MFIX-DEM Phi: Performance and Capability Improvements Towards Industrial Grade Open-source DEM Framework with Integrated Uncertainty Quantification

Presenter: M. Adepu
A. Gel, S. Chen, Y. Jiao, H. Emady, C. Tong and J. Hu

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Pittsburgh, PA
03/20/2017

Lawrence Livermore National Laboratory
Sandia National Laboratories
ASU

Presentation Outline

- ❑ Team members
- ❑ Potential Significance of The Results of The Work
- ❑ Physical Modeling Enhancements
- ❑ Results and Discussion
- ❑ Acknowledgements

MFIX-DEM Phi team: ASU campus

PI: Aytekin Gel

- PhD, West Virginia U. 1999; MBA, ASU, 2007.
- Professor of Practice, School of Computing, Informatics, Decision Systems Engineering (SCIDSE), ASU
- Expertise: HPC, CFD, UQ, multiphase reactive flow, Six Sigma for Quality
- 16 years of startup company experience; Involved with MFIX since 1999
- Award: Team Member of R&D 100, 2007

Co-PI: Heather Emady

- PhD, Purdue U. 2012
- Assistant Professor, School of Engineering, Materials, Transport and Energy (SEMTE), ASU.
- Expertise: particulate processes and product design
- Award: Bisgrove Scholar, 2015

Co-PI: Yang Jiao

- PhD, Princeton U. 2010
- Assistant Professor, School of Engineering, Materials, Transport and Energy (SEMTE), ASU.
- Expertise: computational materials
- Award: DARPA Young Faculty, 2014

GRA: Manogna Adepu

- PhD candidate, SEMTE.
- Focus: Validations

GRA: Shaohua Chen

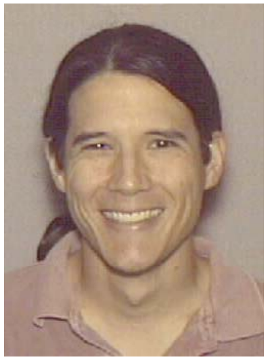
- PhD candidate, SEMTE.
- Focus: Computation

MFIX-DEM Phi Team

Member at
Lawrence Livermore National Laboratory (LLNL)

Co-PI: Charles Tong
- Research Scientist
- Expertise: uncertainty quantification
- Developer of open-source UQ toolbox PSUADE and CCSI Toolkit UQ framework FOQUS

Members at
Sandia National Laboratory (SNL)

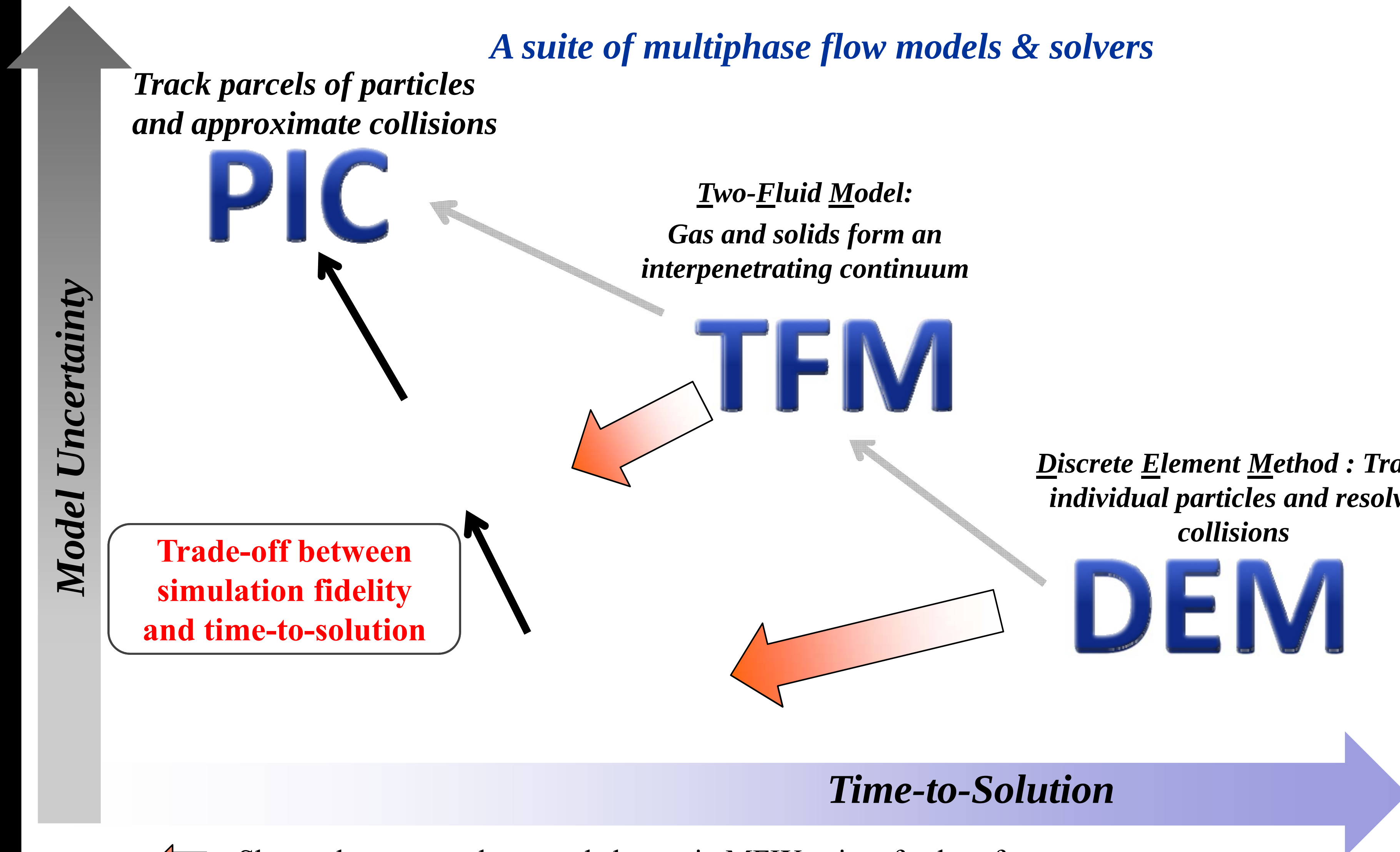


Co-PI: Jonathan Hu
- Principal Member of the Technical Staff at Sandia National Laboratories
- Expertise: highly scalable linear equation solver, developer of Trilinos Project (ML, nextgen ML: MueLu)
- Award: R&D 100 (Trilinos)

Nathan Ellingwood
- Research Staff at Sandia National Laboratories
- Ph.D. in Applied Math & and Computational Sciences, University of Iowa (2014)
- Expertise: Data parallel algorithms for GPU, FEM, CFD, HPC, Digital Lung Project

Overview of MFIX DEM Phi Project Outcomes

MFIX: **M**ultiphase **F**low with **I**nterphase e**X**changes



Shows the proposed targeted change in MFIX suite of solver features.

MFIX-DEM Phi: Performance and Capability Improvements Towards Industrial Grade Open-source DEM Framework with Integrated Uncertainty Quantification

Task 1 Aim:

Demonstrate usability for industrial scale problems and collaboration for industrial adoption.

BASF We create chemistry

ExxonMobil Research and Engineering

P&G Procter&Gamble

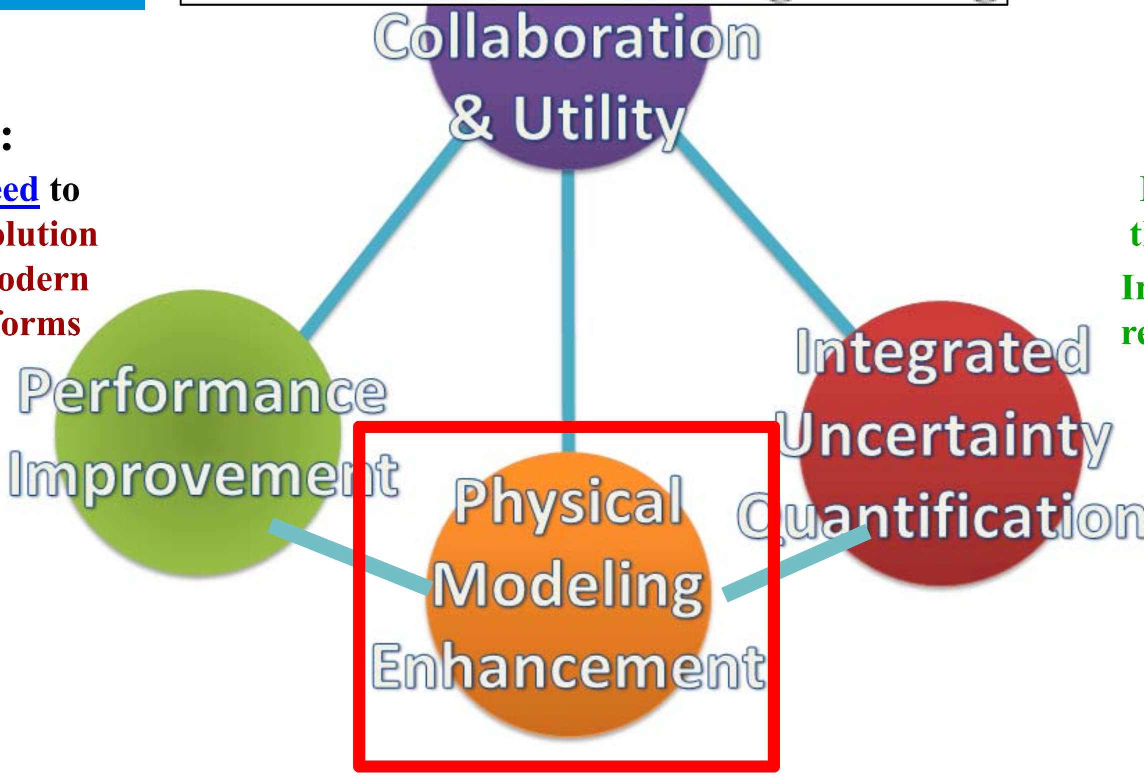
Task 2 Aim:

Increase the speed to reduce time-to-solution by optimizing modern computing platforms

Task 4 Aims:

Ensure the results of the code are accurate.

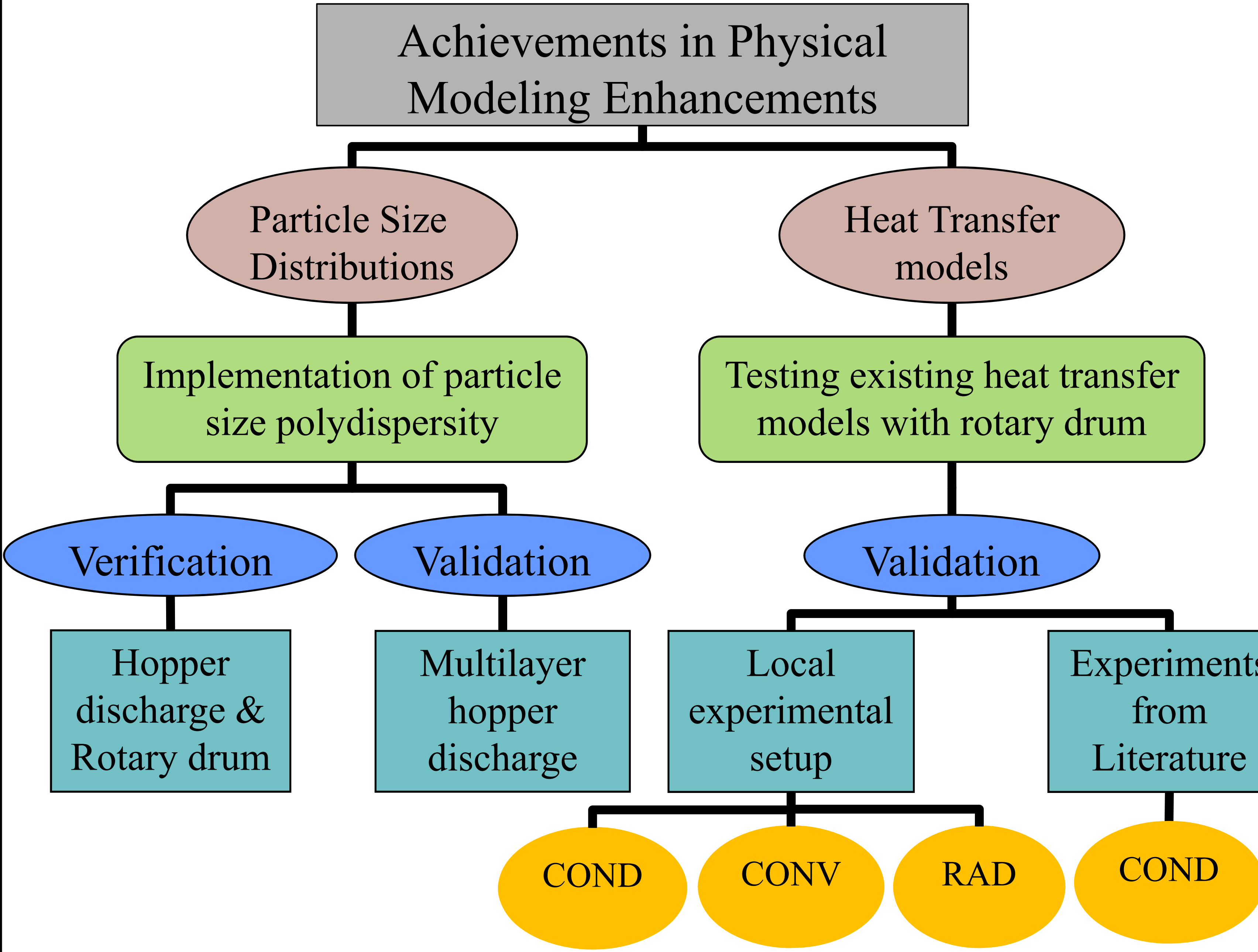
Increase usability by reducing complexity



Task 3 Aim:

Develop physics w.r.t. the targeted application

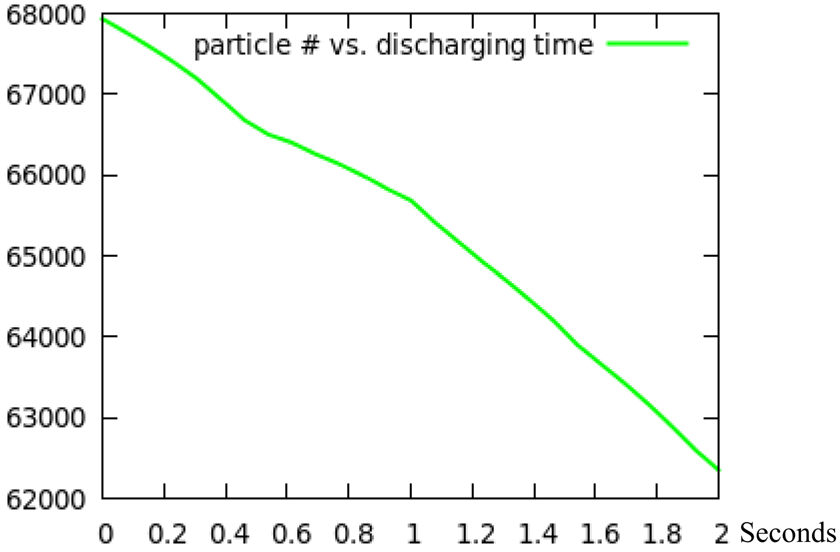
Physical Modeling Enhancement

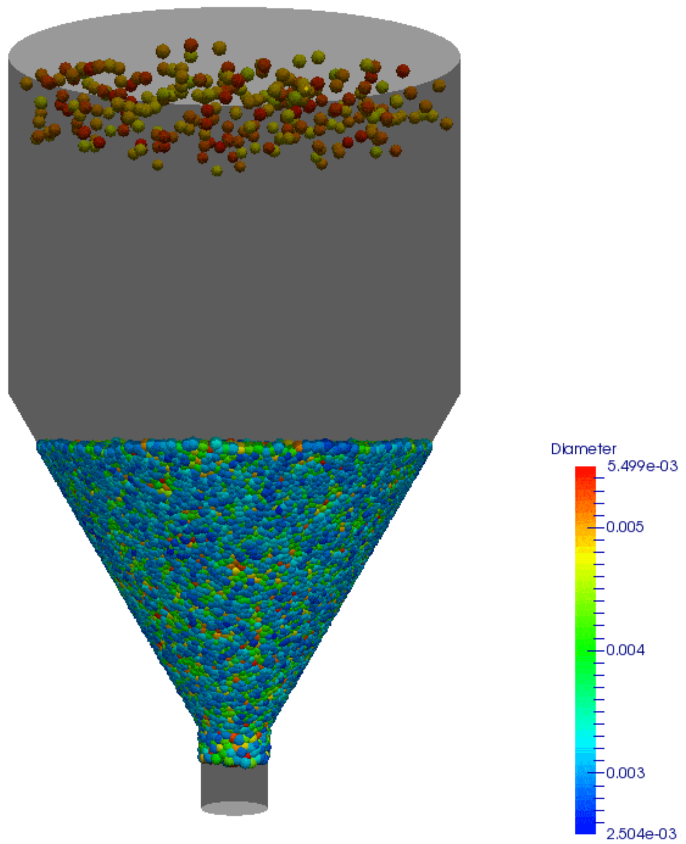


Hopper with mass inflow BC

Three solid phases:

