

# MFiX Development Updates



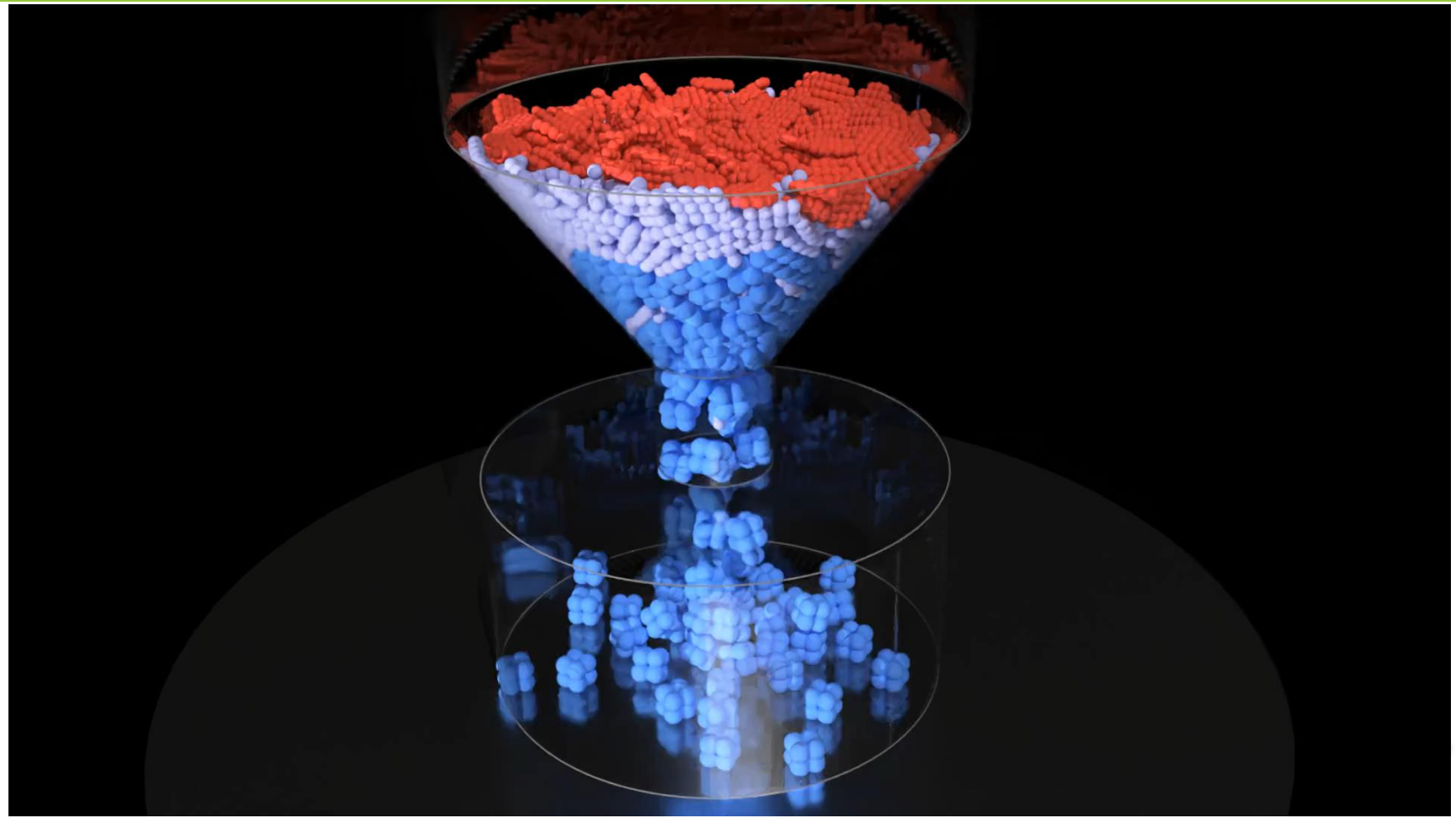
*Software Tools and Expertise To Address Multiphase Flow Challenges in Research, Design, and Optimization*

**Jeff Dietiker**

NETL Support Contractor



NETL 2024 Workshop on Multiphase  
Flow Science  
Aug. 13, 2024



# Disclaimer



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# Authors and Contact Information

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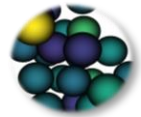
# MFiX Suite of Multiphase Computational Fluid Dynamics Modeling Software

## Capabilities and Benefits

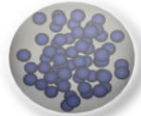
**MFiX** Multiphase Flow with  
Interphase eXchanges



MFiX-TFM (Two-Fluid Model)



MFiX-DEM (Discrete Element Model)



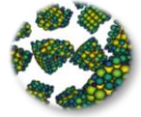
MFiX-PIC (Multiphase Particle In Cell)



MFiX-CGDEM (Coarse Grain DEM)



MFiX-SQP (Super Quadric Particle)



MFiX-GSP (Glued Sphere Particle)

3 Decades  
of development history  
8,800+  
registered users

600+  
downloads per month  
850  
citations per year

- Transport equations for both gas and solids phases
- Requires closure models



- Uses first principles to account for particle interactions
- Computationally expensive



- Computationally efficient, tracks parcels
- Continuum stress model to approximate particle-particle interactions



- Computationally efficient, tracks groups of particles
- Same contact mechanism as DEM



- Non-spherical particles, superquadric shapes
- Contact mechanism more expensive than DEM

