is a continuum and particles are individually tracked, resolving particle-particle-wall collisions

Advantages

- Uses first principles to account for particle interactions, reducing model complexity.
- Fewer complex closures results in less overall model uncertainty.
- Only open-source, fully coupled CFD-DEM code designed for reacting flows.

Technical limitations

- Computationally expensive, limiting the size of systems that can be modeled.
- Fluid-particle interaction is closed using drag models.

Fluid continuity equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) = \mathcal{S}_g$$

Fluid momentum equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g\right)$$

$$= -\varepsilon_g \nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \boldsymbol{g} + \sum_p \boldsymbol{\mathcal{I}}_{g,p}$$

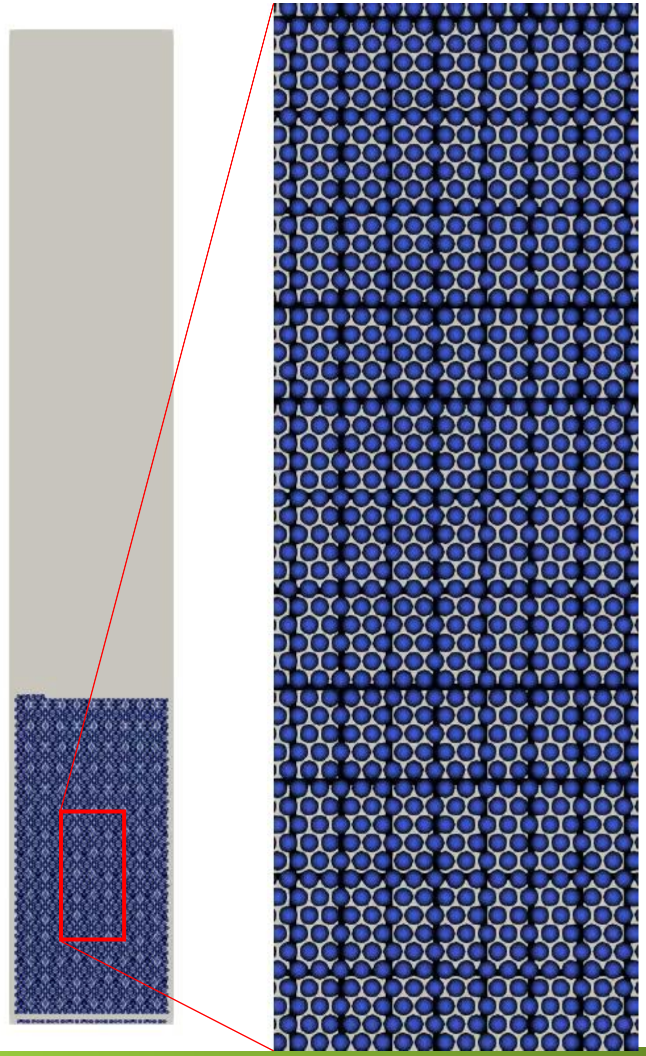
Particle continuity equation:

$$\frac{\partial}{\partial t}\left(m_p\right) = \mathcal{S}_p$$

Particle momentum equations:

$$m_p \frac{\partial \boldsymbol{u}_p}{\partial t} = m\boldsymbol{g} + \boldsymbol{F}_{coll} - \boldsymbol{\mathcal{I}}_{g,p}$$

$$I_p \frac{\partial \boldsymbol{\omega}_p}{\partial t} = \boldsymbol{\mathcal{T}}$$



MFiX-DEM : Discrete Element Model

Fluid is a continuum and particles are individually tracked, resolving particle-particle-wall collisions

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- Computationally expensive, limiting the size of systems that can be modeled.
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Fluid continuity equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) = \mathcal{S}_g$$

Fluid momentum equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g\right)$$

$$= -\varepsilon_g \nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \boldsymbol{g} + \sum_p \boldsymbol{\mathcal{I}}_{g,p}$$

Particle continuity equation:

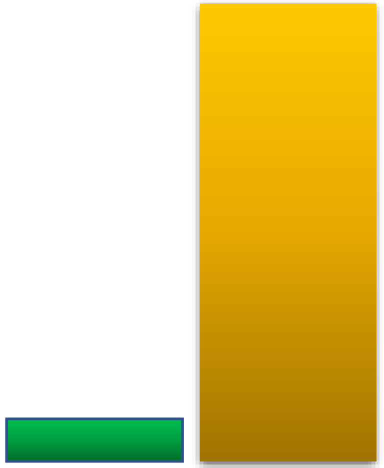
$$\frac{\partial}{\partial t}\left(m_p\right) = \mathcal{S}_p$$

Particle momentum equations:

$$m_p \frac{\partial \boldsymbol{u}_p}{\partial t} = m\boldsymbol{g} + \boldsymbol{F}_{coll} - \boldsymbol{\mathcal{I}}_{g,p}$$

$$I_p \frac{\partial \boldsymbol{\omega}_p}{\partial t} = \boldsymbol{\mathcal{T}}$$

P-P and P-W collisions are resolved (soft sphere)



MFiX-CGDEM : Coarse Grain Discrete Element Model

Fluid is a continuum, particles are grouped into larger particles (CGP). CGP are individually tracked, resolving collisions

Advantages

- Same formulation as DEM
- Runs faster than DEM

Technical limitations

- Loss of accuracy for large statistical weights

Fluid continuity equation:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \boldsymbol{u}_g) = \mathcal{S}_g$$

Fluid momentum equation:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \boldsymbol{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g)$$
$$= -\varepsilon_g \nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \boldsymbol{g} + \sum_p \boldsymbol{\mathcal{J}}_{g,p}$$

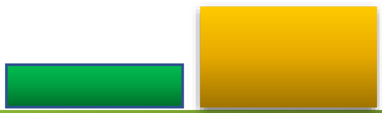
Particle continuity equation:

$$\frac{\partial}{\partial t}(m_p) = \mathcal{S}_p$$

Particle momentum equations:

$$m_p \frac{\partial \boldsymbol{u}_p}{\partial t} = m\boldsymbol{g} + \boldsymbol{F}_{coll} - \boldsymbol{\mathcal{J}}_{g,p}$$
$$I_p \frac{\partial \boldsymbol{\omega}_p}{\partial t} = \boldsymbol{\mathcal{T}}$$

Drag force is based on real particle size



MFiX-PIC : (Multiphase) Particle-in-Cell

Fluid is a continuum and particles are tracked as parcels, solid-stress model approximates collisions

Advantages

- Computationally efficient
- Able to track particle-scale phenomena like time-histories and size distributions
- Only open-source, PIC model

Technical limitations

- Relies on a continuum stress model to approximate particle-particle interactions
- Strong dependence on implementation

Formally released: April, 2019

Fluid continuity equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) = \mathcal{S}_g$$

Fluid momentum equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g\right)$$
$$= -\varepsilon_g \nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \boldsymbol{g} + \sum_p \boldsymbol{\mathcal{I}}_{g,p}$$

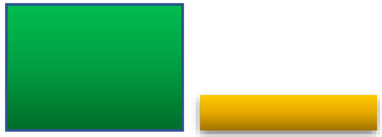
Parcel continuity equation:

$$\frac{\partial}{\partial t}\left(m_p\right) = \mathcal{S}_p$$

Parcel momentum equation:

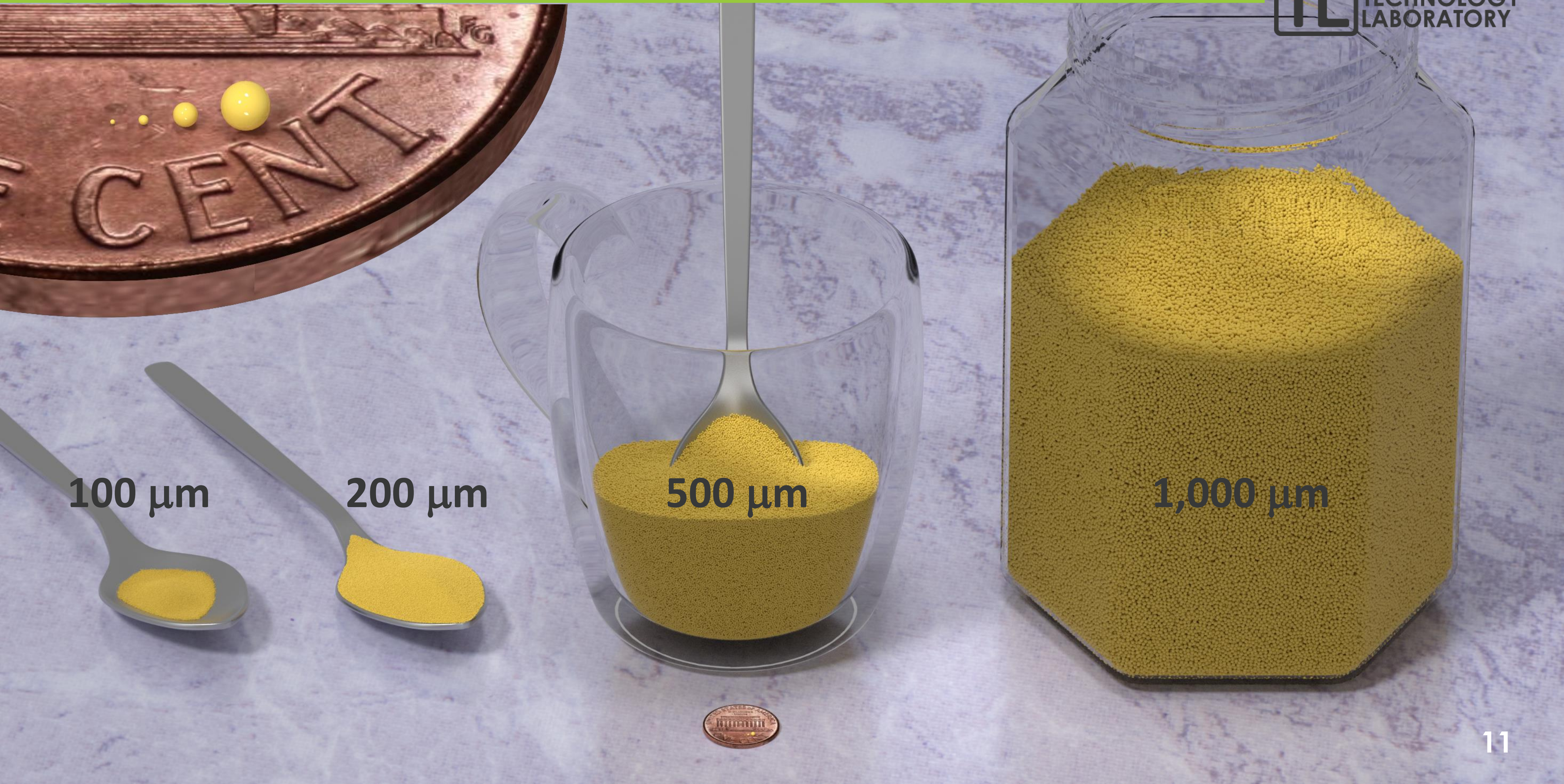
$$m_p \frac{\partial \boldsymbol{u}_p}{\partial t} = m\boldsymbol{g} + \nabla \tau_p - \boldsymbol{\mathcal{I}}_{g,p}$$

Parcel collisions are not resolved



Solver time: Fluid Solid

What can be modeled with 1 Million particles?



Enabling large Scale simulations

DEM example

Height = 0.68 m

Particle diameter = 800 microns

Particle count = 500,000 particles

Enabling large Scale simulations

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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)

Use MP-PIC for computational speed and averaged accuracy

REDUCED ACCURACY

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**	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**	

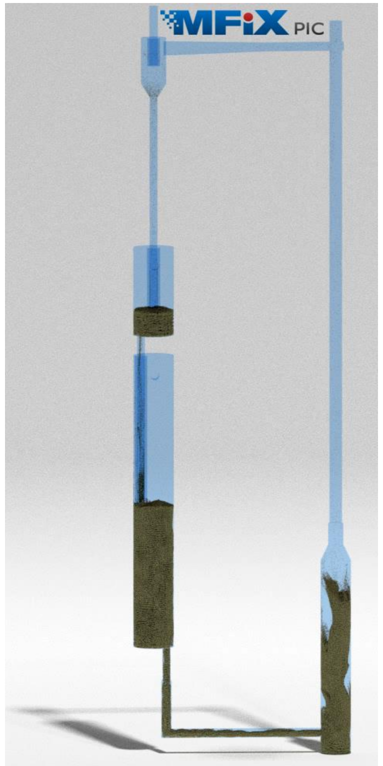
INCREASED COMPUTATIONAL SPEED

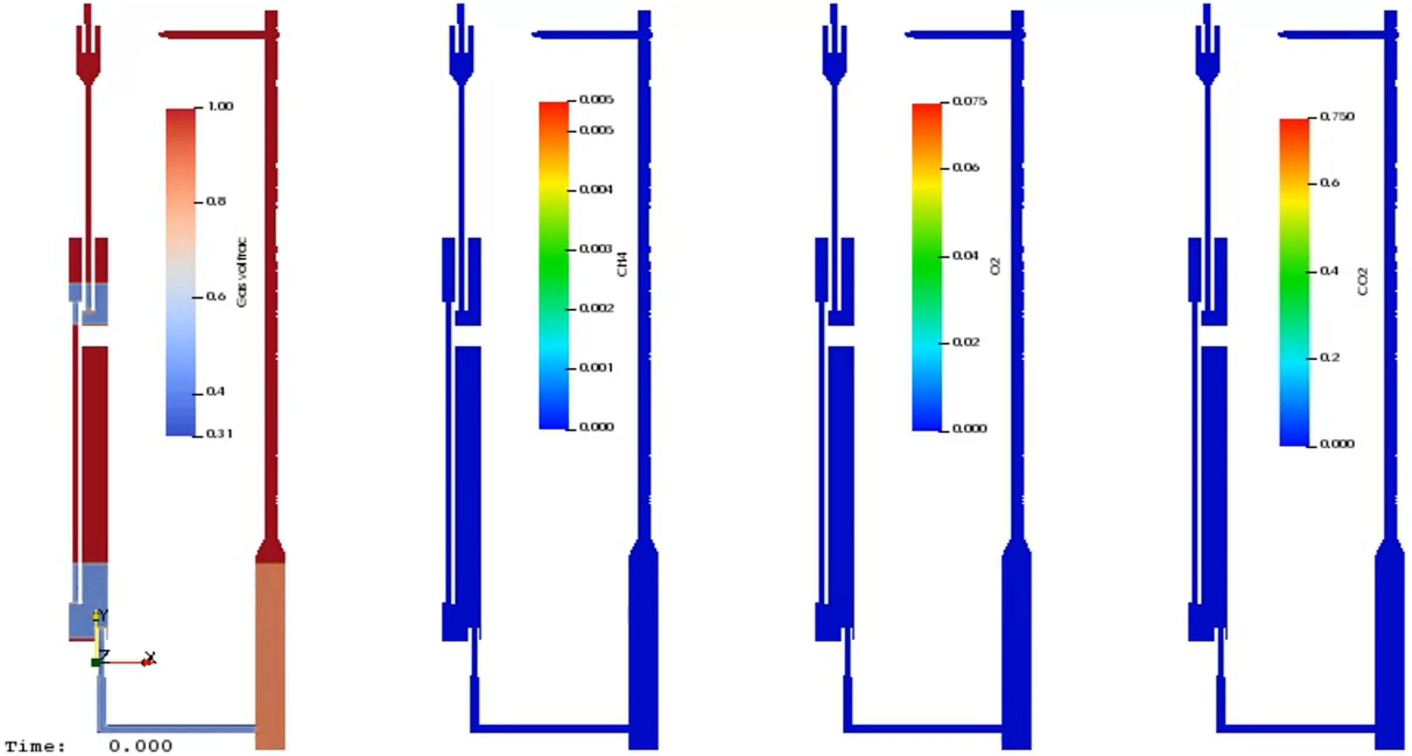
GENERALIZED IDEA FOR PARTICLE INTERACTIONS

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)





- ~4 meters tall
- 650 million particles
- 13 million PIC parcels
- 200 cores on Joule 2
- 15 seconds/day

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.

MFiX Development

Recent developments

- 20.4
  - Coarse Grain DEM
  - PIC collision damping
- 21.1
  - ~ ≈ 2x fluid solver speedup
  - Prodecural STL
  - ≈ 6 new drag laws, 3 new Nusselt number correlations
- 21.2
  - CGDEM specify statistical weight per phase
  - Force chain visualization
  - Reaction rate output
  - Filtering of particle_input.dat/partile_output.dat
- 21.3
  - ≈ Guo-Boyce friction model
  - Residence time output
  - Create animation from GUI
- 21.4
  - Polydispersity for PIC
- 22.1
  - DEM Rolling friction

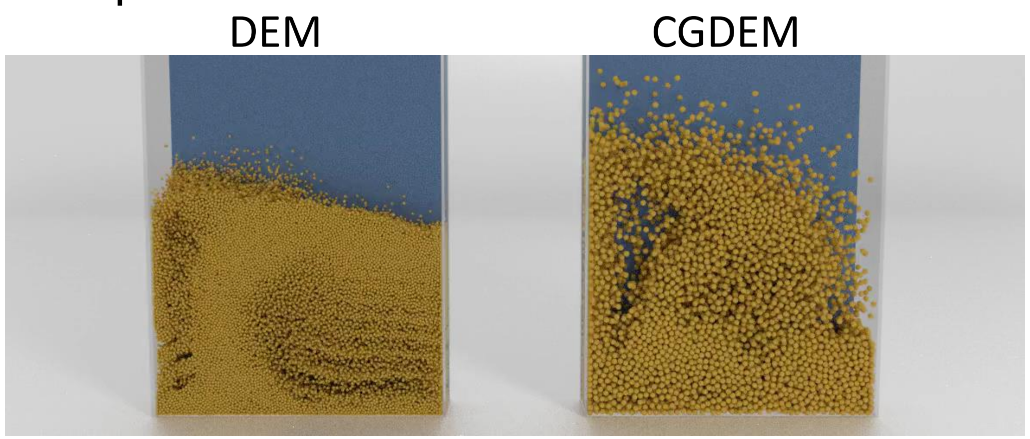
~ Single phase
≈ TFM
DEM
CGDEM
PIC

Workflow
Geometry
Chemistry
Output
Postprocessing

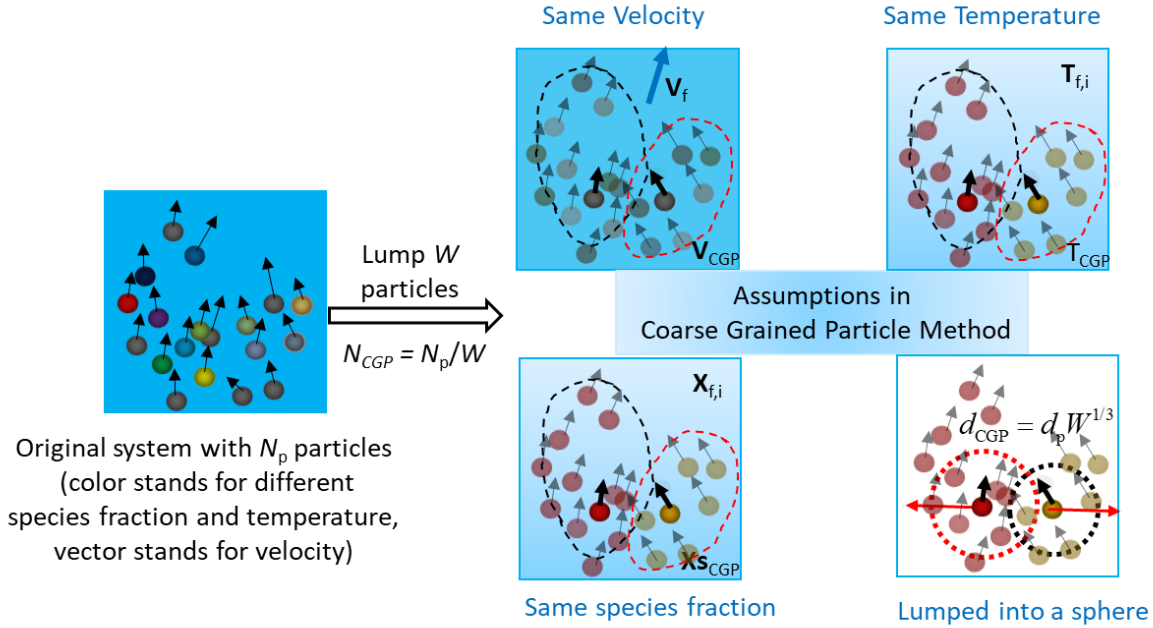
MFiX Development

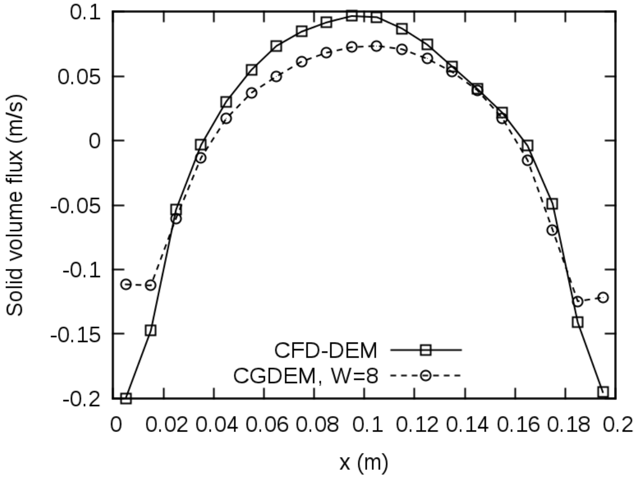
20.4 – Coarse Grain DEM

- Particles are lumped together to create a CG particle
- CG particles collide with each other
- Heat transfer, chemical reactions
- MFiX-CGDEM formal release: 12/31/2020



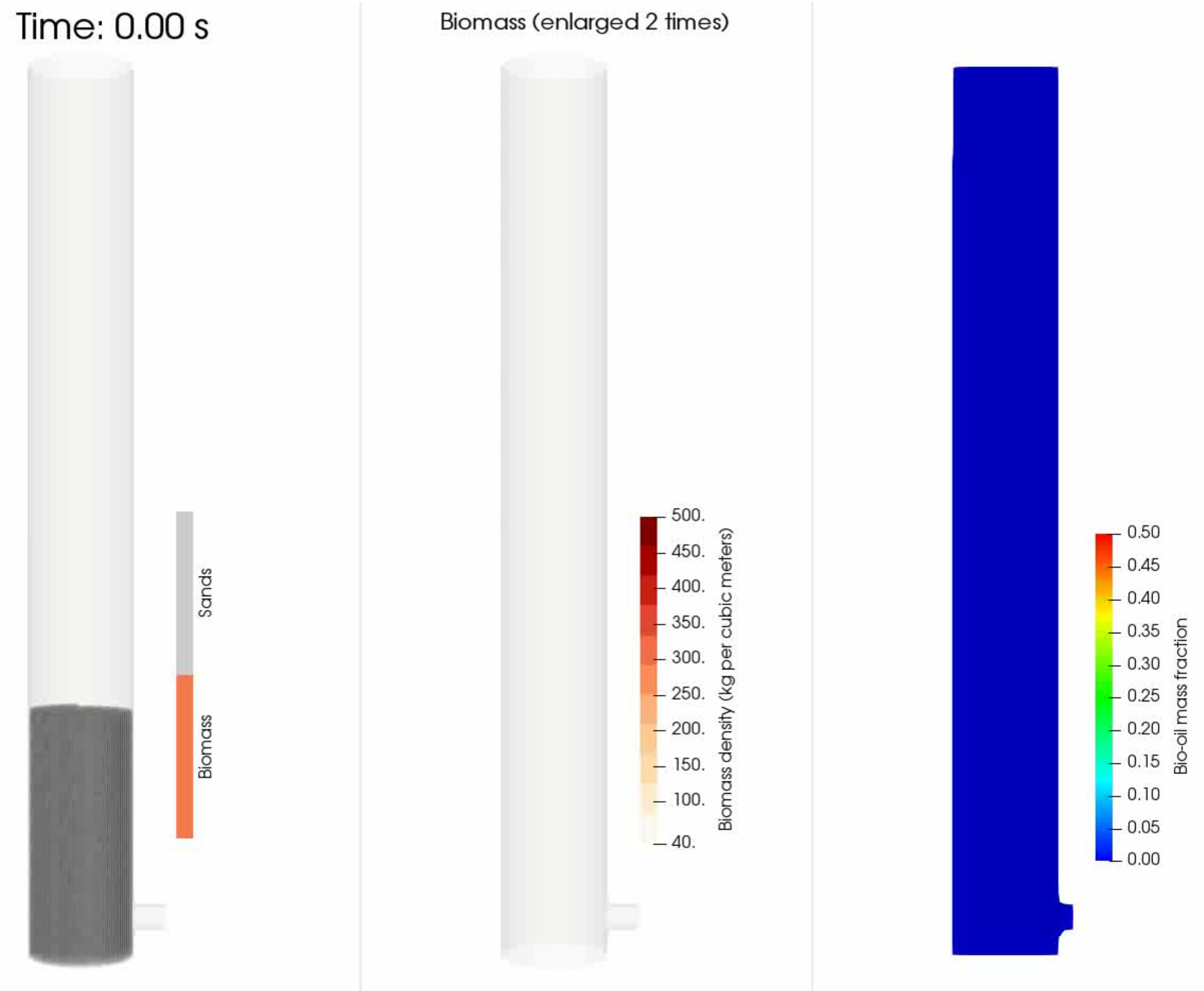
Coarse Grain DEM – **10 to 100x speedup** compared with DEM