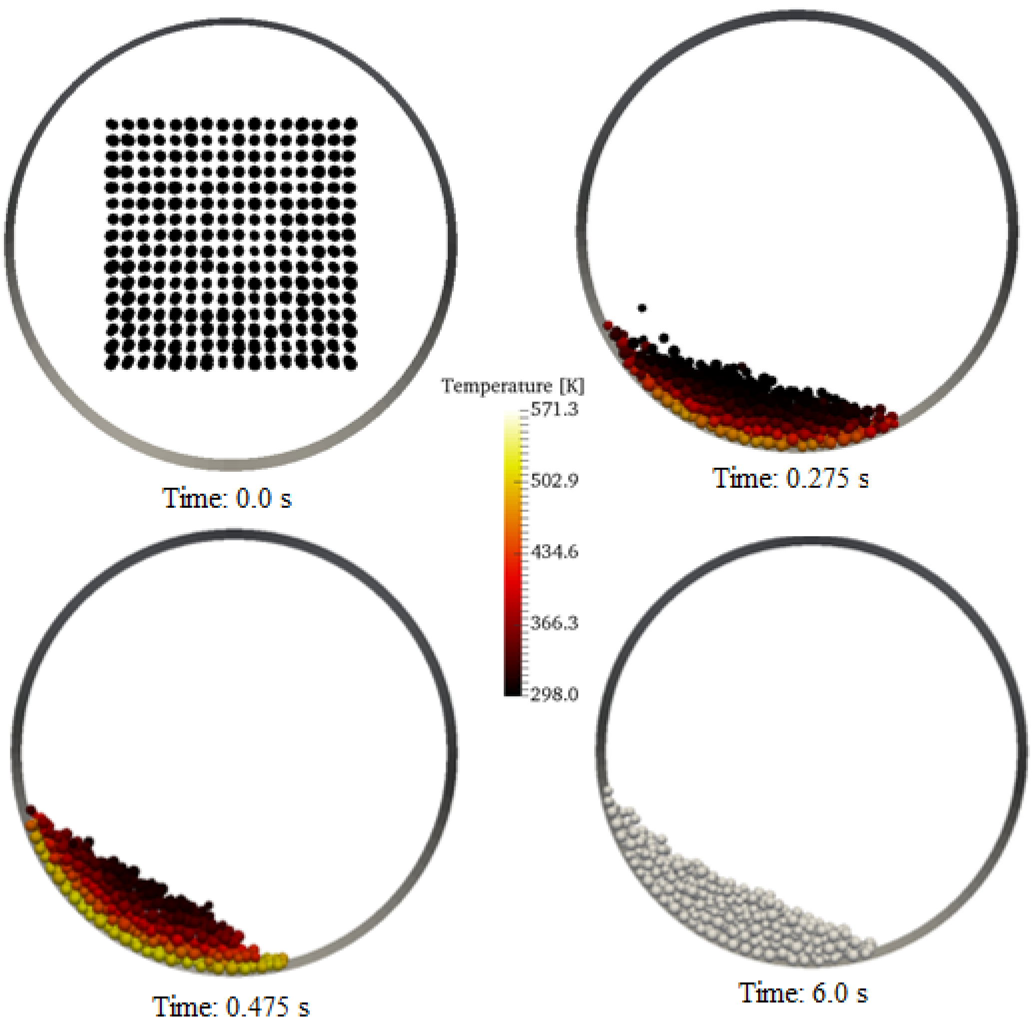
phase 1, μ=5.3 σ=0.05(MI)
phase 2, μ=5.5 σ=0.05
phase 3, μ=5.8 σ=0.05





Enhance the Capability for Handling Particle Size Distributions

Testing polydispersity implementation with conduction heat transfer



Temperature profile

Particle distribution under initial condition

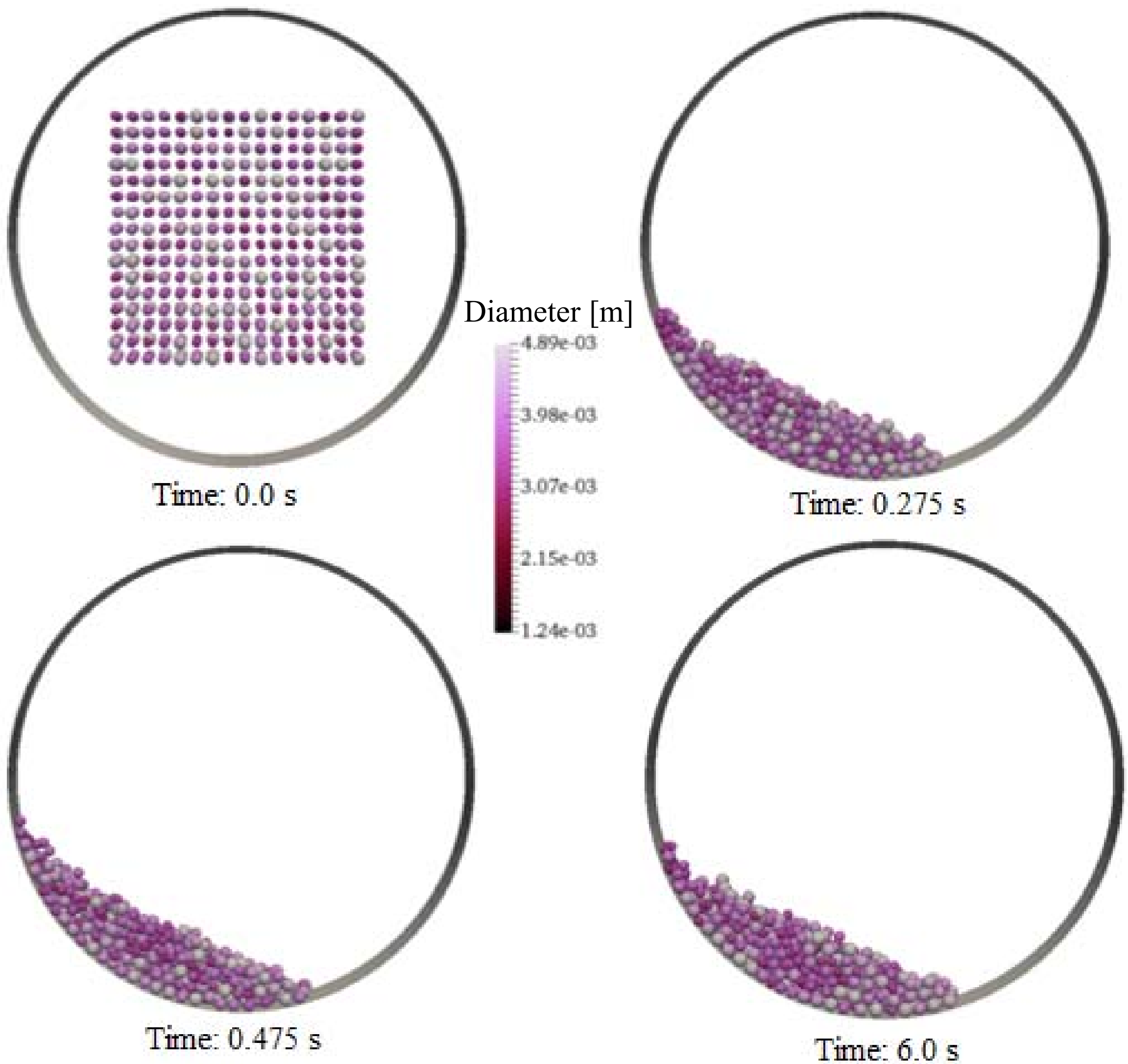
IC_PSD_TYPE	NORMAL
IC_PSD_MEAN_DP	4 mm
IC_PSD_STDEV	0.9
IC_PSD_MIN_DP	3.1 mm
IC_PSD_MAX_DP	4.9 mm

Parameter used for studying HT

Global	Coefficient of restitution	
	particle-particle	0.9
	particle-wall	0.9
	Normal stiffness coefficient	
	Particle/particle	1.0D2 N/m
	Particle/wall	1.0D2 N/m
	DEM time step	1*10-5 s
Particles	Density	3900 kg/m3
	Number of particles	512
	Initial temperature	298 K
	Specific heat	880 J/KgK
	Thermal conductivity	3000 W/mK
Drum	Temperature	600 K
	Diameter	15 cm
	Length	2 cm
	Rotation speed	20 rpm

Enhance the Capability for Handling Particle Size Distributions

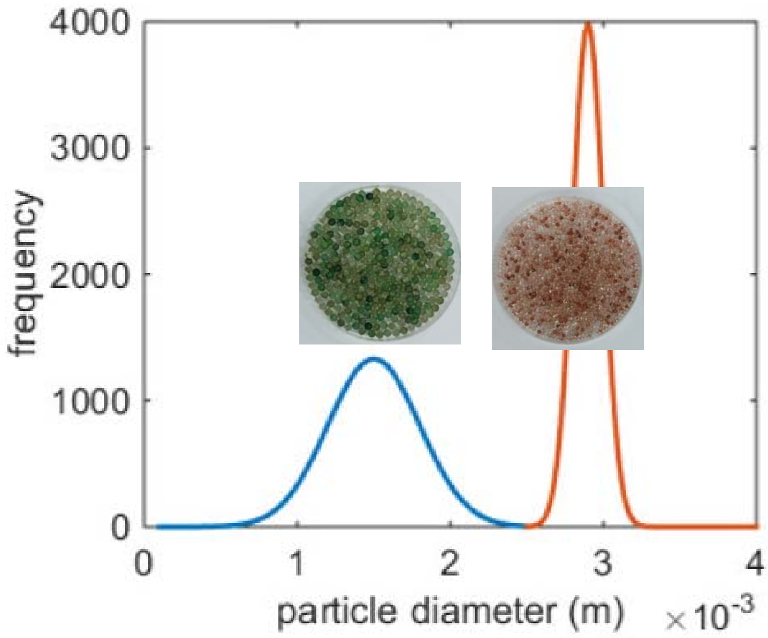
Testing polydispersity implementation with conduction heat transfer



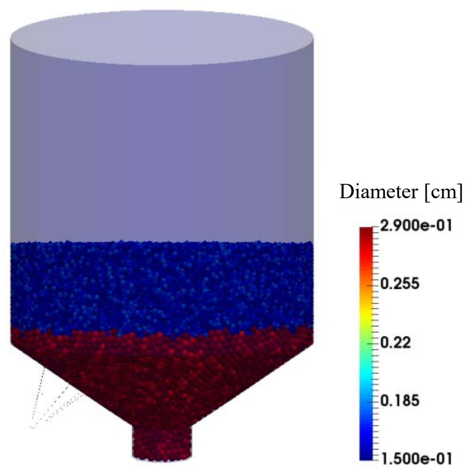
Granular flow in a rotary drum

Enhance the Capability for Handling Particle Size Distributions

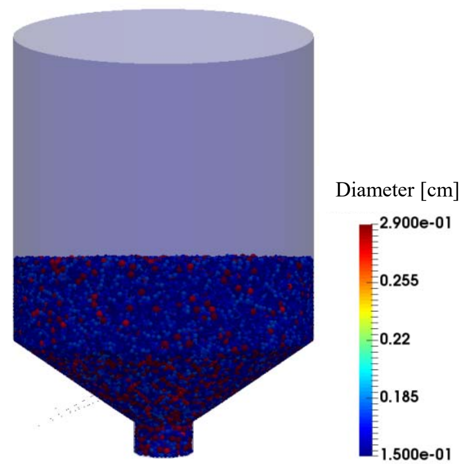
Validation of Polydispersity Implementation



The particles in the hopper possess a bi-modal particle size distribution, which includes two normal distributions for fine and coarse particles.



Initial configuration of the discharge hopper containing a layered packing of spherical beads with a bi-modal size distribution.



Initial configuration of the hopper discharge containing a well-mixed packing of spherical beads with a bi-modal size distribution.

Source: Chen, S. et. al., Enhancing the Capability for Handling Particle Size Polydispersity of Open-Source CFD-DEM Software : Implementation and Validation. Submitted to Powder Technology. (completed first stage of peer review)

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Enhance the Capability for Handling Particle Size Distributions

Validation of Polydispersity Implementation

Sample	mean diameter (m)	max diameter (m)	min diameter (m)	STDV (m)	total mass (g)
Fine	0.0015	0.0017	0.0013	0.0003	580
Coarse	0.0029	0.0031	0.0027	0.0001	420

Coarse particles

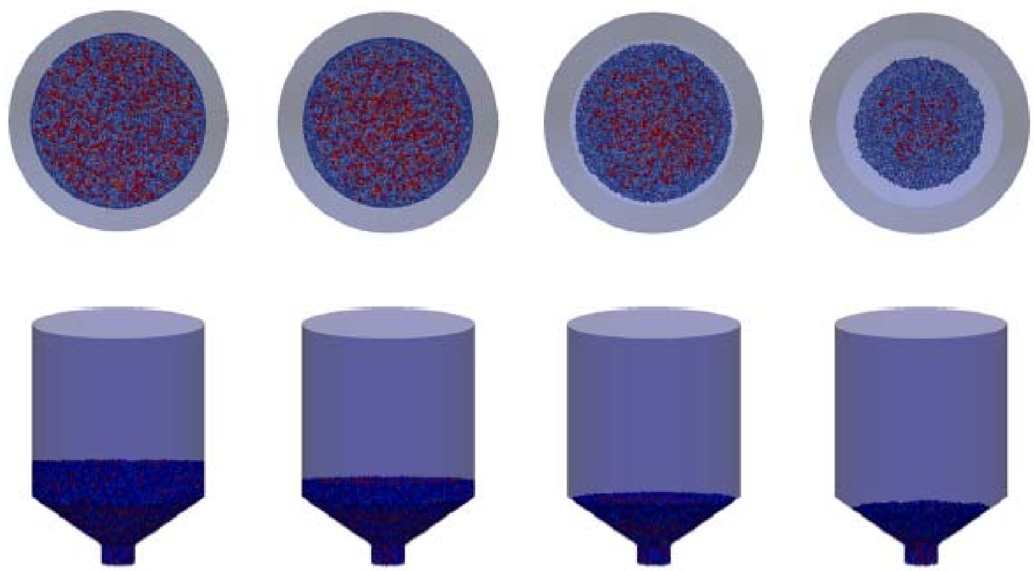
Fine particles

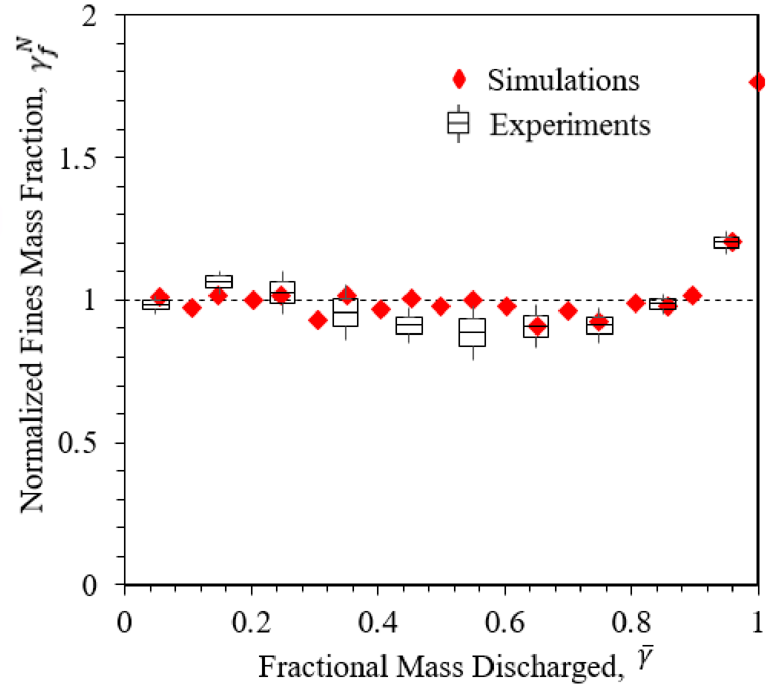
Source: Chen, S. et. al., Enhancing the Capability for Handling Particle Size Polydispersity of Open-Source CFD-DEM Software : Implementation and Validation. Submitted to Powder Technology. (completed first stage of peer review)

Enhance the Capability for Handling Particle Size Distributions

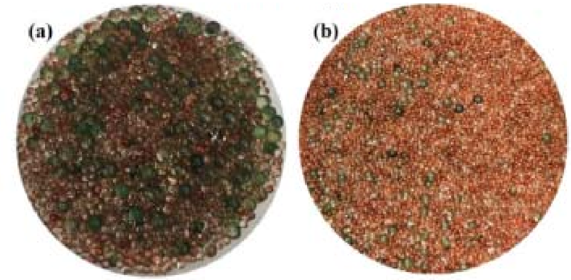
Validation of Polydispersity Implementation

Well-mixed configuration





Snapshots of the discharge simulation of the well-mixed configuration at 6 s, 9 s, 11s and 12 s respectively from left to right. The upper panels show the top view and the lower panels show the side view.