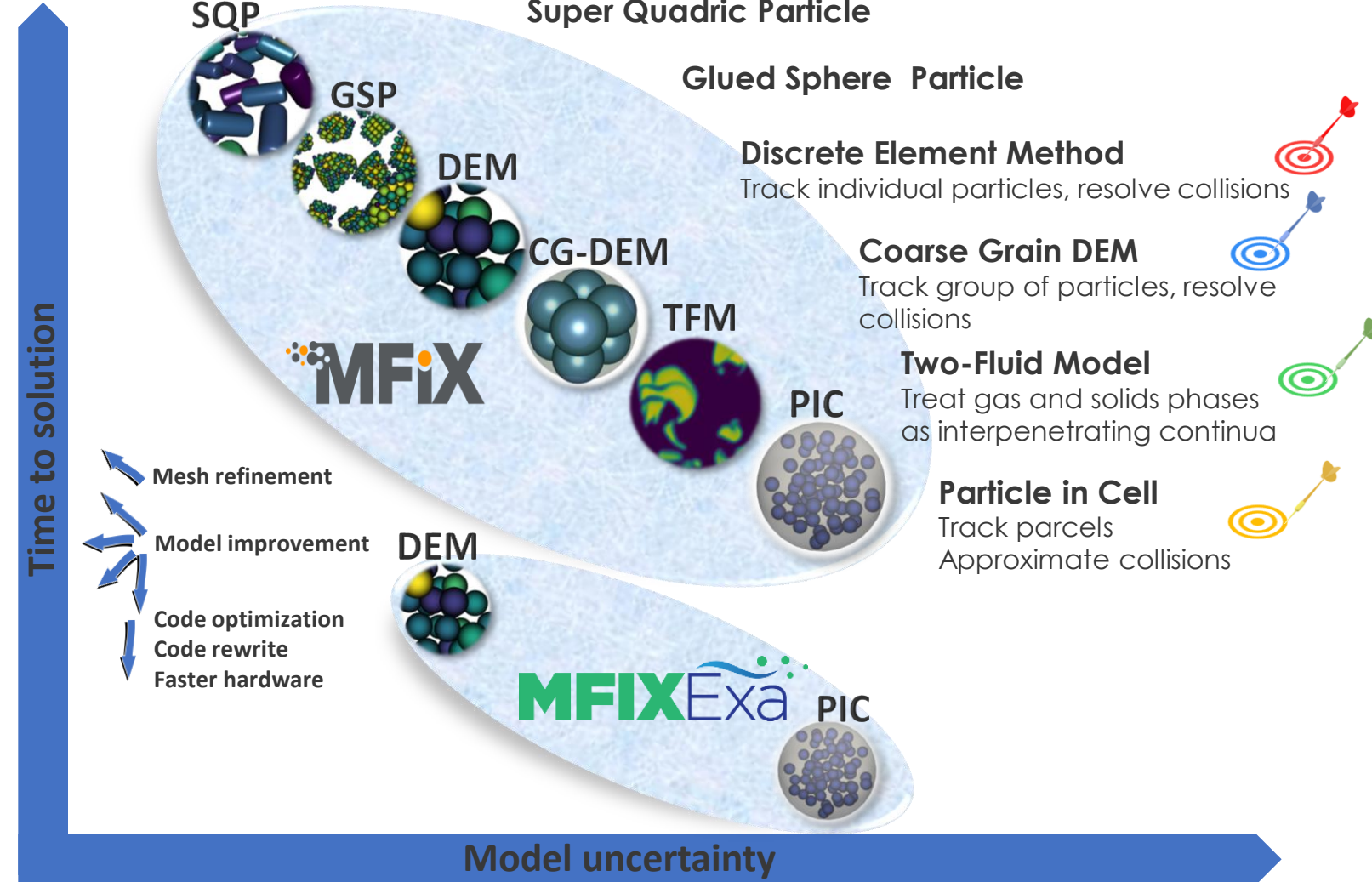


- Non-spherical particles, glued spheres
- Same contact mechanism as DEM



# MFiX Suite of Multiphase CFD Software

## Managing the Tradeoff Between Accuracy and Time to Solution



# Multiphase Models

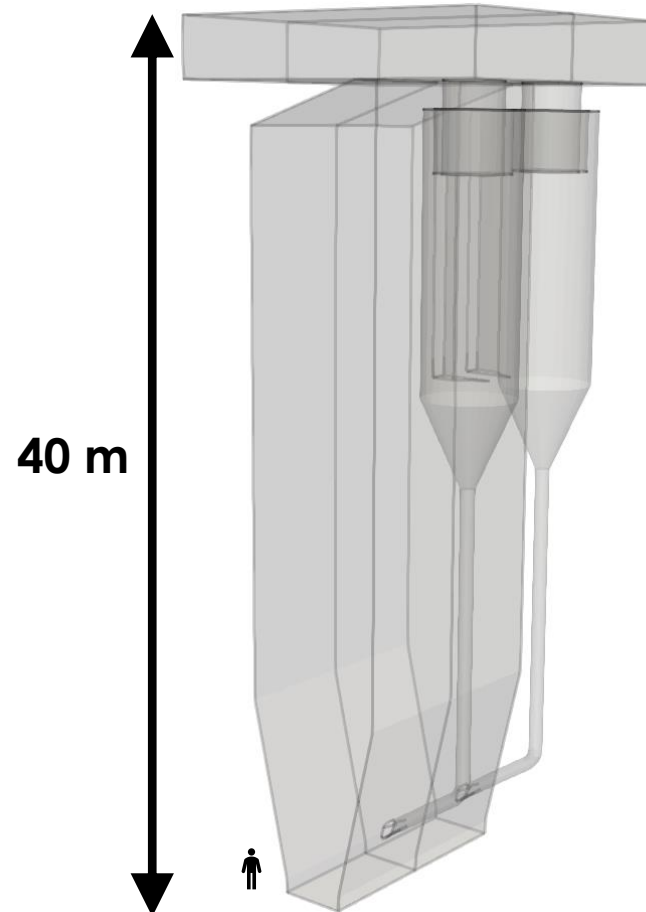
## Example: 10 MWth Industrial-Scale Circulating Fluidized Bed (CFB) Furnace

Miao Yang et al. (2023) **CFD Simulation of Biomass Combustion in an Industrial Circulating Fluidized Bed Furnace**, Combustion Science and Technology, 195:14, 3310-3340

- 40 m tall CFB furnace
- 60 tons of sand + biomass
- OpenFoam
- Coarse Grain DEM and PIC

Fine mesh:

- 600K cells
- 989K sand parcels
- 100K biomass parcels



Refs	Scale	D	Model	subModel	H	T	R
Gu et al. (2020)	12 MWth	3D	E-L	MP-PIC	✓	✓	✓
Kong et al. (2020)	lab-scale	3D	E-L	MP-PIC	✓	✓	✓
Lin et al. (2022)	1 MWth	3D	E-L	MP-PIC	✓	✓	✓
Yang et al. (2020)	0.3 MWth	3D	E-L	MP-PIC	✓	✓	✓
Li and Shen (2021)	lab-scale	3D	E-E	TFM	✓	✓	✓
Cai et al. (2022)	lab-scale	3D	E-E	TFM	✓	✓	✓
Ghadirian, et al. (2019)	lab-scale	3D	E-E	TFM	✓	✓	✓
Wang et al. (2018)	lab-scale	3D	E-L	MP-PIC	✓	✓	✓
Wang et al. (2017)	600 MWth	3D	E-L	DEM	✓	✗	✗
Luo et al. (2015)	lab-scale	3D	E-L	DEM	✓	✗	✗
Lee et al. (2022)	550 MWth	3D	E-L	MP-PIC	✓	✗	✗
Tu and Wang (2018)	lab-scale	3D	E-L	MP-PIC	✓	✗	✗
Kadyrov, et al. (2019)	lab-scale	3D	E-L	MP-PIC	✓	✗	✗
Yang and Wang (2020)	lab-scale	3D	E-L	MP-PIC	✓	✗	✗
Muhammad et al. (2019)	lab-scale	3D	E-L	MP-PIC	✓	✗	✗
Ma et al. (2017)	lab-scale	3D	E-L	MP-PIC	✓	✗	✗
Li et al. (2021)	lab-scale	3D	E-L	MP-PIC	✓	✗	✗
Liu et al. (2002)	lab-scale	3D	E-E	TFM	✓	✗	✗
Lu et al. (2018)	lab-scale	2D	E-E	TFM	✓	✗	✗
Deng et al. (2021)	350 Mw	1D	✗	✗	✓	✓	✓

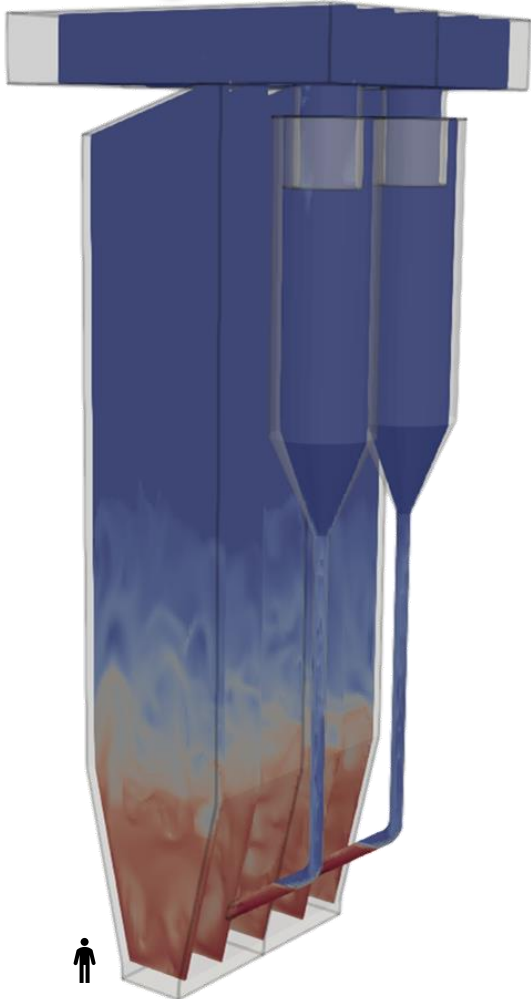
H- Hydrodynamic, T- thermo-, R- gasification/combustion

# Multiphase Models

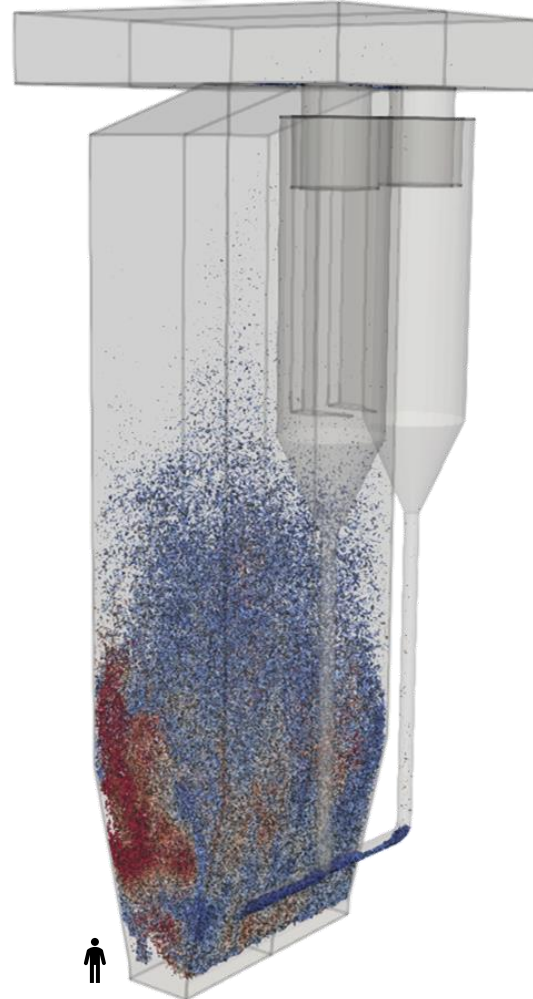
## Example: 10 MWth Industrial-Scale CFB Furnace