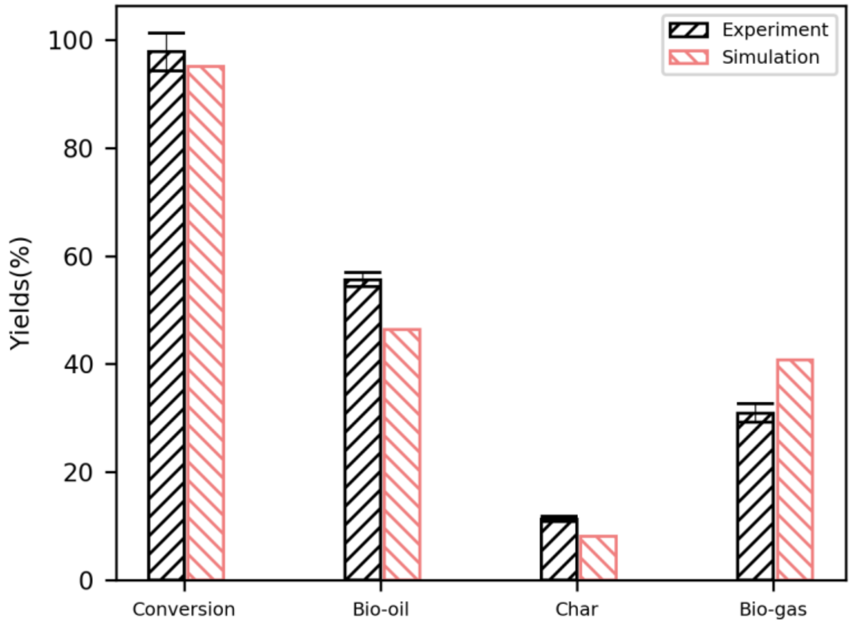


MFiX Development

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



MFiX Development

21.1 PIC Collision Damping

parcel

- Update parcel velocity (regular PIC algorithm)

cell

- Compute mean velocity $$\overline{v_i} = \frac{\iint f m v_i \, dm \, dv_j}{\iint f m \, dm \, dv_j}$$
- Compute std.dev $$\sigma = \left[\frac{\iint f m (v_i - \overline{v_i})^2 \, dm \, dv_j}{\iint f m \, dm \, dv_j} \right]^{1/2}$$
- Compute Sauter mean radius $$r_{32} = \frac{\iint f r^3 \, dm \, dv_j}{\iint f r^2 \, dm \, dv_j}$$
- Compute radial dist. function $$g_0(\theta) = \frac{\theta_{cp}}{\theta_{cp} - \theta}$$
- Compute collision frequency $$\frac{1}{\tau_D} \rightarrow \frac{16}{\sqrt{3\pi}} \frac{\theta \sigma}{r_{32}} g_0 \eta (1 - \eta)$$

parcel

- If collision frequency is not zero: replace regular PIC velocity with $$v_p^{n+1} = \frac{v_p^n + (\delta t / 2\tau_D) \overline{v_i}}{1 + (\delta t / 2\tau_D)}$$

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Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

An improved collision damping time for MP-PIC calculations of dense particle flows with applications to polydisperse sedimenting beds and colliding particle jets

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- Restitution coefficient e_p controls amount of damping

$$\eta = \frac{1 + e_p}{2}$$

Setting e_p = 1 turns off damping

- Introduced a new keyword `pic_cd_e` instead or reusing `mppic_coeff_en1`
- If collision frequency is very large, we “replace” parcel velocity with the average velocity

MFiX Development

Test case: Jet collision

- Collision of gas–solid jets
- 2 jets colliding
- Solids fraction = 0.1, velocity = 20m/s
- No energy loss at walls (e_w = 1)
- Statistical weight = 1
- Without collision damping, the two jets do not interact
- Polydisperse system, particle diameter:
  - Mean=650 μm, σ=25 μm, clipped at mean±2σ
  - Mean=350 μm, σ=25 μm, clipped at mean±2σ

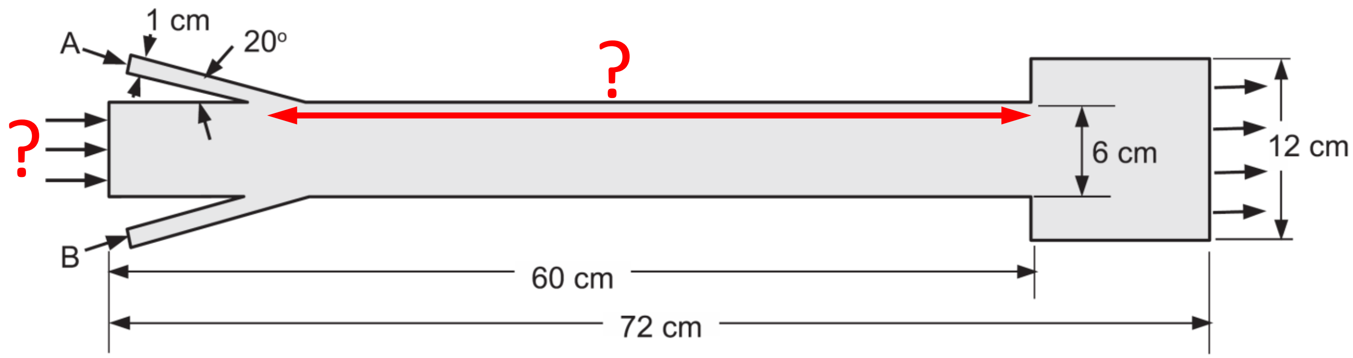
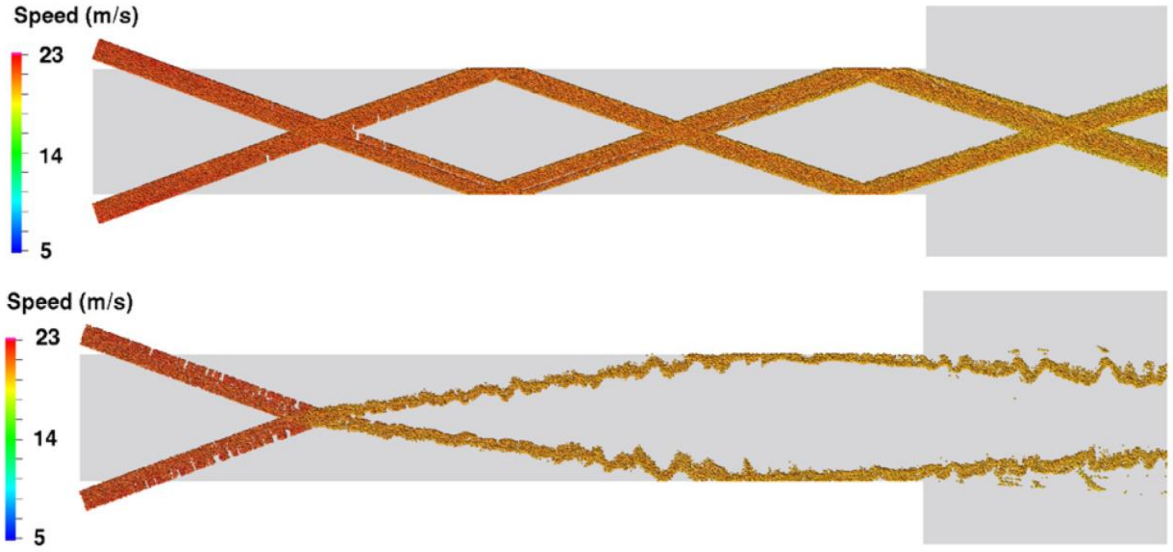
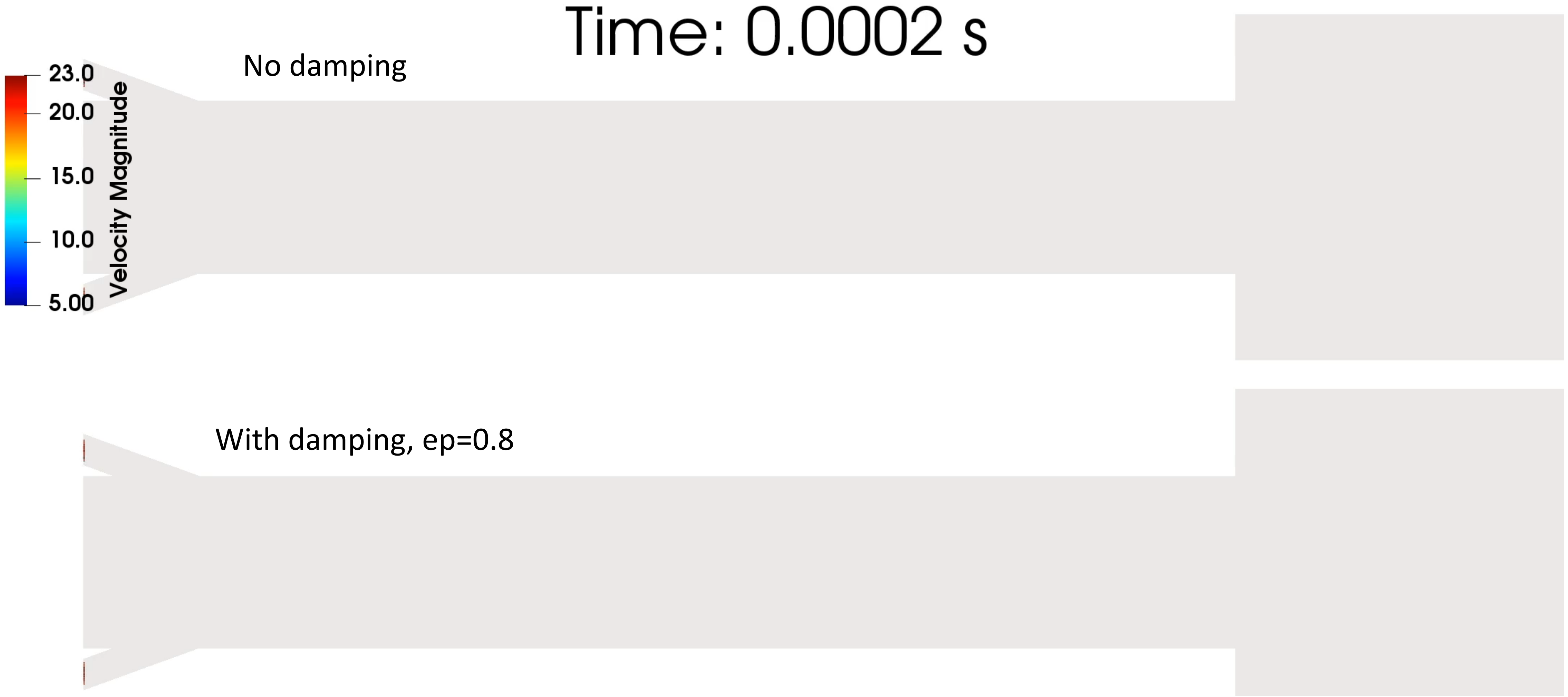


Fig. 5. Channel geometry used for the calculations of two impinging gas-particle jets.



MFiX Development

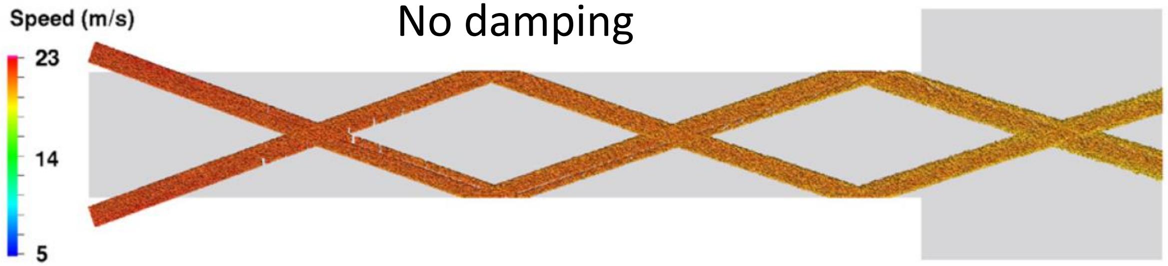
Mean=650 μm, σ=25 μm, clipped at mean±2σ



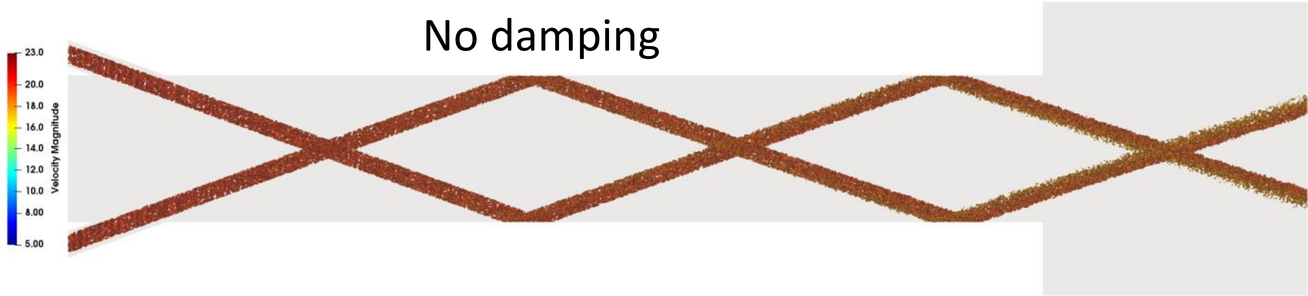
MFiX Development

Mean=650 μm, σ=25 μm, clipped at mean±2σ

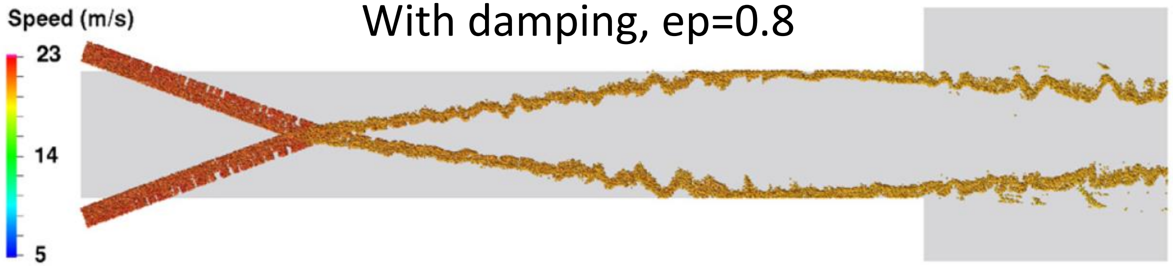
No damping



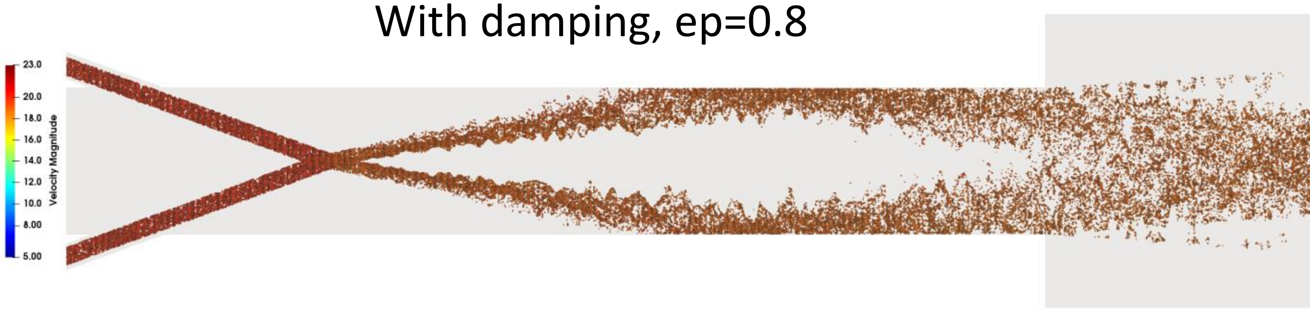
No damping



With damping, ep=0.8



With damping, ep=0.8

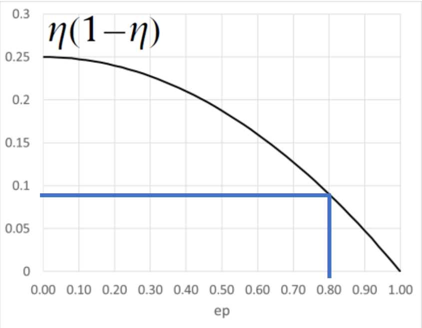


Barracuda (Paper)

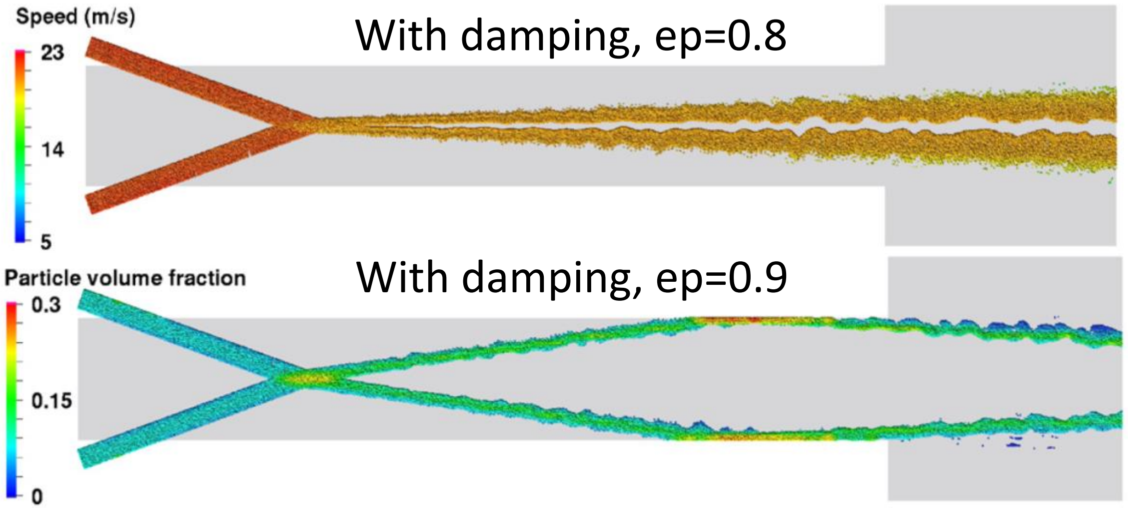
MFiX

MFiX Development

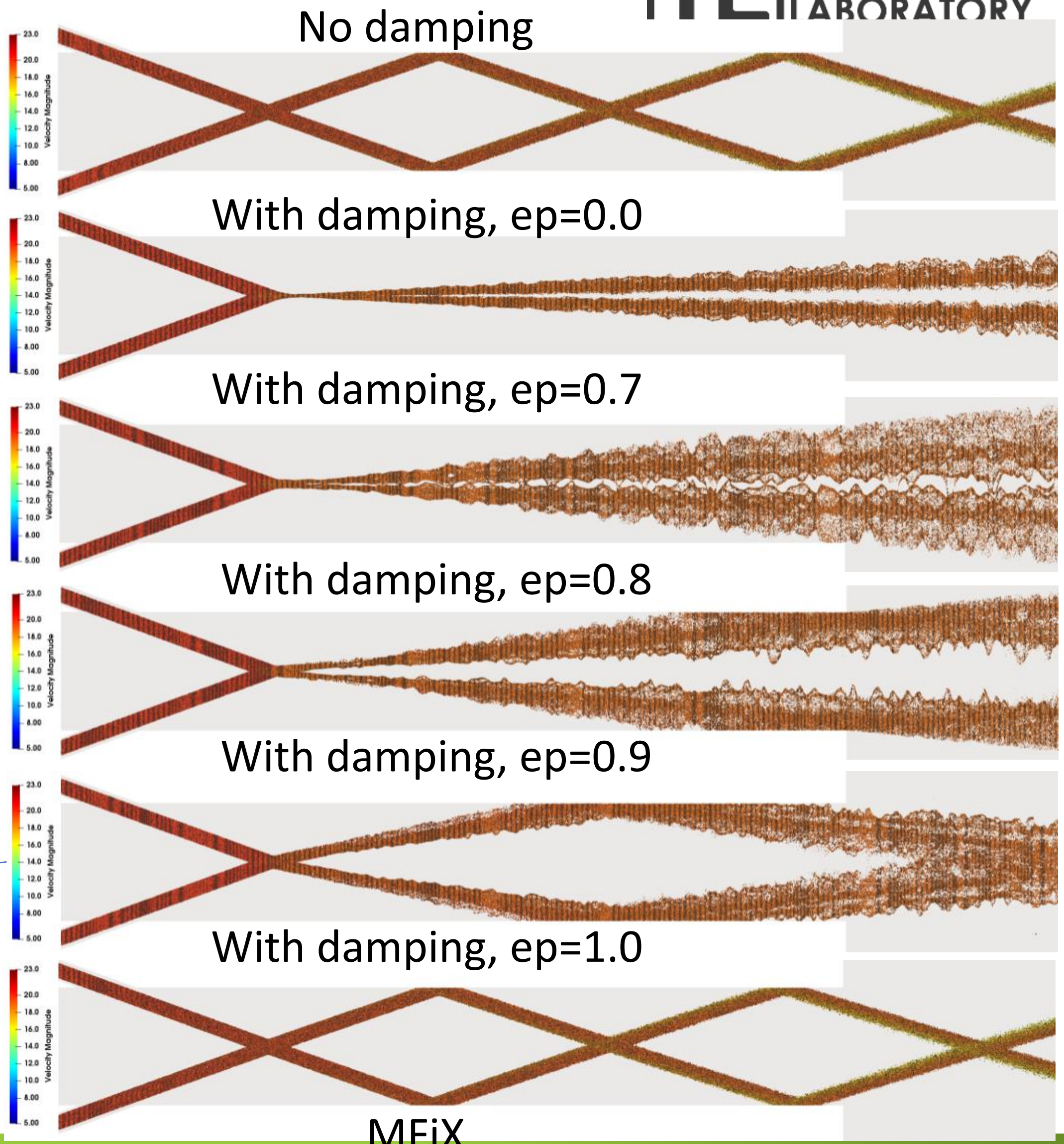
Mean=350 μm, σ=25 μm, clipped at mean±2σ



$$\frac{1}{\tau_D} \rightarrow \frac{16}{\sqrt{3\pi}}\frac{\theta\sigma}{r_{32}} g_0 \eta(1-\eta)$$



Barracuda (Paper)



MFiX

MFiX Development

21.1 Fluid solver 2x speedup

- Single Phase benchmarks
  - SQUARE PIPE: Steady State
  - BLUFF BODY
  - SQUARE PIPE DYNAMIC: Unsteady, transient inlet BC
- MFiX tutorials
  - FLD VORTEX SHEDDING
  - TFM HOPPER 3D
  - TFM HOPPER 2D
  - DEM CYCLONE
  - PIC LOOPSEAL

- Timing based on 1 to 3 repeats, manually launched on a dedicated node on Joule

- 21.1 Milestone: Accelerate fluid solver by a factor of 2

MFiX Development

21.1 Fluid solver 2x speedup

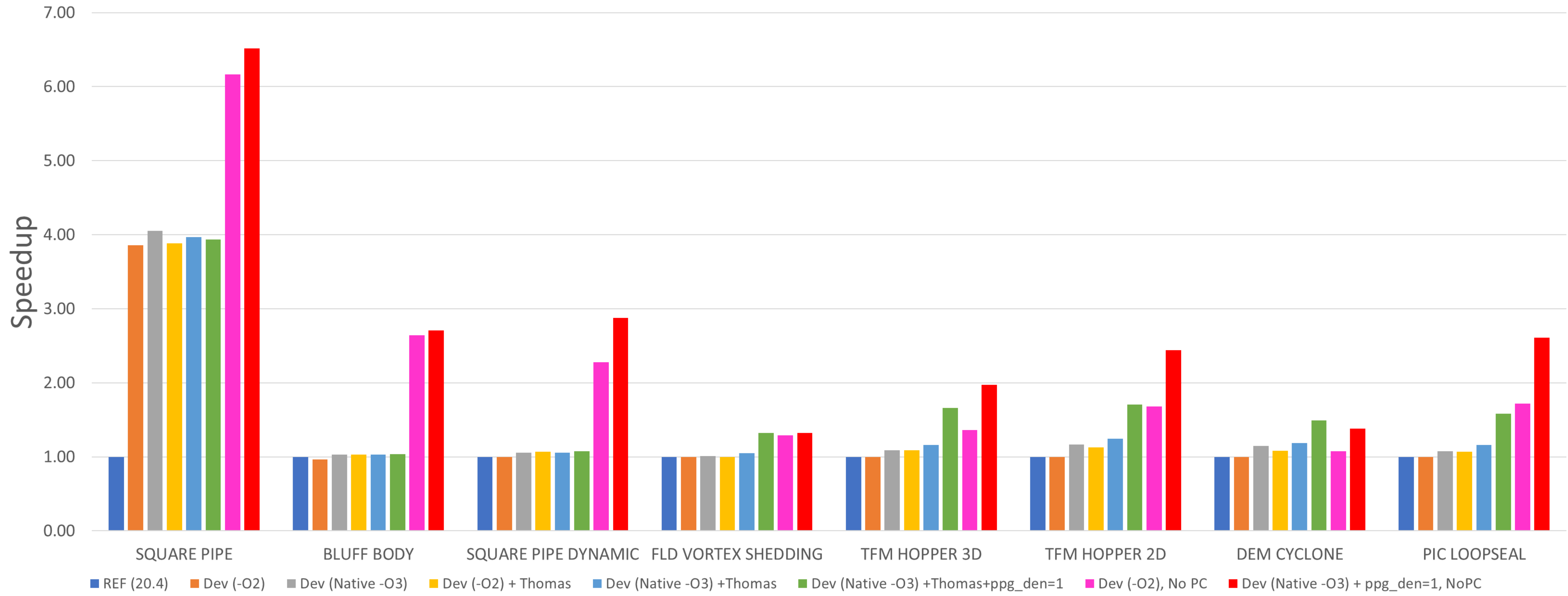
- Reference: MFiX 20.4, "-O2", Line PC, ppg_den=10, epp_den=10
- Dev: Feb 2021 develop version:
  - Code change: SS convergence criteria: only affects Steady State simulations
  - Regular vs Optimized Thomas algorithm: only affects simulation with Line PC (Charles Waldman)
  - New control for PPG and EPP residual scaling (ppg_den, epp_den): loosen convergence when norm_g=0, norm_s=0; default values: ppg_den=10, epp_den=10
- Optimization flag: "-O2" (default) vs "-march=native –O3"
- Line PC: On vs OFF

REF (20.4)
Dev (Native -O3) +Thomas
Dev (-O2)
Dev (Native -O3) +Thomas+ppg_den=1
Dev (Native -O3)
Dev (-O2), No PC
Dev (-O2) + Thomas
Dev (Native -O3) +ppg_den=1, NoPC

MFiX Development

21.1 Fluid solver 2x speedup

Speedup: Higher is better

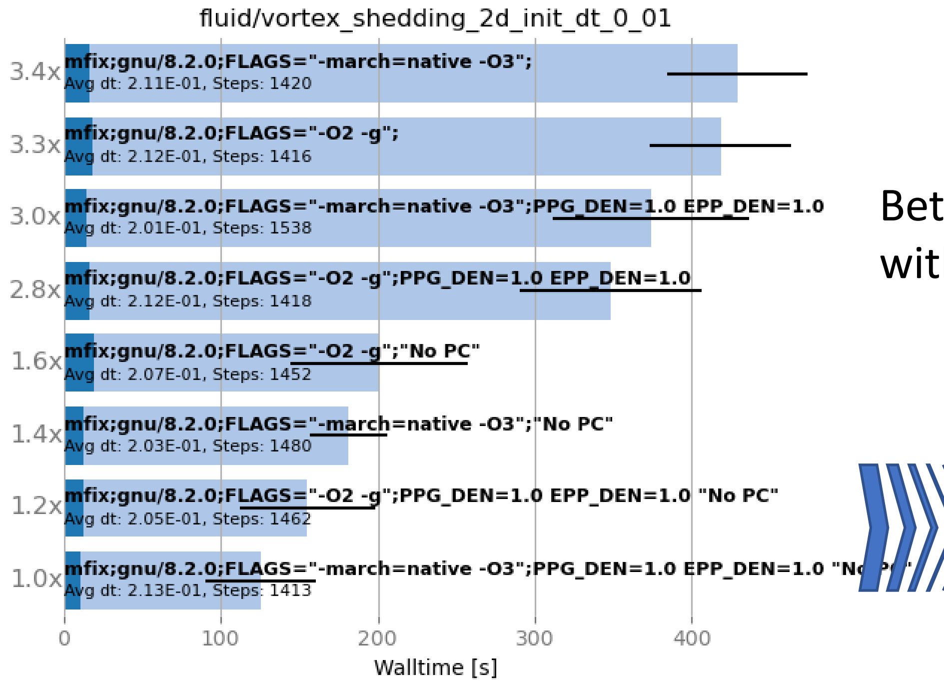


MFiX Development

21.1 Fluid solver 2x speedup

- 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**



Better to start with small DT

Faster than real time!!