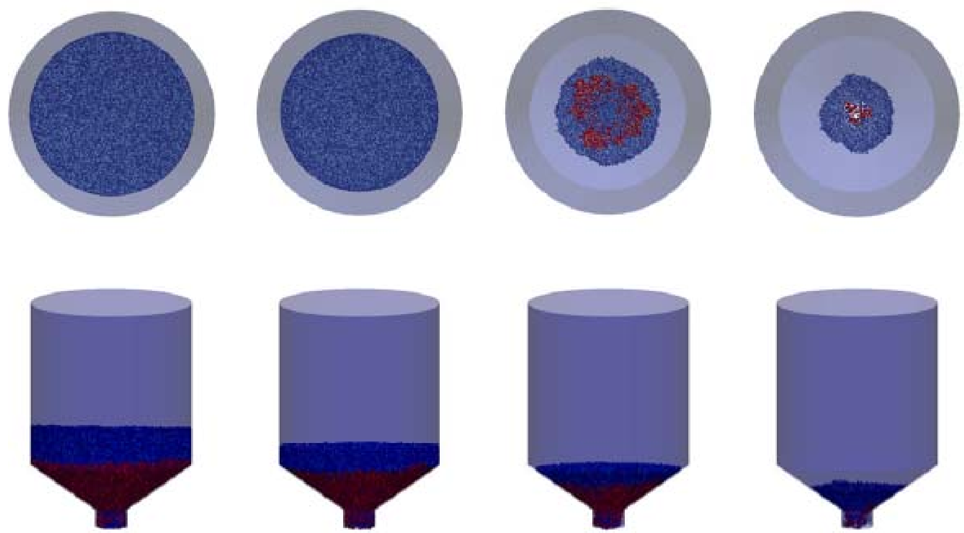


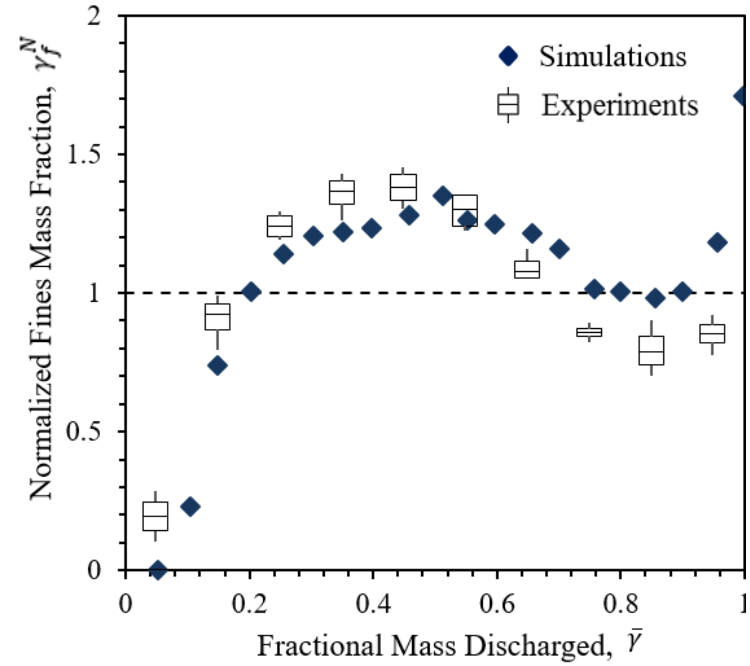
Source: Chen, S. et. al., Enhancing the Capability for Handling Particle Size Polydispersity of Open-Source CFD-DEM Software : Implementation and Validation. Submitted to Powder Technology. (completed first stage of peer review)

Enhance the Capability for Handling Particle Size Distributions

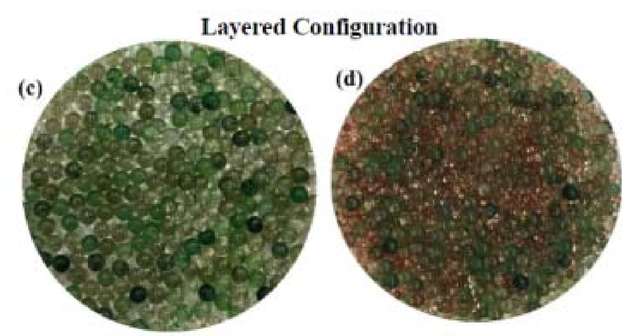
Validation of Polydispersity Implementation

Layered configuration





Snapshots of the discharge simulation of the layered configuration at 6 s, 9 s, 11 s and 12 s respectively from left to right. The upper panels show the top view and the lower panels show the side view.



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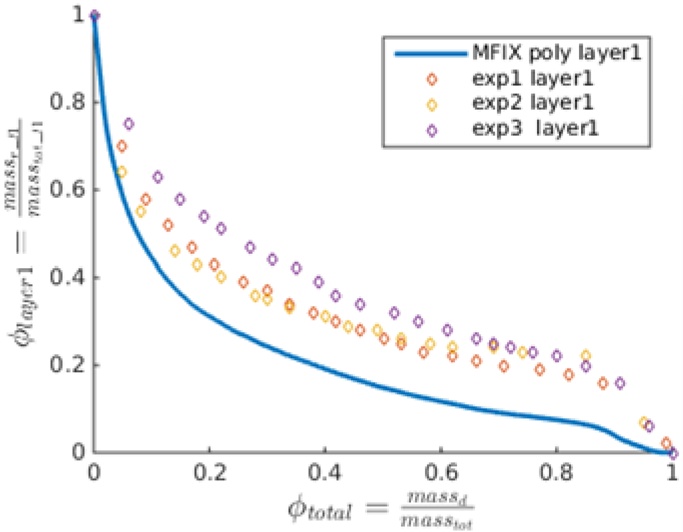
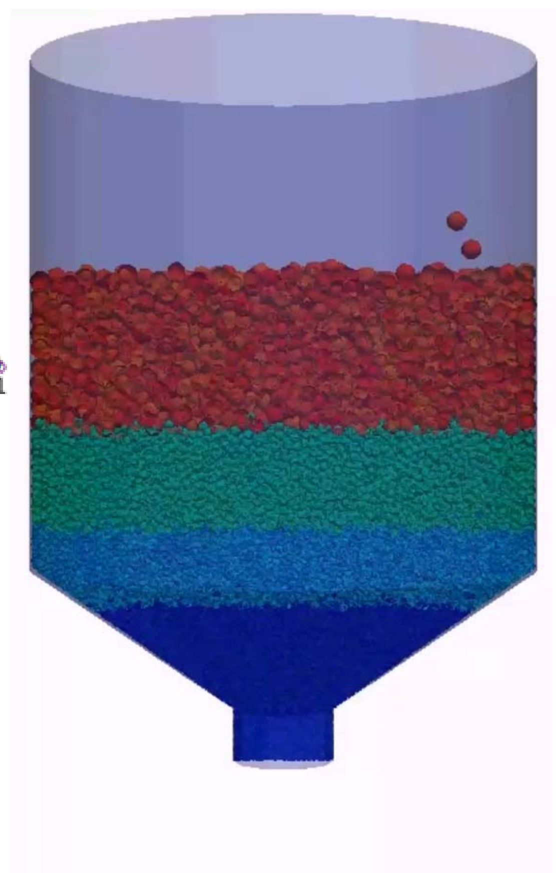
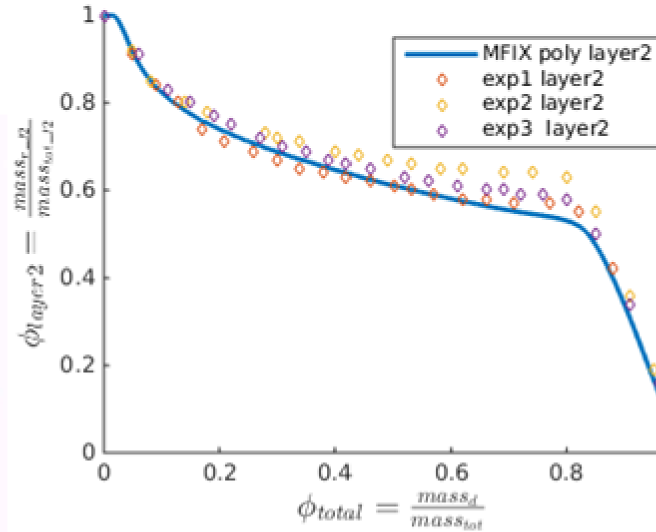
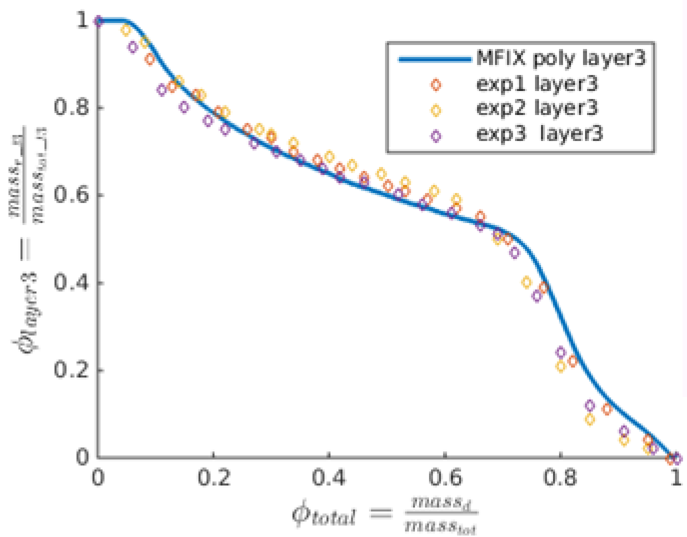
Enhance the Capability for Handling Particle Size Distributions

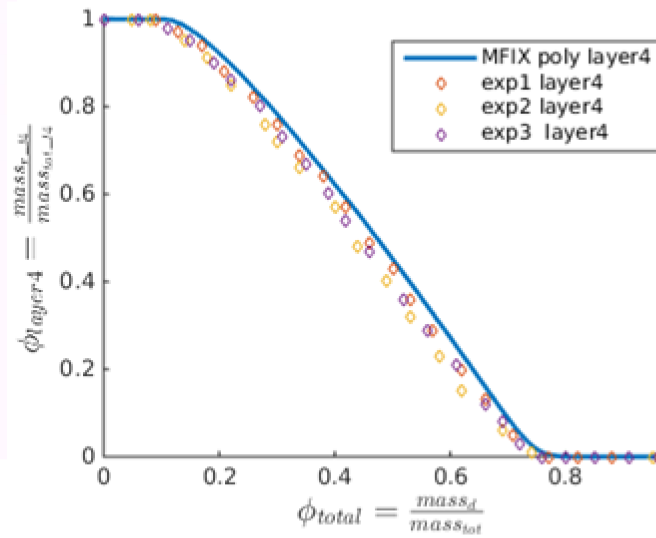
Multilayer Discharge Segregation result: MFIX Vs Experiments





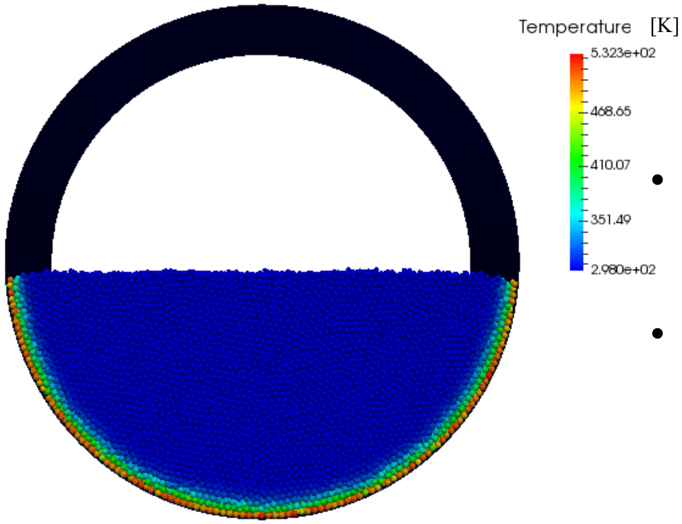






Enhance the Capability for Handling Heat Transfer

Wall heat transfer in a rotary drum



Snapshot of wall HT after 2 sec of simulation.

- Conduction, convection, and radiation occur in many multiphase processes. Particle-particle conduction is now commonly used in DEM codes, but more complex heat transfer nodels are necessary to more accurately simulate these processes.

- Current serial version of MFIX-DEM has codes for each of these, but they remain to be tested and validated.

- Whether drying, mixing, granulating, coating or heating, rotary drum systems are among the most common process equipment, offering efficient economical solutions. Thus, a rotary drum was selected for validating heat transfer models.

Source : http://www.muzzio.rutgers.edu/

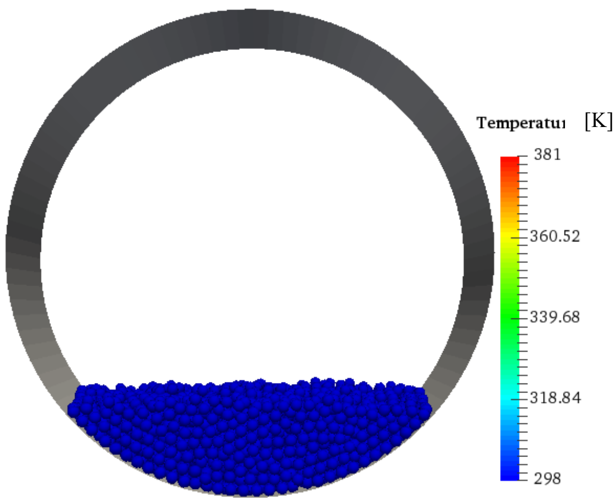
Enhance the Capability for Handling Heat Transfer

Testing all modes of HT implemented in MFIX-DEM

- Simulations were done to test the implementation of all the three modes of HT.
- The drum was held at a fixed hot temperature of 1000 K and particles are initially placed in the drum with a temperature of 298K.