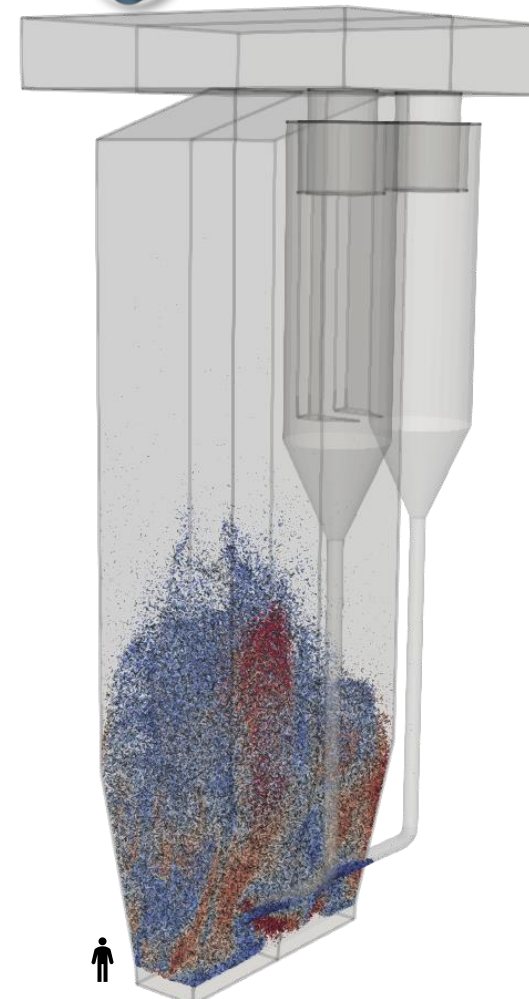
MFiX-TFM



MFiX-PIC



MFiX-CGDEM



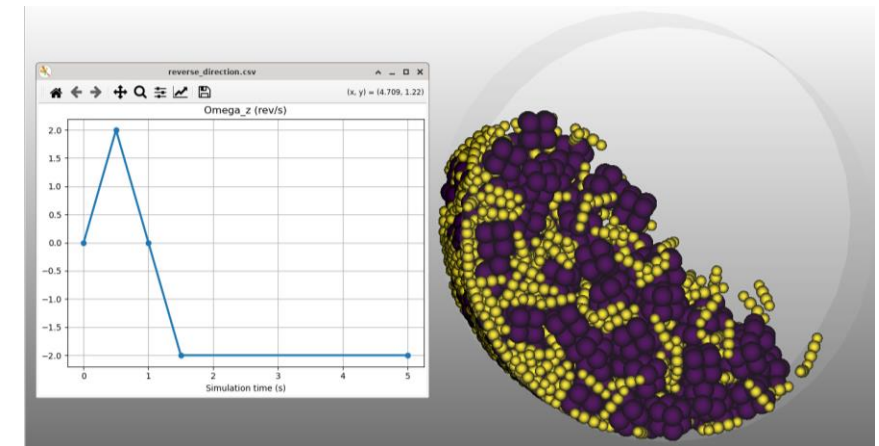
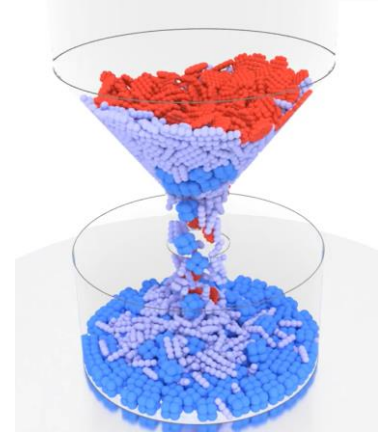
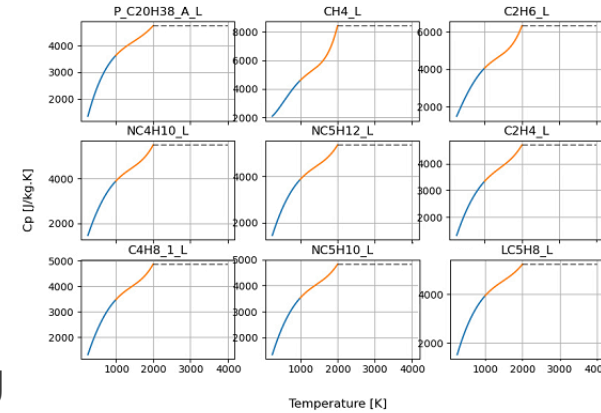
### MFiX:

- 1.7M cells
- 1.4M parcels/CGP

# MFiX Development

## 4 Releases in EY23 (See [mfix.netl.doe.gov](https://mfix.netl.doe.gov) for Full Release Note)

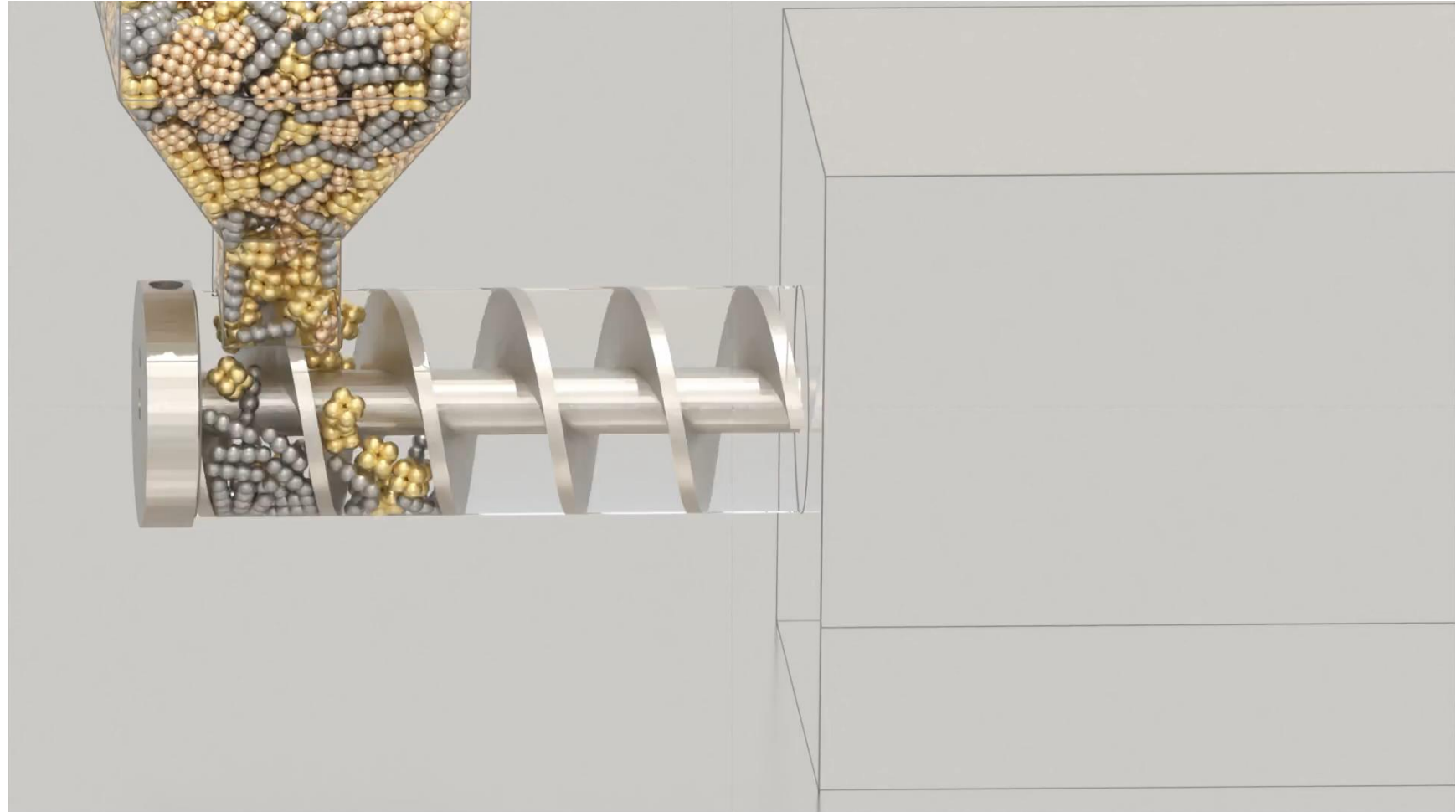
- **23.2:** - Support for Chemkin thermodynamic data  
- Chemical species and reaction equation import
- **23.3:** - Stiff solver for DEM simulations  
- Default Shared Memory and Distributed Memory solvers  
- Keyword control of floating-point exception handling
- **23.4:** - New adaptive time step option (nice dt)
- **24.1:** - Glued Sphere Particle model  
- Non-Newtonian viscosity model (Herschel-Bulkley)  
- Mass inlet ramps
- **24.2:** - New keyframe data workflow  
- DEM rigid motion