MFiX Development

21.2 – Force chain visualization

Ability to visualize force chain

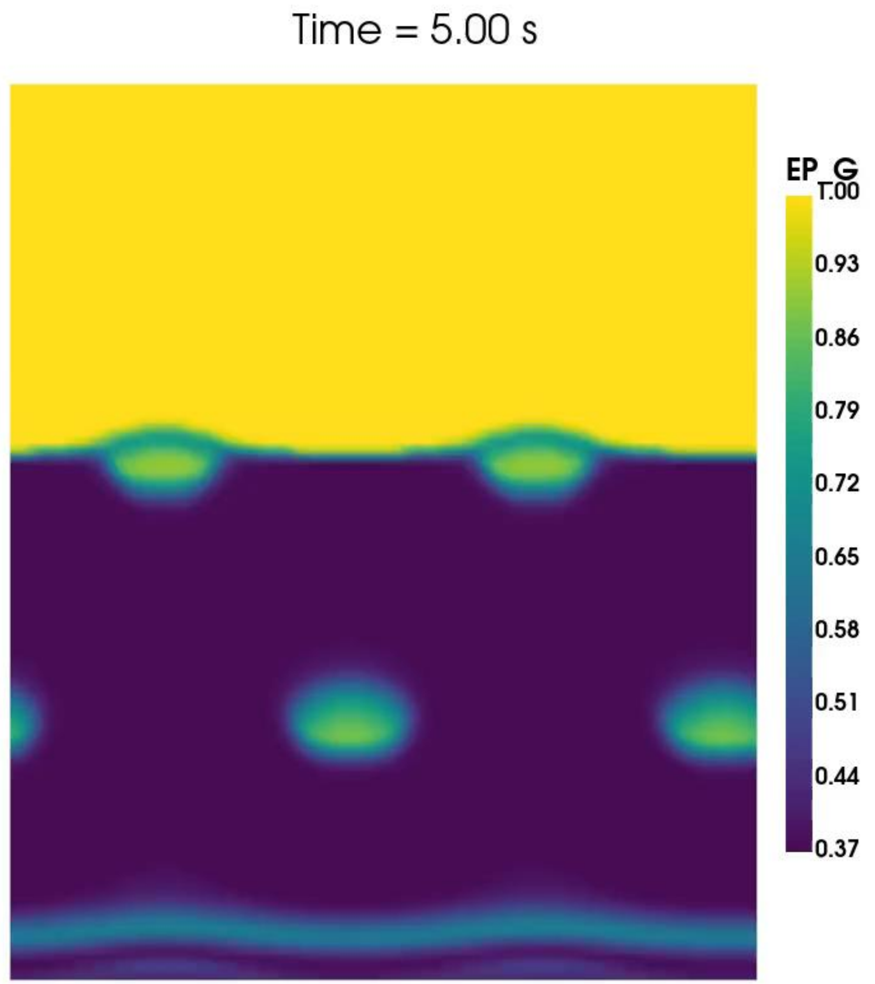
Between particles (DEM)

MFiX Development

21.3 – Guo-Boyce friction model (TFM)

- This model was graciously provided by researchers from Columbia University, NY.
- Allows to correctly predict bubble pattern in a pulsating fluidized bed.

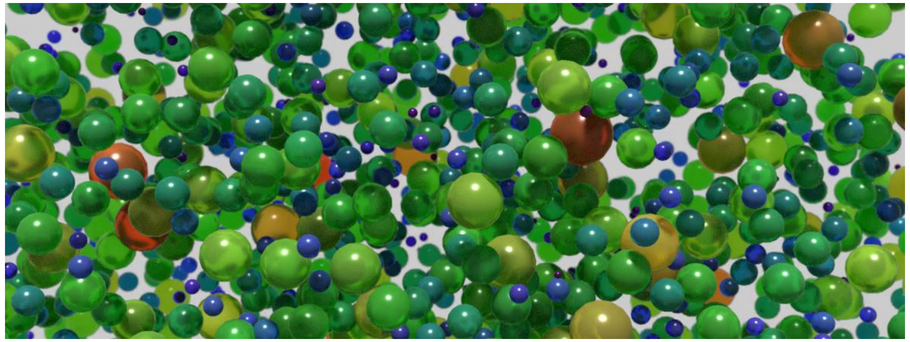
Qiang Guo, Yuxuan Zhang, Azin Padash, Kenan Xi, Thomas M. Kovar, Christopher M. Boyce, "Dynamically structured bubbling in vibrated gas-fluidized granular materials", Proceedings of the National Academy of Sciences Aug 2021, 118 (35) e2108647118; DOI: 10.1073/pnas.2108647118

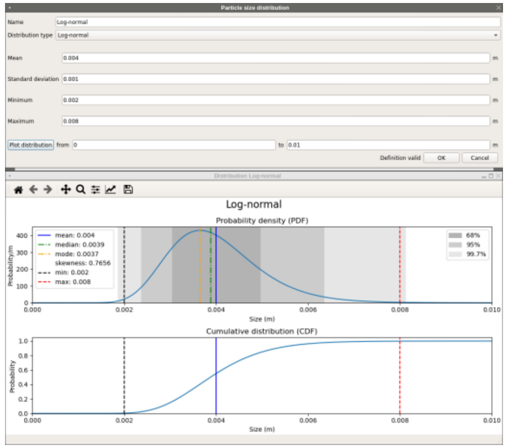


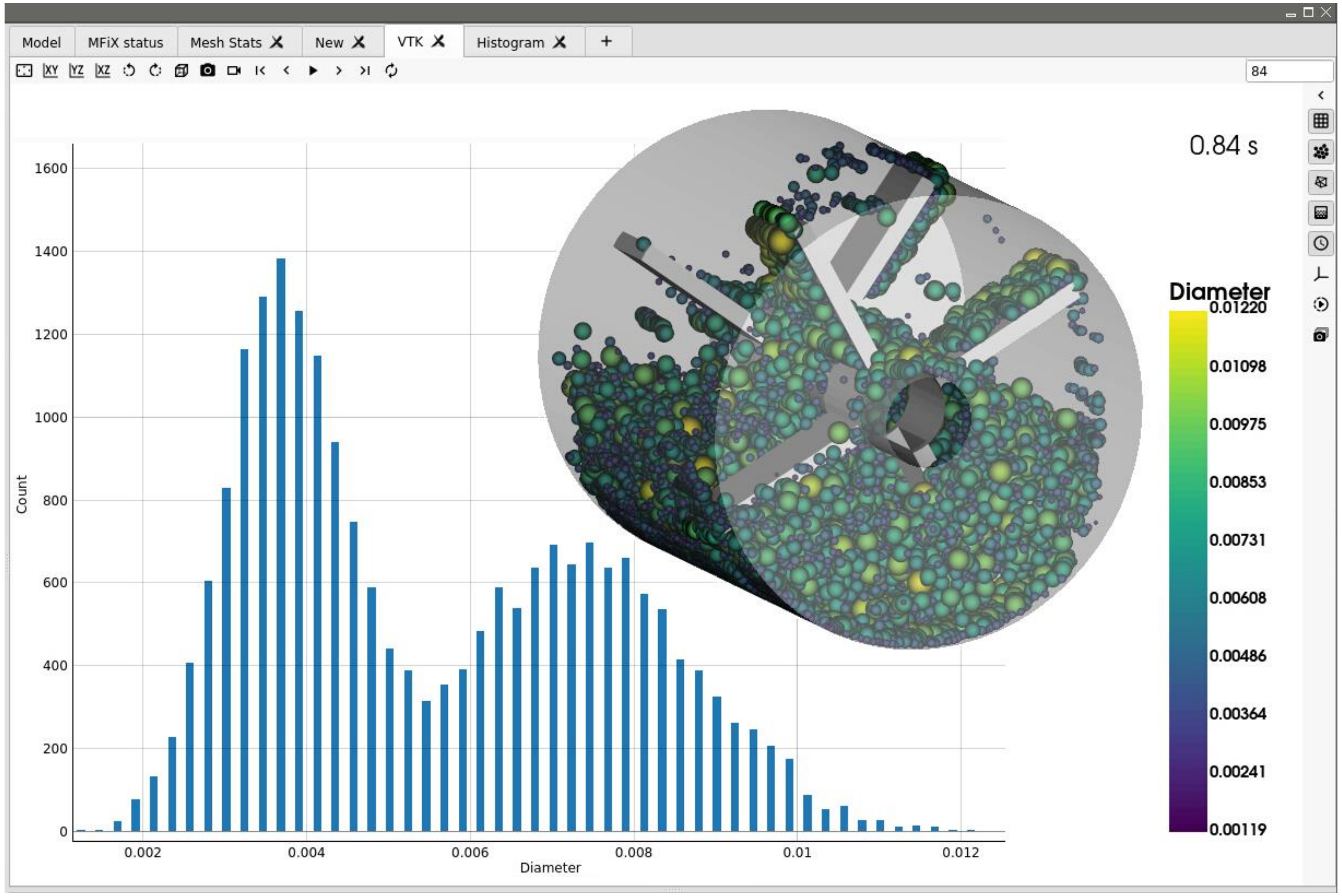
MFiX Development

21.4 Polydispersity for PIC

- Extension of DEM polydispersity
- Normal distributions
- log-normal distributions
- Custom distributions
- Boundary condition and initial condition

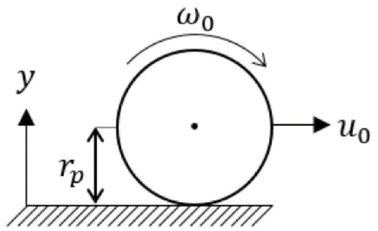


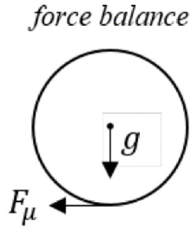


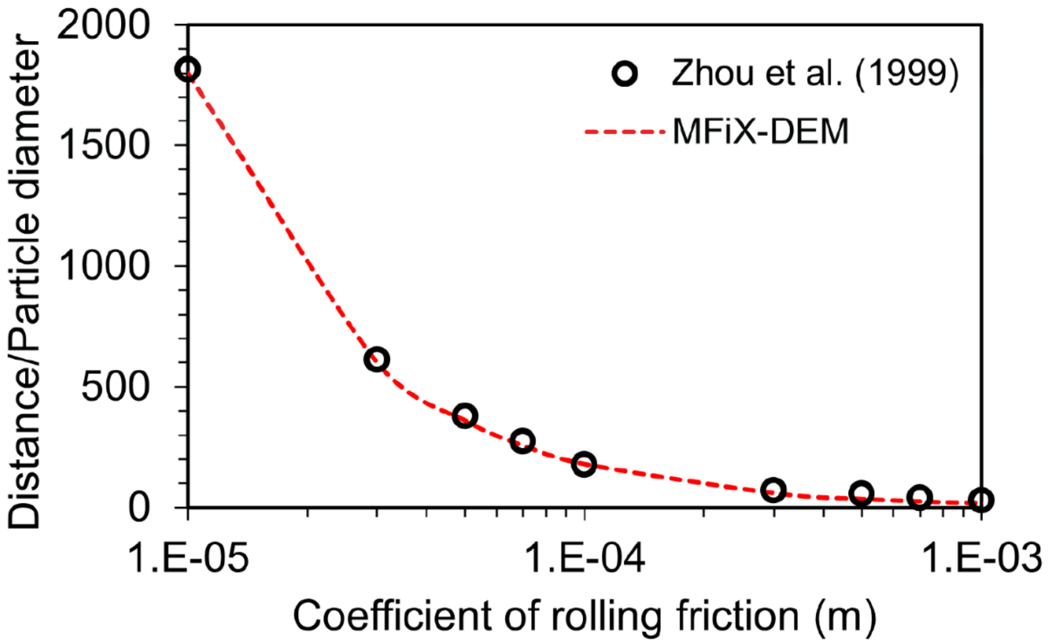


MFiX Development

22.1 DEM Rolling friction





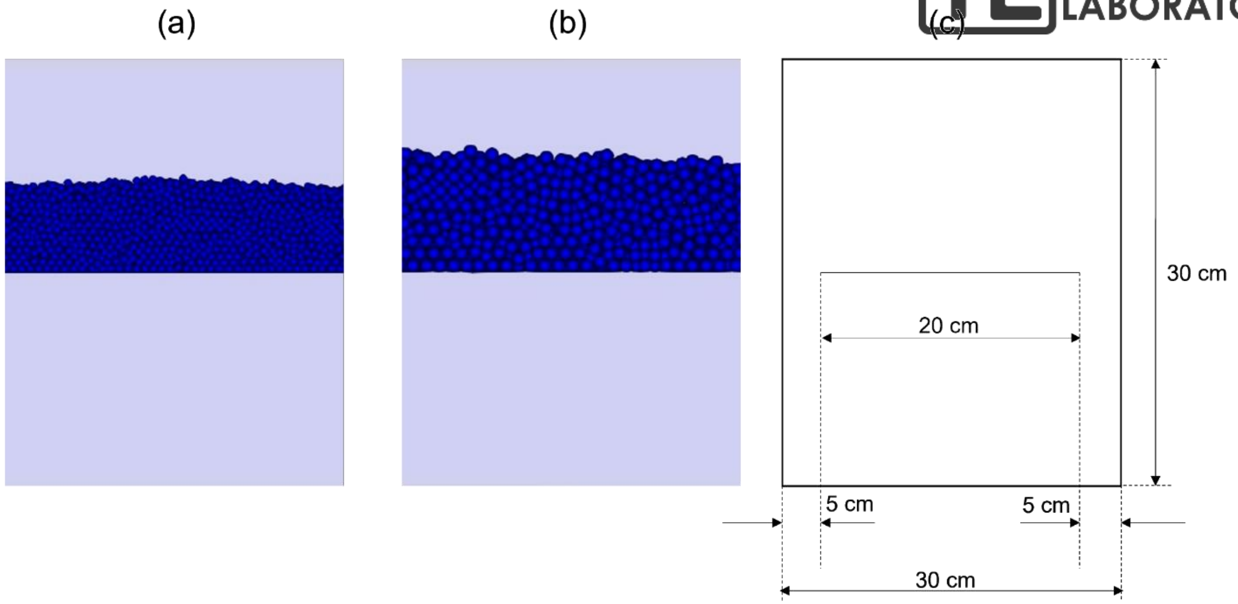


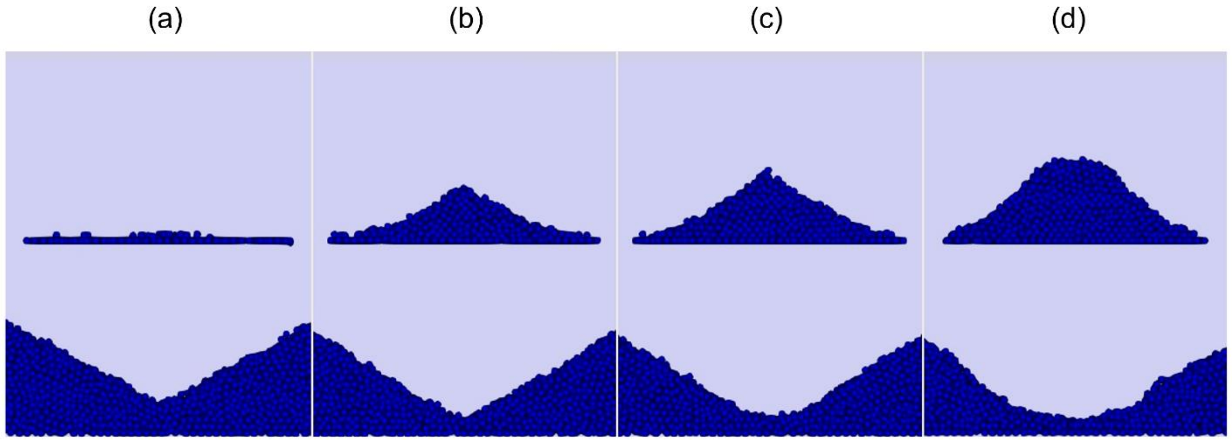
NATIONAL ENERGY TECHNOLOGY LABORATORY

22.1 DEM Rolling friction

Test case 2: Formation of a stagnant zone

- Particles initially in the top half
- Particle sizes = 6 mm and 10 mm
- Particles collect at the bottom once the ends are opened.
- A stagnant zone at the midplane is formed whose characteristics depend on the value of the rolling friction coefficient
- As the value is increased, more particles accumulate in the stagnant zone. In our case, we obtain reasonable results while using μr = 1.0E-4 m.
- Good qualitative comparison of final particle locations between MFiX-DEM predictions and the work of Zhou et al.





Formation of stagnant zone along the midplane with 6 mm particles using a rolling friction coefficient of (a) 0 m, (b) 2.5E-5 m, (c) 5.0E-5 m and (d) 1.0E-4 m.

Y.C. Zhou, B.D. Wright, R.Y. Yang, B.H. Xu, A.B. Yu, "Rolling friction in the dynamic simulation of sandpile formation", Physica A: Statistical Mechanics and its Applications, Volume 269, Issues 2–4, 1999, Pages 536-553

Non-spherical particles (SuperDEM)

- Superquadrics are a family of geometric shapes defined as

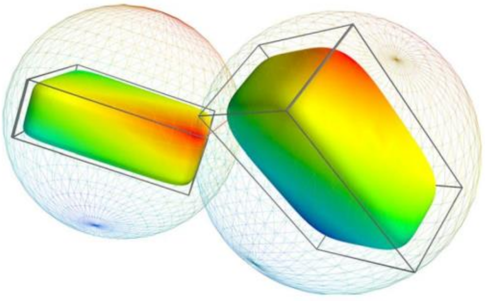
$$\left[\left(\frac{x}{a_1}\right)^{\frac{2}{\varepsilon_2}} + \left(\frac{y}{a_2}\right)^{\frac{2}{\varepsilon_2}}\right]^{\frac{\varepsilon_2}{\varepsilon_1}} + \left(\frac{z}{a_3}\right)^{\frac{2}{\varepsilon_1}} = 1$$

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

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

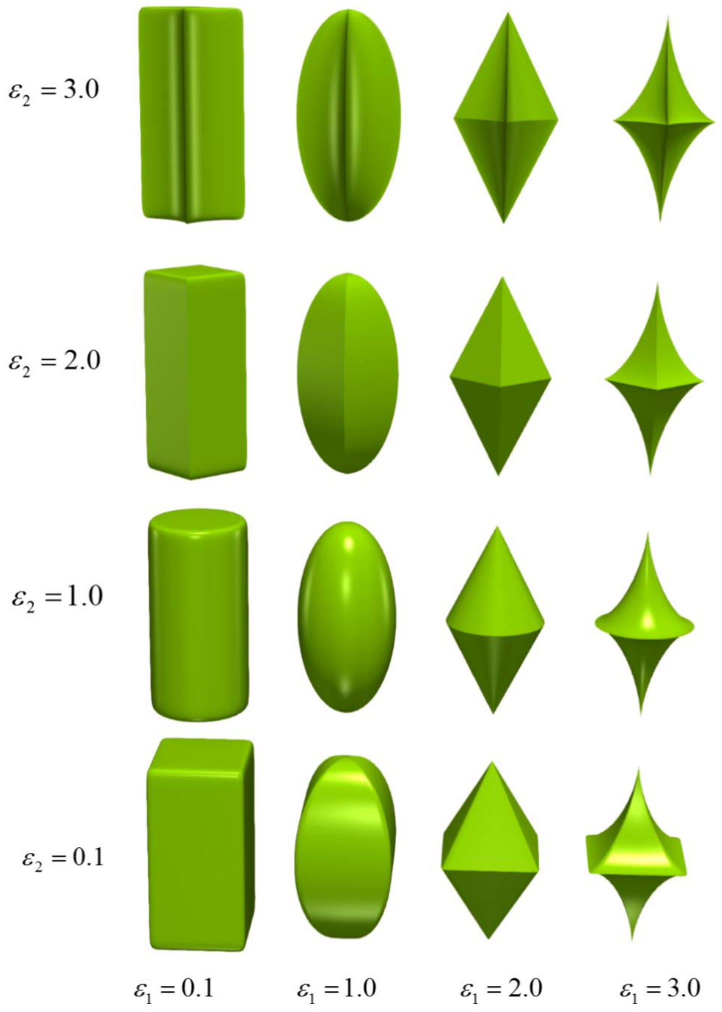
Semi-axis

roundness parameters



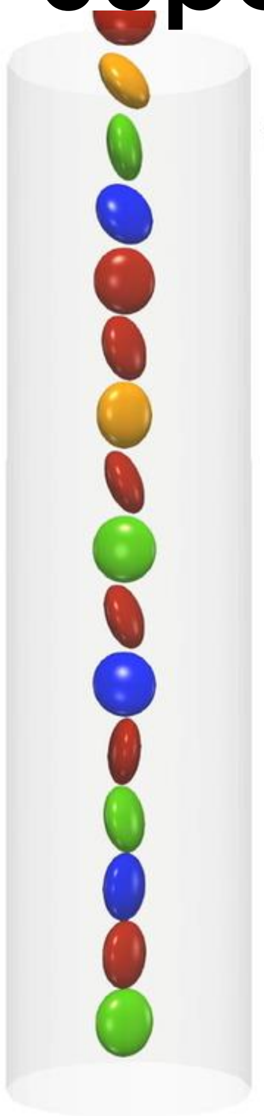
Bounding spheres and oriented bounding boxes