Simulations demonstrates:

1. particle-wall and particle-fluid-wall heat transfer
2. Radiation heat transfer



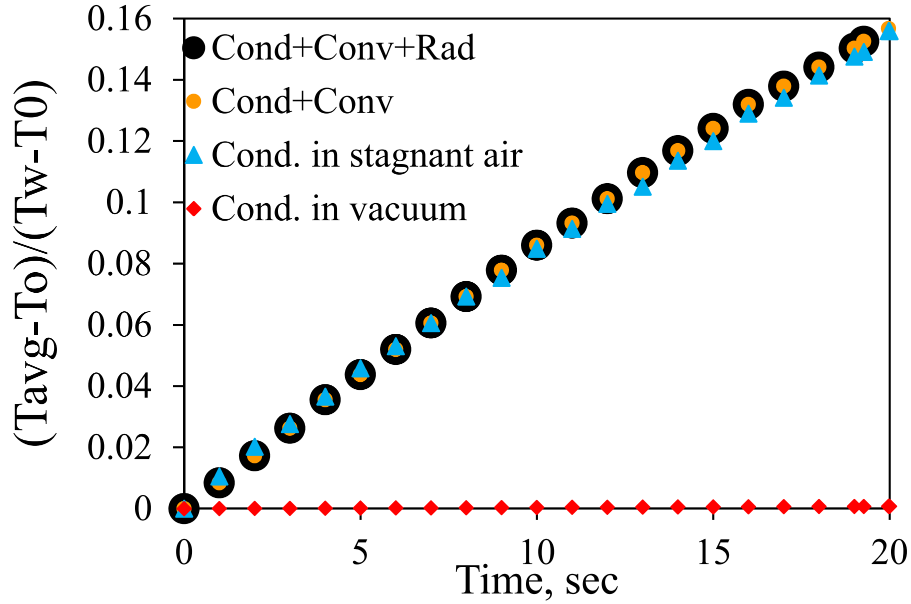
Settled particles: Used as the initial setup

Global	Coefficient of restitution, PP, PW	0.9
	Friction coefficient, PP, PW	0.1
	Stiffness coefficient, PP, PW [N/m]	1.0D2
	DEM time step [s]	1*10-5
Geometry	Diameter [cm]	15.24
	Length [cm]	7.62
	Rotation speed [rpm]	45
	Boundary condition	CG_NSW
	Temperature(fixed) [K]	1000
Solid phase (Silica balls/glass)	Density [Kg/m³]	2500
	Number of particles	3583
	Initial temperature [K]	298

Parameters employed for the simulations

Enhance the Capability for Handling Heat Transfer

Testing all modes of HT implemented in MFIX-DEM using a rotary drum

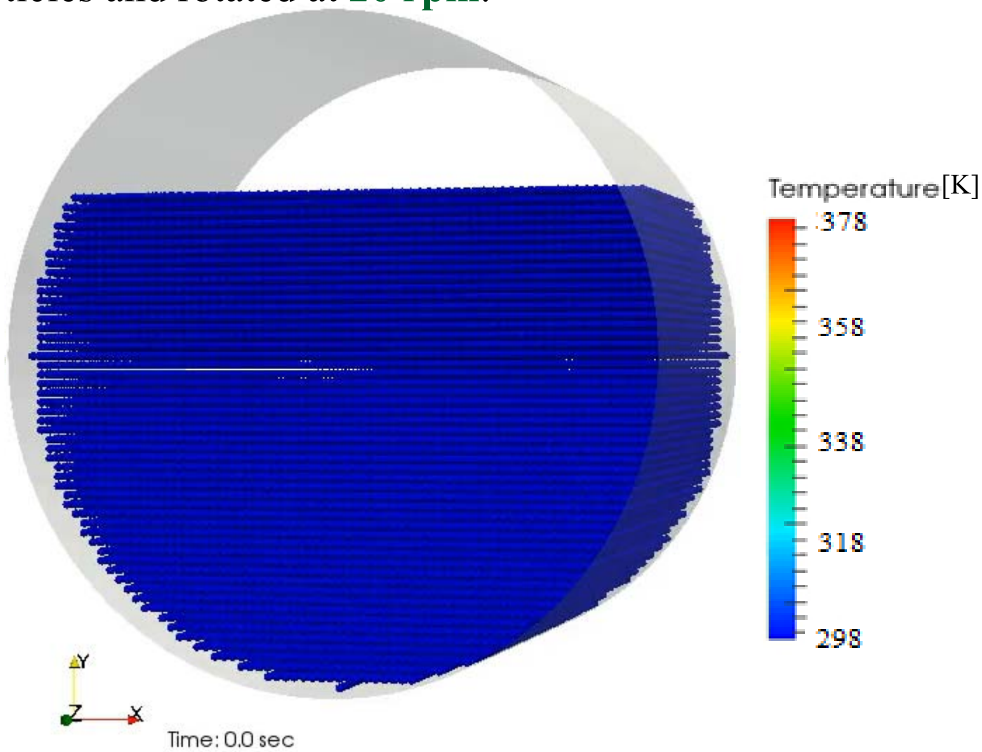


	Parameters	Conduction in vacuum	Conduction in stagnant air	Convection & Conduction	Conduction, convection and radiation
Solid Phase	Specific heat [J/KgK]	840	840	840	840
	Thermal conductivity [W/mK]	1.05	1.05	1.05	1.05
	Thermal emissivity	0	0	0	0.8
Coupling	Drag model	-	-	SYAM_OBRIEN	SYAM_OBRIEN
Gas phase	Specific heat [J/Kg-K]	0	1000.7	1000.7	1000.7
(air)	Thermal conductivity [W/mK]	0	0.0261	0.0261	0.0261

Enhance the Capability for Handling Heat Transfer

Validation of conduction heat transfer

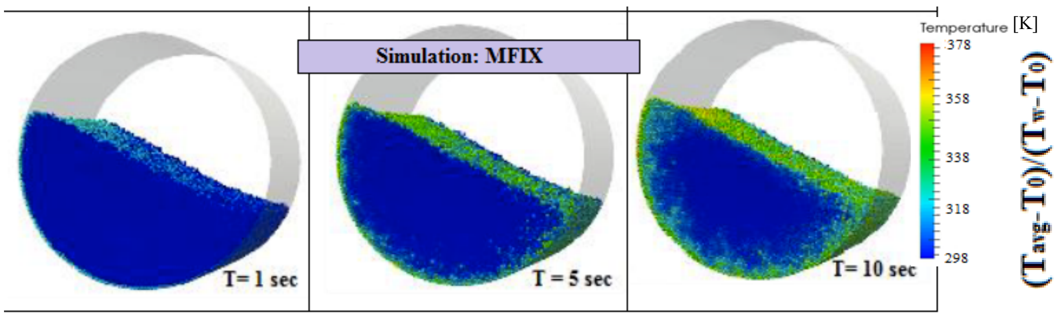
- *Bodhisattwa Chaudhuri, et al. "Experimentally validated computations of heat transfer in granular materials in rotary calciners". Powder Technology 198 (2010) 6–15.*
- A cylindrical drum with **6" diameter and 3" long** was held at 398 K.
- Drum is **half filled** with **2 mm alumina** particles and rotated at **20 rpm**.
- All the parameters and setup was **based on the experimental works** published by *Chaudhuri et al., 2010.*
- Particles are loaded and allowed to fall under gravity.
- **Particles move due to friction** between the wall and particles.
- Heat is transferred simultaneously from wall to particles.



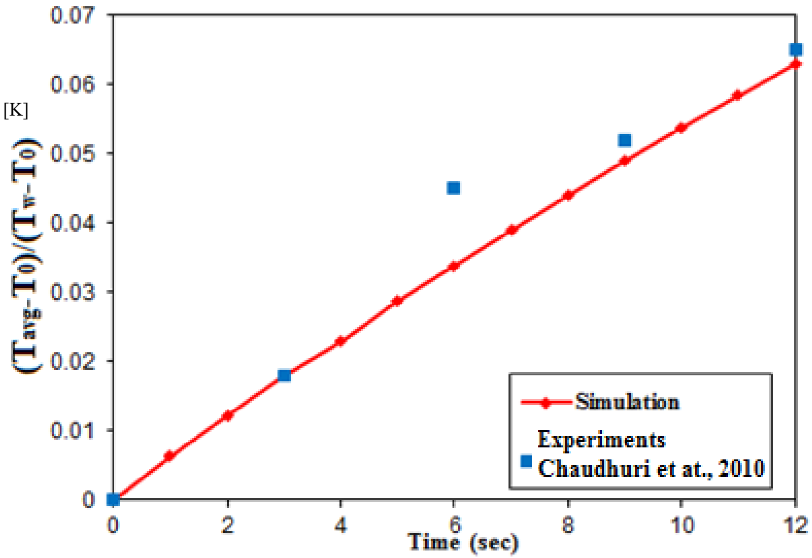
Animation of conduction wall heat transfer (20 sec)

Validation of conduction heat transfer

- To validate MFIX, the **normalized temperature curve** was compared to the experimental results.
- **Good agreement** of temperature profile between the MFIX simulations and paper experiments was observed.
- For a better quantitative comparison the thermal time constant was estimated.



A time sequence of axial snapshots of temperature profile



Evolution of average bed temperature. The fill level of the drum is 50% and is rotated at 20 rpm.

***Source**: *Bodhisattwa Chaudhuri, et al. "Experimentally validated computations of heat transfer in granular materials in rotary calciners". Powder Technology 198 (2010) 6–15.*

Enhance the Capability for Handling Heat Transfer

Validation of conduction heat transfer

Estimation of the thermal time constant-simulations and experimental results

- The heat transfer from the wall to the particles can be calculated from the heat balance equation:

$$M_s C_{ps} \frac{d}{dt}(T_s) = \alpha e_s A_s L (T_W - T_s)$$

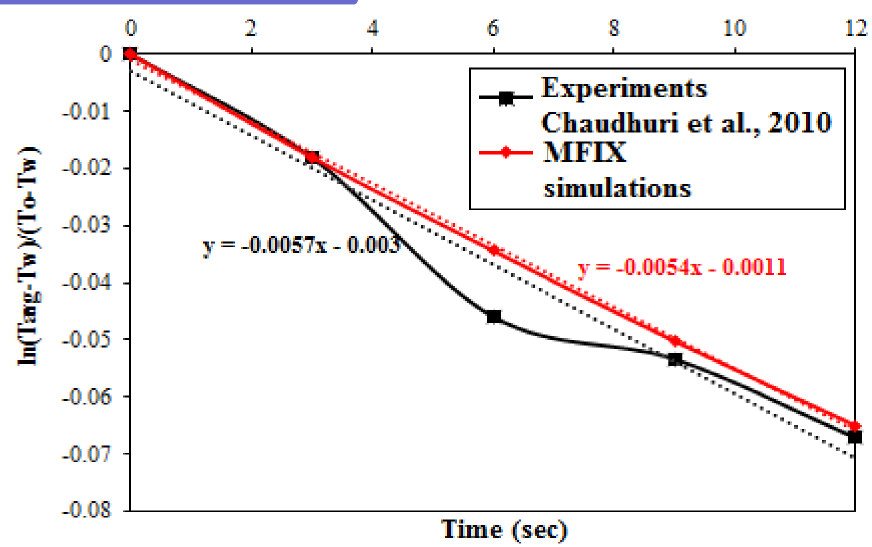
$$ln\left(\frac{T_W - T_s}{T_W - T_s^{\circ}}\right) = -\frac{\alpha e_s A_s L}{M_s C_{ps}} t = -\frac{t}{\tau}$$

From the graph, slope = -1/τ = - 0.0057 (paper experiments)
slope = -1/τ = - 0.0054 (MFIX simulations)

- The thermal time constant is estimated,

τ (experiments) = 175 s
τ (MFIX) = 185 s

- A discrepancy of **5.6%** is observed.



Variation of scaled temperature difference of MFIX and experimental results

***Source**: *Bodhisattwa Chaudhuri, et al. "Experimentally validated computations of heat transfer in granular materials in rotary calciners". Powder Technology 198 (2010) 6–15.*

Enhance the Capability for Handling Heat Transfer

Local experimental setup for Validation all modes of heat transfer

- A stainless steel drum with 6” inner diameter and 3” long was constructed for the HT experiments.

- One side is a sapphire window, capable of transmitting IR radiations, and one side is quartz for internal view.

- The system was constructed to handle 1000° C.

- Temperature profile can be monitored using an IR camera and thermocouples.

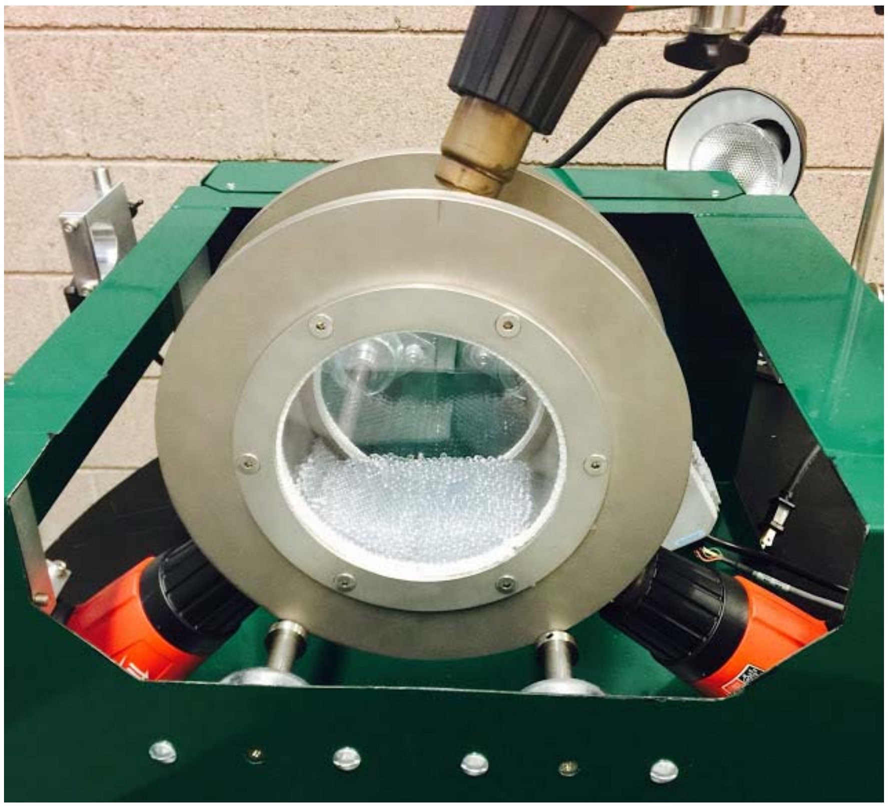
- All heat transfer modes will be tested and validated using this setup.

Rotary drum for validation studies

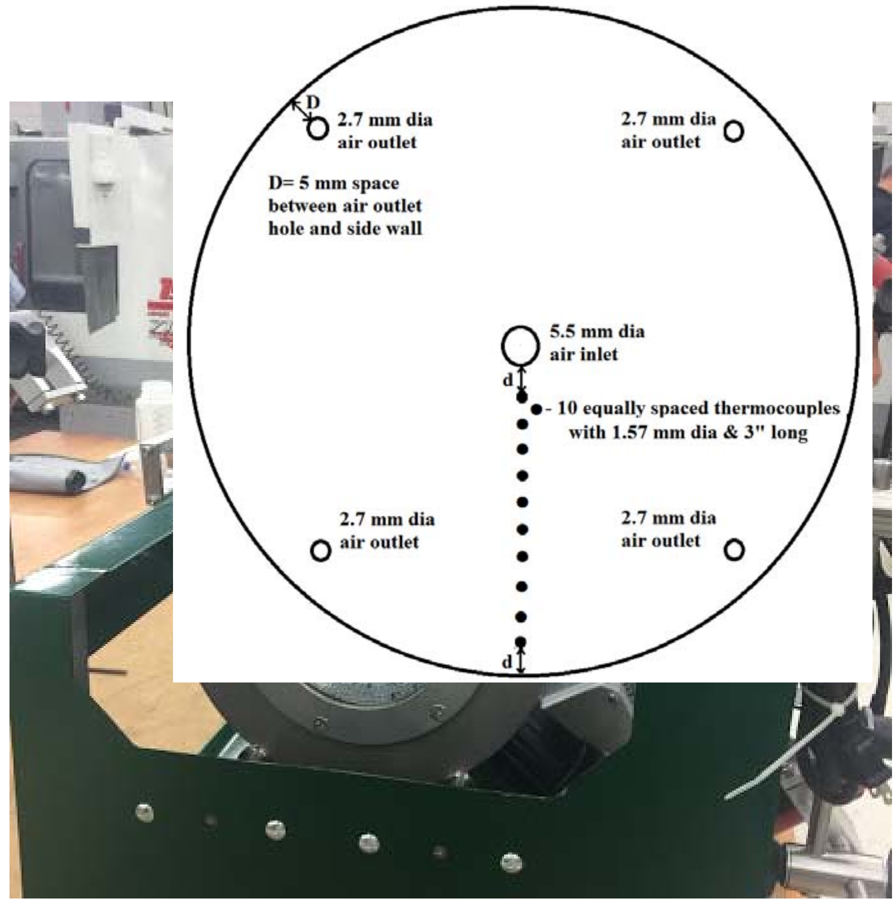
Drum design with Titanium wheel supporting the IR sapphire window, and the quartz glass with air inlet and outlet holes.