## 23.2 Example

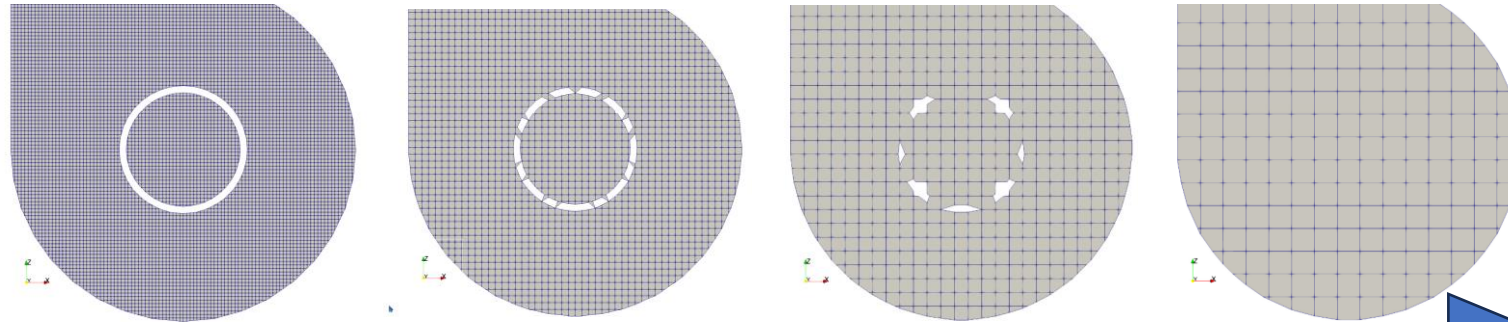
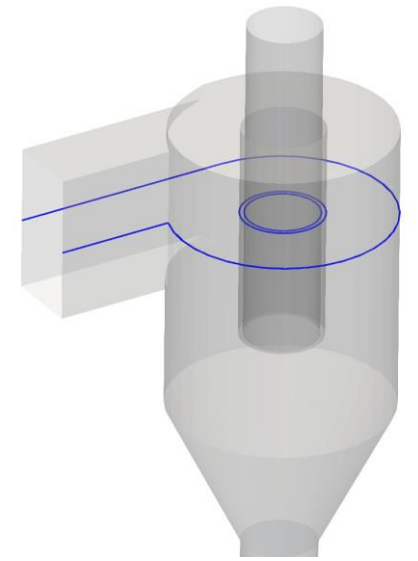
- **Screwfeeder**
  - Glued sphere DEM
  - Moving STL
  - Keyframe data



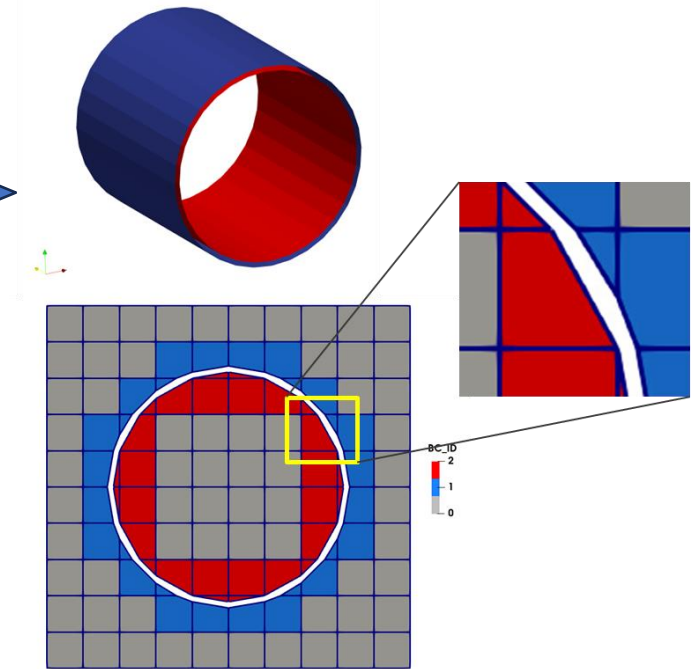
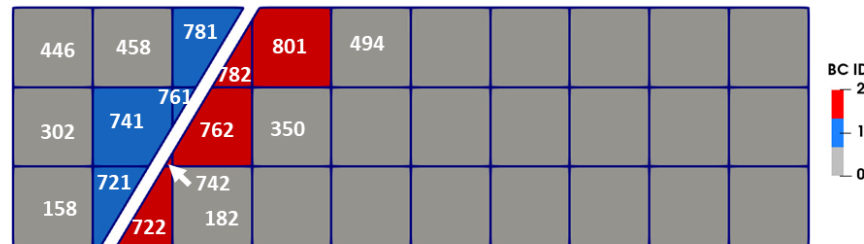
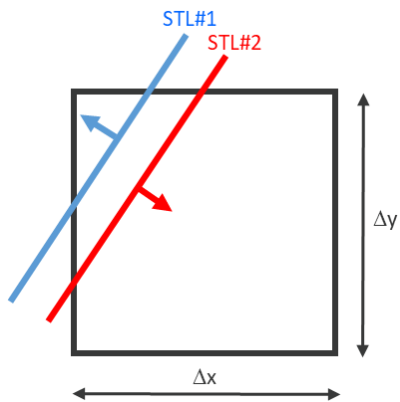
# Thin Wall Boundary Conditions

## Motivation

- Cut cell approach cannot resolve geometric details smaller than cell size
- Internal walls must be at least 2-3 times thicker than cell size
- Not always feasible to refine the mesh

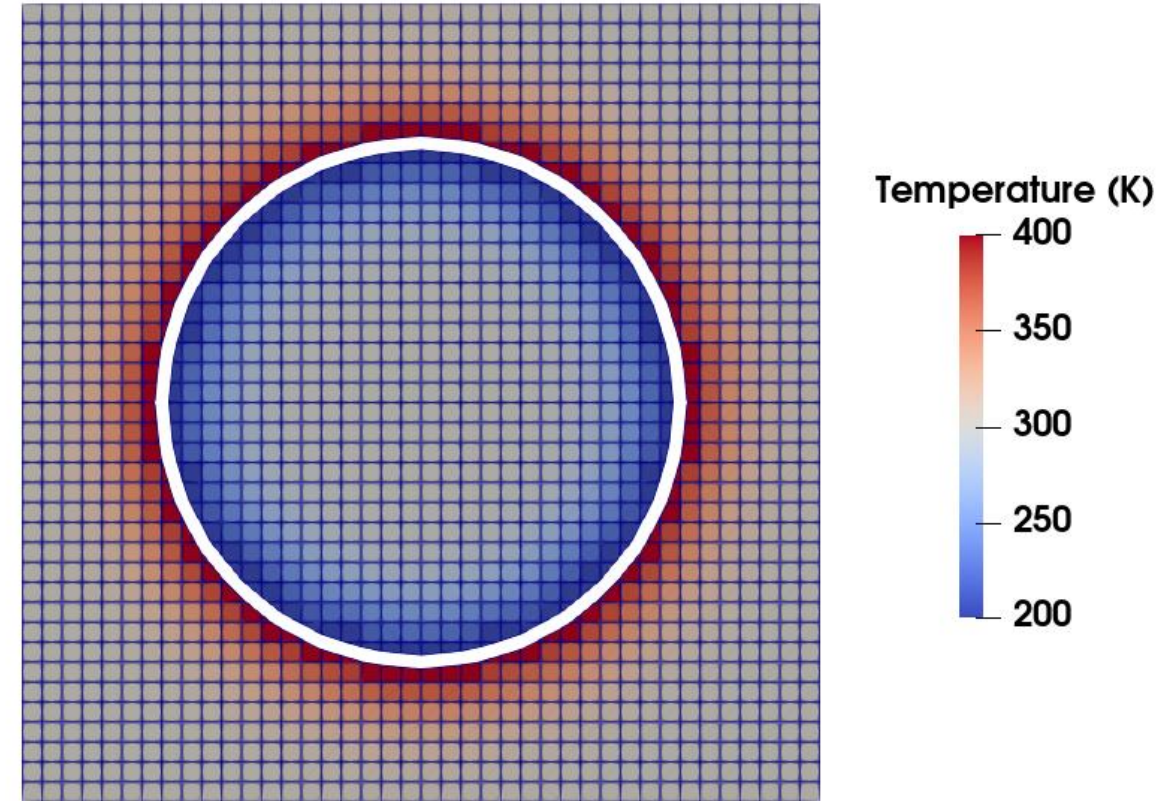
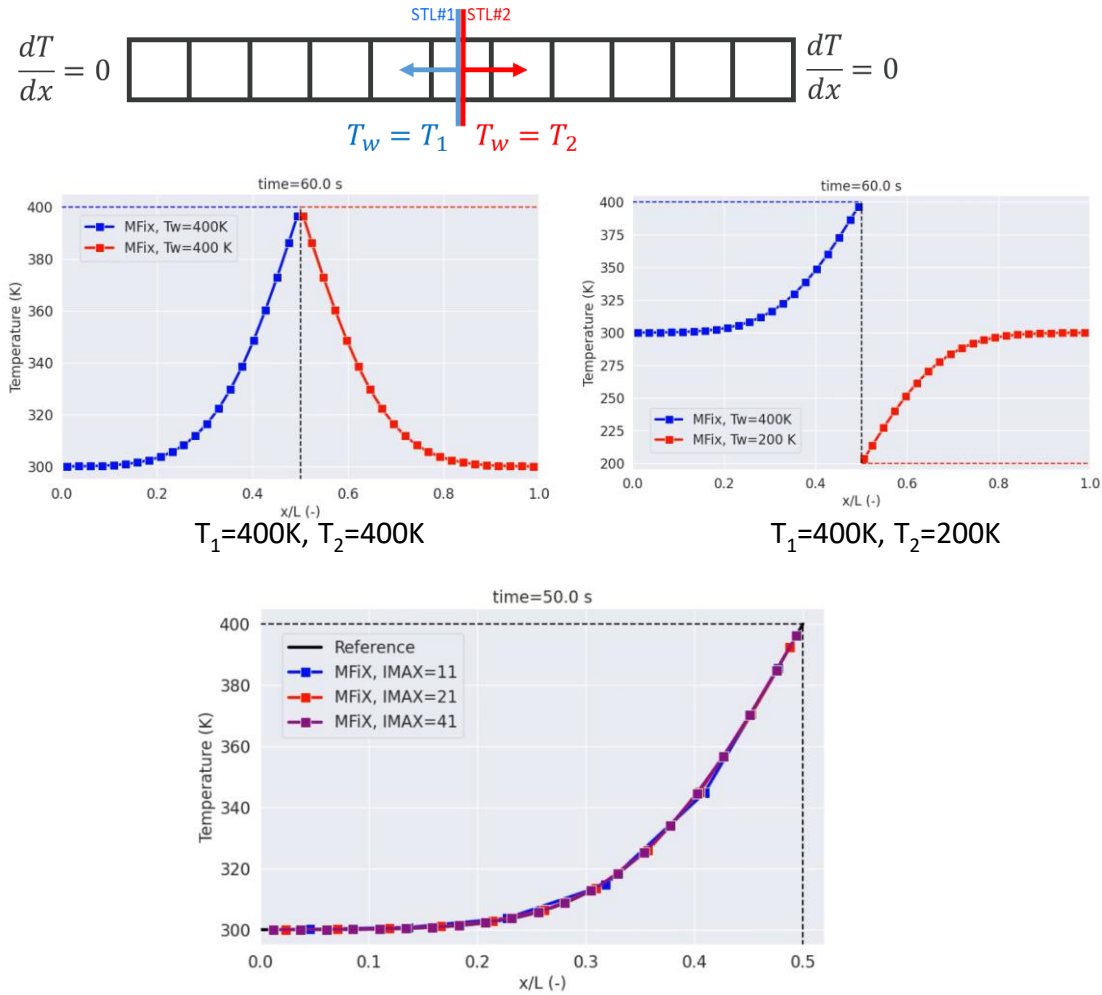