Superquadric particles

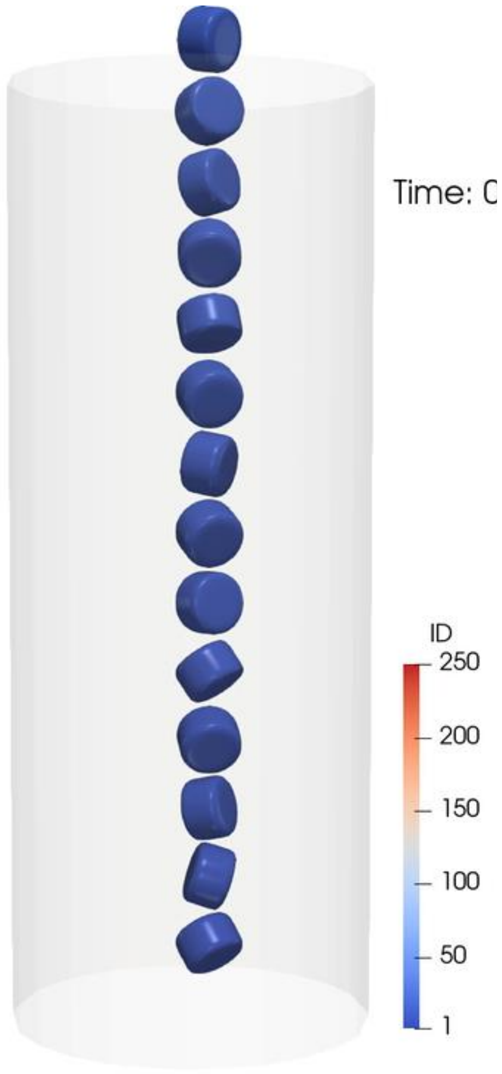


a1=2
a2=2
a3=4

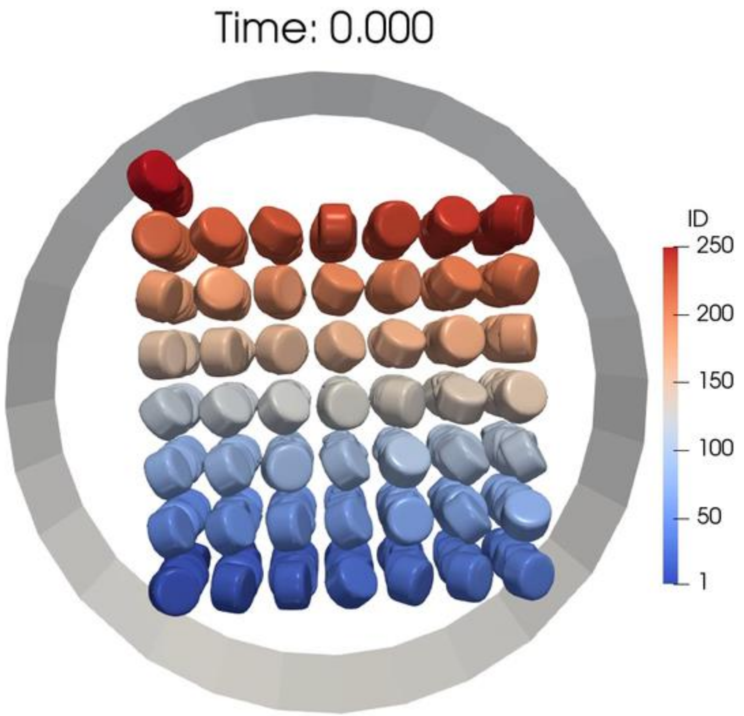
SuperDEM examples



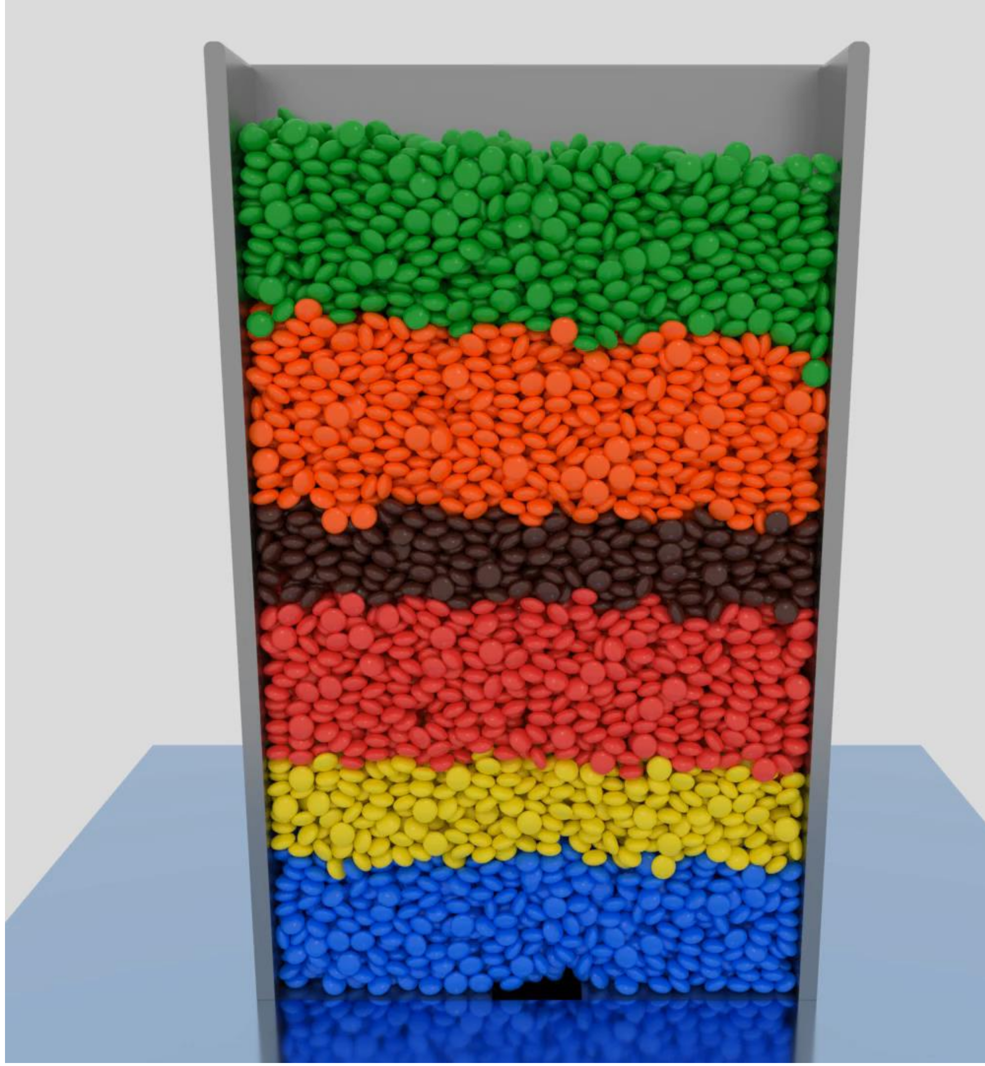
M&M candy
static packing



Cylinder candy
static packing

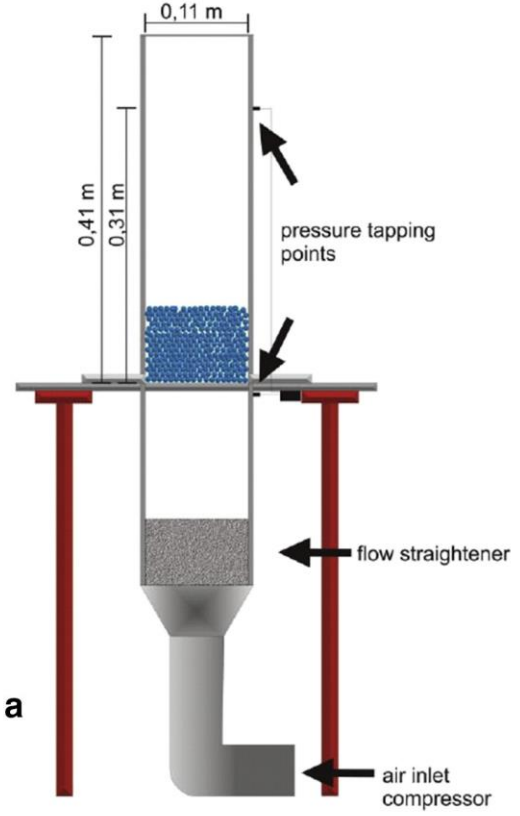


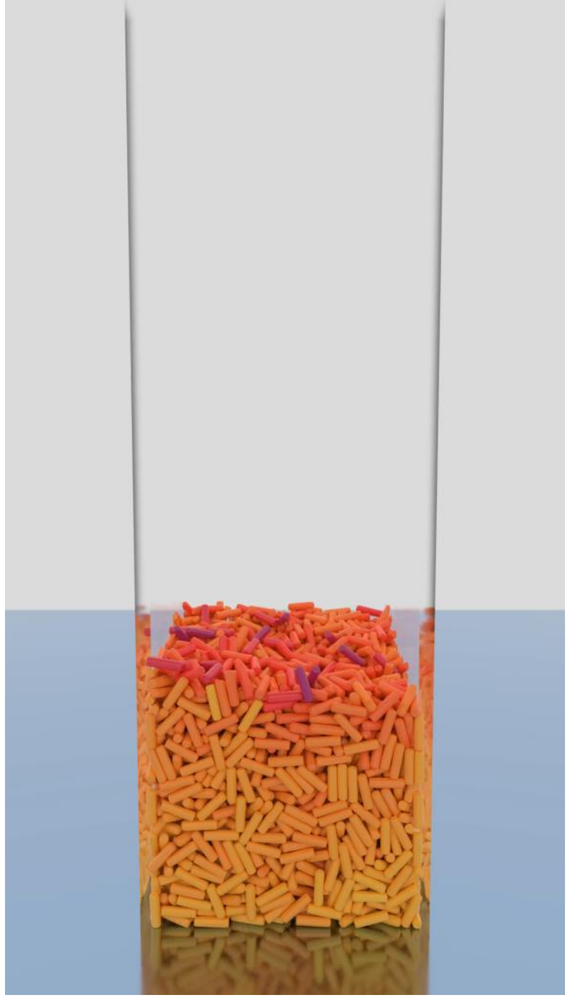
Cylinder rotating drum



M&M candy discharging from a hopper

Validation experiment



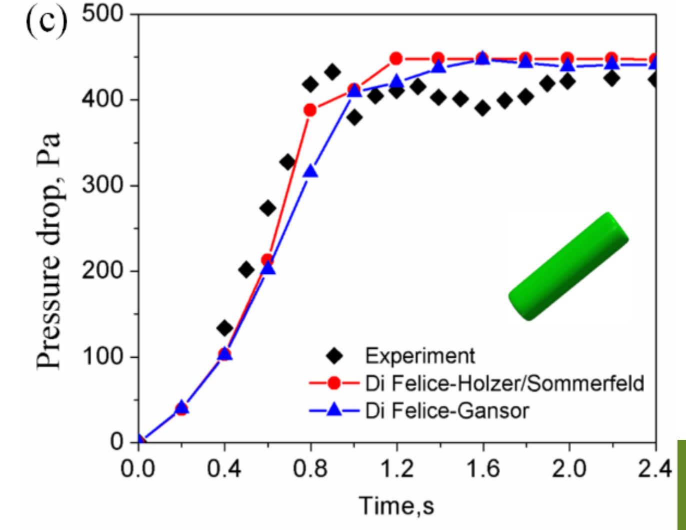


Particle properties including the volume equivalent diameter d_e-class, the particle dimensions, the sphericity ϕ, the particle density ρ_p, the bed height L and the averaged porosity ε for the initial, unfluidized setup.

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

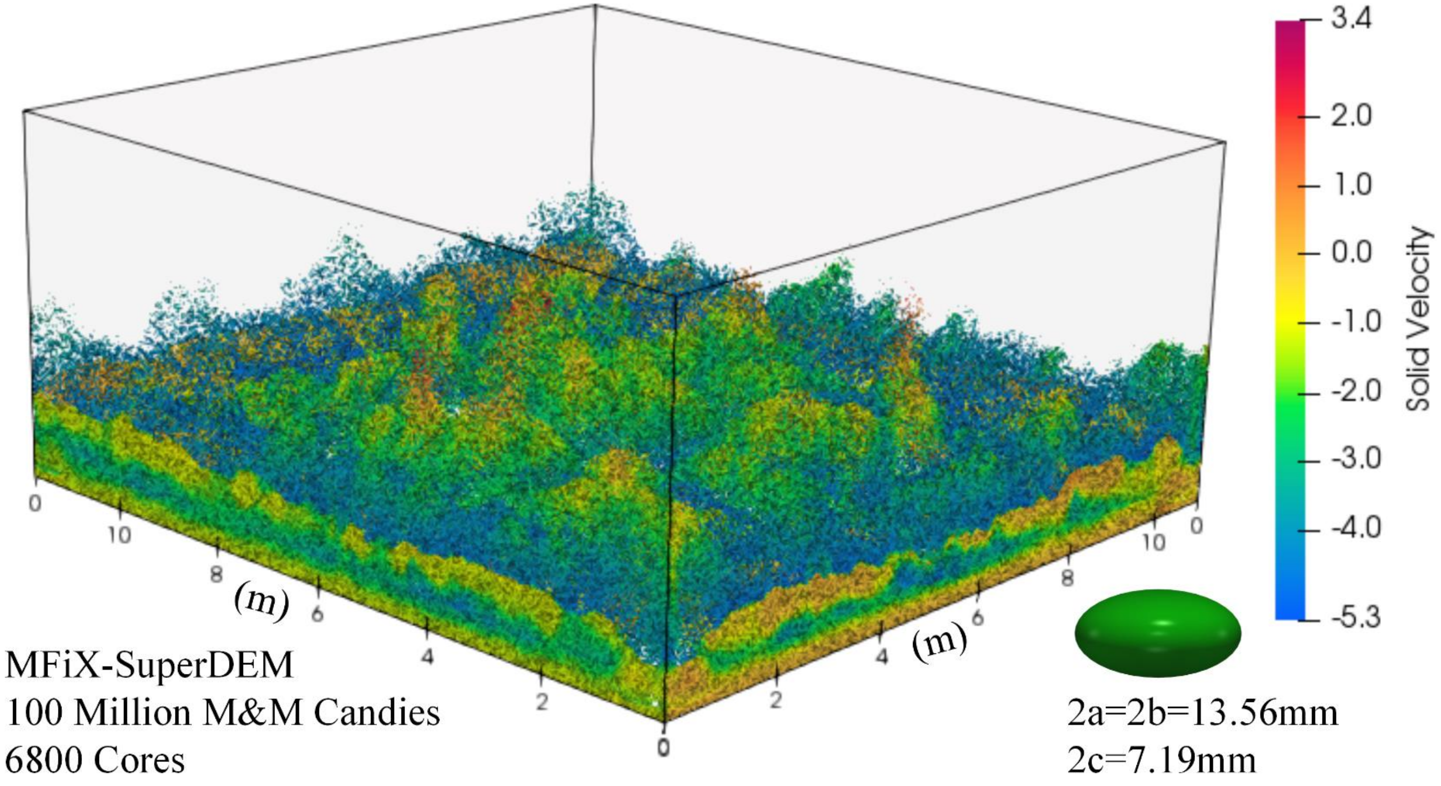
Shape	Elongated Cylinder	Elongated Cuboid	Elongated Cuboid	Plate	Elongated Plate
d_e–class [mm]	7	5	7	5	5
Size [mm]	3.9 14.0	3.0 3.0 7.1	4.2 4.2 11.4	2.0 4.9 6.0	2.0 4.0 8.0
ϕ [–]	0.75	0.75	0.73	0.71	0.69
ρ_p [kg/m³]	764.4	745.6	639.7	754.1	756.6
L_{fb} [mm]/$\bar{\varepsilon}$ [–]	103 0.44	103 0.42	115 0.40	102 0.43	108 0.46

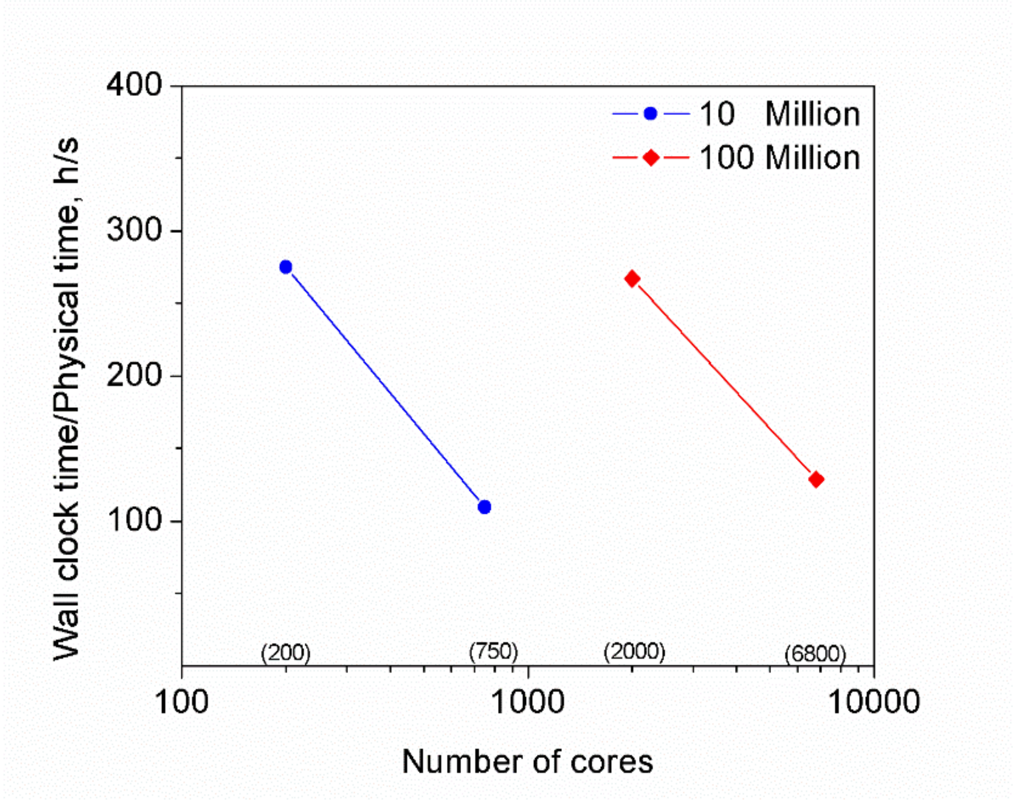
Shape	Elongated Cuboid	Plate
d_e–class [mm]	5	7
Size [mm]	2.0 3.0 11.0	2.2 9.0 9.8
ϕ [–]	0.64	0.63
ρ_p [kg/m³]	728.1	672.8
L_{fb} [mm]/$\bar{\varepsilon}$ [–]	117 0.48	121 0.46



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.

Massively Parallel SuperDEM Simulation





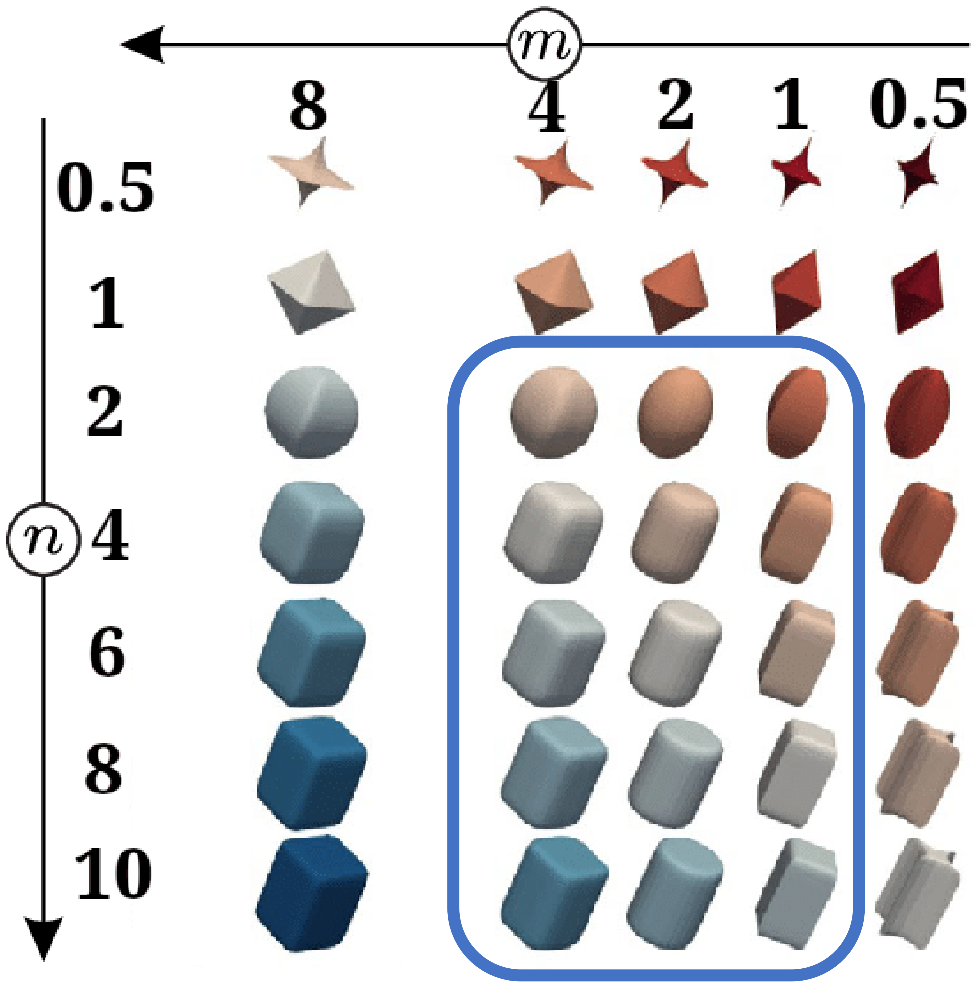
- The solver was parallelized using MPI.
- Simulation on NETL supercomputer Joule 2 (80K cores) , World Top 60, 2020
- Non-spherical particles fluidization simulation, 100 million (6800 cores)

SuperDEM

Non-spherical particles code acceleration

$$\left(\left|\frac{x}{a}\right|^m + \left|\frac{y}{b}\right|^m\right)^{n/m} + \left|\frac{z}{c}\right|^n$$

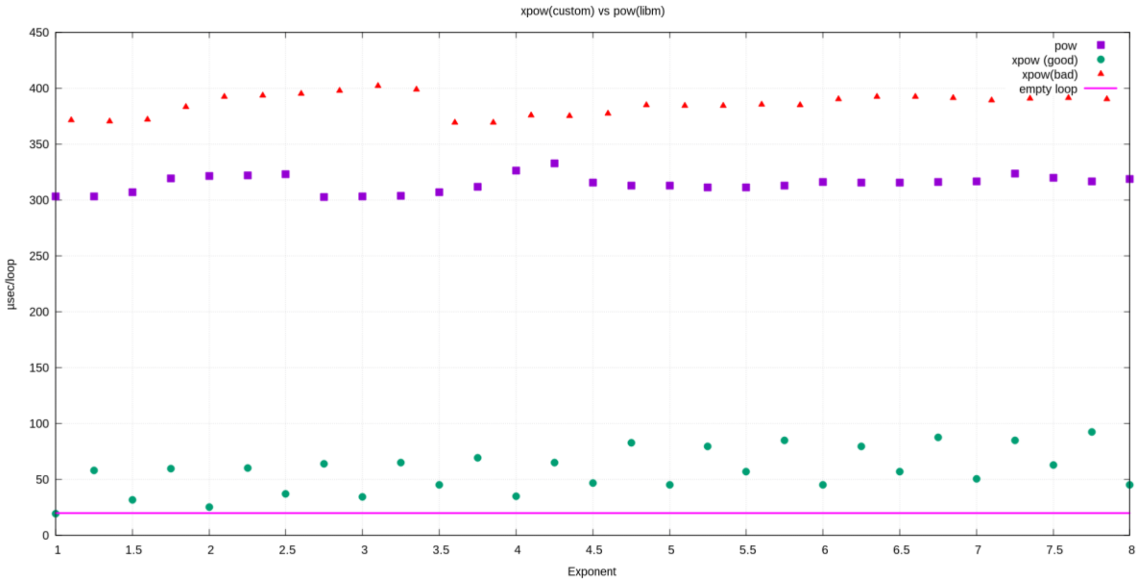
- Need to compute x^y for non-integer x *and* y.
- Range $0 \le x \le 2$ *and* $y \ge 1$.
- 70% code spent on exponentiations
- Integer powers and square roots are computationally inexpensive
- We can compute certain powers quickly, e.g $x^{2.5}$ is x*x*sqrt(x) (not an approximation)
- Constrain m and n to be integers or dyadic rationals
- Does not guarantee that the ratio n/m is similarly nice
- Restricting values on m and n such that m,n and the ratio n/m are lead to an efficient exponent computations



SuperDEM

Non-spherical particles code acceleration

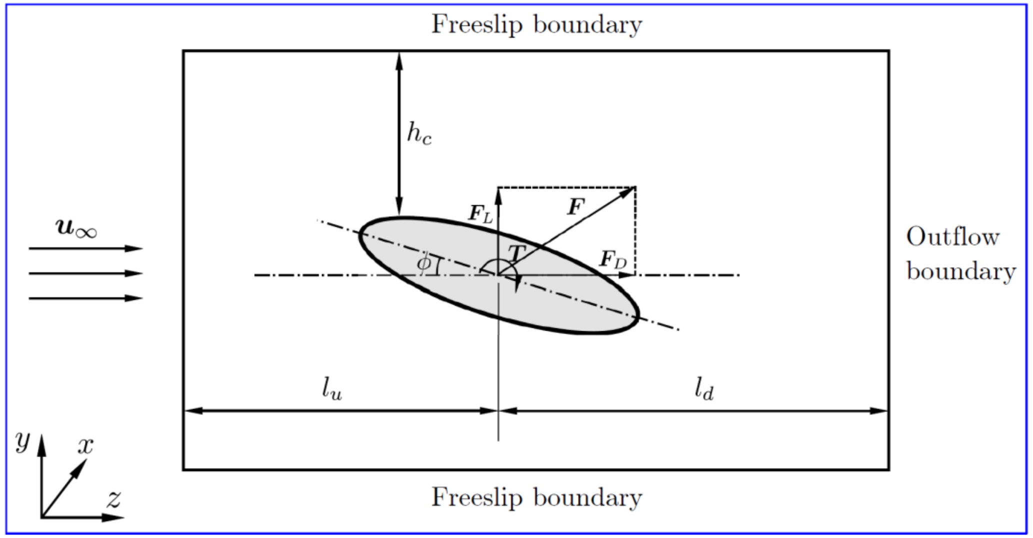
- Prototype function xpow
- Checks for integer exponents or exponents of the form a+b/4
- Efficient methods based on squaring and square roots
- 6x speedup compared with built-in math library
- Overall speedup on hopper benchmark is about 2.1x

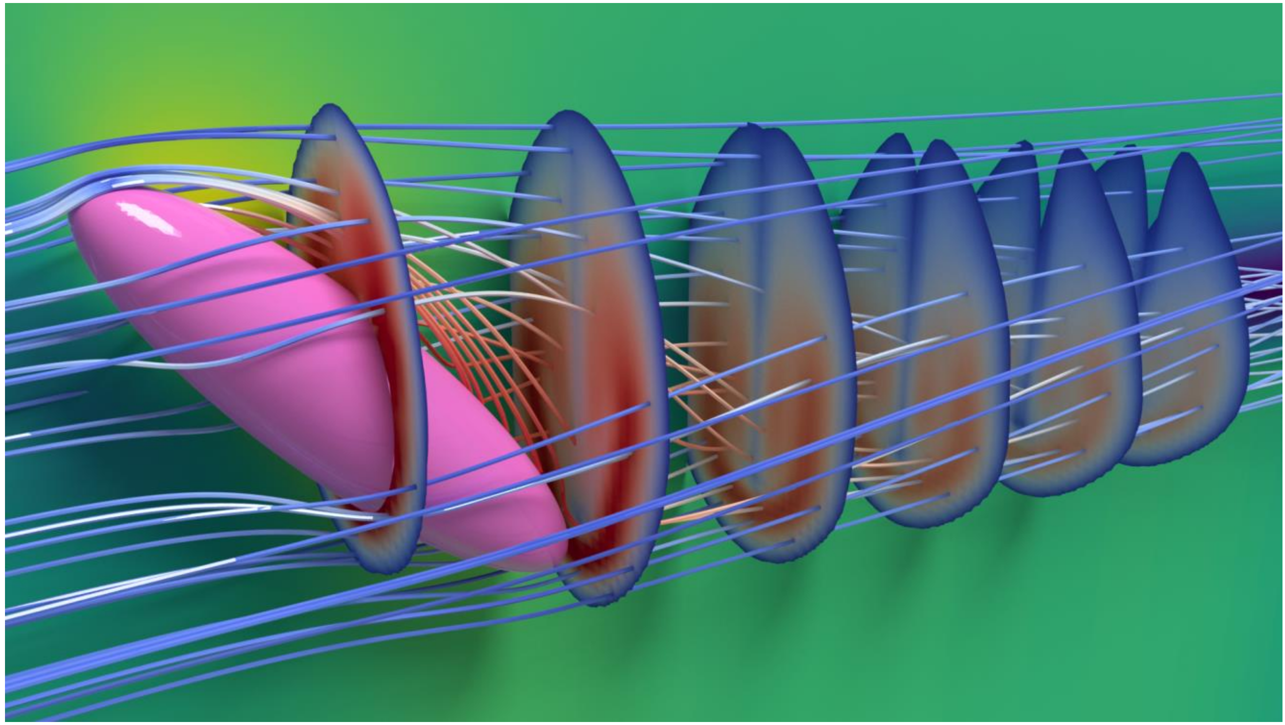


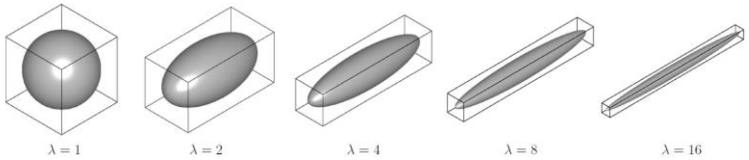
Non-spherical particle drag

Non-spherical particle drag law

- Detailed simulations of flow around prolate spheroids
- Lattice Boltzmann method (LBM).
- Reynolds numbers range $0.1 \leq Re \leq 2000$
- Incident angles $0° \leq \Phi \leq 90°$
- Aspect ratios $1 \leq \lambda \leq 16$.
- Accurate correlations for average drag, lift and torque coefficients are proposed.