Enhance the Capability for Handling Heat Transfer

Local experimental setup for Validation all modes of heat transfer



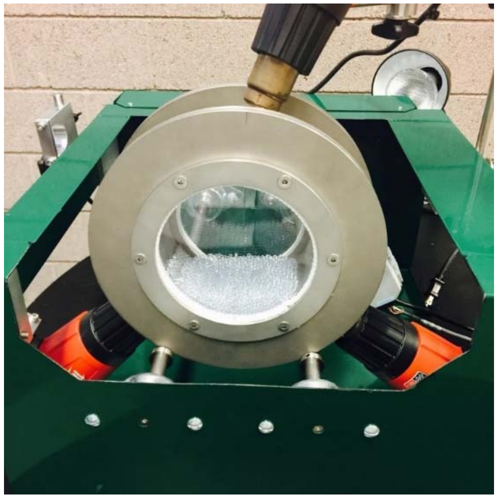
Indirect heating with heat guns

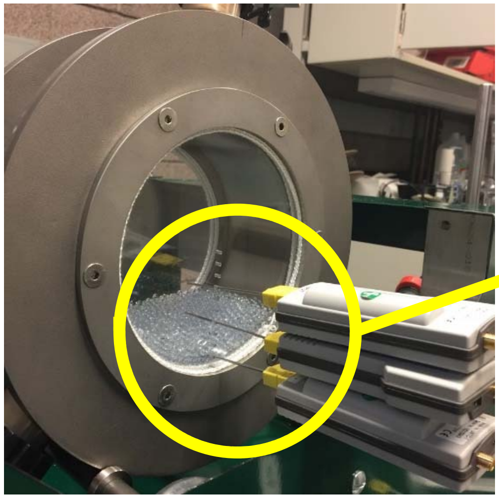


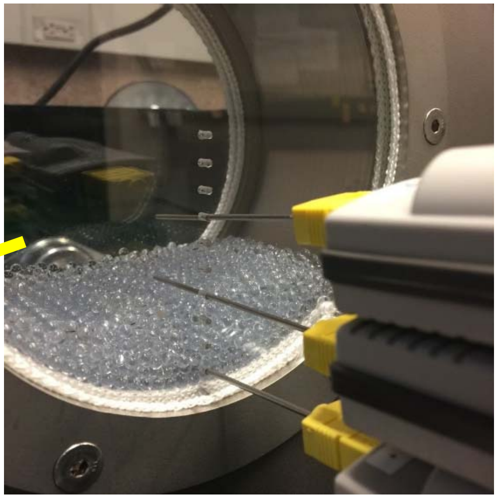
Heating with hot air injection

Local experimental setup for Validation all modes of heat transfer

Heating and temperature recoding





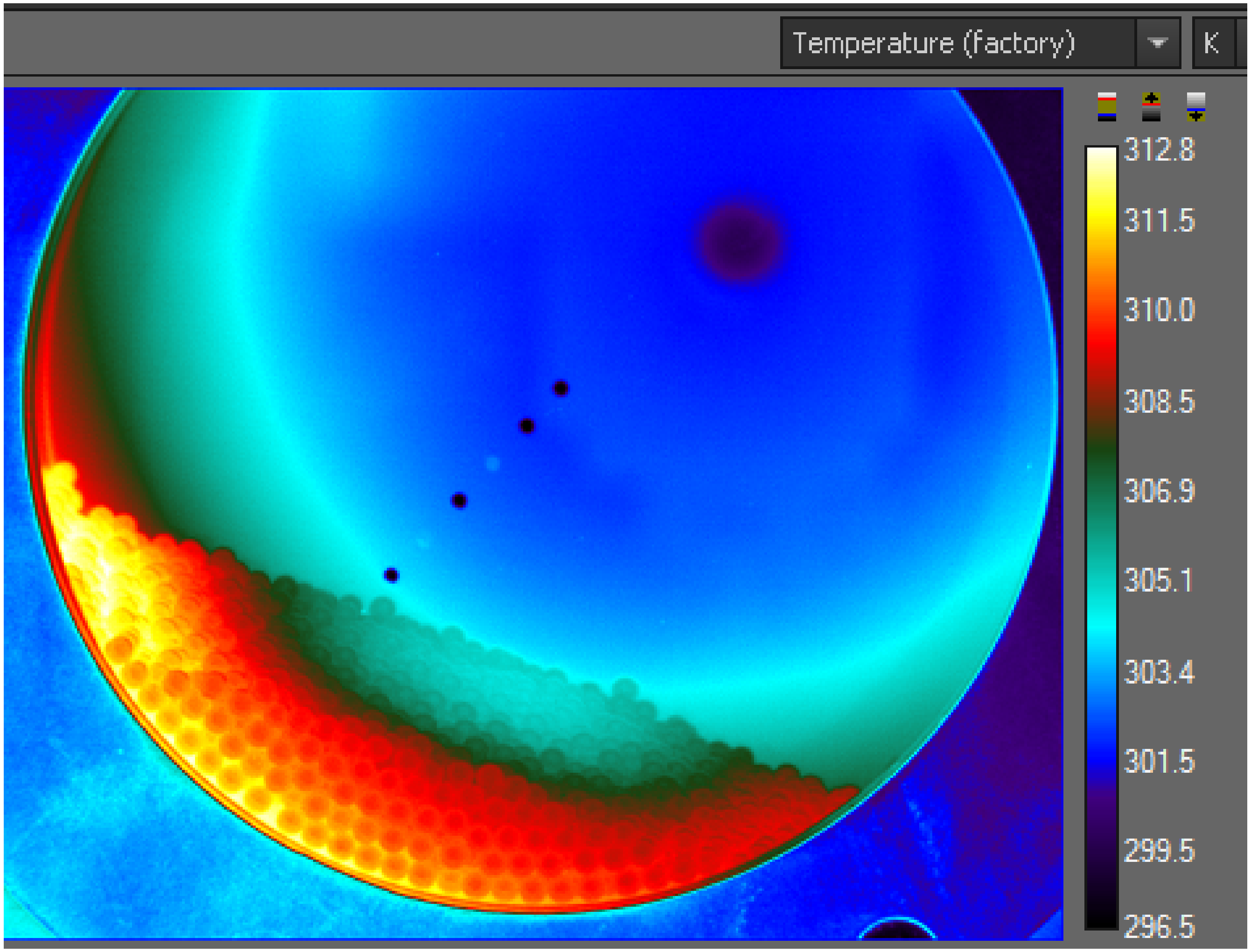


- Three heat guns will be used for maintaining the wall at the desired constant temperature.
- Current design can have up to 5 heat guns.

- Drum is stopped and the thermocouples are inserted to record the temperature.
- The response time is less than 2 s.

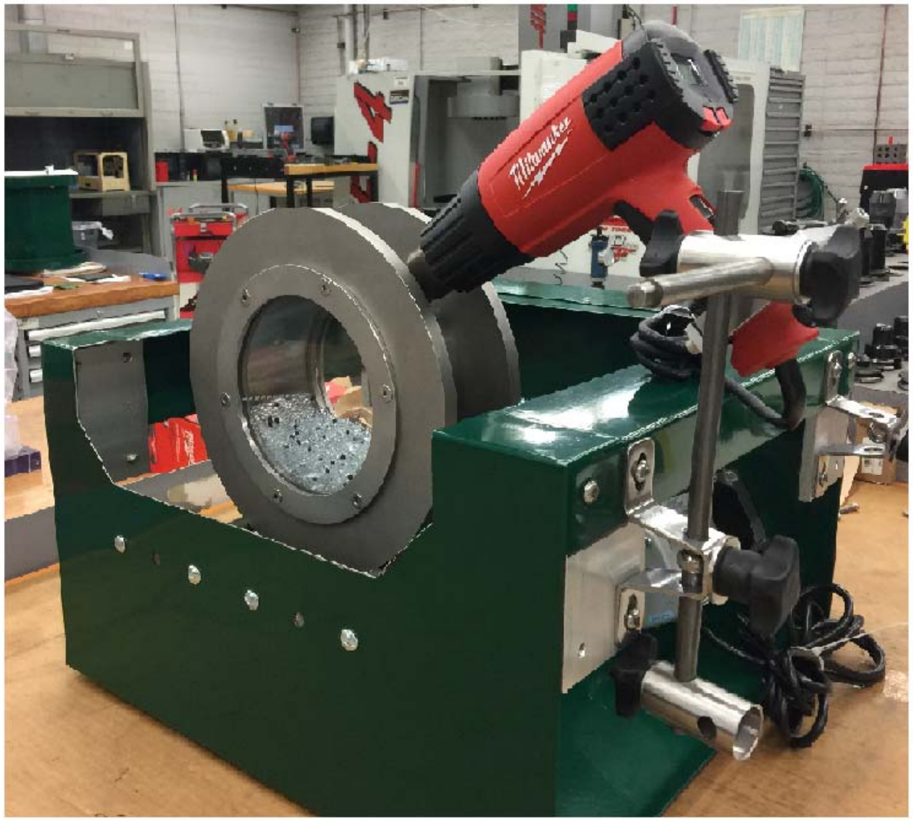
Enhance the Capability for Handling Heat Transfer

Validation of conduction heat transfer: Temperature recoding



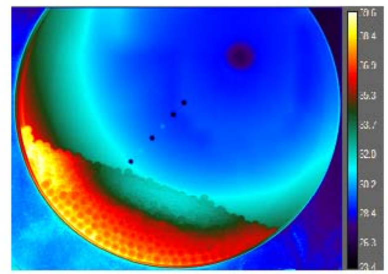
Capability to capture heat transfer profile using an IR camera.

Capabilities

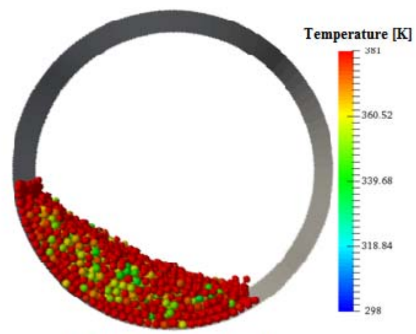


Experimental setup: Rotating stainless steel drum with heat gun to heat the drum walls

Image analysis to validate granular flow



Experimental infrared image to validate heat transfer



MFIX simulations

Conclusions

Physical Modeling Enhancement

Particle Size Distributions

Successful:

- Implementation
- Verification
- Validation

Using benchmark cases:

- Multilayer hopper discharge
- Rotary drum

- Available in Git repository at bitbucket.org
- Beta testing in progress by several NETL members

Heat Transfer models

Successful:

- Testing using multi-particle system.
- Validation of conduction HT using Literature

Using rotary drum wall-particles heat transfer

The overarching goal is for MFIX-DEM-Phi to be able to solve industrial-scale problems, and to encourage its adoption by industry.

Acknowledgments

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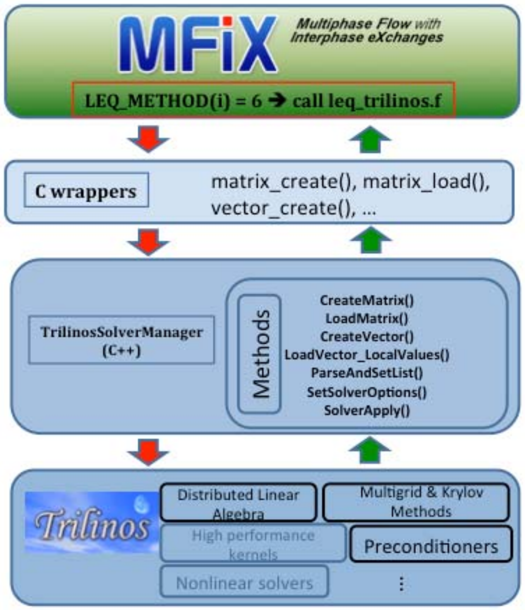
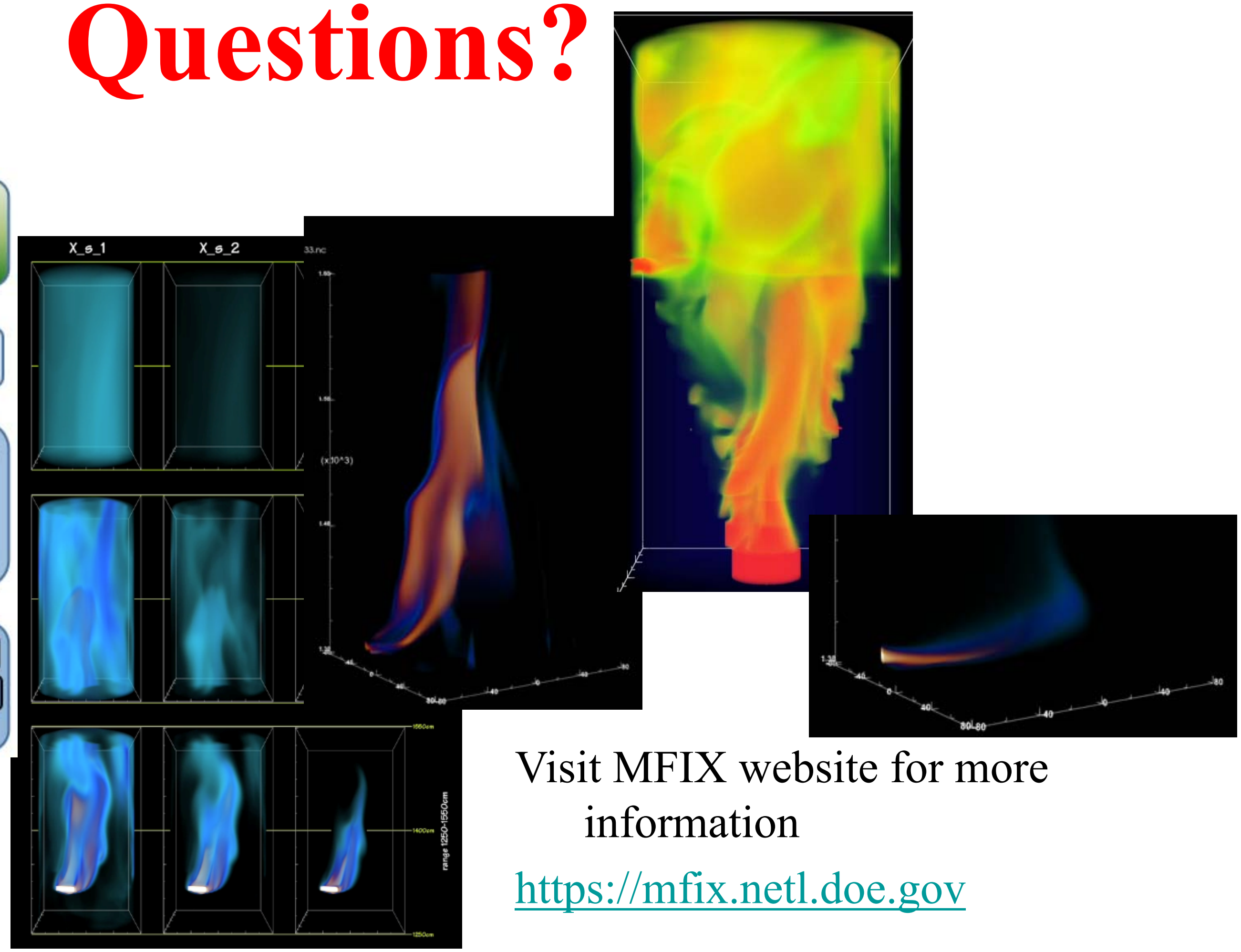
- Valuable feedback from MFIX Development Team at NETL is acknowledged.

- This work used the Extreme Science and Engineering Discovery Environment (XSEDE) at Texas Advanced Computing Center, which is supported by National Science Foundation grant number ACI-1053575.

- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Questions?





Visit MFIX website for more information

https://mfix.netl.doe.gov

Source: Visualizations prepared by A. Gel & OLCF Visualization Support for Commercial Scale Gasifier Simulations with MFIX as part of INCITE award (2010)
https://mfix.netl.doe.gov/results.php#commercialscalegasifier

APPENDIX

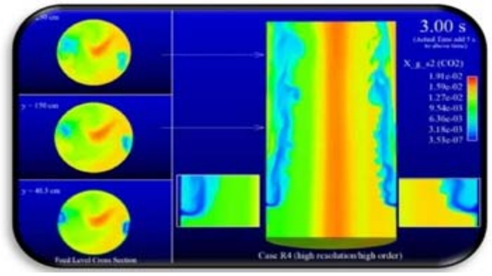
Technical Background/Motivation for The Project

MFIX: **M**ultiphase **F**low with **I**nterphase e**X**changes

MFIX Open Source Suite (https://mfix.netl.doe.gov)

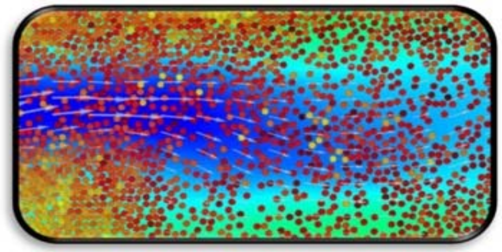
(1) MFIX-TFM (Eulerian-Eulerian)

	Serial	†DMP	‡SMP
Momentum Equations	●	●	●
Energy Equations	●	●	●
Species Equations	●	●	●
Chemical Reactions	●	●	
Cartesian cut-cell	●	●	□



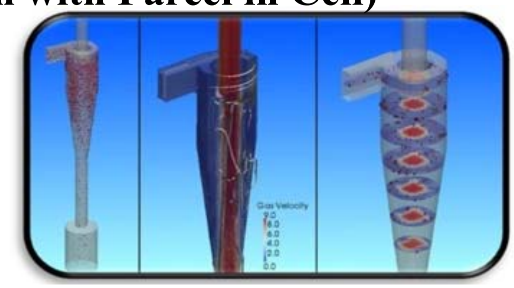
(2) MFIX-DEM (Eulerian-Lagrangian with CFD+DEM or DEM only)

	Serial	†DMP	‡SMP
Momentum Equations	●	●	●
Energy Equations	●		
Species Equations	●		
Chemical Reactions	●		
Cartesian cut-cell	○	○	



(3) MFIX-PIC (Eulerian-Lagrangian with Parcel in Cell)

	Serial	†DMP	‡SMP
Momentum Equations	●		○
Energy Equations			
Species Equations			
Chemical Reactions			
Cartesian cut-cell	○		□



(4) MFIX-Hybrid (Eulerian-Lagrangian-Eulerian blend of TFM + DEM)

● – implemented and fully tested
○ – implemented with limited testing
□ – not tested or status unknown

MFIX* Open Source Multiphase Flow Solver Suite

MFIX Two-Fluid Model (TFM) Equations Solved:

Mass conservation for phase m (m=g for gas and s for solids)

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m) = \sum_{l=1}^{N_m} R_{ml}$$

https://mfix.netl.doe.gov

Momentum conservation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m \vec{v}_m) = \nabla \cdot \overline{\overline{S}}_m + \varepsilon_m \rho_m \vec{g} + \sum_n \vec{I}_{mn}$$

Granular energy conservation (m ≠ g)

$$\frac{3}{2}\varepsilon_m \rho_m \left(\frac{\partial \Theta_m}{\partial t} + \vec{v}_m \cdot \nabla \Theta_m \right) = \nabla \cdot \vec{q}_{\Theta_m} + \overline{\overline{S}}_m : \nabla \vec{v}_m - \varepsilon_m \rho_m J_m + \prod_{\Theta_m}$$

R&D100 Award 2007

Energy conservation

$$\varepsilon_m \rho_m C_{pm} \left(\frac{\partial T_m}{\partial t} + \vec{v}_m \cdot \nabla T_m \right) = -\nabla \cdot \vec{q}_m + \sum_n \gamma_{mn} (T_n - T_m) - \Delta H_{rm}$$

Species mass conservation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{ml}) + \nabla \cdot (\varepsilon_m \rho_m X_{ml} \vec{v}_m) = R_{ml}$$

Tech-Transfer Award 2006

* MFIX: **M**ultiphase **F**low with **I**nterphase e**X**changes

Sources:

- Syamlal et al. "MFIX Documentation, Theory Guide,“ DOE/METC-94/1004, NTIS/DE94000087 (1993)
- Benyahia et al. “Summary of MFIX Equations 2005-4”, From http://www.mfix.org/documentation/MfixEquations2005-4-3.pdf, July 2007.