Grid coarsening



# Thin Wall Boundary Conditions

- Scalar cell meshing
- Test with simple Heat Transfer

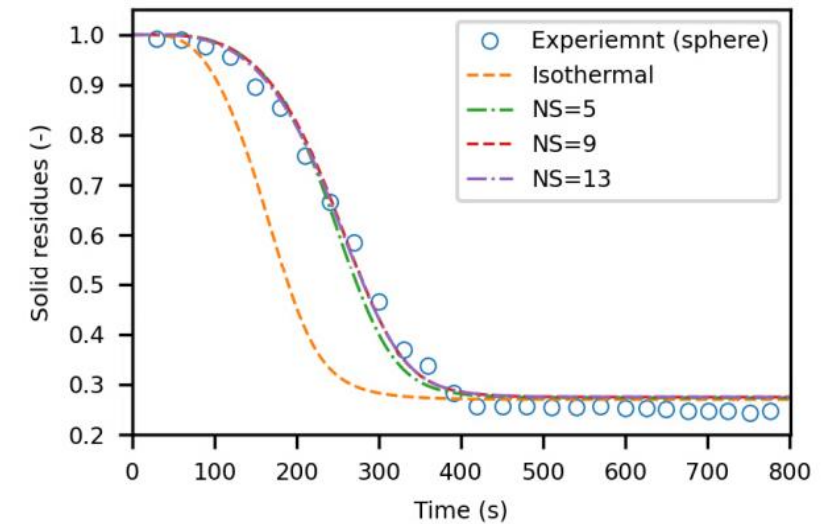
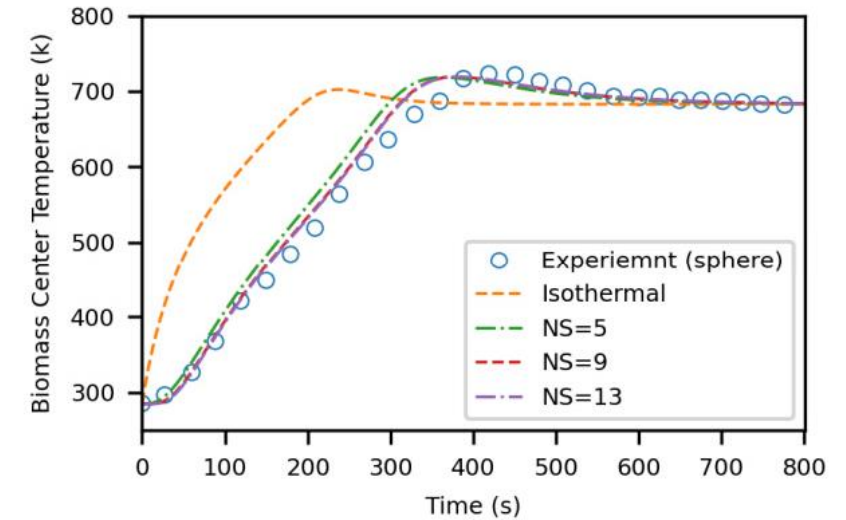
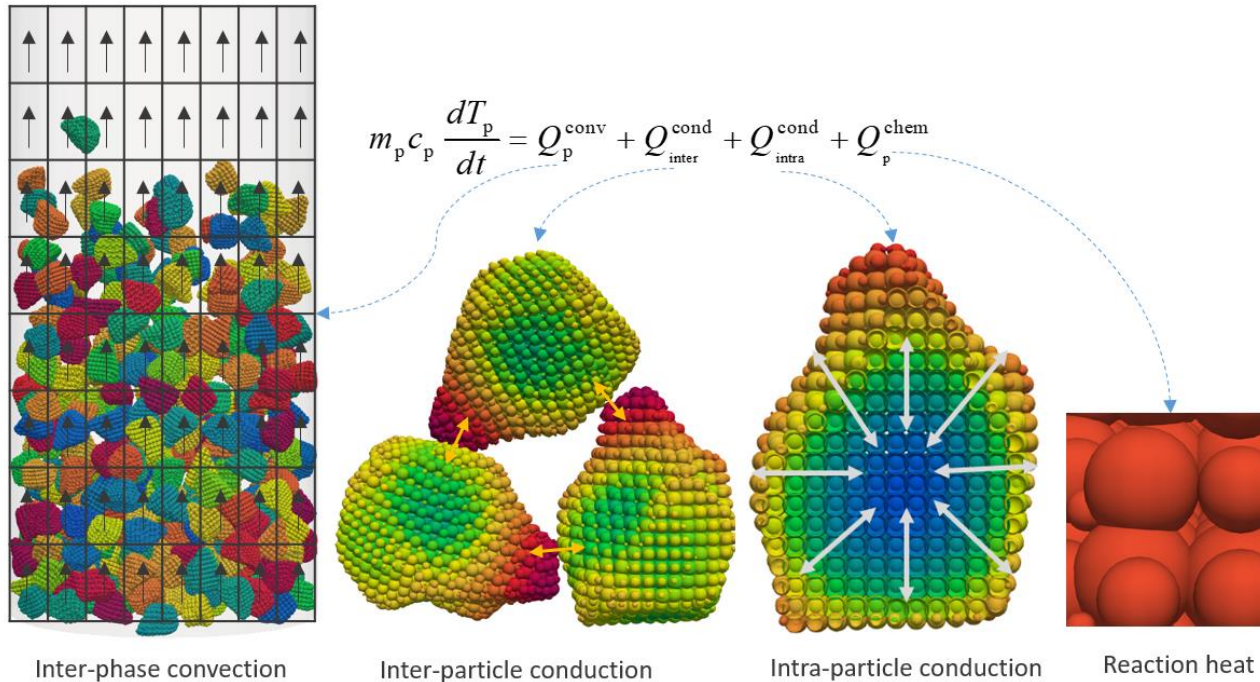