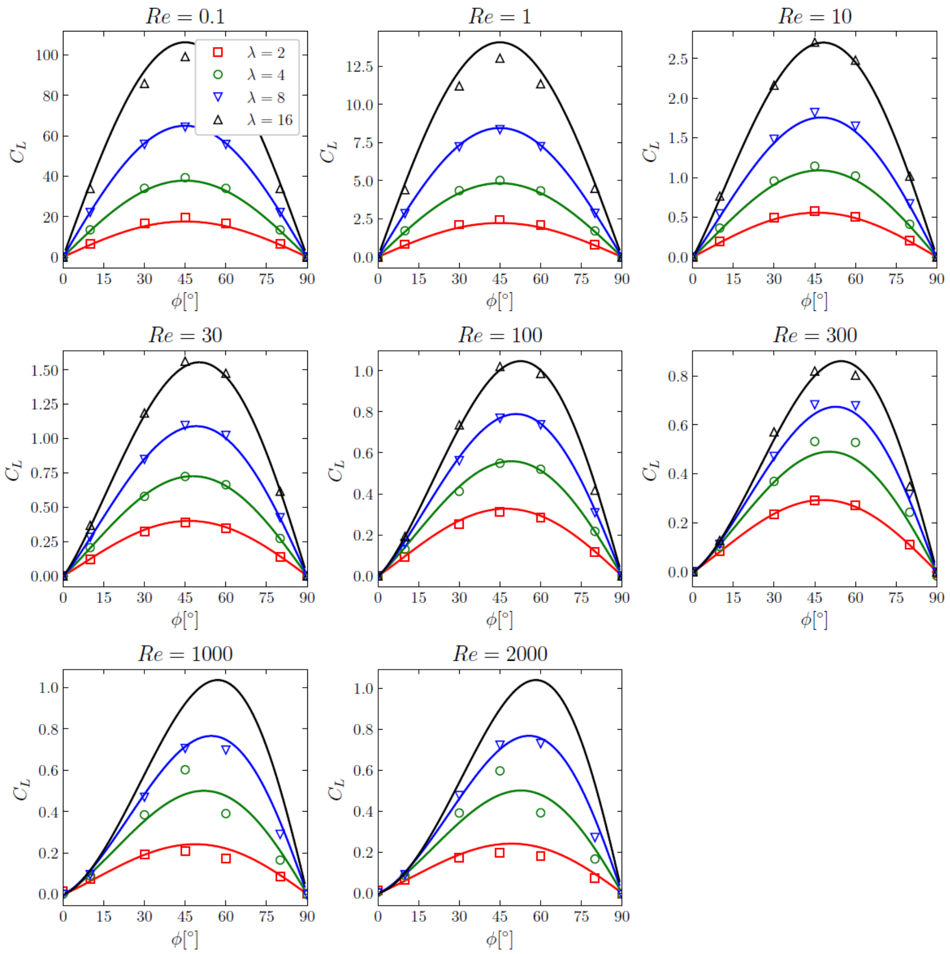


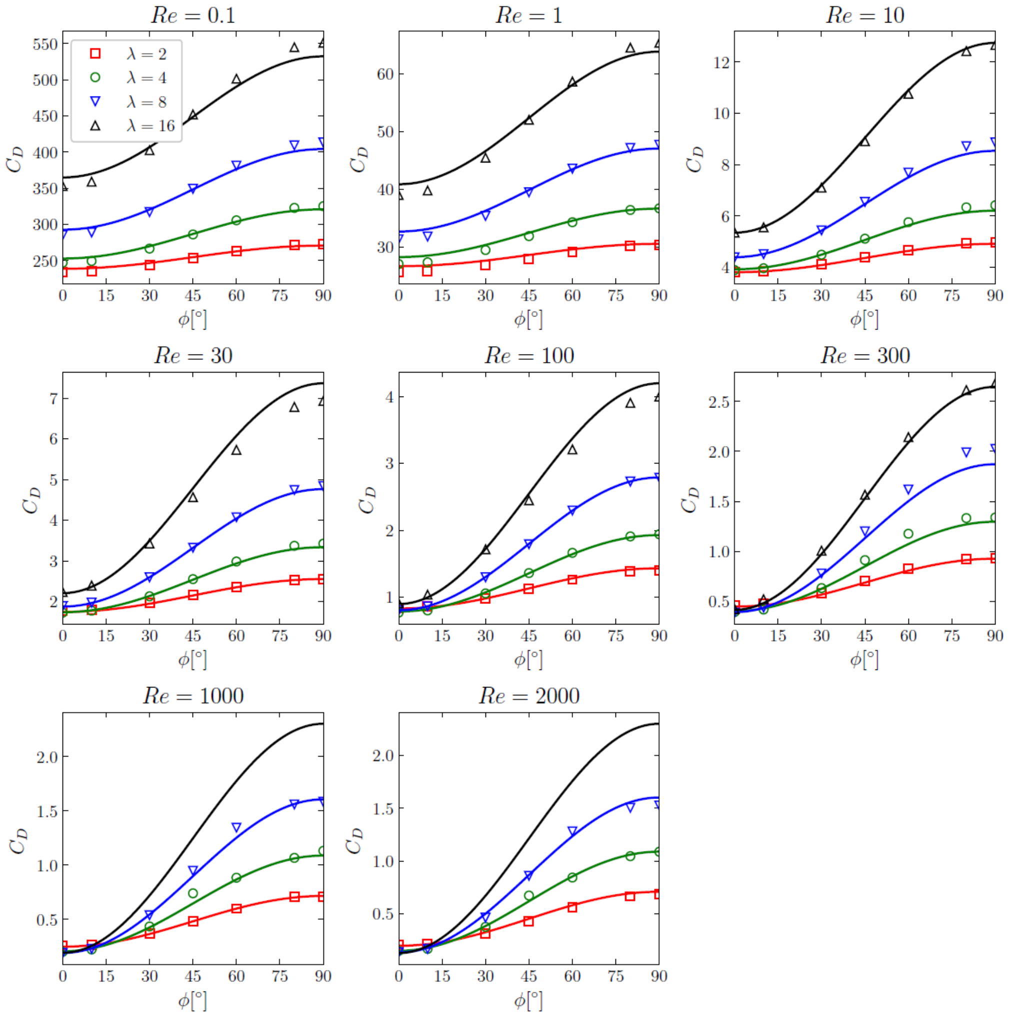
Sathish Sanjeevi, Jean-F. Dietiker, and Johan T. Padding, "Accurate hydrodynamic force and torque correlations for prolate spheroids from Stokes regime to high Reynolds numbers ", accepted for publication, Chemical Engineering Journal

Non-spherical particle drag

Non-spherical particle drag law

Lift and drag





Non-spherical particle drag

Non-spherical particle drag law

Lift and drag

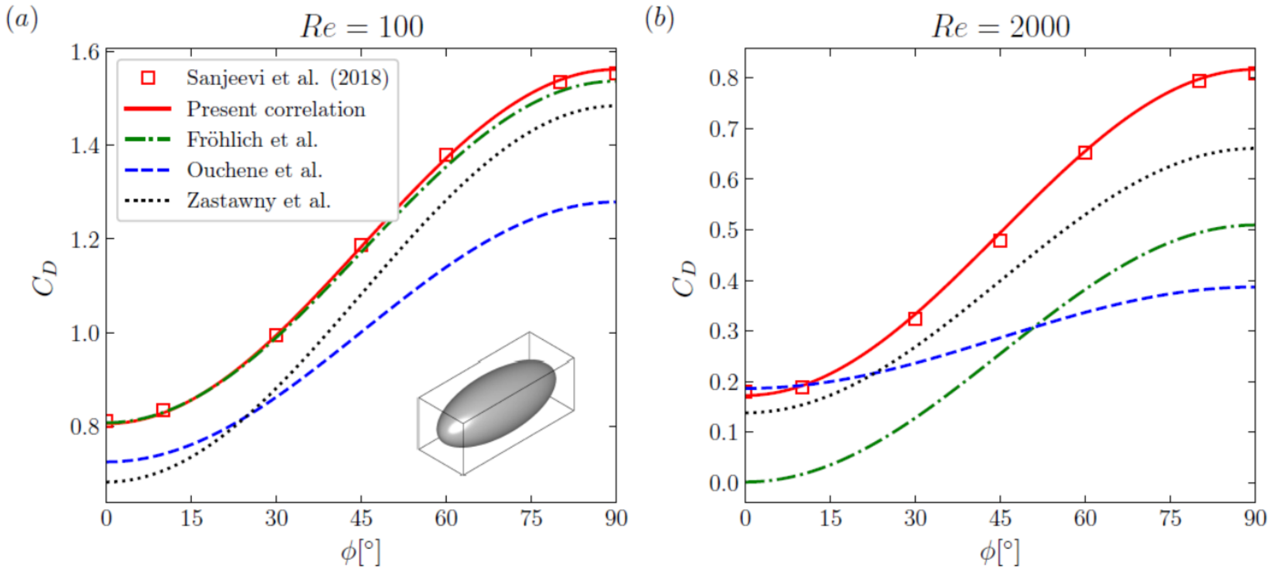


Figure 12: Comparison of C_D against ϕ for $\lambda = 2.5$ at (a) $Re = 100$ and (b) $Re = 2000$.

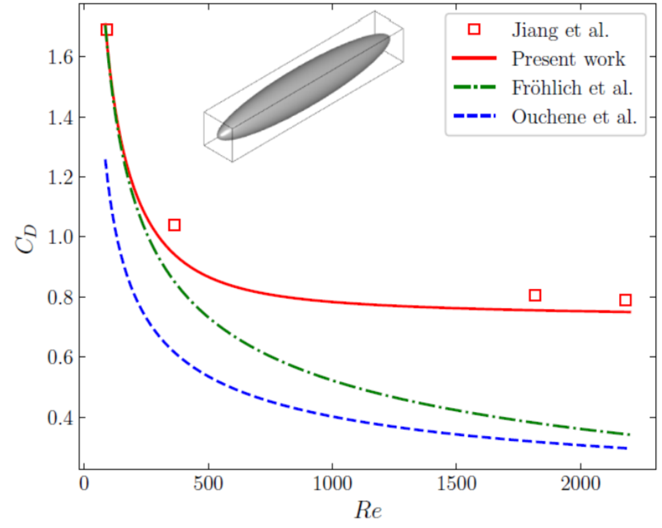
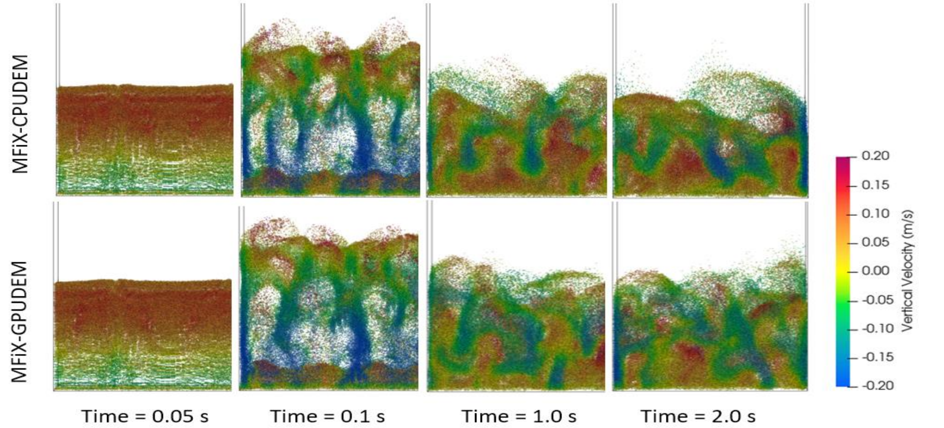


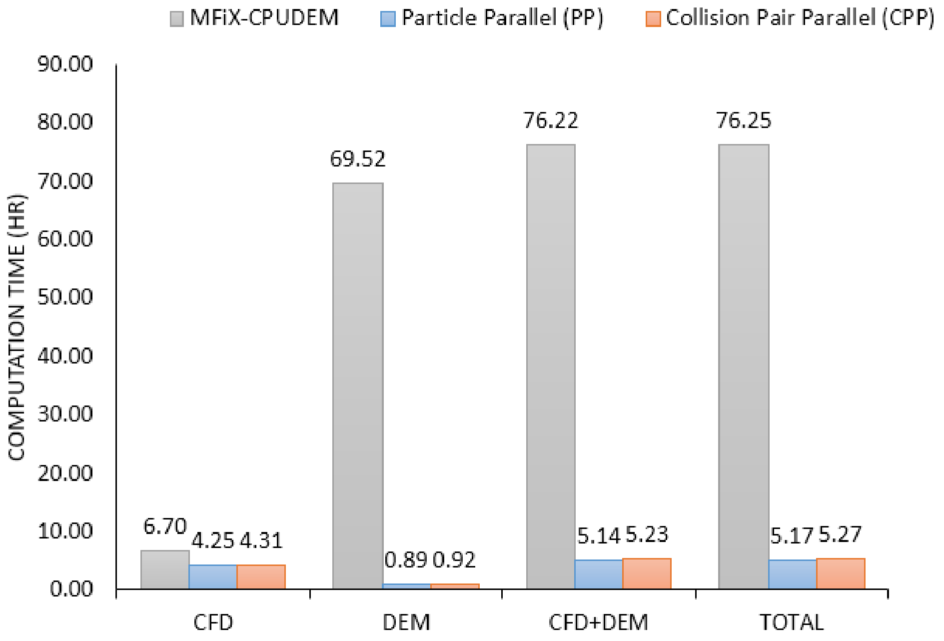
Figure 13: Comparison of C_D for a particle of $\lambda = 6$ at $\phi = 45°$ from different correlations with the DNS data of Jiang et al. [21, 22].

Hundredfold Speedup of MFiX-DEM using GPU

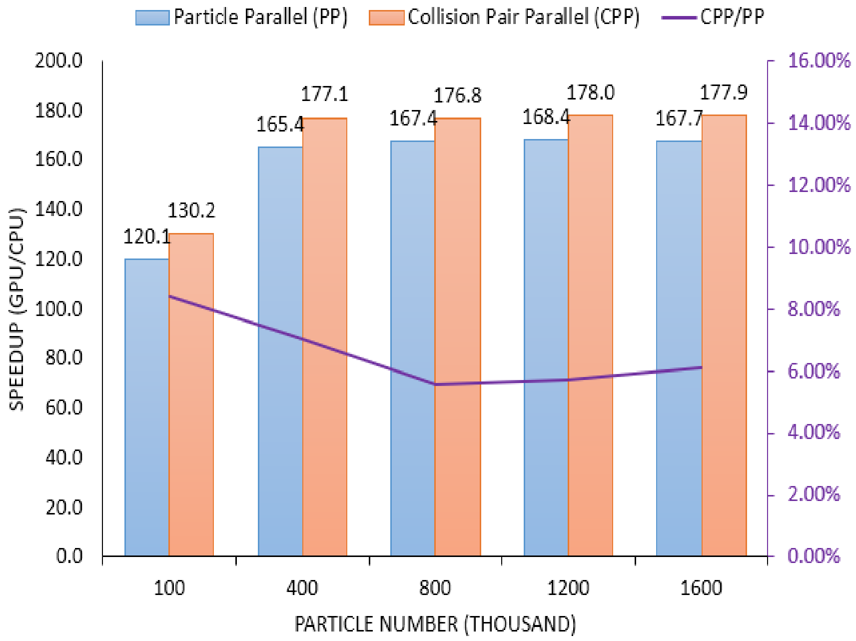
DEM solver was ported to GPU (prototype)

- 170 fold speedup with double precision, 243 fold with single precision
- Re-use CFD, interphase coupling, and chemical reaction modules in MFiX

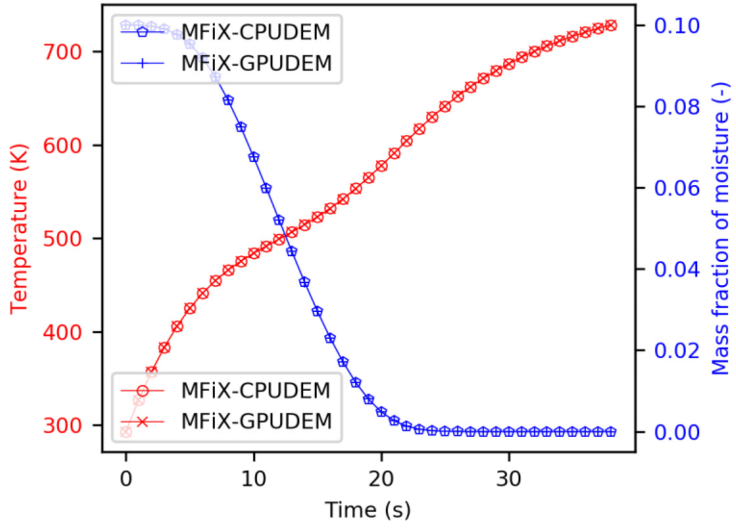




Fluidized bed Speedup



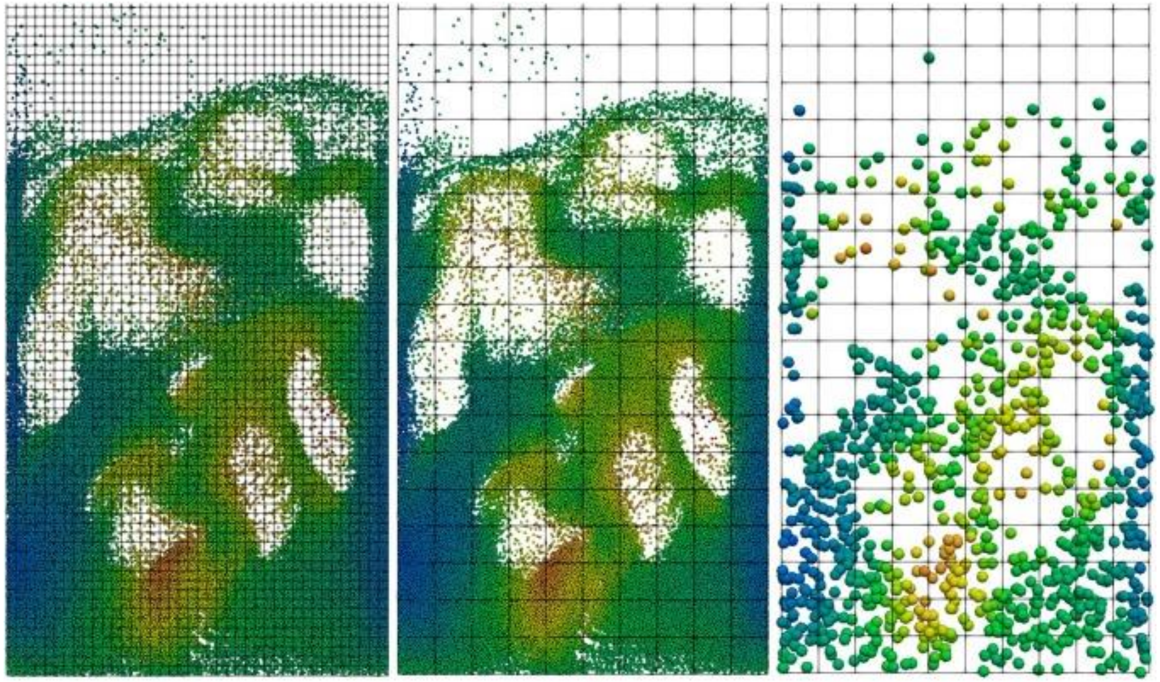
Particle packing Speedup



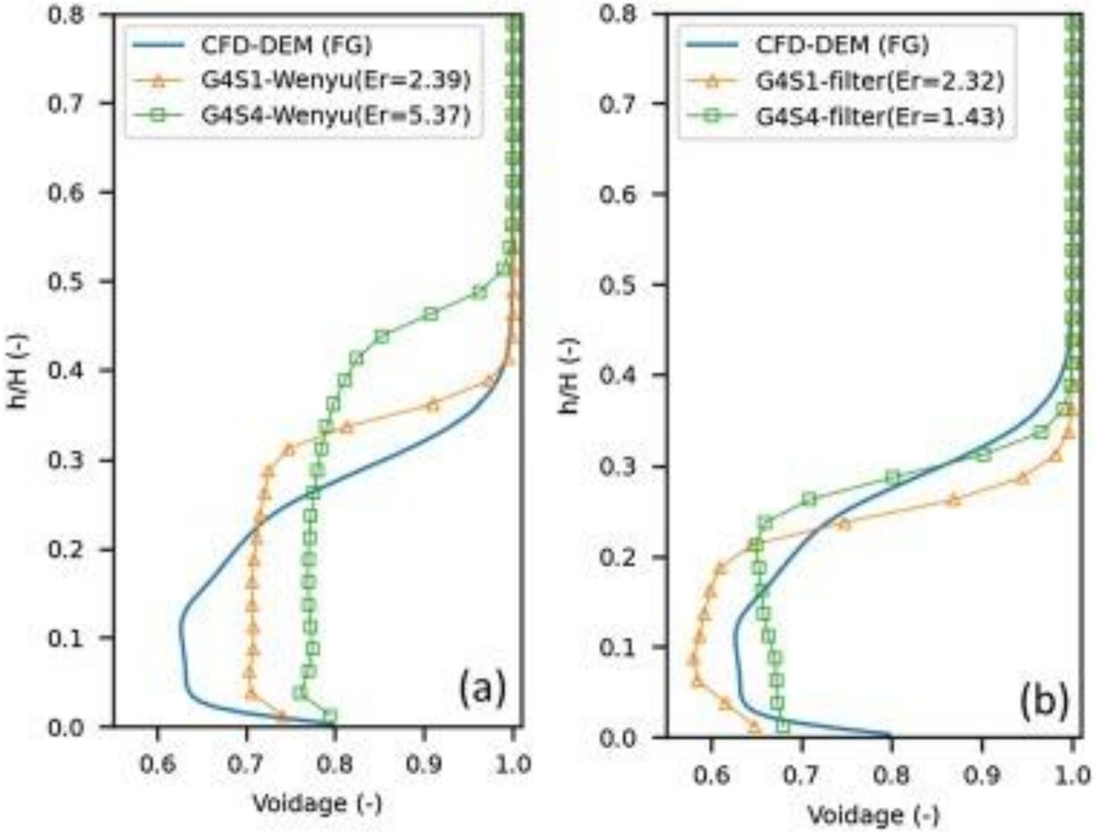
Heat transfer & chemical reactions (biomass drying)

Hundredfold Speedup of MFiX-DEM using GPU

Effect of coarse graining



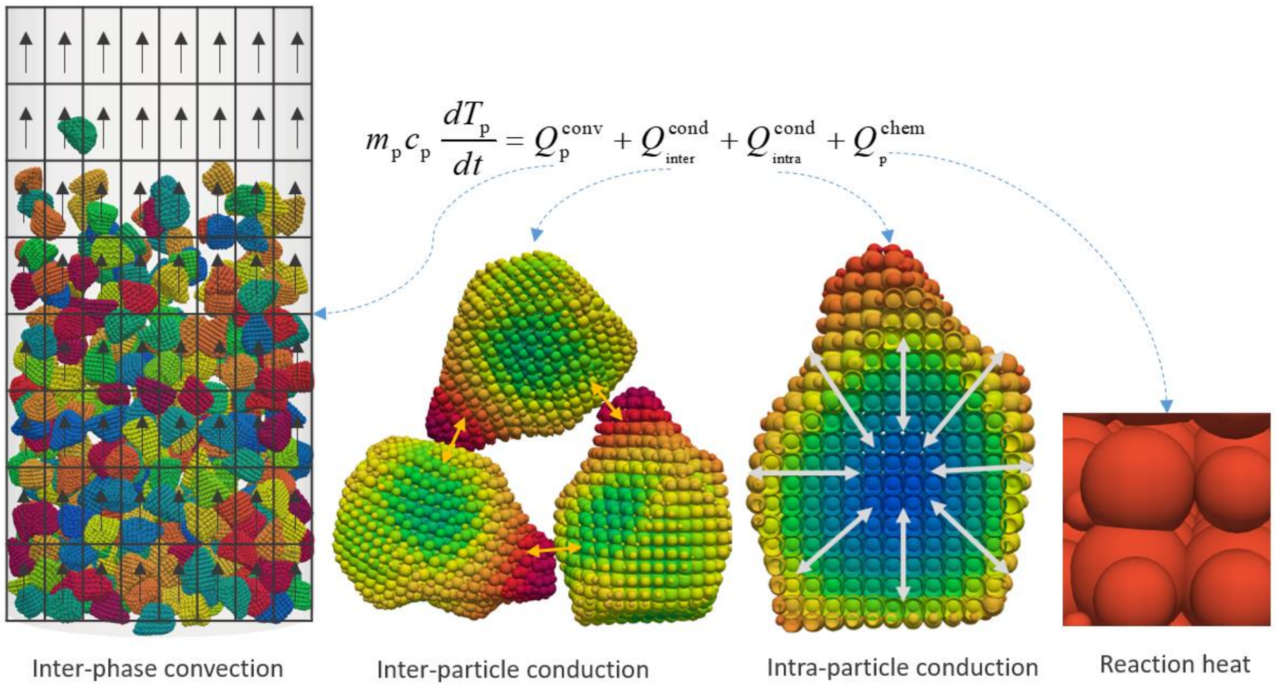
(a) Fine grid CFD-DEM (b) Fluid Coarse-graining (c) Fluid-Particle Coarse-graining