MFIX Discrete Element Method (DEM) Equations:

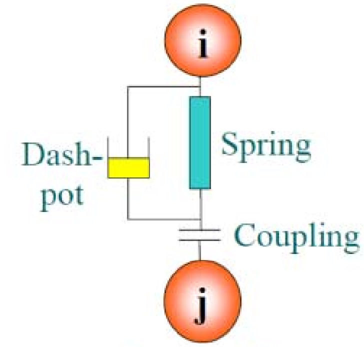
https://mfix.netl.doe.gov

Newtonian Equations for Particles

$$\frac{d\mathbf{X}^{(i)}(t)}{dt} = \mathbf{V}^{(i)}(t),$$

$$m^{(i)}\frac{d\mathbf{V}^{(i)}(t)}{dt} = \mathbf{F}_{\mathrm{T}}^{(i)} = m^{(i)}\mathbf{g} + \mathbf{F}_{\mathrm{d}}^{(i\in k,m)}(t) + \mathbf{F}_{\mathrm{c}}^{(i)}(t),$$

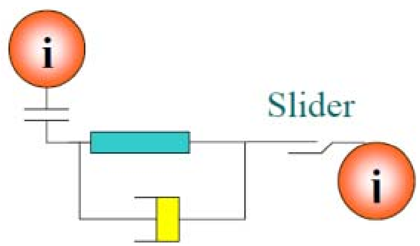
$$I^{(i)}\frac{d\boldsymbol{\omega}^{(i)}(t)}{dt} = \mathbf{T}^{(i)}$$



Normal force

Particle Contact Force Models

$$\mathbf{F}_{\mathrm{n}ij}(t) = \mathbf{F}_{\mathrm{n}ij}^{\mathrm{S}}(t) + \mathbf{F}_{\mathrm{n}ij}^{\mathrm{D}}(t) \qquad \mathbf{F}_{\mathrm{t}ij}(t) = \mathbf{F}_{\mathrm{t}ij}^{\mathrm{S}}(t) + \mathbf{F}_{\mathrm{t}ij}^{\mathrm{D}}(t)$$



Tangential force

Drag Forces on Particles

$$\mathbf{F}_{\mathrm{d}}^{(i\in k,m)} = -\nabla P_{\mathrm{g}}(\mathbf{x}_k)\mathcal{V}_{\mathrm{m}} + \frac{\beta_{\mathrm{m}}^{(k)}\mathcal{V}_{\mathrm{m}}}{\varepsilon_{sm}}\left(\mathbf{v}_{\mathrm{g}}(\mathbf{x}_k) - \mathbf{v}_{sm}(\mathbf{x}_k)\right)$$

Solid-Fluid Momentum Transfer

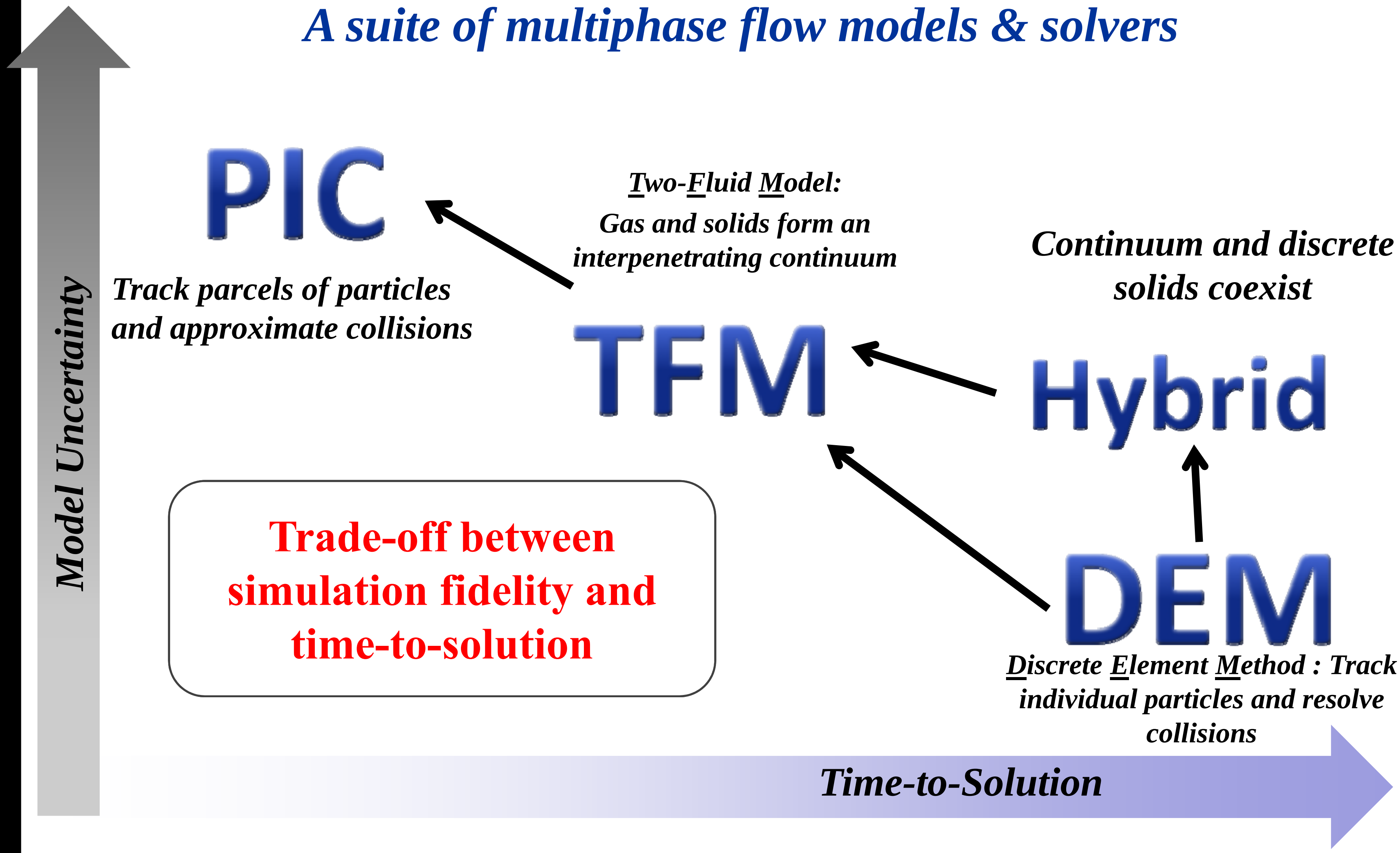
$$\mathbf{I}_{gm}^{k} = -\varepsilon_{sm}\nabla P_{\mathrm{g}}(\mathbf{x}_k) + \beta_{\mathrm{m}}^{(k)}\left(\mathbf{v}_{\mathrm{g}}(\mathbf{x}_k) - \mathbf{v}_{sm}(\mathbf{x}_k)\right)$$

Sources:

- R Garg, J Galvin, T Li, S Pannala, “Documentation of open-source MFIX–DEM software for gas-solids flows” (2010)

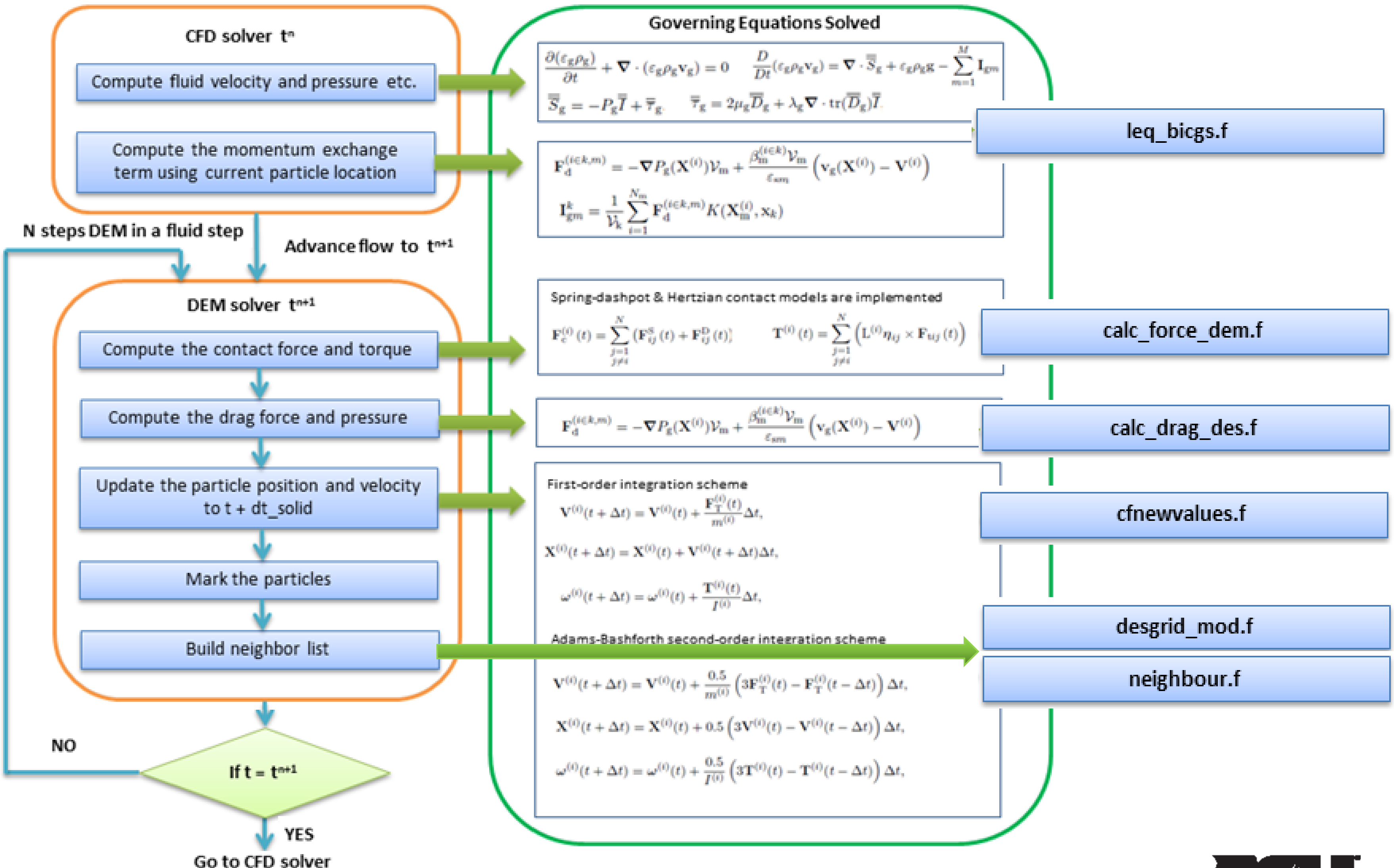
MFIX Overview (Today)

A suite of multiphase flow models & solvers



Source: Musser et al. "MFIX Update", 2014 NETL Workshop on Multiphase Flow Science (2014)

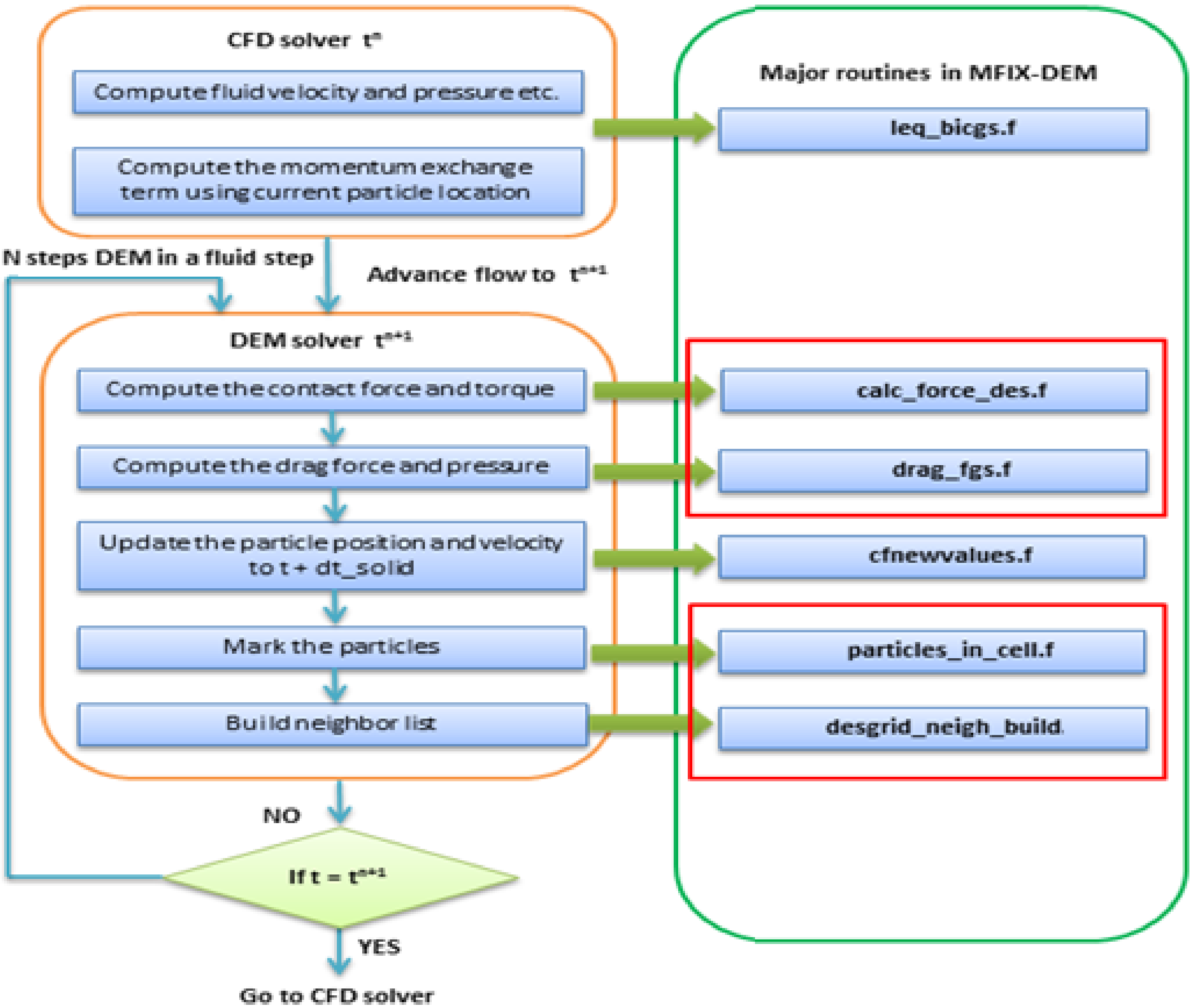
Flow chart illustrating the key solution processes coupling the CFD & DEM solvers and the associated governing equations