# Glued Sphere Model (Non-Spherical Particles)

## Irregular Shape of Particles



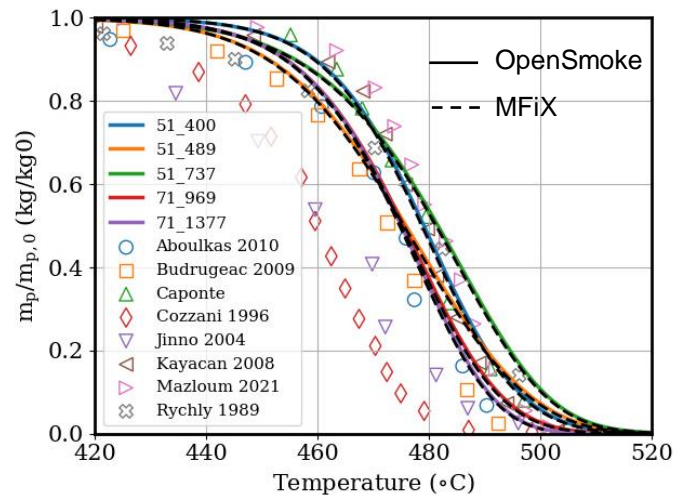
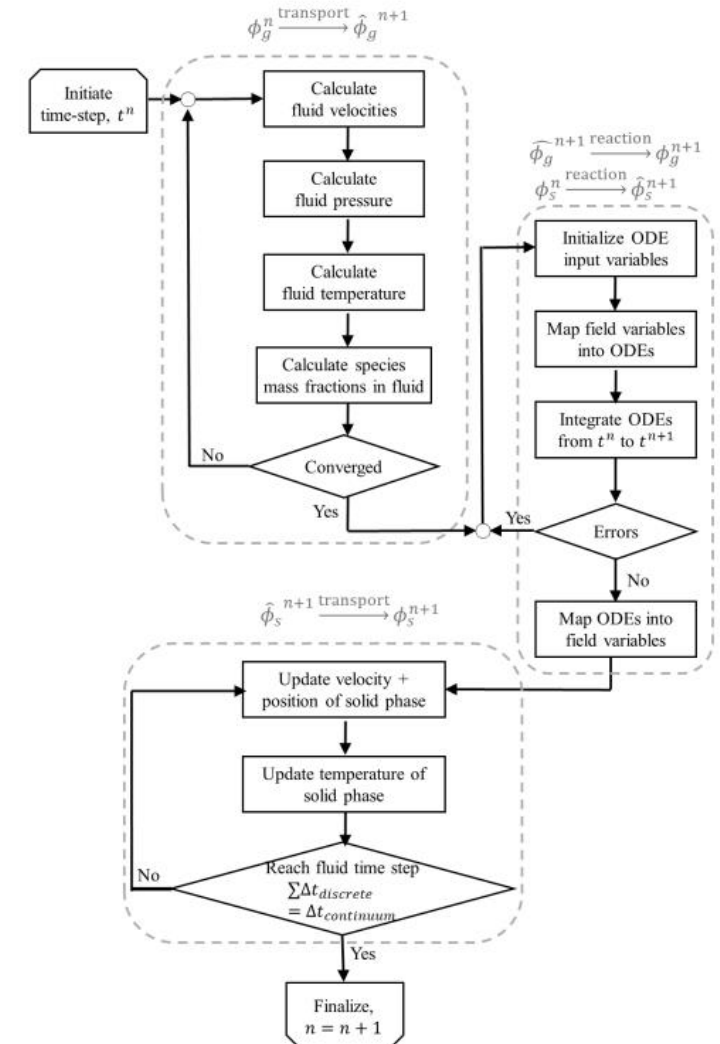
- Composite spheres
- Intra-particle temperature distribution



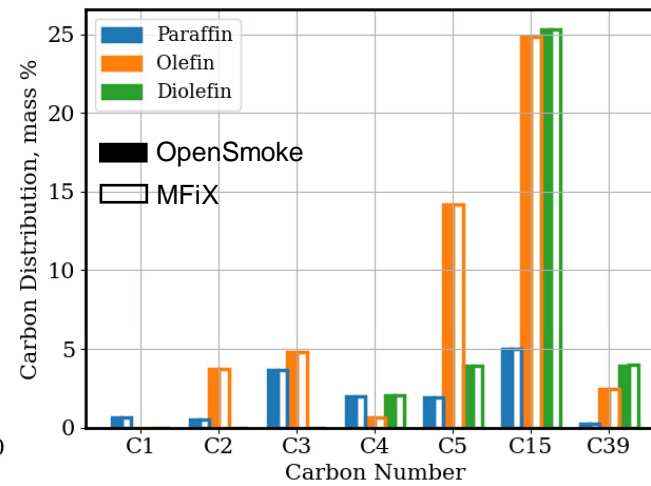
# Chemistry Management

## DEM Stiff Solver (10x to 100x Speedup)

- Stiff solver (fractional-step method) was extended to all discrete particle models (DEM, GSP, SQP, CGP, PIC)
- Improves the ability to deal with detailed chemical mechanisms
- Separates chemical reactions from transport phenomena
- Tested with pyrolysis mechanism from Politecnico di Milano (400 to 1,377 reactions)
- MFiX predicts the same particle mass change and species productions as OpenSMOKE and experimental data



(a) Particle Mass Change



(b) Gas Species Production

## Implementation of CHEMKIN Mechanism in MFiX

```
# Chemical reaction section
@(RXNS)
Reaction_1 {
  chem_eq = "A + B --> 2*C + 3*D"
  dh = 1e3
  fracdh(0) = 1
  arrhenius_coeff = 1000 0.0 2e3
  reverse_calc = fromForwardRateConstant
  rxn_order = A:2 B:1.5
  third_body_param = M_all "A:2 E: 0.5"
  press_rxn_param = Troe_coeff "press_coeff: 0.1 0.2 0.3 &
    Arrhenius_press: 100 -2.0 3e5"
  lt_coeff = 200 500
  fit_coeff = JAN "coeff: 1 2 3 4 5 6"
}
@(END)

@(DES_RXNS)
Reaction_DES_1{
  chem_eq = "F + 2*G --> H + 3*J"
  dh = 2e3
  fracdh(0) = 0.5
  fracdh(1) = 0.5
  arrhenius_coeff = 1e3 -1.0 3e5
  reverse_calc = fromForwardRateConstant
  rxn_order = F: 0.3 G: 2.0
}
@(DES_END)
```

```
ARRHENIUS_RATES_FLUID = .True.
ARRHENIUS_RATES_DES = .True.
```

Two ways to give the reaction rates:

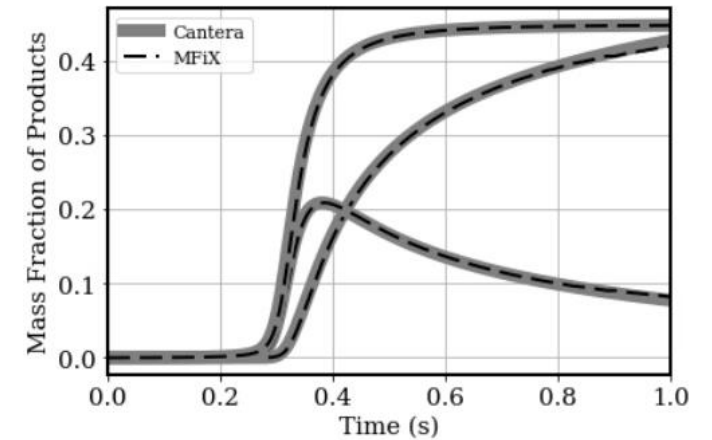
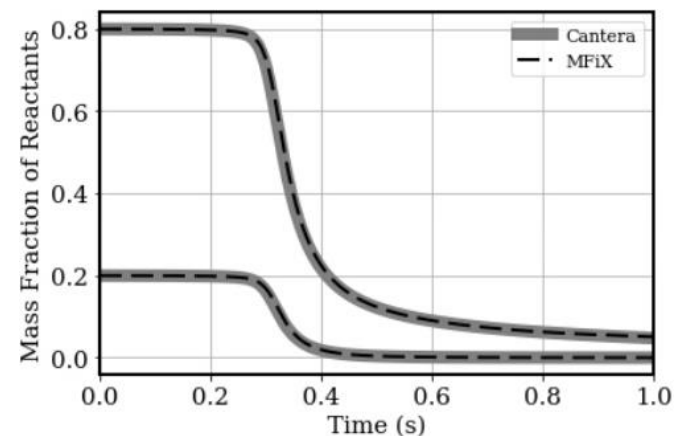
1. User-defined functions (UDF): `usr_rates.f` and `usr_rates_des.f`
2. Give parameters used for reaction rates in the input file (no UDF is required):
  - 1) Input the CHEMKIN mechanism file
  - 2) Add the parameters manually using the corresponding keywords

It could be applied to single gas phase and multiphase models in MFiX, like TFM, DEM, CGDEM, and PIC.

It is helpful when the users want to use CHEMKIN mechanisms directly, especially for detailed chemical mechanisms.


CH<sub>4</sub> combustion in a batch reactor using CHEMKIN **GRI-30 mechanism**:

- Constant temperature:  $T_0 = 1000K$
- Initial composition: CH<sub>4</sub>: 20 wt.%, O<sub>2</sub>: 80 wt.%



# Integrating Machine Learning into MFiX

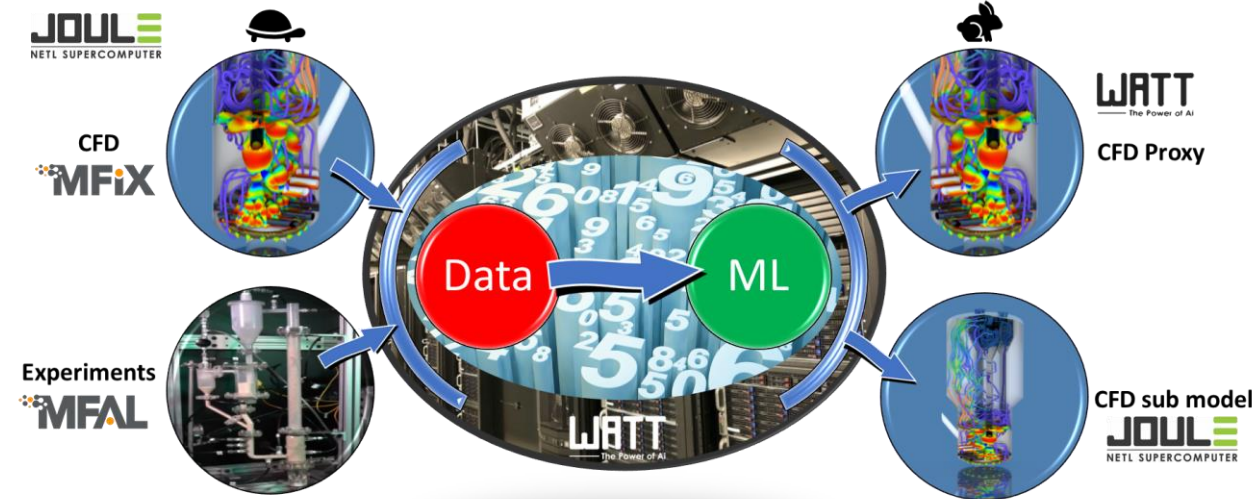
## CFD & Machine Learning Workflow

- Data Generation 
  - Setup
  - Customize output
  - Run CFD
  - Archive/transfer data
- Data Preparation
  - Data cleanup
  - Data compression/dim. reduction
  - Data labeling
  - Remove outliers
  - Normalization
  - One-hot encoding
- ML Training
  - Feature selection and engineering
  - Model + hyperparameters
  - Hyperparameter optimization
  - Training
  - Cross-validation
- User-Defined Function (UDF) hook to use ML During Simulation
  - Call ML model at run time