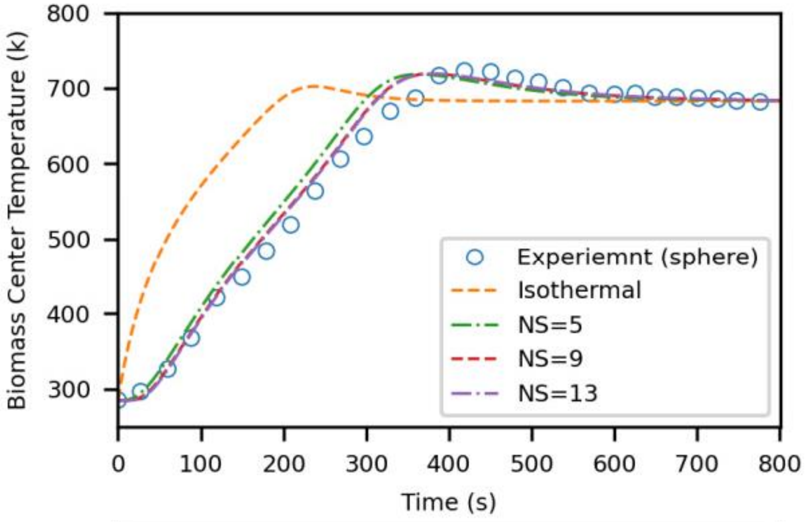
Glued-sphere DEM

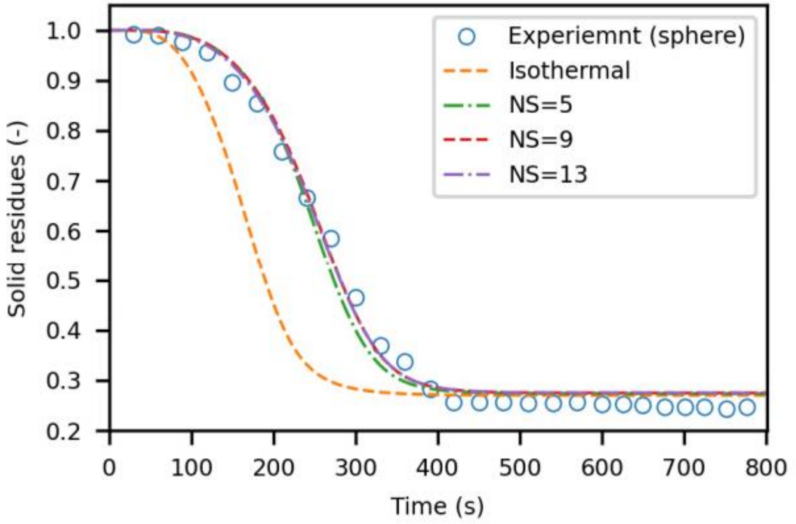
Irregular Shape of Particles

- Composite spheres
- Intra-particle temperature distribution



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





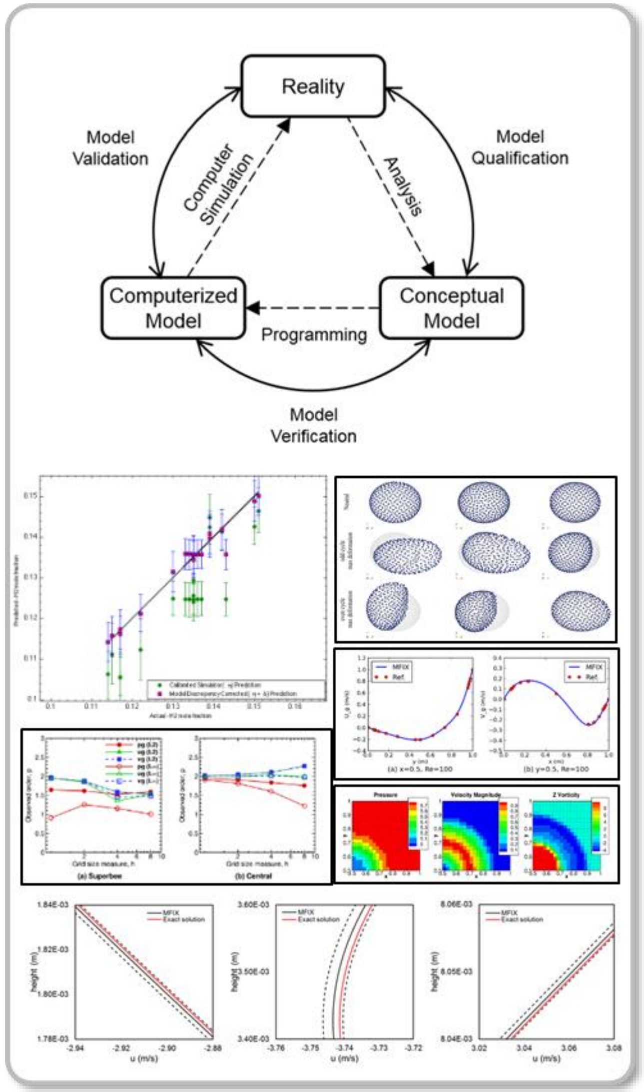
MFiX Quality Assurance

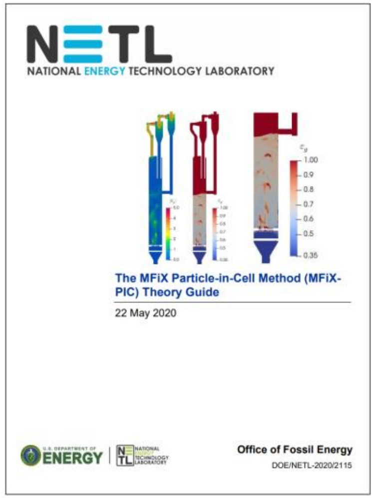
Building Confidence in Simulation Results

- **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 (https://mfix.netl.doe.gov/mfix/mfix-documentation**)**

- 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

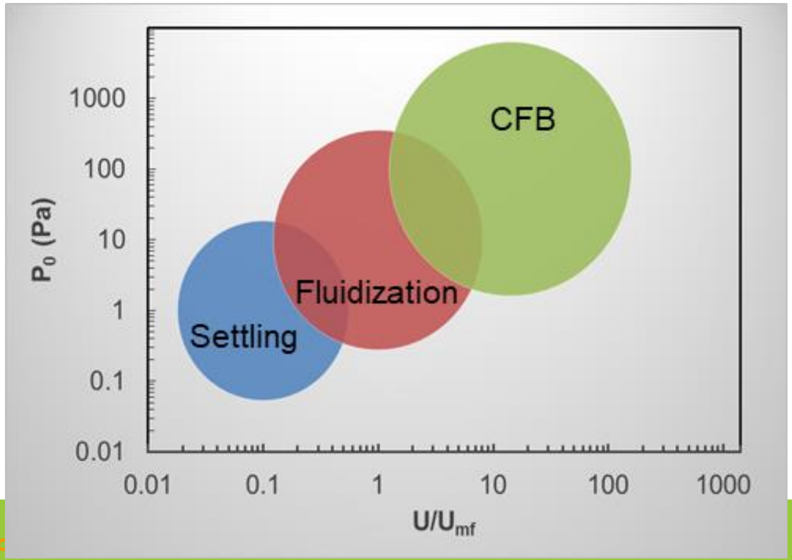
Cases selected to cover a broad range of flow conditions

- 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: $U/U_{mf} >> 1.0$ ($P_0 \sim 100$)

Parcel momentum equation

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

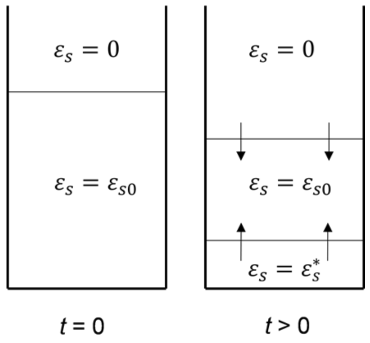
$$\tau_p = \frac{P_0 \varepsilon_p^{\beta}}{\max\left(\varepsilon_{cp} - \varepsilon_p, \delta(1 - \varepsilon_p)\right)}$$

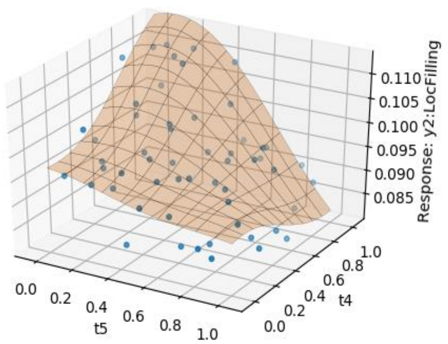


C1: Particle settling

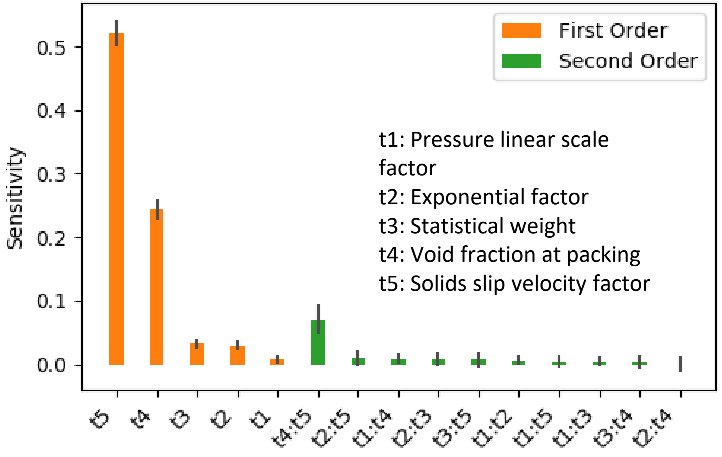
Sensitivity analysis and Deterministic calibration

- Response surface(55 samples)
- Sobol indices show:
  - main effects (first oder)
  - interactive effects (second order)





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

MFiX Development

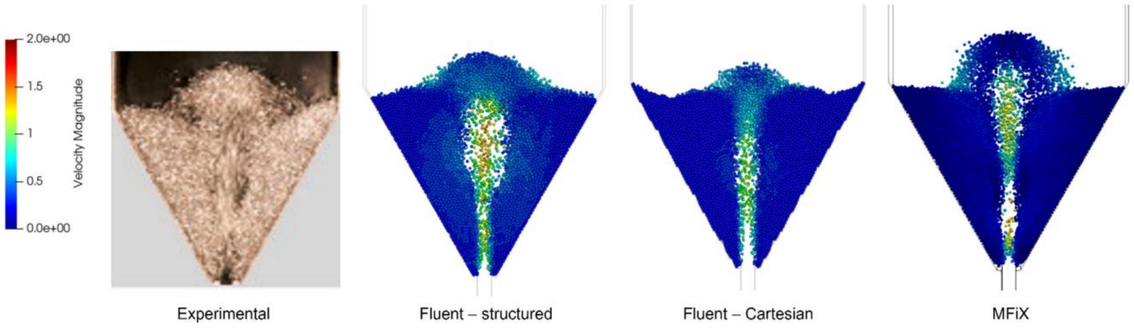
EY22 plans

- Validation and formal release of superDEM particle capability
  - **Step-change** from the typical approximation of spherical particle shape
  - Code optimization for faster turn-around time on large supercomputing systems
  - These capabilities allow for accurate modeling of mixed feedstocks of large, reacting particles
- Validation and Formal release of multiphase radiation modeling capability
  - This work incorporates the development work performed by University of Wyoming under NETL support
  - New radiation models available for all multiphase modeling approaches (TFM, DEM, PIC)
  - Enhanced accuracy of heat transfer in high temperature FE reactors
- Development of conjugate heat transfer capability in MFiX
  - Accurate modeling of internal heat transfer surfaces critical to industrial scale reactors
  - Critical capability for Hydrogen production and Oxygen separation technologies
- Continued development of the Graphical User Interface (GUI)
  - Improved usability, reduced user setup error, faster overall workflow
  - Contributes to a larger MFiX community worldwide and better visibility of NETL's multiphase modeling expertise
- Continued Verification and Validation efforts
  - Improved confidence in new implemented models
  - Documentation of parameters sensitivity and best practices for simulation setups

Comparison with other codes

MFiX – Ansys Fluent (2021)

Marchelli, F.; Di Felice, R. A Comparison of **Ansys Fluent** and **MFiX** in Performing CFD-DEM Simulations of a Spouted Bed. Fluids **2021**, 6, 382. https://doi.org/ 10.3390/fluids6110382



"Both programs can provide acceptable qualitative predictions when employing standard settings. If the Di Felice drag model is applied, MFiX yields better results and provides a very good quantitative reproduction of the experimental particle velocity profile. Moreover, despite employing similar mesh and time steps and the same number of particles, MFiX is about 17 times faster. However, Fluent seems to respond slightly more efficiently to an increase in the particle number and appears to have better parallelisation functionalities. "

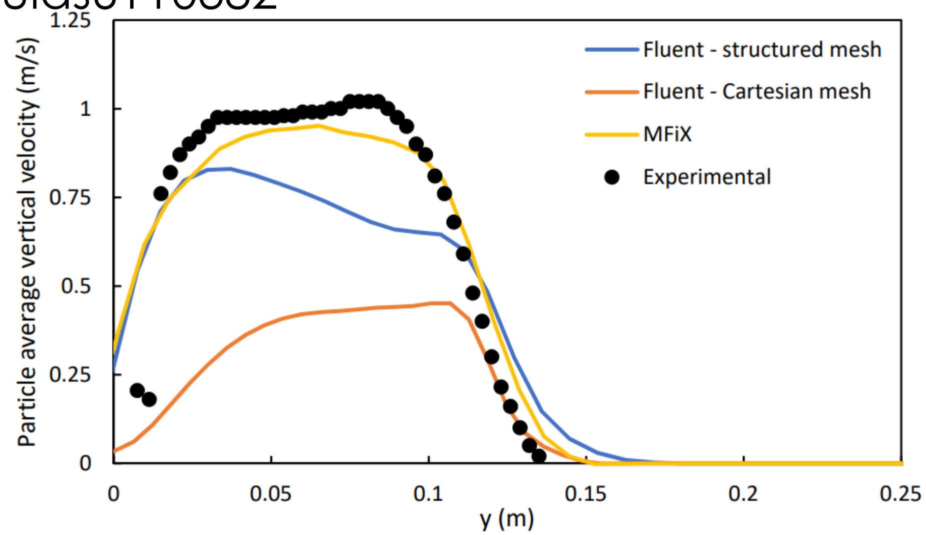


Figure 6. Time-averaged vertical profiles of the particles' vertical velocity when employing the Di Felice drag model.

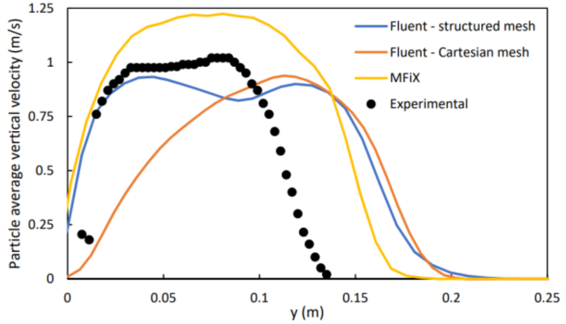


Figure 3. Time-averaged vertical profiles of the particles' vertical velocity when employing the Gidaspow drag model.

MFiX publications

Publications/ Presentations

- 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, Li, Cheng, Ashfaq, Huda, Rowan, Steven L, Rogers, William A, and Wu, Xiongjun. Geometric Scale-up Experiments on Fluidization of Geldart B Glass Beads. United States: N. p., 2020. Web. doi:10.2172/1648031.
- 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.
- Gel, Aytekin, Vaidheeswaran, Avinash, & Clarke, Mary Ann (2021). Deterministic Calibration of MFiX-PIC, Part 1: Settling Bed. NETL Technical Report Series; U.S. Department of Energy, National Technology Laboratory: Morgantown, WV, 2021; p. 72. https://doi.org/10.2172/1764832
- Vaidheeswaran, A., Gel, A., Clarke, M. A., & Rogers, W. A., “Assessment of model parameters in MFiX particle-in-cell approach”, Advanced Powder Technology, Vol. 32 (8), 2021, 2962-2977, https://doi.org/10.1016/j.apt.2021.06.011.
- Gel, A.; Weber, J.; Vaidheeswaran, A. Sensitivity Analysis of MFiX-PIC Parameters Using Nodeworks, PSUADE, and DAKOTA; DOE.NETL-2021.2652; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2021; p 52. https://edx.netl.doe.gov/dataset/sensitivity-analysis-of-mfix-pic-parameters-using-nodeworks-psuade-and-dakota, DOI: 10.2172/1809024.
- Lu, L., “GPU accelerated MFiX-DEM simulations of granular and multiphase flows”, Particuology, 2022, 62: 14-24, https://doi.org/10.1016/j.partic.2021.08.001
- Gel, A., Vaidheeswaran, A., Clarke, M., “Calibration of a particle-in-cell simulation model for gravitational settling bed application,” 2021 NETL Multiphase Flow Workshop, on-line, Morgantown, WV, August 2021.
- Gel, A., Weber, J., and Vaidheeswaran, A., “Sensitivity Analysis of MFiX-PIC Parameters Using Nodeworks, PSUADE, and DAKOTA”, 2021 NETL Multiphase Flow Workshop, on-line, Morgantown, WV, August 2021.
- Liqiang Lu, Xi Gao, Jean-François Dietiker, Mehrdad Shahnam, William A. Rogers, MFiX based multi-scale CFD simulations of biomass fast pyrolysis: A review, Chemical Engineering Science, Vol. 248, Part A, 2022, 117131, ISSN 0009-2509, https://doi.org/10.1016/j.ces.2021.117131.
- Liqiang Lu, Xi Gao, J.-F. Dietiker, Mehrdad Shahnam, William A. Rogers, Machine Learning Accelerated Discrete Element Modeling of Granular Flows, Chemical Engineering Science, 2021, 116832, ISSN 0009-2509, https://doi.org/10.1016/j.ces.2021.116832.
- Xi Gao, Jia Yu, Liqiang Lu, William A. Rogers, Coupling particle scale model and SuperDEM-CFD for multiscale simulation of biomass pyrolysis in a packed bed pyrolyzer. AIChE Journal, 2021, e17139. https://aiche.onlinelibrary.wiley.com/doi/abs/10.1002/aic.17139
- Xi Gao, Jia Yu, Ricardo J.F.Portal, Jean-François Dietiker, Mehrdad Shahnam, William A.Rogers, Development and validation of SuperDEM for non-spherical particulate systems using a superquadric particle method, Particuology, January 2021. ISSN 1674-2001, https://doi.org/10.1016/j.partic.2020.11.007.
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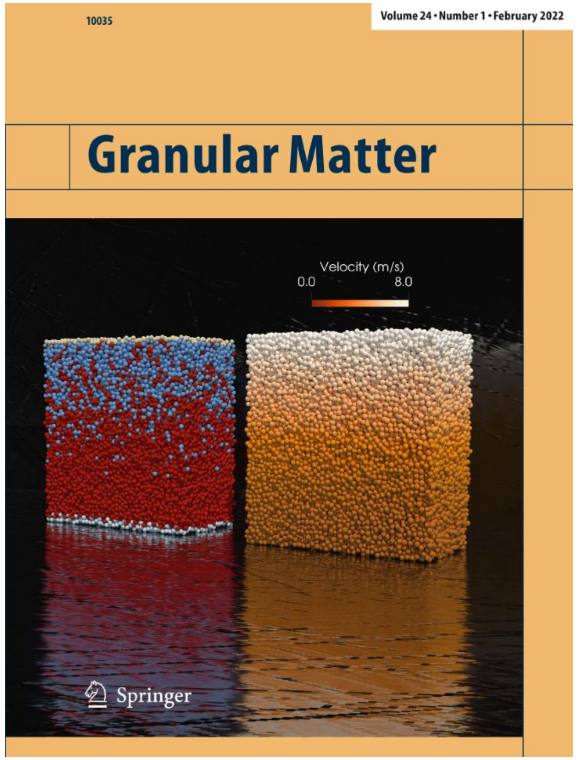
- Lu, L, Gao, X, Shahnam, M, Rogers, WA. Open source implementation of glued sphere discrete element method and nonspherical biomass fast pyrolysis simulation. AIChE J. 2021; 67:e17211. https://doi.org/10.1002/aic.17211
- Liqiang Lu, Xi Gao, Mehrdad Shahnam, William A. Rogers, Simulations of biomass pyrolysis using glued-sphere CFD-DEM with 3-D intra-particle models, Chemical Engineering Journal, Volume 419, 2021, 129564, ISSN 1385-8947, https://doi.org/10.1016/j.cej.2021.129564.

MFiX featured on Journal covers

NATIONAL ENERGY TECHNOLOGY LABORATORY

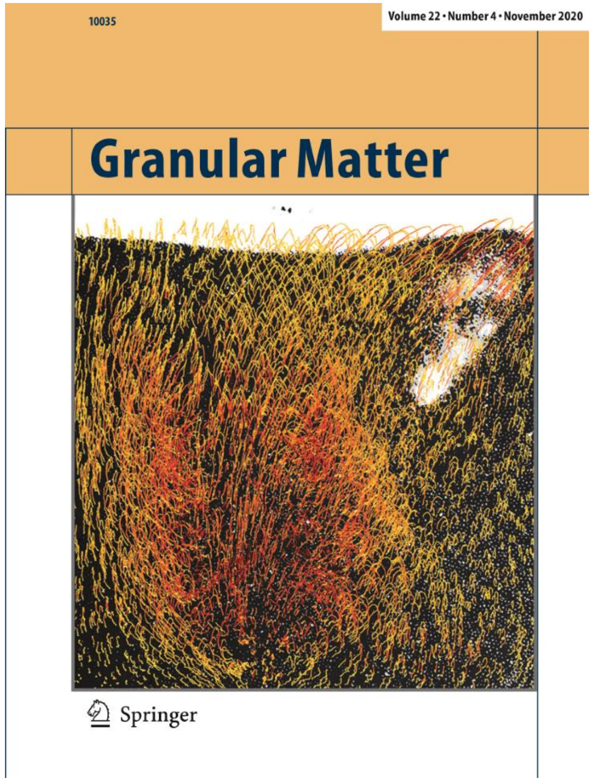


[Investigating the rheology of fluidized and non-fluidized gas-particle beds: implications for the dynamics of geophysical flows and substrate entrainment]()

By Breard C. P. Eric, Fullard Luke, Dufek Josef, Tennenbaum Michael, Fernandez-Nieves Alberto & Dietiker Jean-François

[GPU accelerated MFiX-DEM simulations of granular and multiphase flows]()

By L. Lu



[Using a proper orthogonal decomposition to elucidate features in granular flows]()

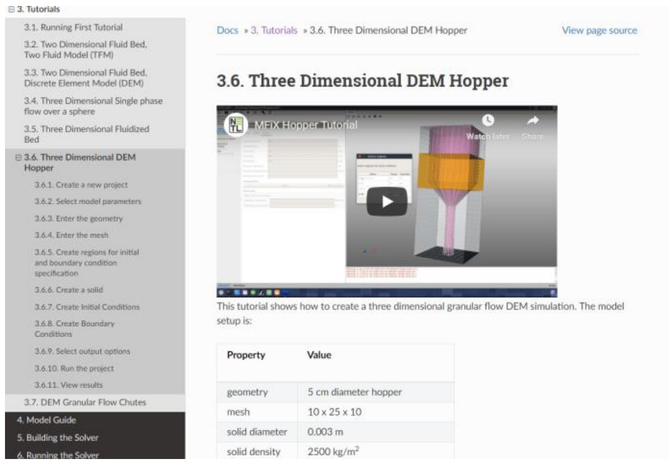
By J. E. Higham, M. Shahnam & A. Vaidheeswaran

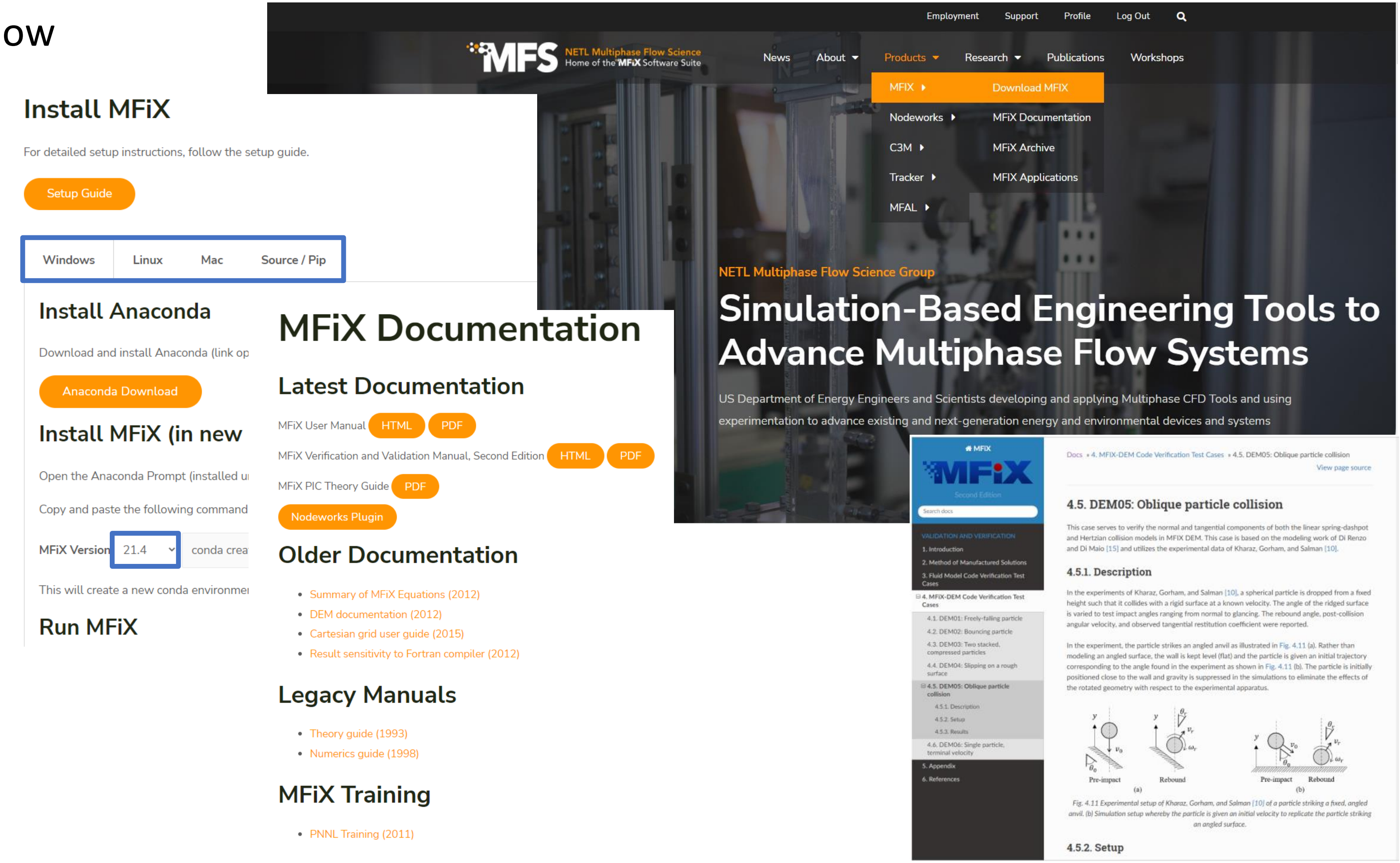
Resources – MFiX website

https://mfix.netl.doe.gov

NATIONAL ENERGY TECHNOLOGY LABORATORY

- Showcase NETL's Multiphase Flow Science (MFS) team
  - MFS software
  - Documentation
  - Forum
  - Experimental data (Challenge pbs)
  - Publications
  - Workshop proceedings
  - News, announcements





Resources – MFiX website

https://mfix.netl.doe.gov

NATIONAL ENERGY TECHNOLOGY LABORATORY

List of Publications

Sort by: Year (Newest to Oldest)

Total: 663

Publication Year 2022

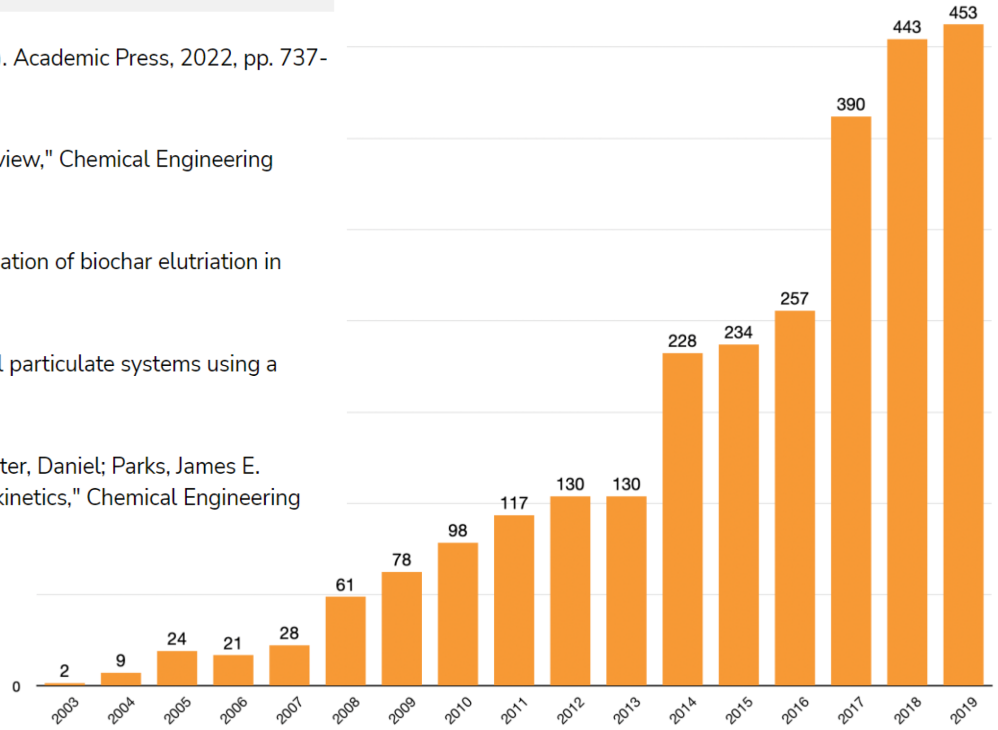
1. Modest, M. F. M., Sandip. "Chapter 20 - The Monte Carlo Method for Participating Media," Radiative Heat Transfer (Fourth Edition). Academic Press, 2022, pp. 737-773.