No need for external coupling of multiple software

Enhance the Capability for Handling Particle Size Distributions

Summary of subroutine modification



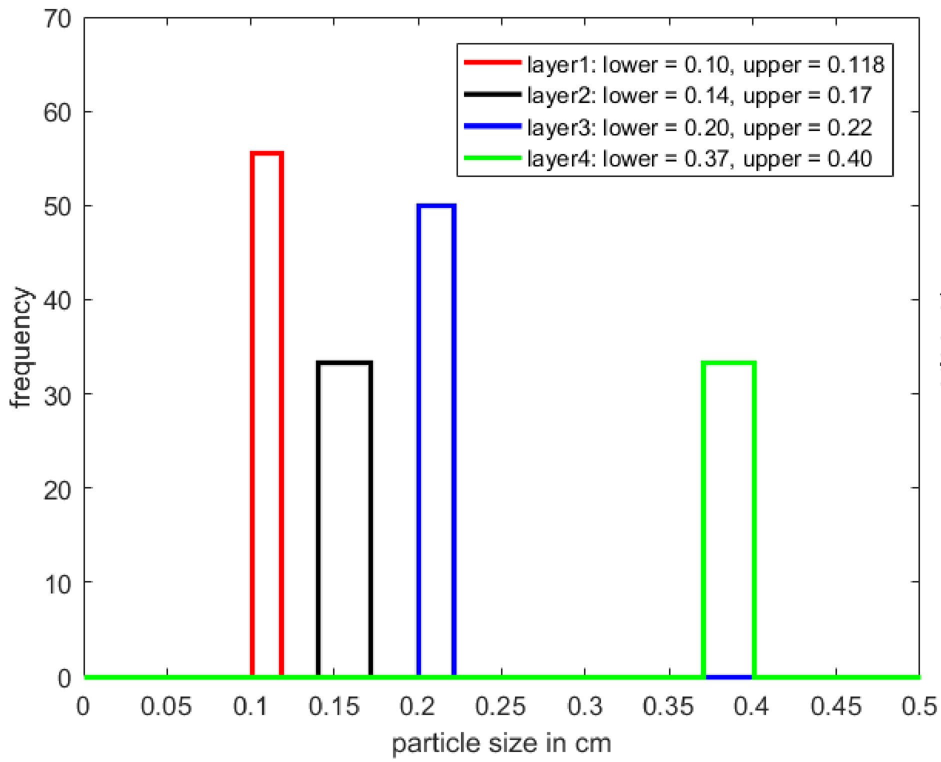
Implemented distribution types:
Uniform, Normal(Gaussian), Lognormal

Added commands for ICs:
IC_PSD_TYPE(ICV, Phase)
IC_PSD_MEAN_DP(ICV, Phase)
IC_PSD_STDEV(ICV, Phase)
IC_PSD_MAX_DP(ICV, Phase)
IC_PSD_MIN_DP(ICV, Phase)

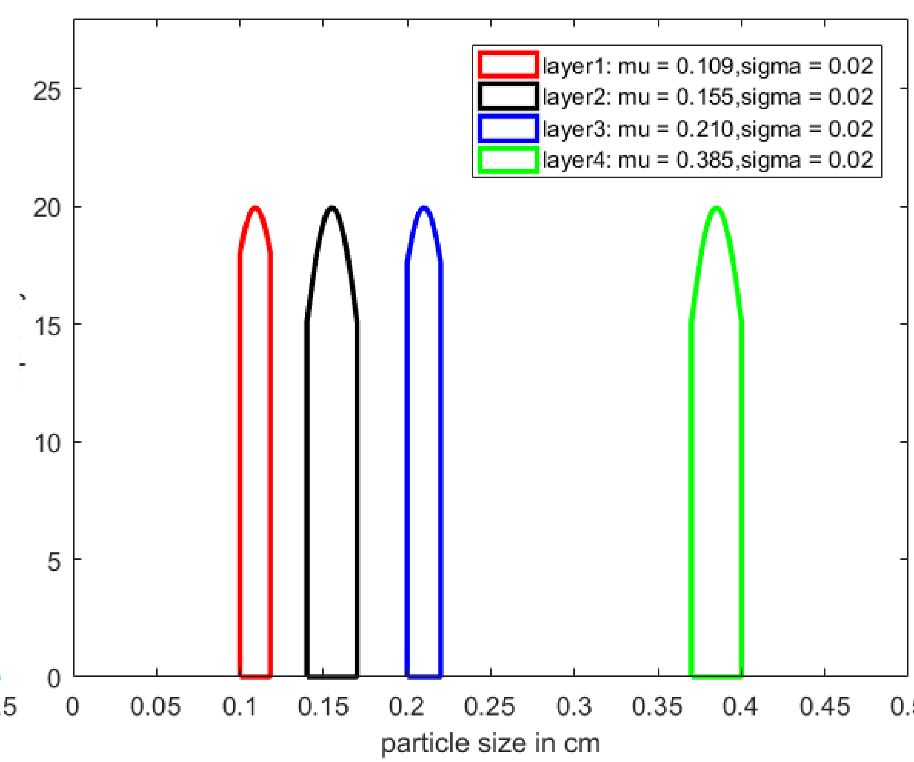
Added commands for BCs:
BC_PSD_TYPE(BCV, Phase)
BC_PSD_MEAN_DP(BCV, Phase)
BC_PSD_STDEV(BCV, Phase)
BC_PSD_MAX_DP(BCV, Phase)
BC_PSD_MIN_DP(BCV, Phase)

Enhance the Capability for Handling Particle Size Distributions

Particle size distributions



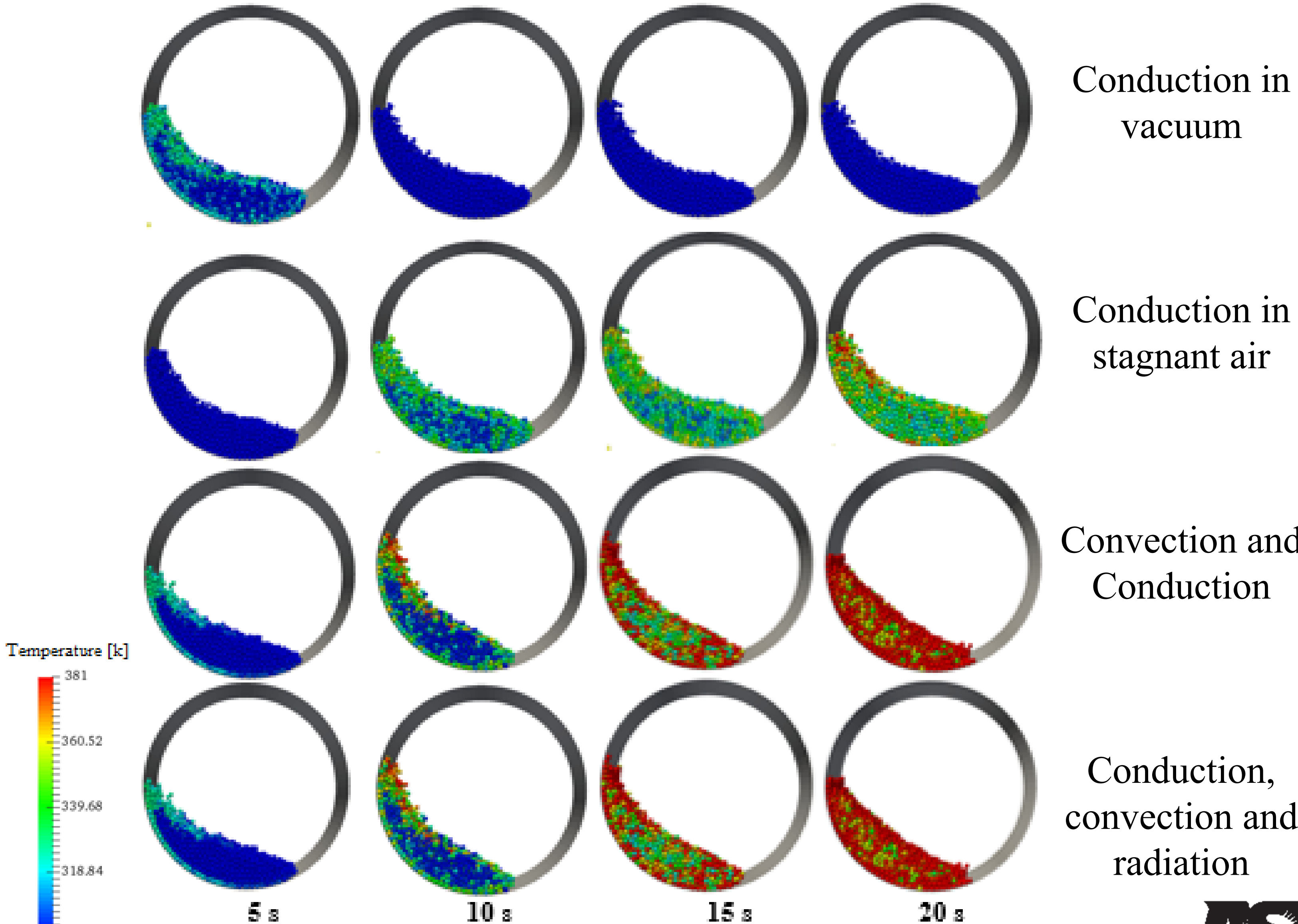
Uniform distribution



Segmented normal distribution

Enhance the Capability for Handling Particle Size Distributions

Testing all modes of HT implemented in MFIX-DEM using a rotary drum

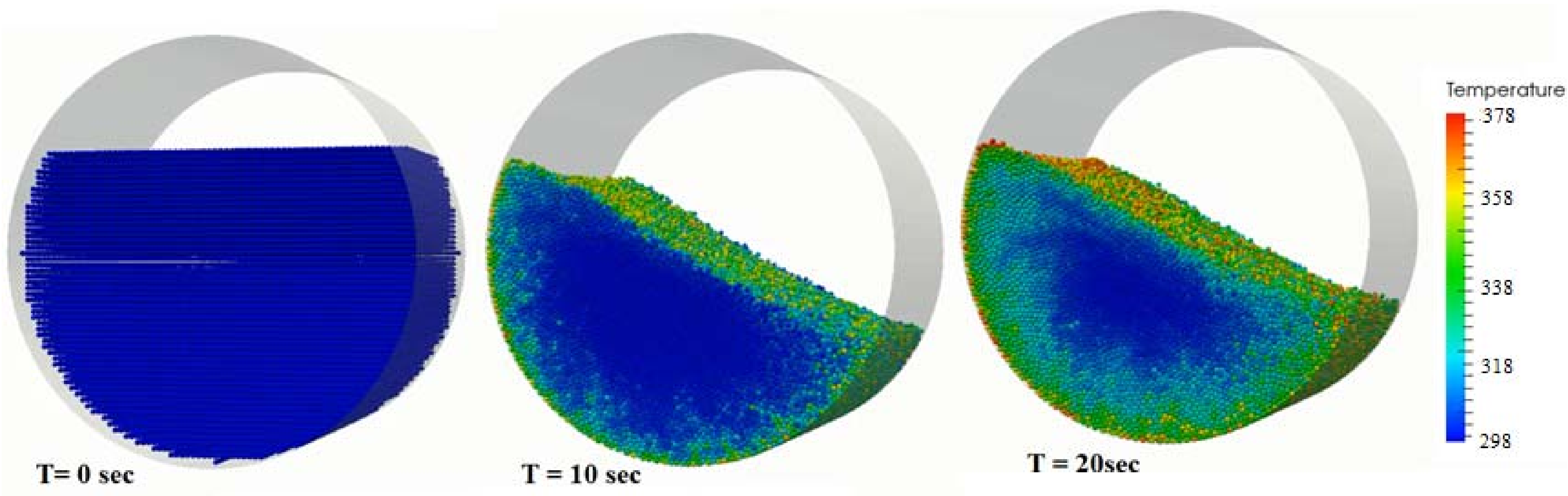


Snapshots showing particles colored by temperature

Enhance the Capability for Handling Particle Size Distributions

Validation of conduction heat transfer

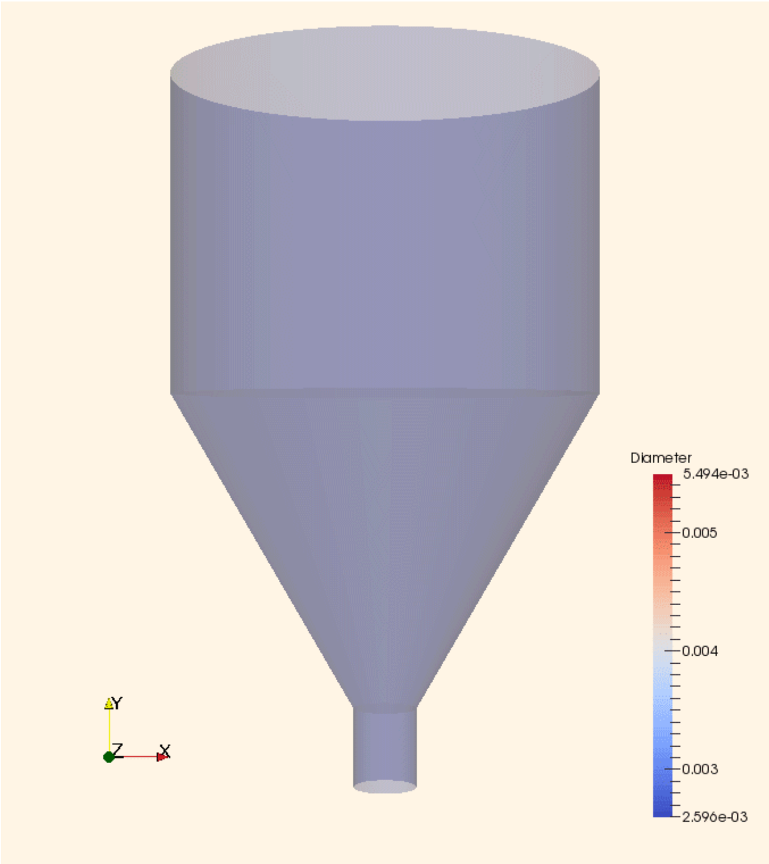
- As time progresses, **temperature of particles inside the drum increases**.
- The particles are heated first along the boundary of the drum forming a cool middle core and hot outer layer.
- DEM tracks temperature of every individual particles after each time step and the average temperature of the particle bed is calculated as a mean of temperature of all the particles.