Python scripting

or

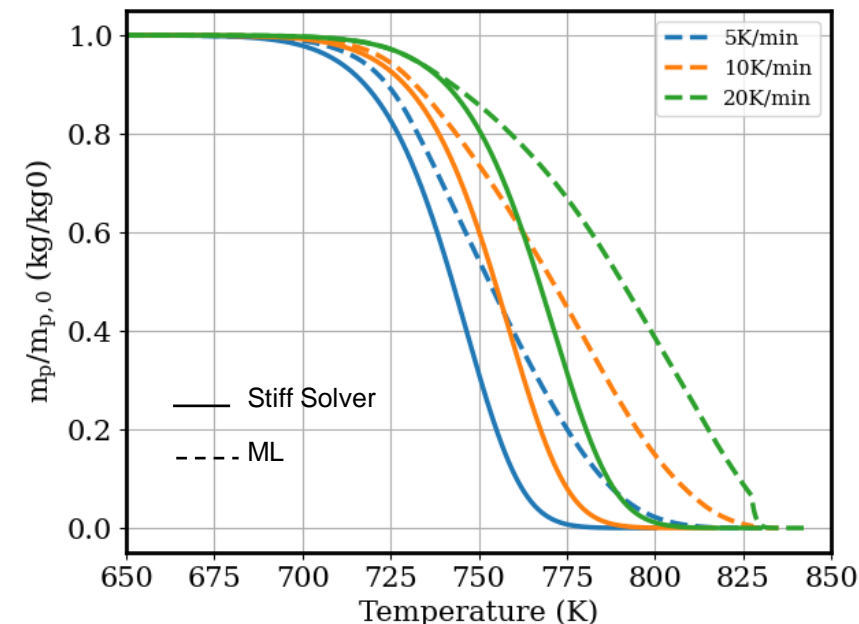
In-house ML tools



# Chemistry ML acceleration

## Stiff Solver ML Proxy

- ML model is integrated into MFIX to replace the stiff solver
- The mechanism for the pyrolysis of high-density polyethylene (HDPE) from Politecnico di Milano is applied to develop and test the ML model
- Data generated by MFIX
- Timing for the reaction terms are compared under three heating rates of particles. Two time-steps are tested
- Current preliminary ML model gives reasonable predictions of particle mass change
- ML model is much faster than the stiff solver, especially with high heating rate and smaller time steps



Time step:  $dt = 0.5s$

	5K/min	10K/min	20K/min
Stiff Solver	276 min	217 min	132 min
ML Model	18 min	10 min	5 min
<b>Speedup</b>	<b>15.3</b>	<b>21.7</b>	<b>26.4</b>

Time step:  $dt = 0.01s$

	5K/min	10K/min	20K/min
Stiff Solver	882 min	441 min	227 min
ML Model	24 min	12.5 min	8 min
<b>Speedup</b>	<b>36.8</b>	<b>35.3</b>	<b>28.4</b>

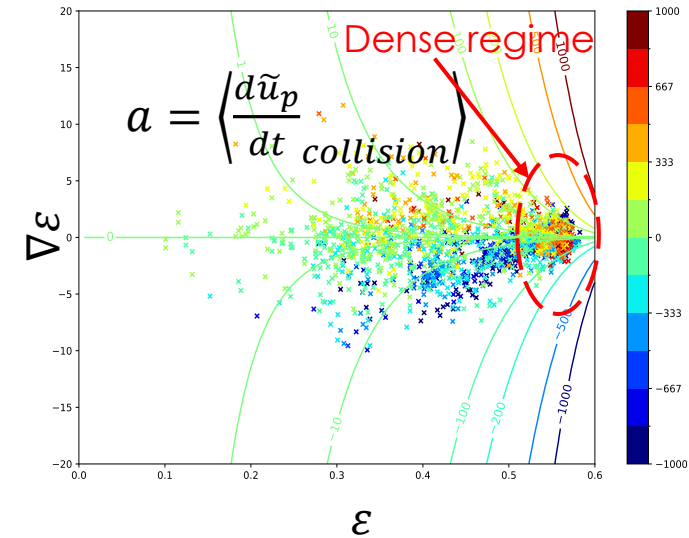
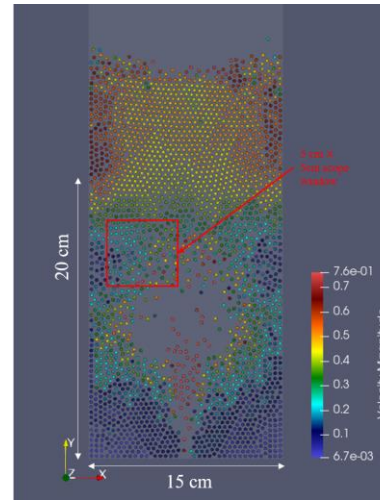


# PIC Stress ML Modeling Using DEM Data

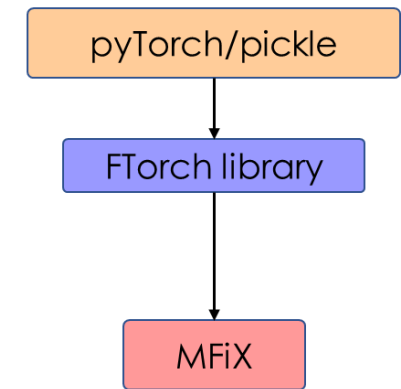
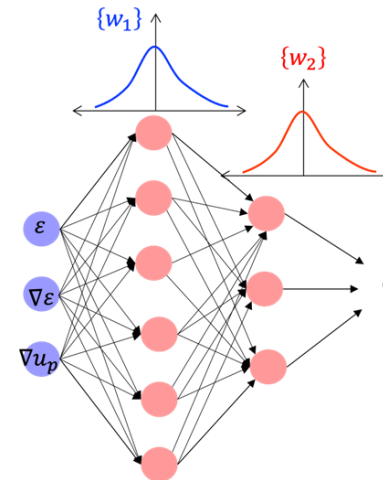
## Data Collection



- DEM fluidized bed with various inlet velocities
- Spatially sample average particulate properties:
- Volume fraction ( $\varepsilon$ ), Gradient of volume fraction ( $\nabla\varepsilon$ ), Granular temperature ( $\theta$ )
  - Average particle velocity ( $u_p$ ), its gradient ( $\nabla u_p$ ), Deceleration due to collisions ( $a$ )
- Temporal averaging of the spatially sampled data is performed over 50 DEM timesteps



- Distinct dense and dilute regimes are observed. Compaction of particles in the dense region and high deceleration magnitudes
- Sampled DEM deceleration term is different from the Harris and Crighton (1994) model used in PIC approach
- Combining Harris & Crighton criteria with sampled datapoints using Bayesian approach
- Incorporating trained BNN model in MFIX code



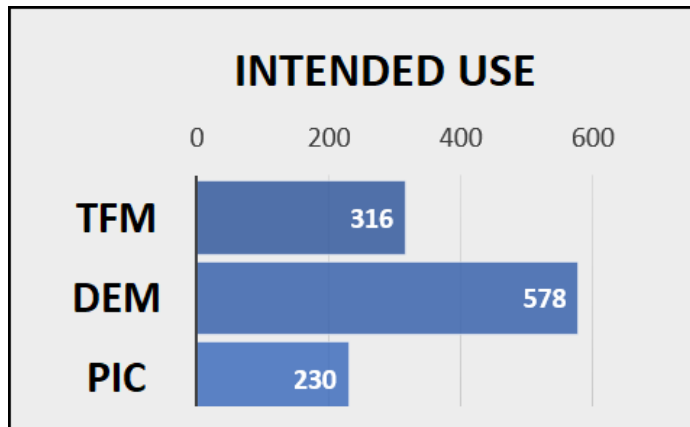
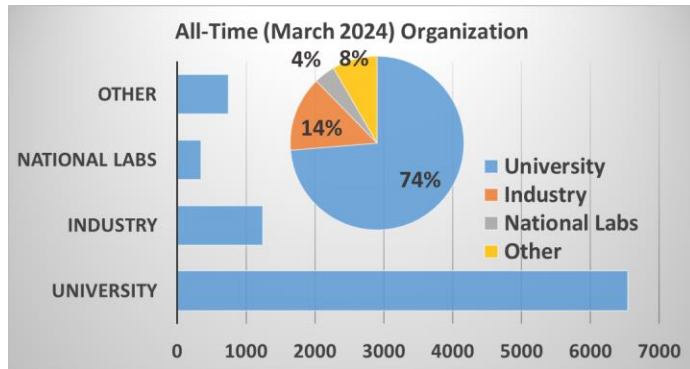
# Outreach: MFiX Stats