2. Lu, L. Q. G., X.; Dietiker, J. F.; Shahnam, M.; Rogers, W. A. "MFiX based multi-scale CFD simulations of biomass fast pyrolysis: A review," Chemical Engineering Science Vol. 248, 2022, p. 26.

3. Lu, L. Q. L., C.; Rowan, S.; Hughes, B.; Gao, X.; Shahnam, M.; Rogers, W. A. "Experiment and computational fluid dynamics investigation of biochar elutriation in fluidized bed," Aiche Journal Vol. 68, No. 2, 2022, p. 11.

4. Gao, X. Y., J.; Portal, R. J. F.; Dietiker, J. F.; Shahnam, M.; Rogers, W. A. "Development and validation of SuperDEM for non-spherical particulate systems using a superquadric particle method," Particuology Vol. 61, 2022, pp. 74-90.

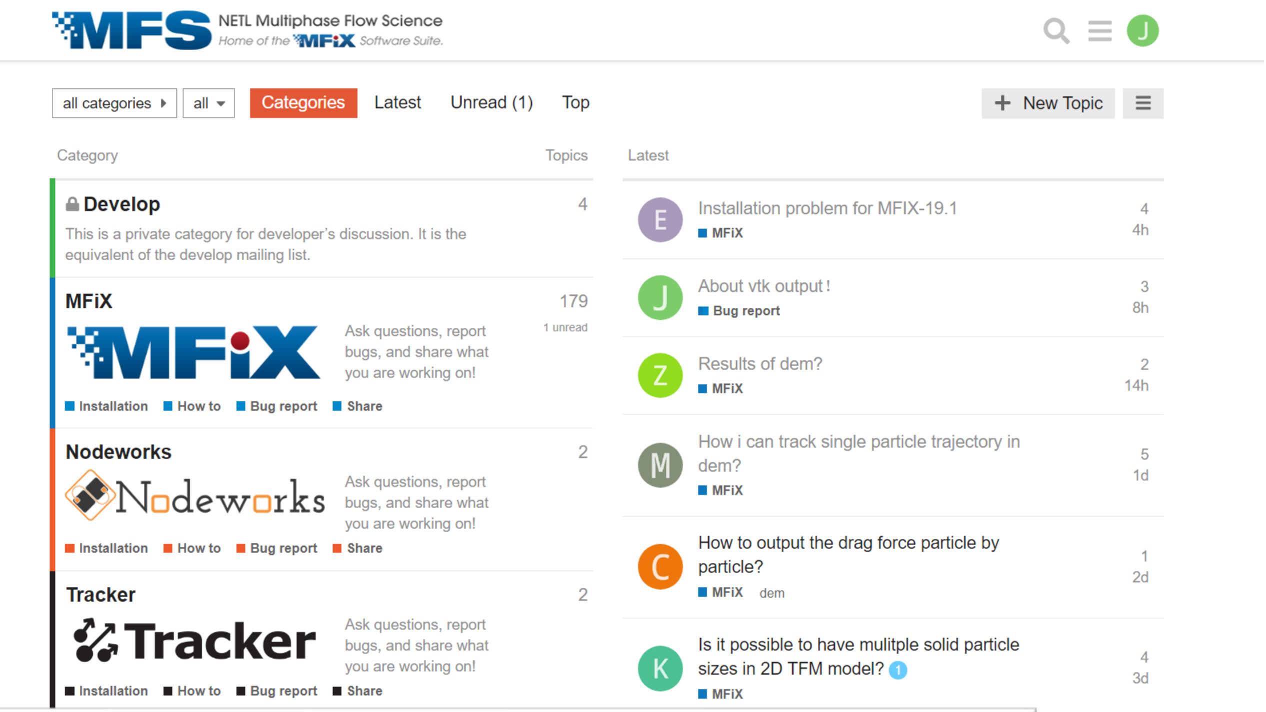
5. Lu, L. Brennan Pecha, M.; Wiggins, Gavin M.; Xu, Yupeng; Gao, Xi; Hughes, Bryan; Shahnam, Mehrdad; Rogers, William A.; Carpenter, Daniel; Parks, James E. "Multiscale CFD simulation of biomass fast pyrolysis with a machine learning derived intra-particle model and detailed pyrolysis kinetics," Chemical Engineering Journal Vol. 431, 2022, p. 133853.

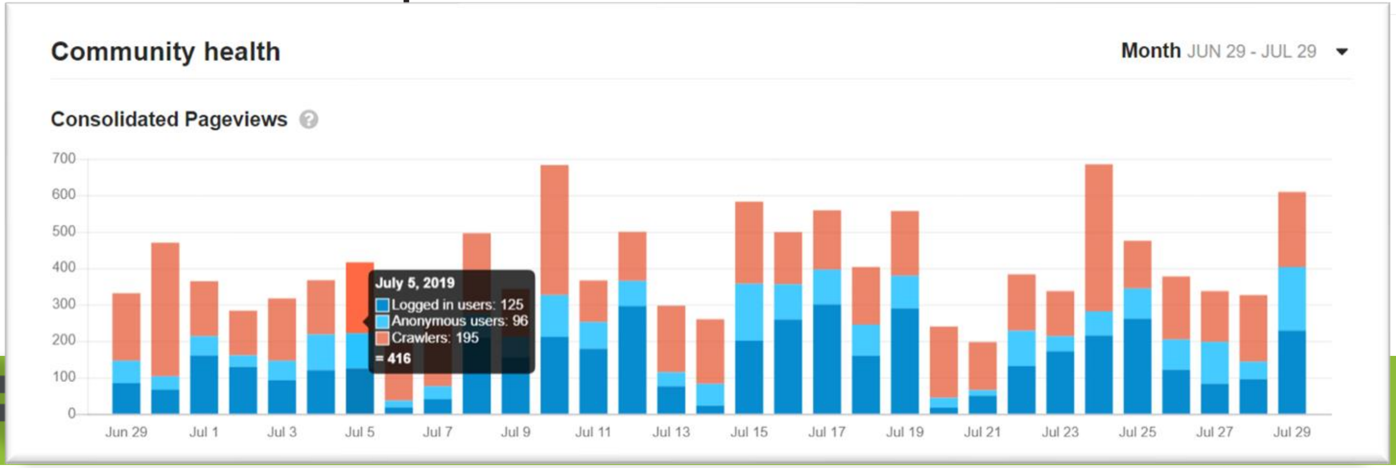


MFiX Forum

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

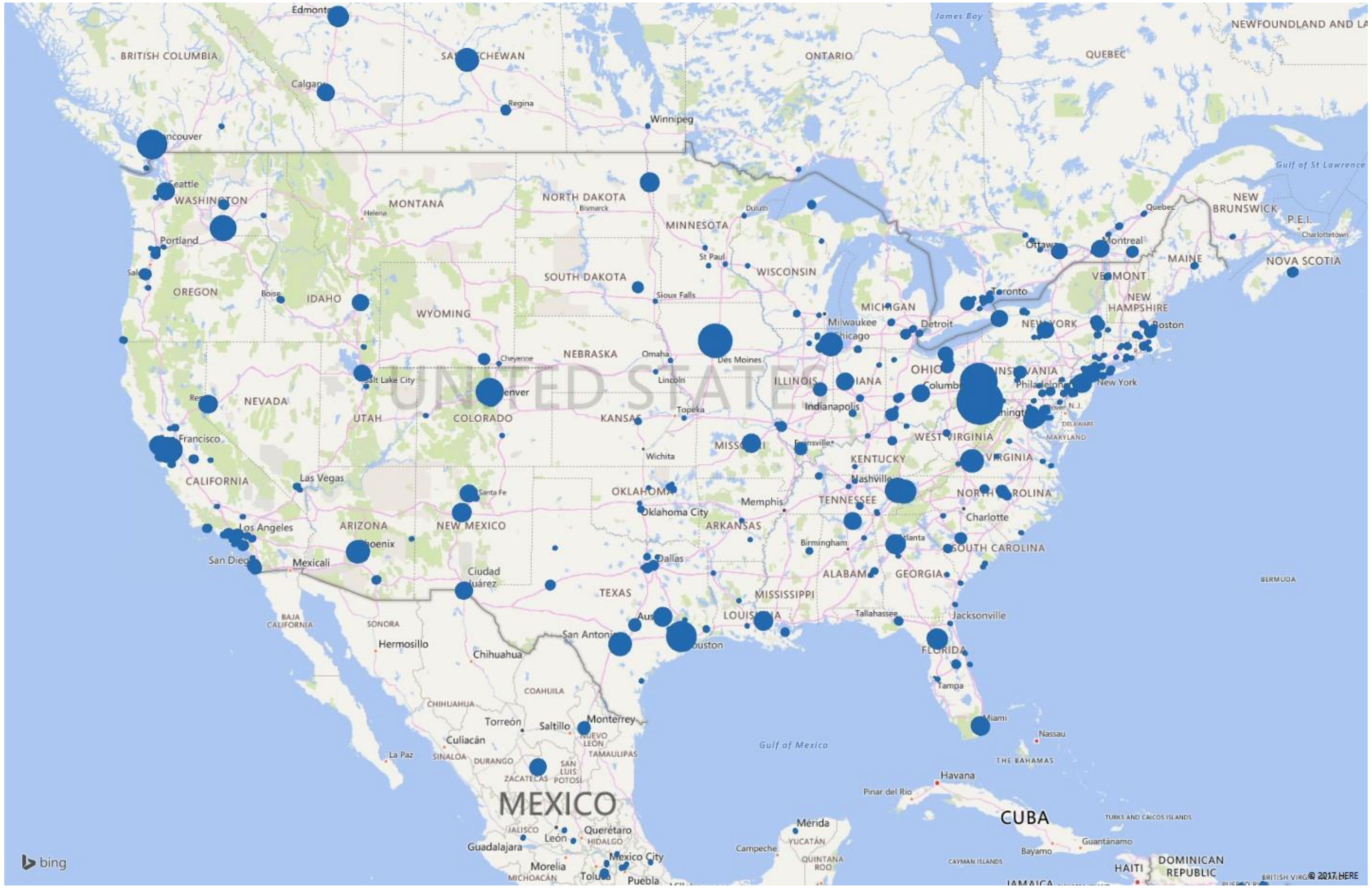
- User support
- Categories
  - Installation
  - How to
  - Bug report
  - Share
- Topics (threads)
- File attachment
- Searchable

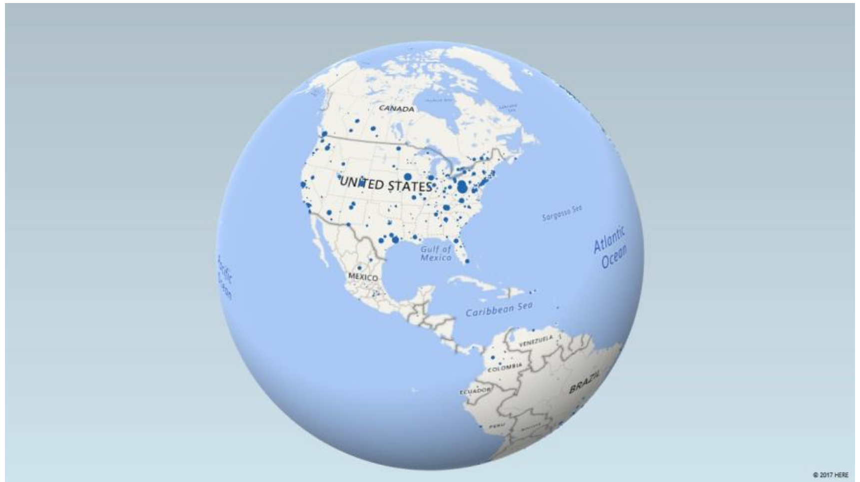




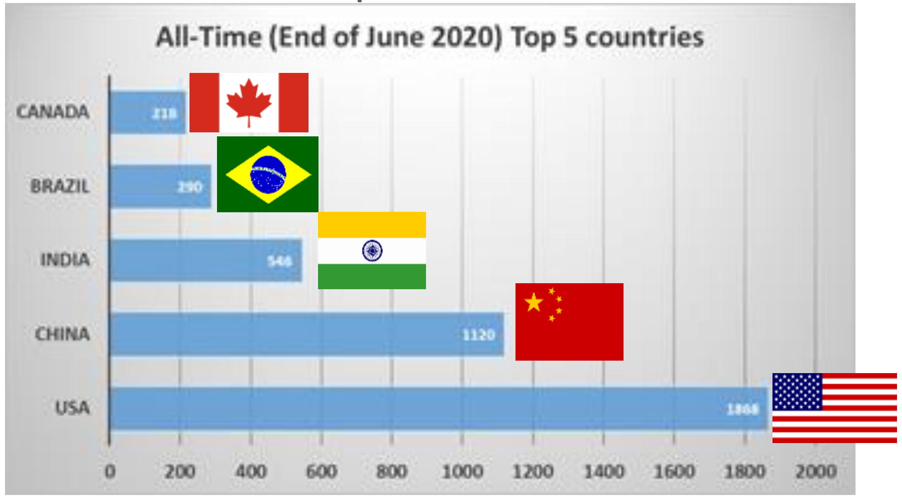
MFiX User Community

7,000+ all-time MFIX registrations





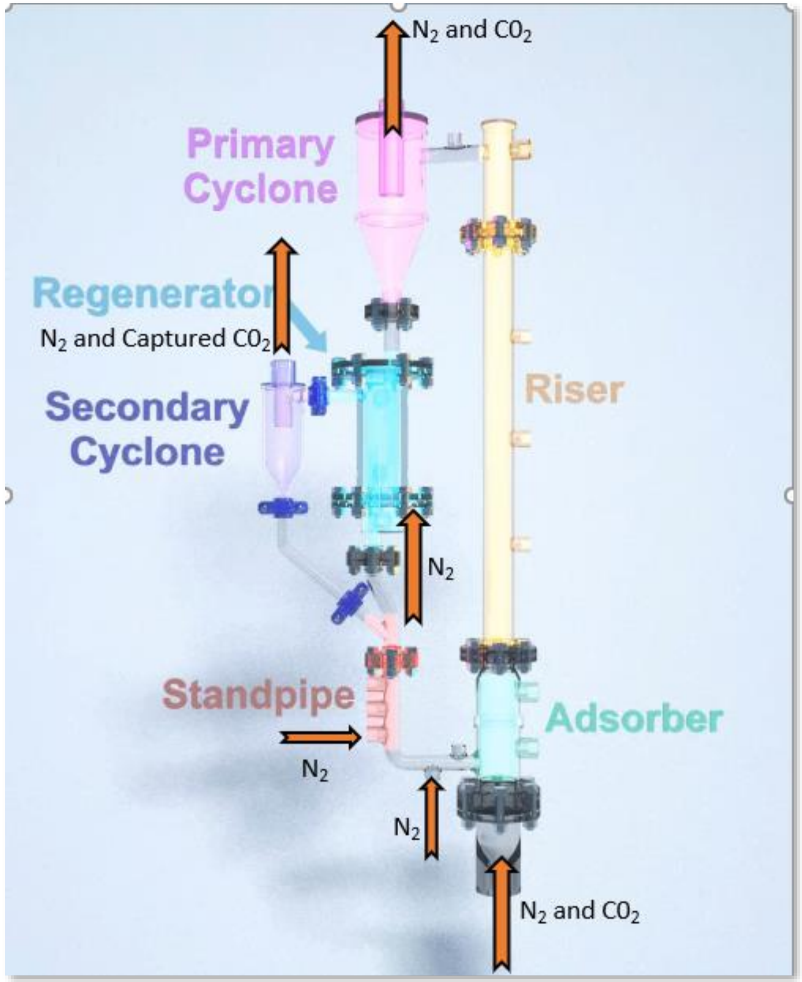
Top 5 Countries



Sorbent-based Carbon Capture - MFiX-DEM

Compare Simulations to Small-Scale, Reacting Flow Measurements

Simulation Results:
MFiX-DEM

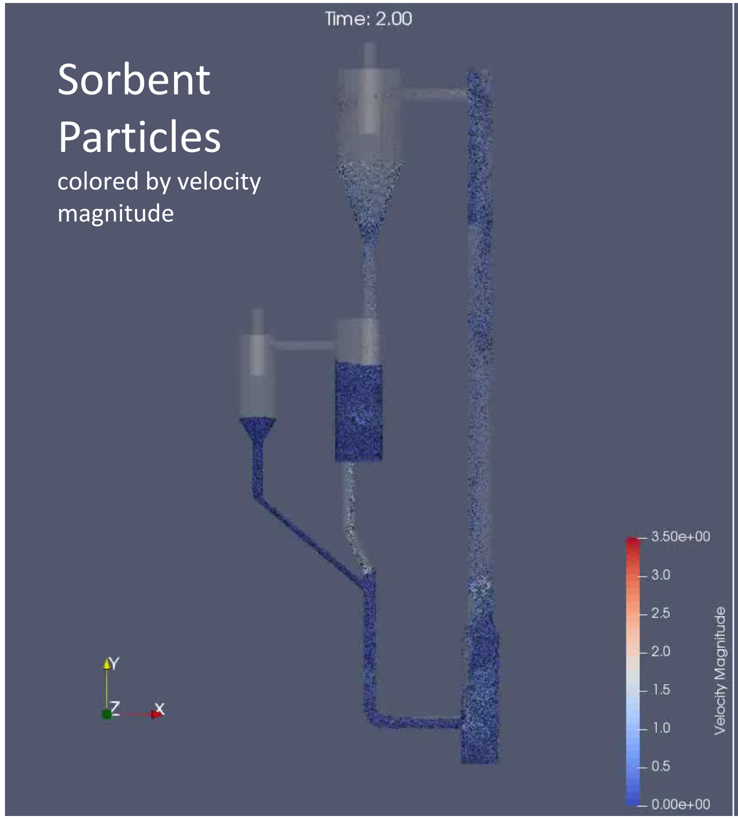


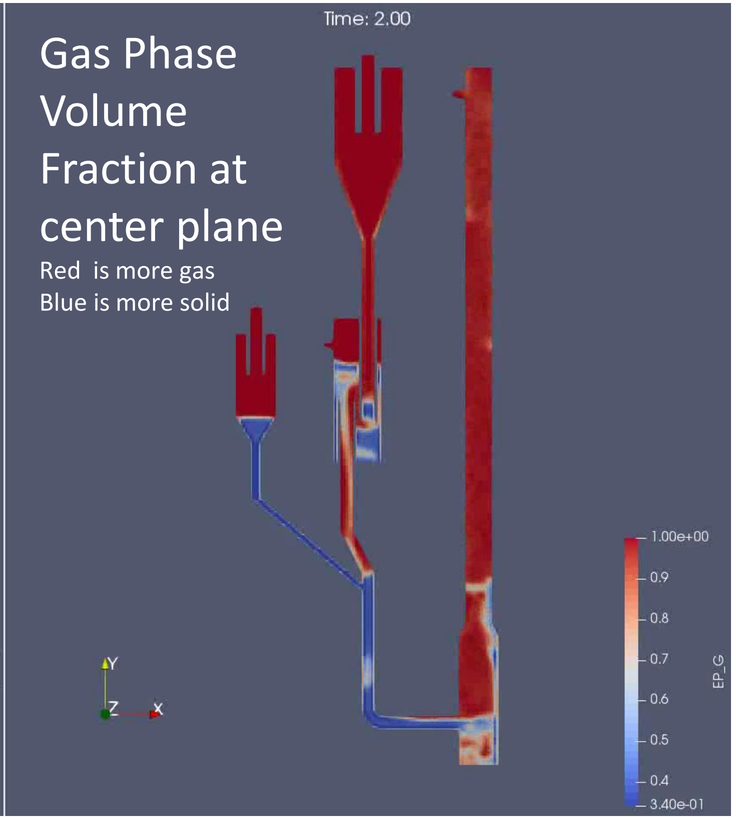
NETL CO_2 Capture Rig

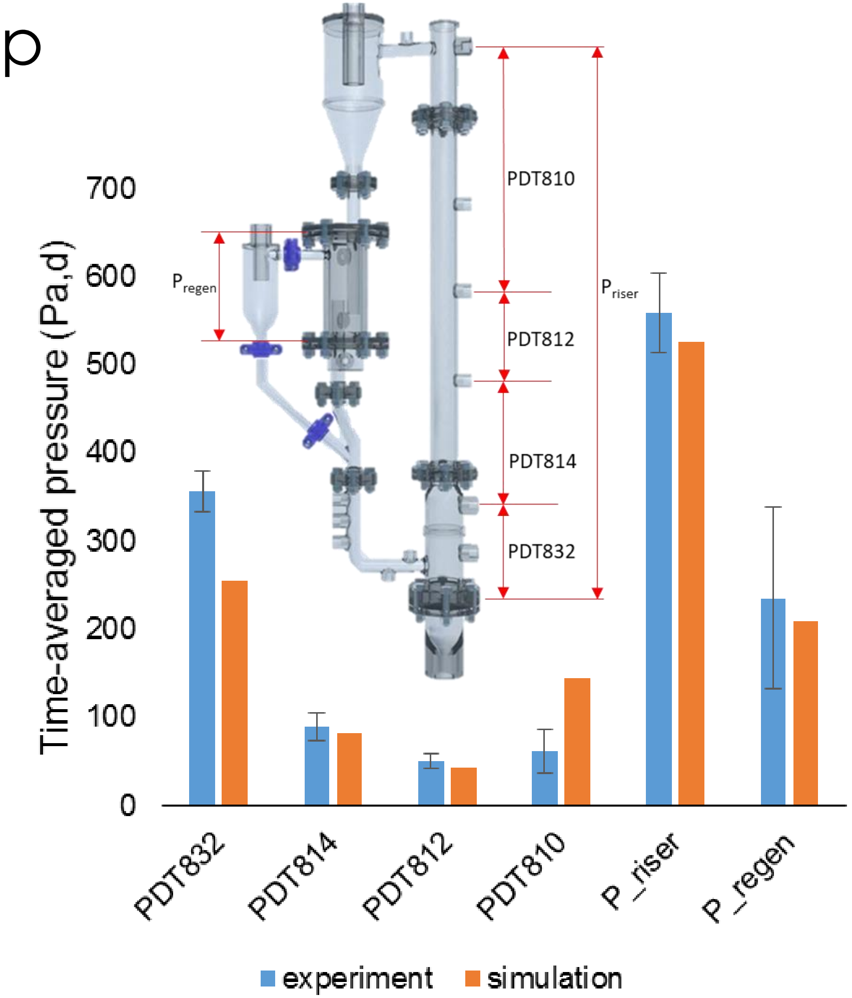
Sorbent-based Carbon Capture - MFiX-DEM

Cold Flow Hydrodynamics

Excellent comparison between modeled and measured solids holdup(pressure drop values) around the flow loop







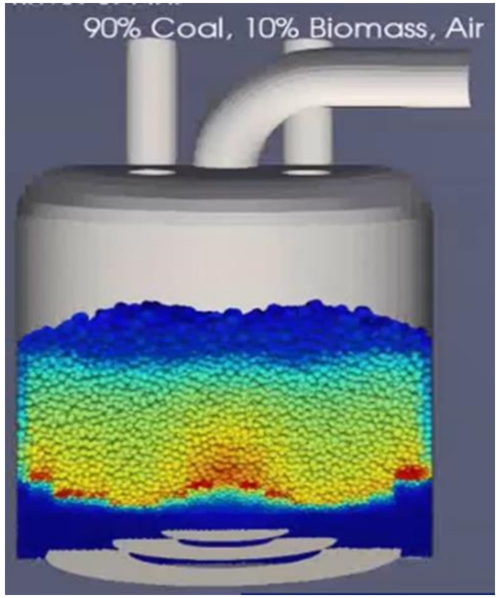
Advanced Reactor System – MFiX CGDEM

Decarbonization through gasification of coal, Biomass and MSW

Commercial-scale gasifier design (22MW)

Accomplishments

- Support the University of Alaska-Fairbanks Modular Gasification project
- Model validated with Sotacarbo pilot scale data
- 3D, transient simulation of prototype gasifier compares well to UAF design
- Transient response of gasifier to load variations, ramp-rate and turndown
- Gasifier performance for coal-biomass co-feed conditions to explore novel Net Zero Carbon, BECCS, and H2 production has been modeled



Impact: NETL's model predicts gasifier performance relative to feedstocks and operating conditions

- Predicted syngas data will provide key information for design of downstream components including engines for generators
- Modeling effort will significantly de-risk the design of the **$46million facility**