## Stakeholders and Technology Transfer

All-time MFiX registrations = **8,800+**

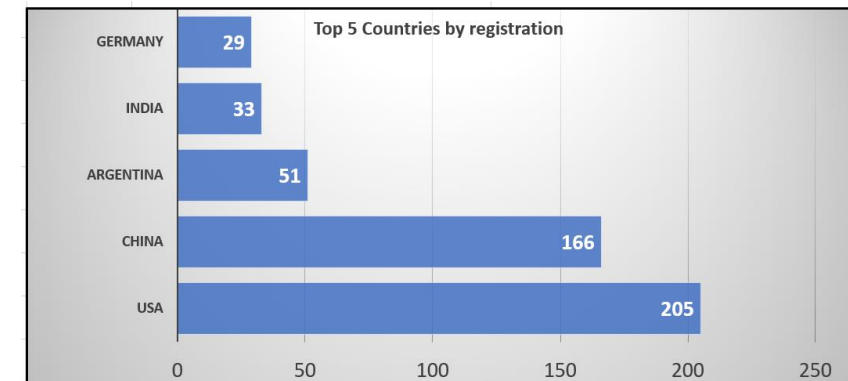
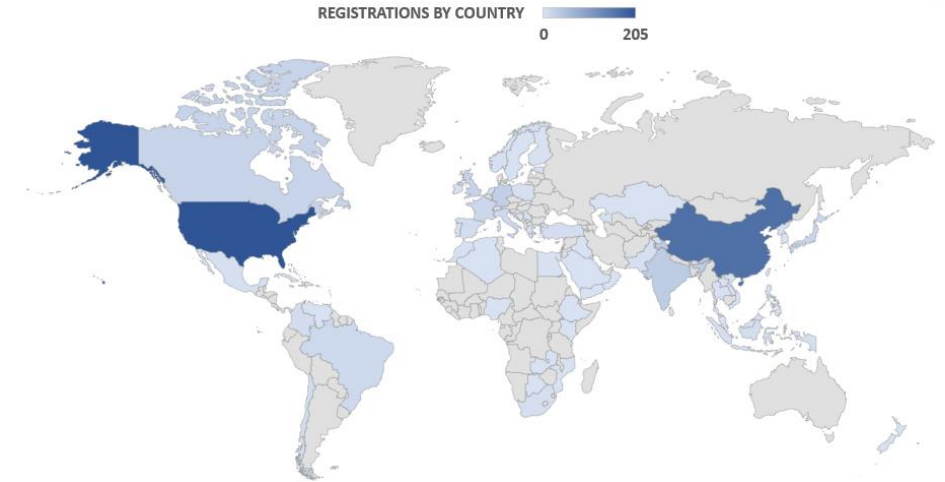
EY23 Registrations = 725

EY23 Downloads = 9,200



Universities using MFiX in their curriculum:

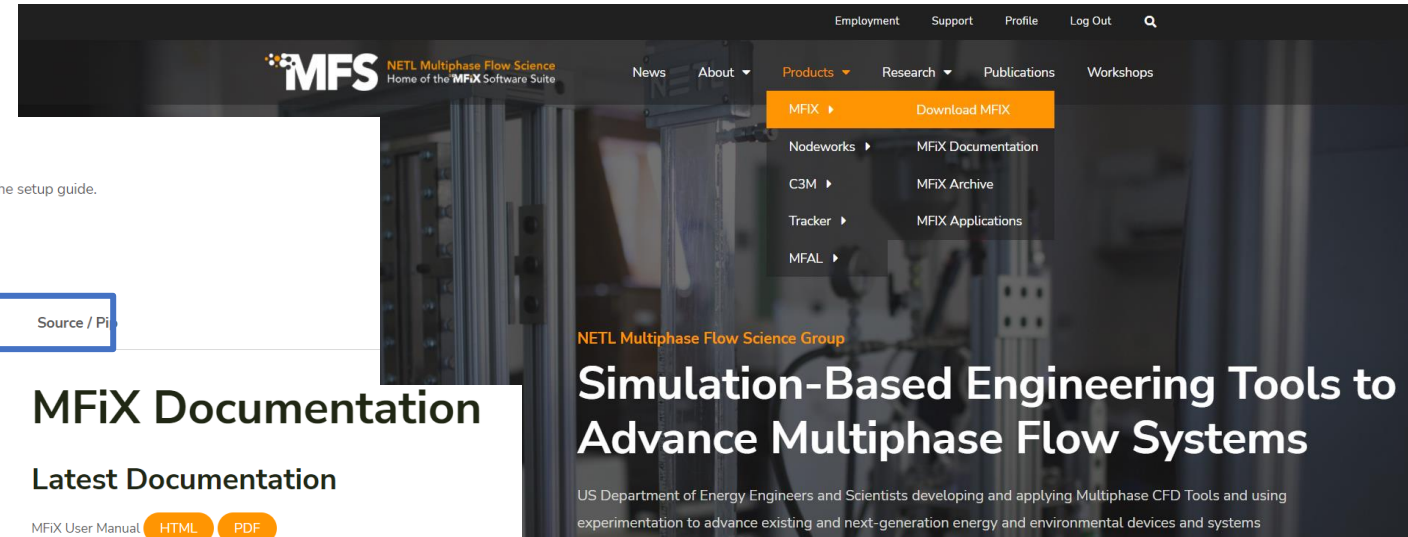
- Arizona State University
- Pennsylvania State University
- Hamburg University of Technology, Germany
- Universidad de La Serena, Chile
- Universidad Nacional de La Plata, Argentina



# Resources – MFiX Website

<https://mfix.netl.doe.gov>

- Showcase NETL's Multiphase Flow Science (MFS) team
  - MFS software
  - Documentation
  - Forum
  - Experimental data (challenge problem)
  - Publications
  - Workshop proceedings
  - News and announcements



## Install MFiX

For detailed setup instructions, follow the setup guide.

[Setup Guide](#)

[Windows](#) [Linux](#) [Mac](#) [Source / Pkgs](#)

## Install Anaconda

Download and install Anaconda (link)

[Anaconda Download](#)

## Install MFiX (in new environment)

Open the Anaconda Prompt (install)

Copy and paste the following command

```
conda create --name mfix --channel=netl mfix
```

This will create a new conda environment

## Run MFiX

## MFiX Documentation

### Latest Documentation

MFiX User Manual [HTML](#) [PDF](#)

MFiX Verification and Validation Manual, Second Edition [HTML](#) [PDF](#)

MFiX PIC Theory Guide [PDF](#)

[Nodeworks Plugin](#)

### Older Documentation

- [Summary of MFiX Equations \(2012\)](#)
- [DEM documentation \(2012\)](#)
- [Cartesian grid user guide \(2015\)](#)
- [Result sensitivity to Fortran compiler \(2012\)](#)

### Legacy Manuals

- [Theory guide \(1993\)](#)
- [Numerics guide \(1998\)](#)

### MFiX Training

- [PNNL Training \(2011\)](#)

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

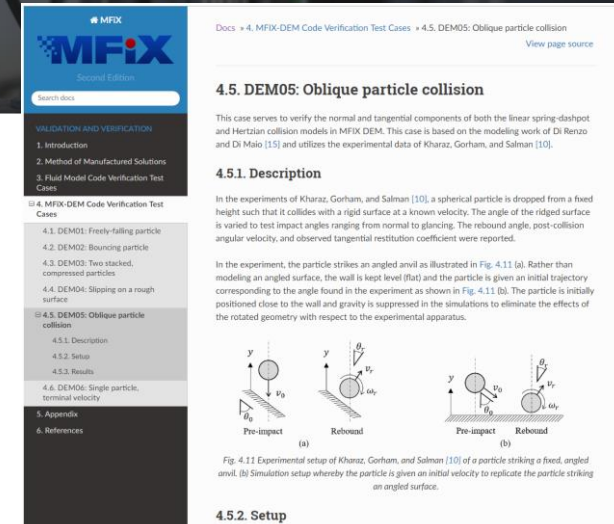
Docs » 3. Tutorials » 3.6. Three Dimensional DEM Hopper [View page source](#)

### 3.6. Three Dimensional DEM Hopper



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

Property	Value
geometry	5 cm diameter hopper
mesh	10 x 25 x 10
solid diameter	0,003 m
solid density	2500 kg/m <sup>3</sup>



4.5. DEM05: Oblique particle collision

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

#### 4.5.1. Description

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

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

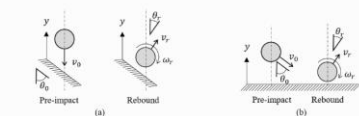


Fig. 4.11 Experimental setup of Kharaz, Gorham, and Salman [10] of a particle striking a fixed, angled anvil. (a) Simulation setup whereby the particle is given an initial velocity to replicate the particle striking an angled surface.

#### 4.5.2. Setup



Thank you.  
Questions?



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