Reactor dimensions : **3.05 m diameter x 4.5 m height**

Solids inventory: **>10 tons**

Number of CG particles: **~130,000**

Time scale (physical time):**>10 hours**

UNIVERSITY OF ALASKA FAIRBANKS

SOTACARBO SUSTAINABLE ENERGY RESEARCH CENTRE

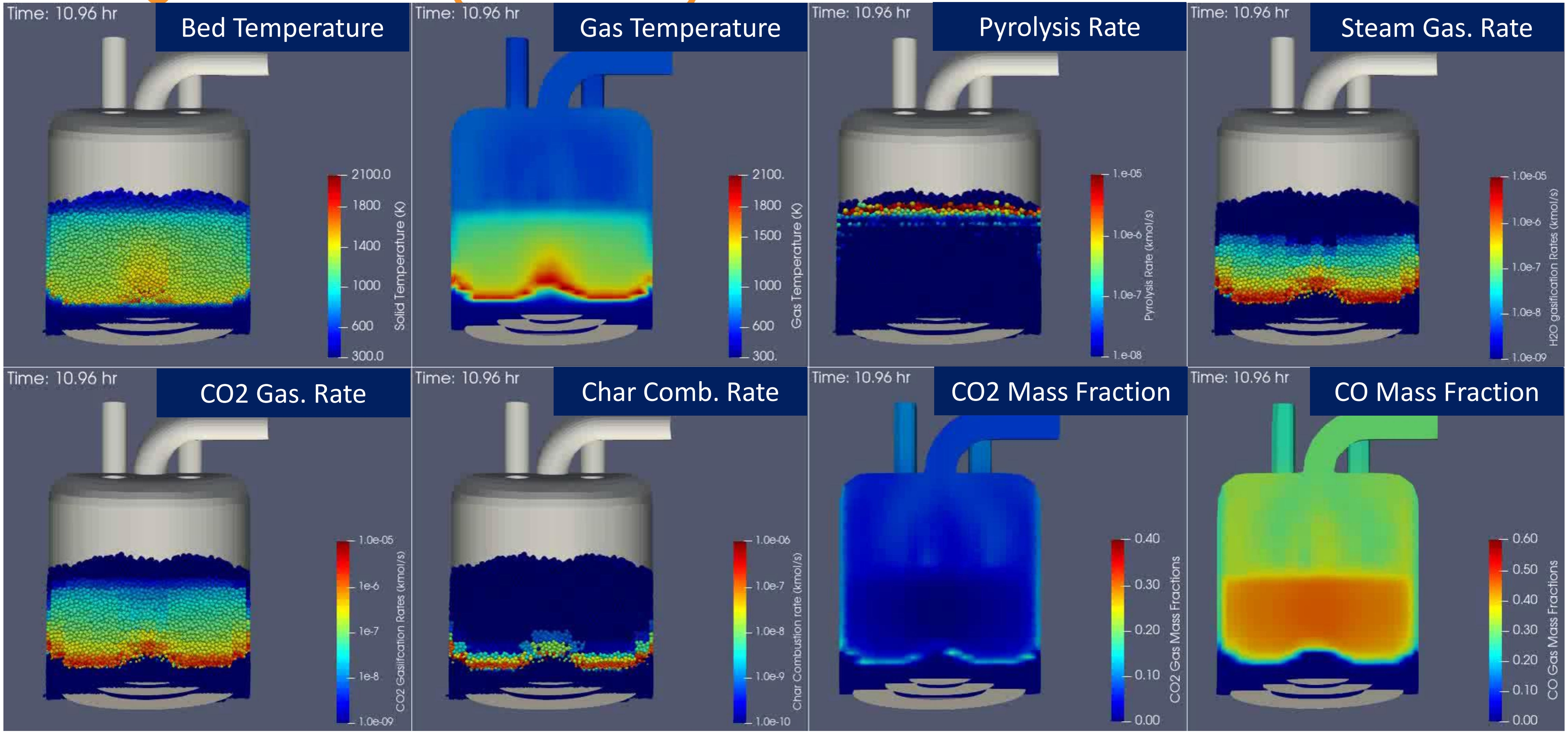
PARSONS

Hamilton-Maurer International

Jia Yu, Liqiang Lu, Yupeng Xu, Xi Gao, Mehrdad Shahnam, and William Rogers, Coarse-Grained CFD-DEM Simulation and the Design of an Industrial-Scale Coal Gasifier, Industrial Engineering and Chemistry Research, 2022, Volume 61, No. 1, 866–881, https://doi.org/10.1021/acs.iecr.1c03386

Advanced Reactor System – MFiX CGDEM

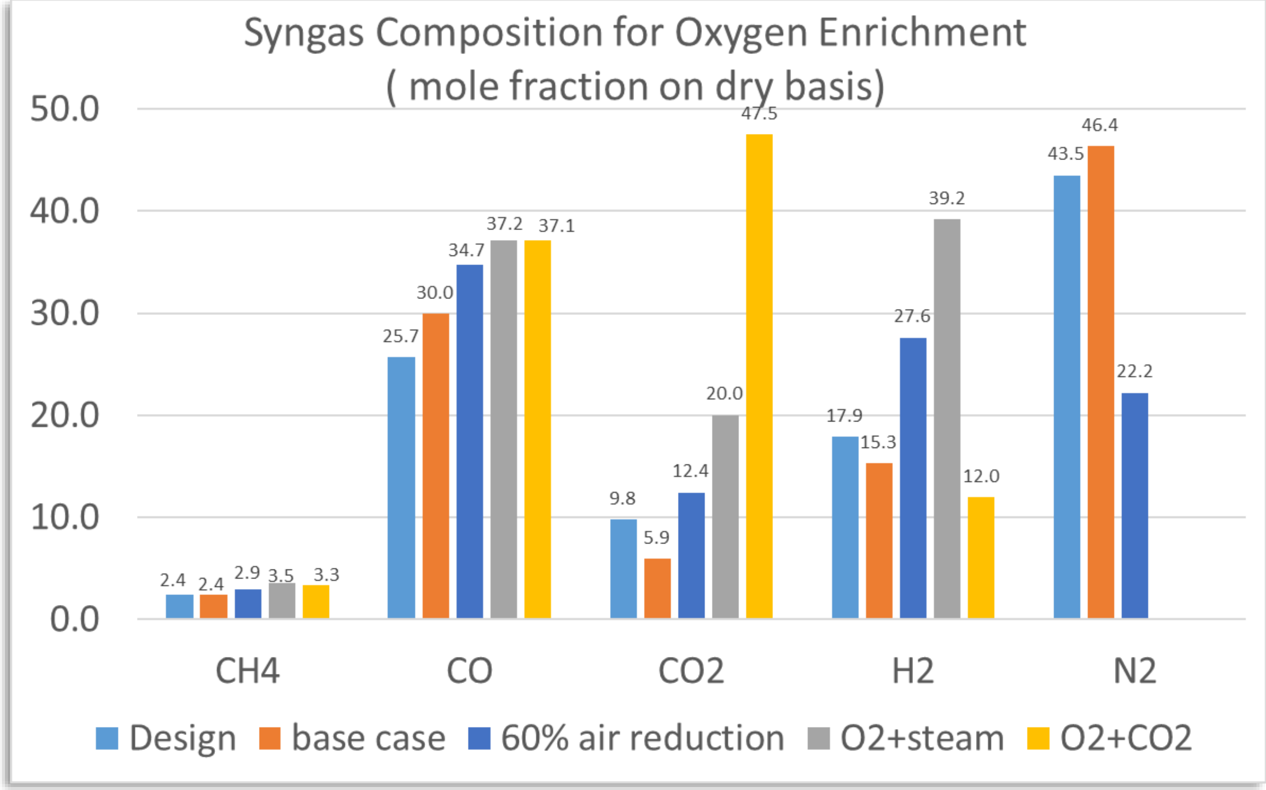
Plant Design Conditions (100% load)



Advanced Reactor System – MFiX CGDEM

Syngas Exit Composition with Oxygen Enrichment

- Simulations show that the prototype gasifier is adaptable to a wide range of oxygen enriched conditions with steam and CO_2 diluents
  - This meets key requirements for candidate gasifiers for Net Zero Carbon and H_2 production
- Oxygen-blown with steam produces higher H_2 as expected



Biomass gasification – MFiX CGDEM

FABER (Fluidized Air Blow Experimental Gasifier Reactor)

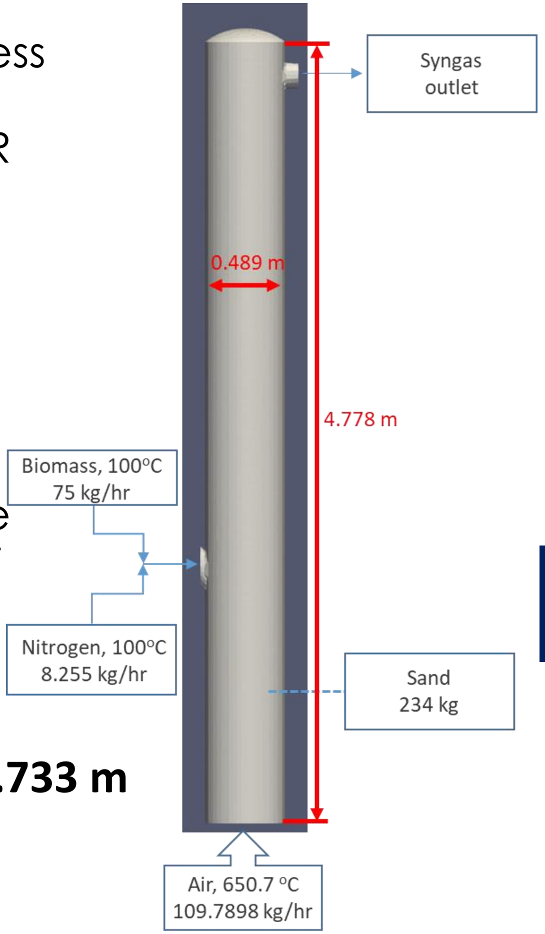
Project Goals:

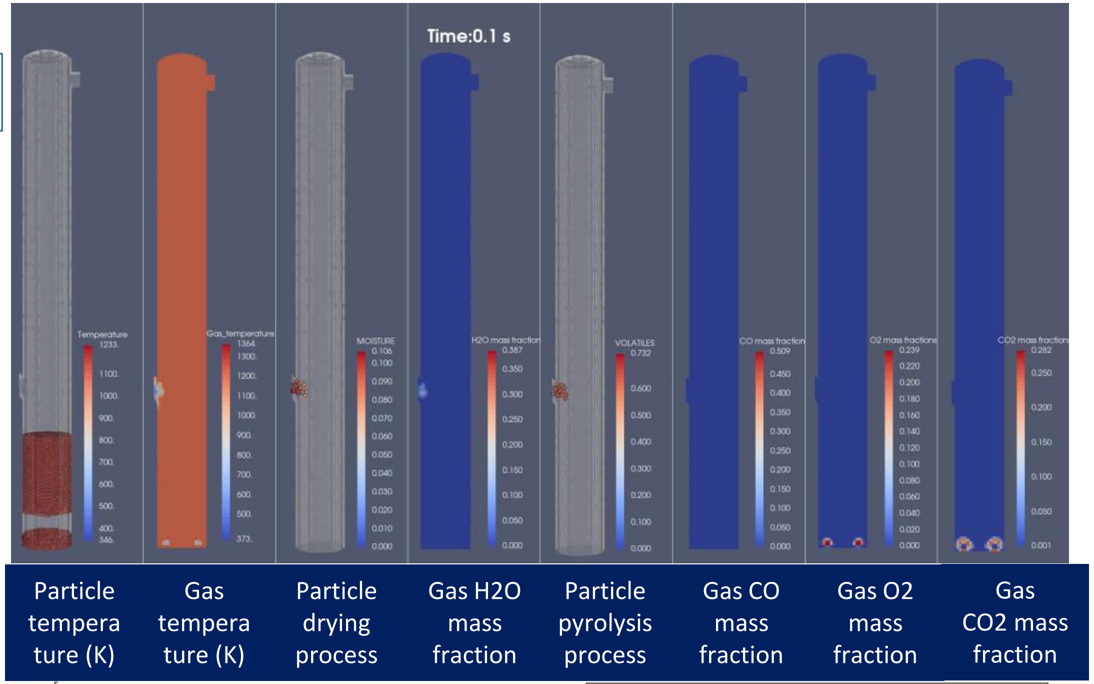
- Develop reaction kinetic for Cypress Biomass gasification
- Validate reaction kinetic for FABER
- Design and optimization of the fluidized bed reactor

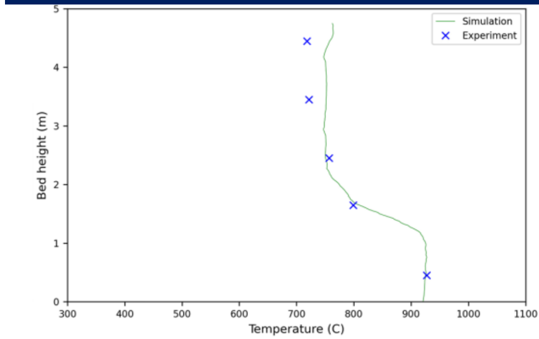
Accomplishments

- Gasification of Cypress biomass in FABER was simulated.
- Gasification reaction kinetics were developed and validated against experimental results.

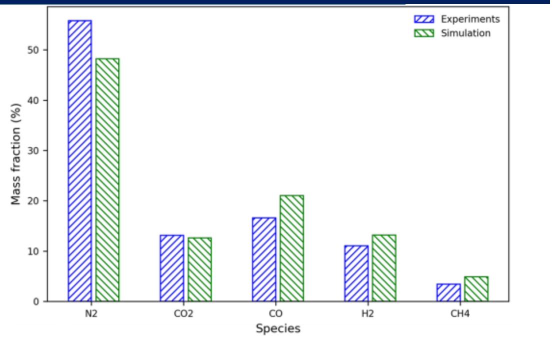
Reactor dimensions: ID = **0.489 m, height = 5.733 m**
Number of CG particles: **~64,000**
Solids inventory: **Sand 234 Kg, Biomass 25 Kg**







Axial bed temperature



Syngas composition

CFB Combustor – MFiX-PIC

NETL and Natural Resources Canada-CanmetENERGY have teamed to study CFB combustion systems with coal-biomass co-feed with potential for carbon capture

Accomplishments:

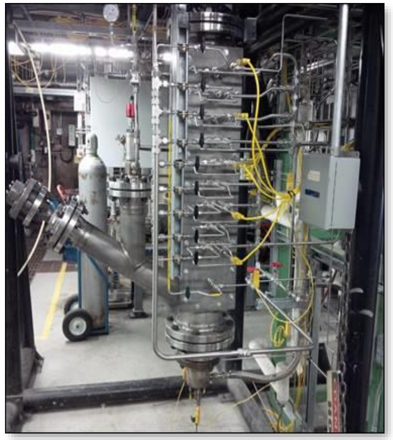
- NETL is simulating the 50kWth pilot CFB system being operated at NRCan over a range of coal-biomass blends and oxygen-enrichment conditions
- The collaboration provides NETL with high quality, detailed data describing rig operations which is critical information for validating the model
- The model is providing NRCan with valuable insight on conditions inside the system to help guide system optimization

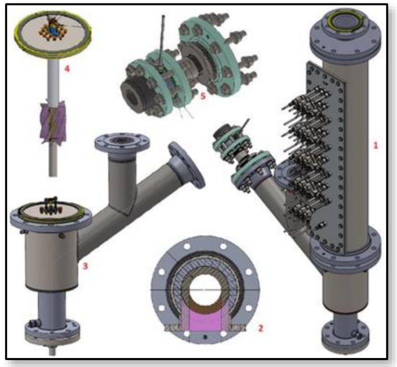
Impact:

- Once validated at the small pilot scale, these MFiX models running on FE's JOULE2 Supercomputer will be used to study scale-up and performance optimization of coal-biomass CFB combustion systems designed for negative CO2 emissions

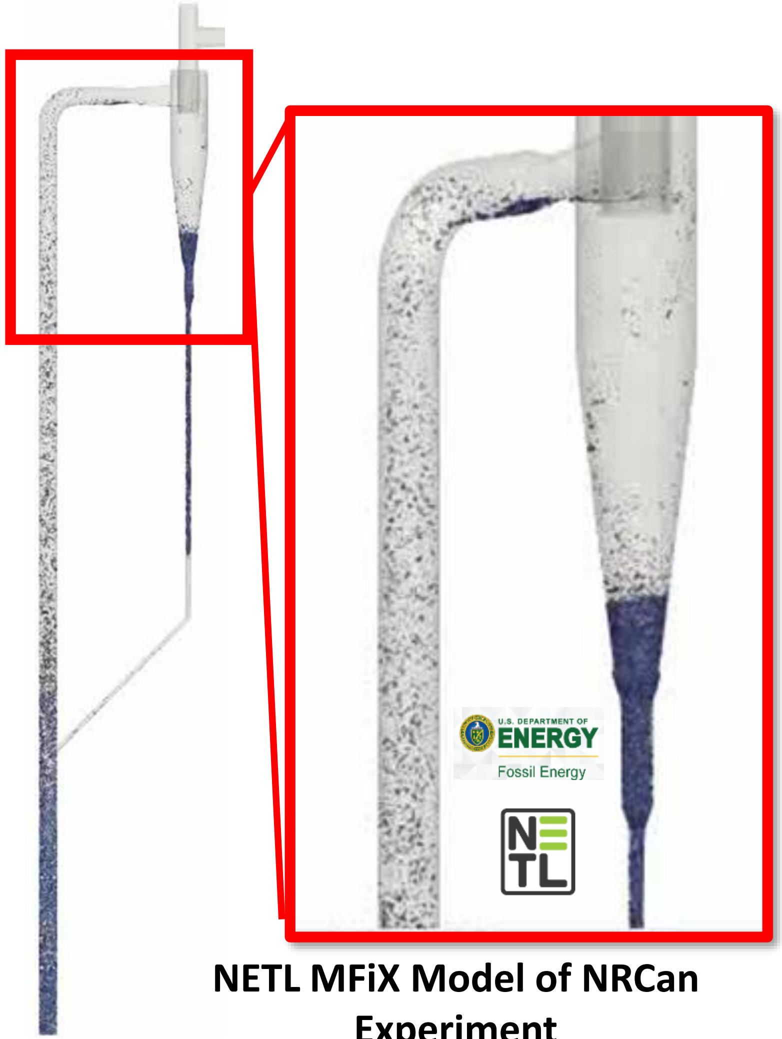
Natural Resources Canada / Ressources naturelles Canada

Canada





NRCan 50kWth CFB Test Facility

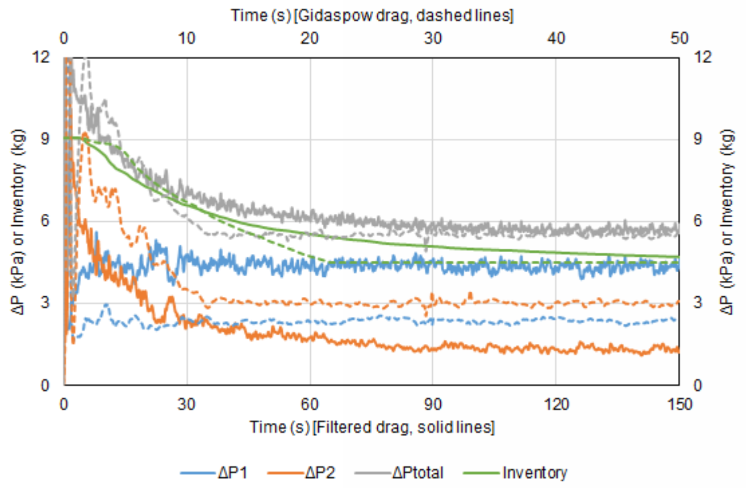


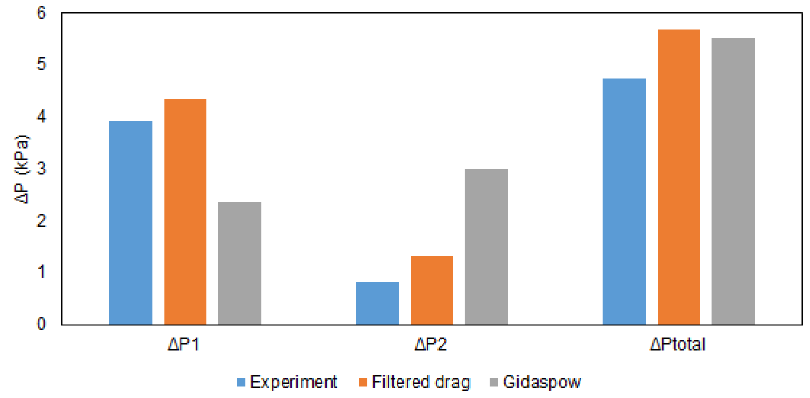
NETL MFiX Model of NRCan Experiment

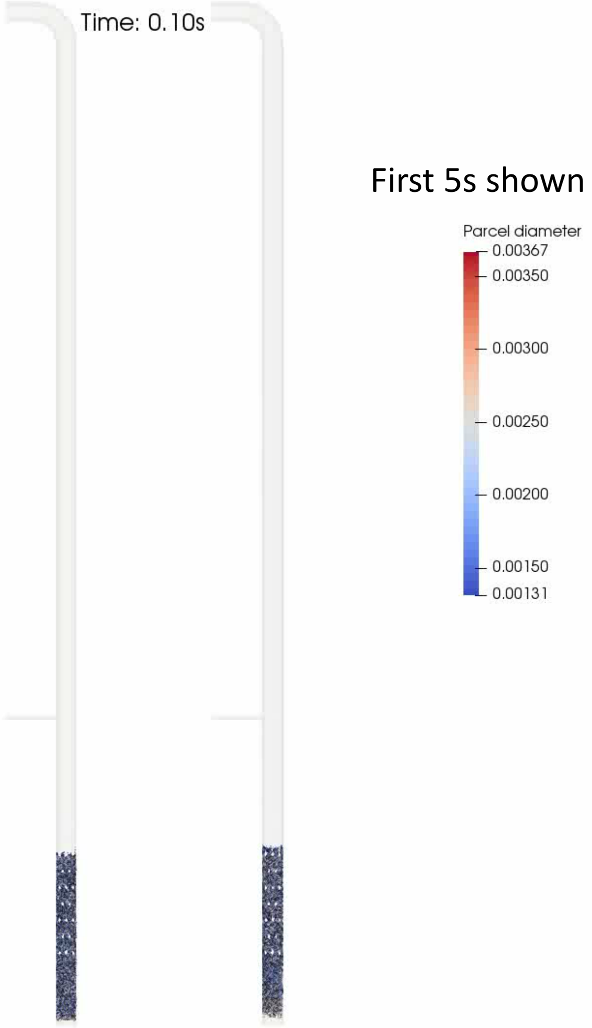
50kWth CFB Combustor – MFiX PIC

Hydrodynamics Benchmarking – Effect of Drag Model

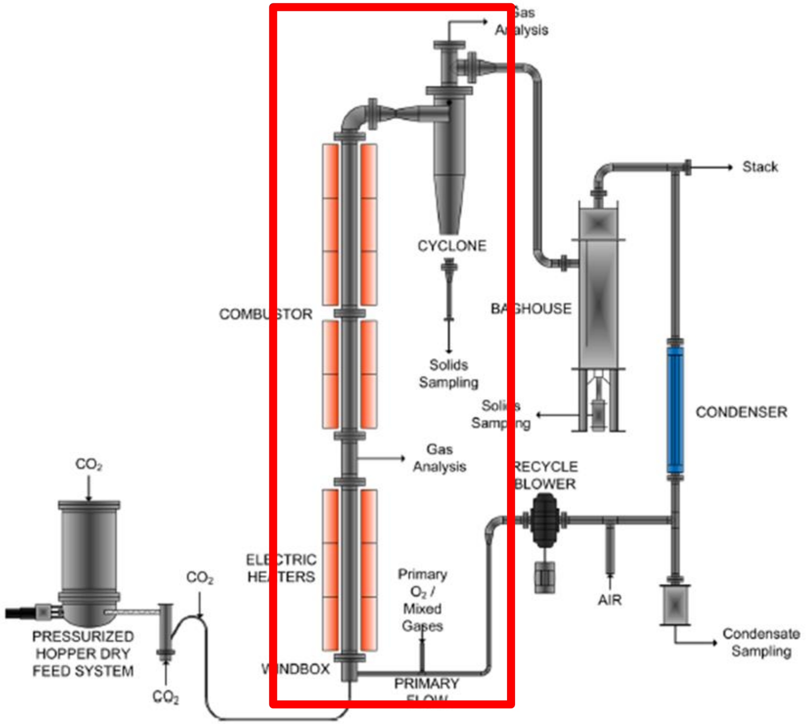
- First step: validate hydrodynamics
- Riser-only simulations
- Fluidization is impeded by applying the filtered drag model, so more particles are retained in the lower riser
- Circulation rate is reduced, reflected in the average mass of recirculated particles in the side inlet
- Pressure drop distribution and overall pressure drop using the filtered drag model show better agreement with the experimental results (P_p = 10, γ = 3)

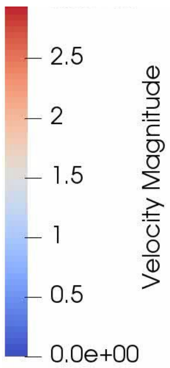


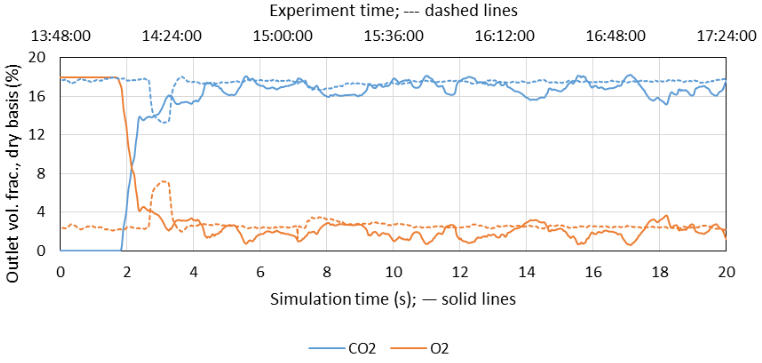


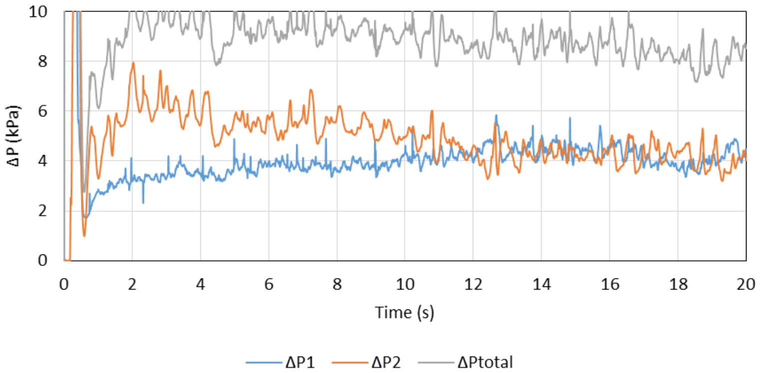


CFB Combustor – MFiX-PIC

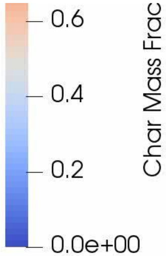








Biomass particles enlarged 50x for visualization of shrinking particle due to pyrolysis and char combustion



Thank you!