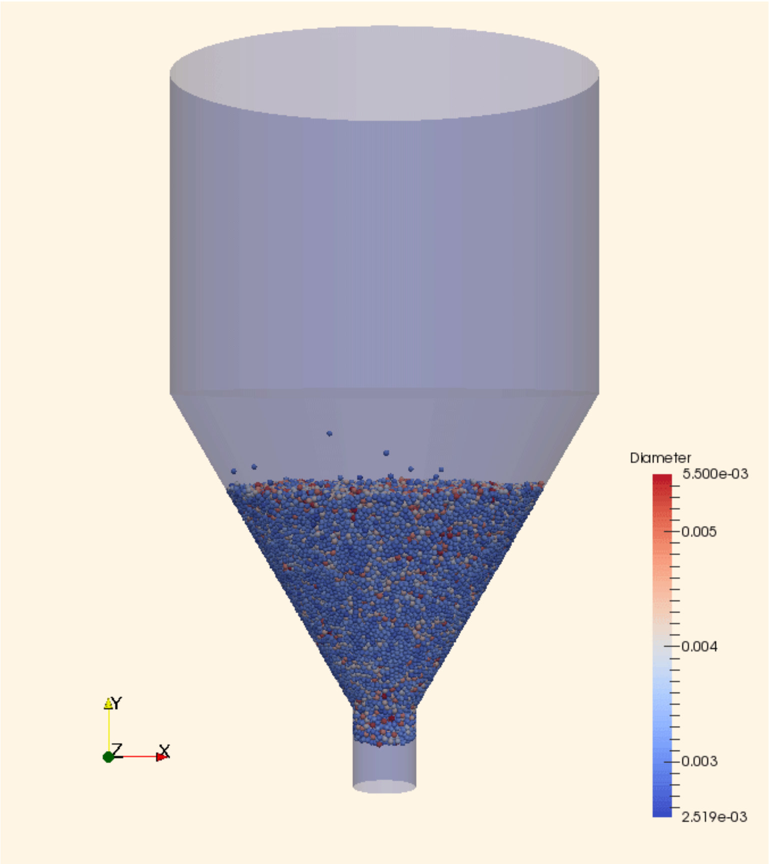
Snapshots of temperature profile at different time intervals

Enhance the Capability for Handling Particle Size Distributions

Preliminary Results for Bin Flow Case



Particle injection (0.4s) and settling (0.3s)



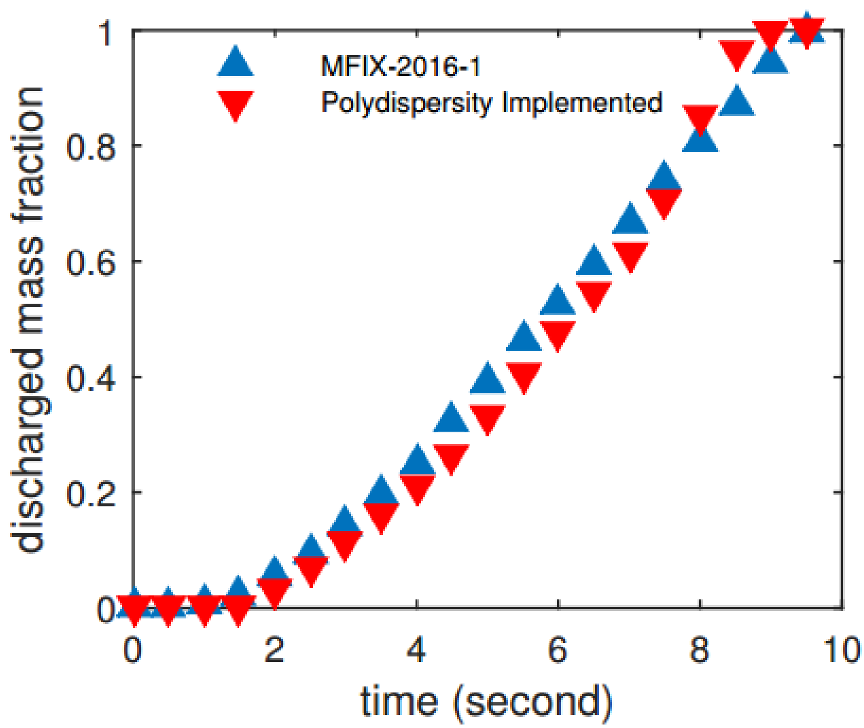
Particle discharge (4.0 s)

Enhance the Capability for Handling Particle Size Distributions

Verification of Polydispersity Implementation

Discharge dynamics for a 3D hopper with equal-sized spherical beads.

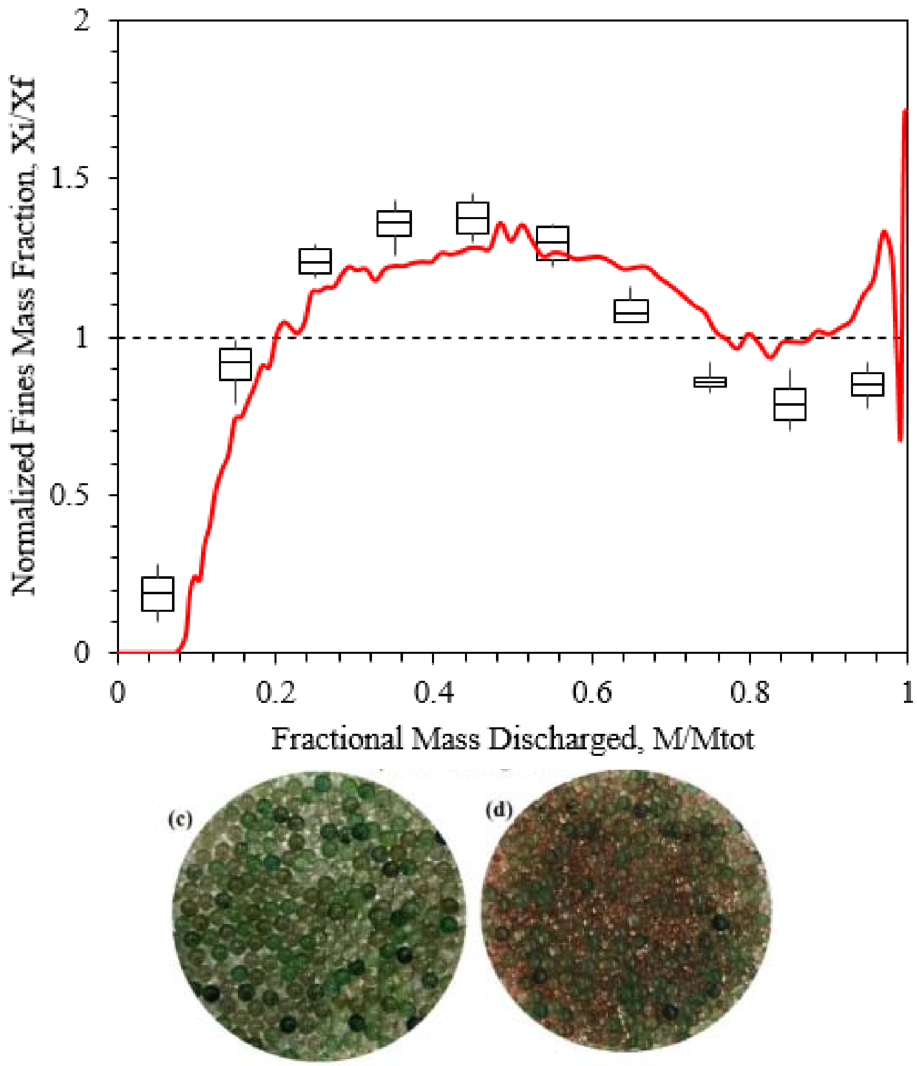
	Domain Decomposition Configuration	Total Number of Particles	CPU hours
MFIX-DEM 2016-1	$2 \times 2 \times 2$	15544	5.45
Our implementation	$2 \times 2 \times 2$	15540	5.44



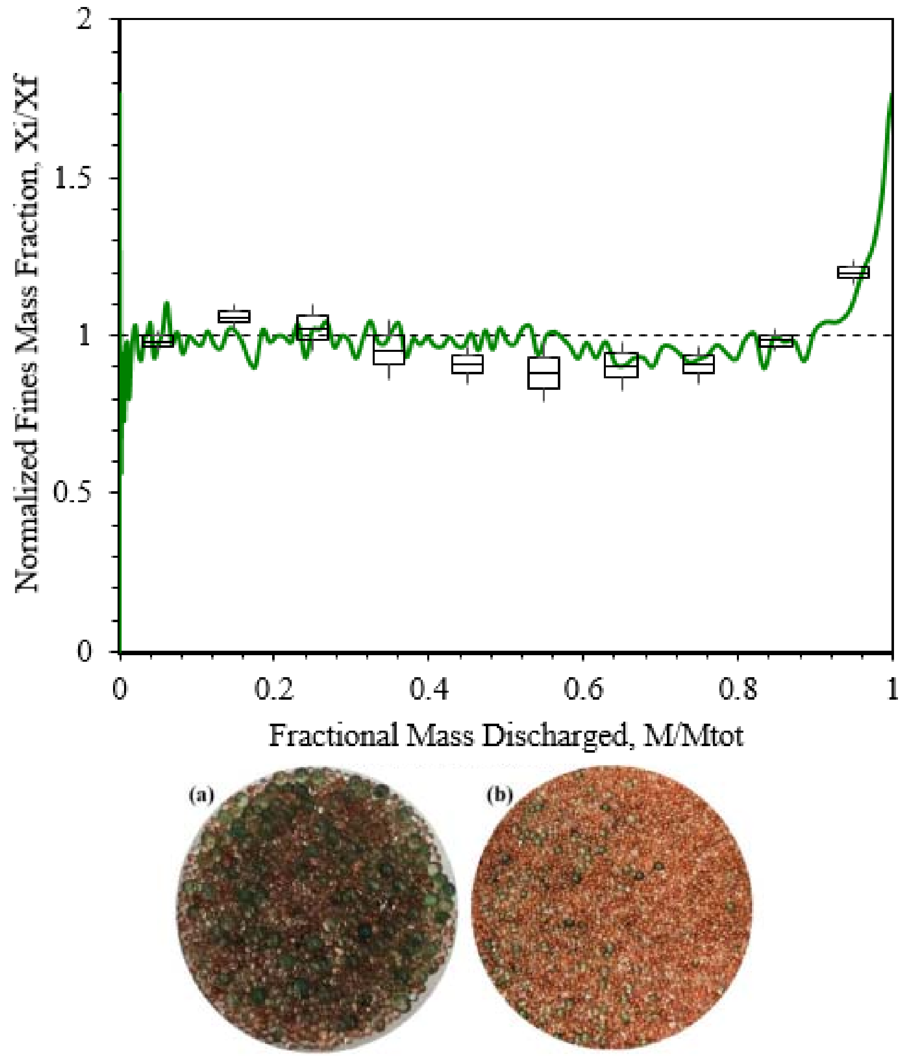
- The discharged mass vs. discharge time curves obtained from both the 2016-1 MFIX and our new implementation agree well with one another.
- The total computational cost in terms of wall-clock CPU hours for the simulations are also comparable in the two cases.
- Hence, these results verify the correctness of our new implementation.

Enhance the Capability for Handling Particle Size Distributions

Validation of Polydispersity Implementation



Layered configuration

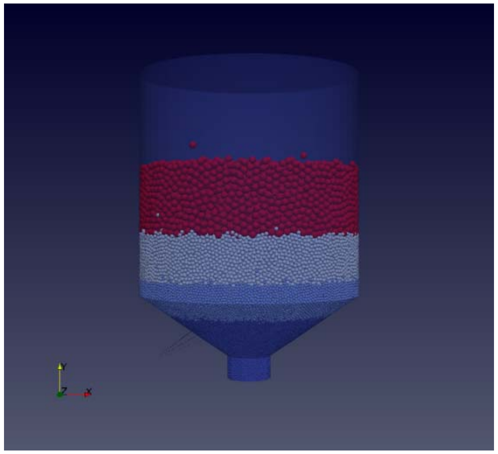


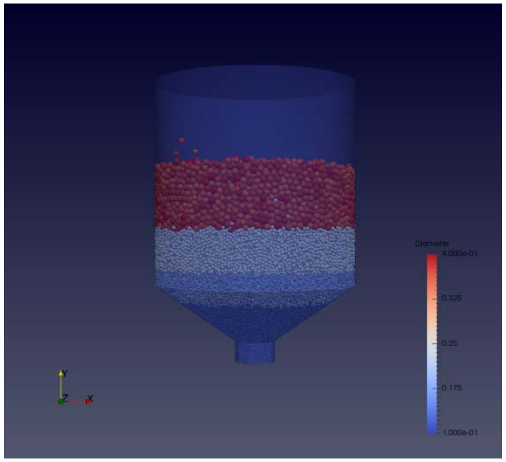
Well-mixed configuration

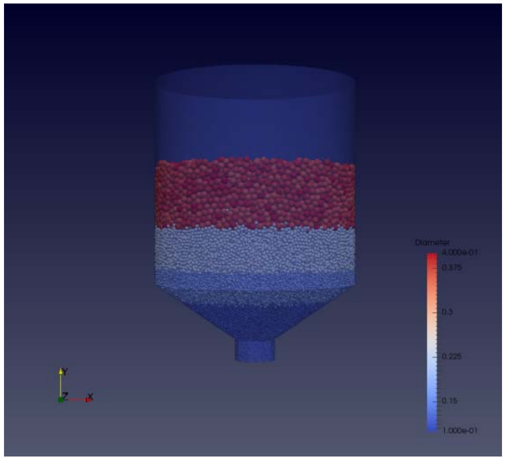
Segregation results for the discontinuous discharge methods in experiment and mfix simulation..

Enhance the Capability for Handling Particle Size Distributions

Multilayer Discharge Simulation







Monodispersed

- 1^{st} layer: 0.10cm
- 2^{nd} layer : 0.15cm
- 3^{rd} layer: 0.21 cm
- 4^{th} layer: 0.38cm
- 199442 particles

Polydispersed distributed

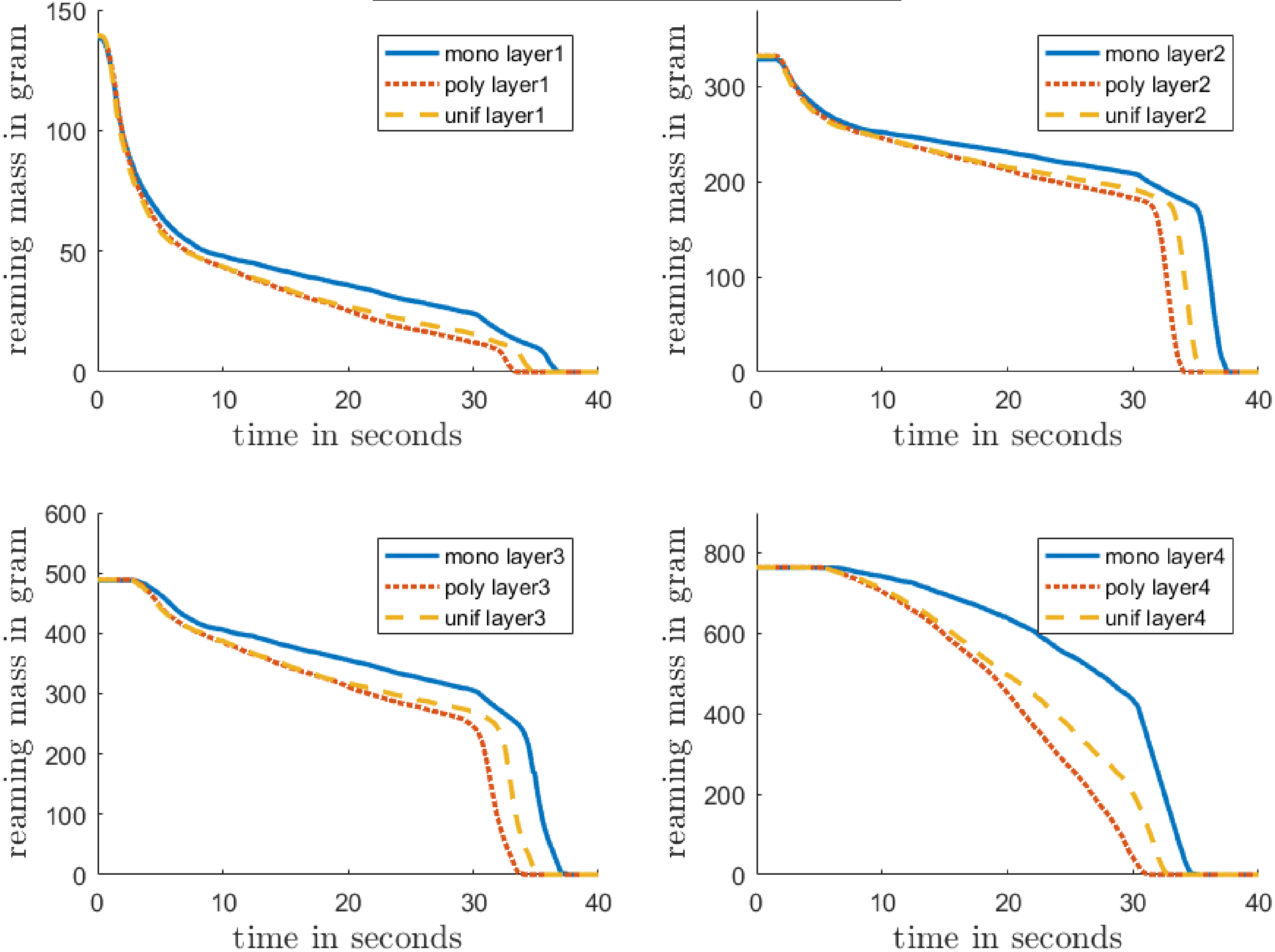
- 1^{st} layer: $\mu = 0.10$cm; σ=0.02 cm
- 2^{nd} layer : $\mu = 0.15$cm; σ=0. 02 cm
- 3^{rd} layer: $\mu = 0.21$cm; σ=0. 02 cm
- 4^{th} layer: $\mu = 0.38$cm; σ=0. 02 cm
- 199442 particles

Uniform distributed

- 1^{st} layer: 0.1~0.118cm
- 2^{nd} layer : 0.14~0.17cm
- 3^{rd} layer: 0.20~0.22 cm
- 4^{th} layer: 0.37~0.40cm
- 199442 particles

Enhance the Capability for Handling Particle Size Distributions

Multilayer Discharge Simulation



Validation and Implementation of particle size polydispersity

Enhancing Capability for Handling Particle Size Distributions

- New data structures have been implemented to separate geometrical and physical parameters of each particles of a solid phase, and to allow each solid phase to possess a different size distribution.

- New subroutines have been written to generate initial particle configurations with built-in distributions, including Gaussian, Log-Normal, and Uniform.

Implemented distribution types:
Uniform, Normal(Gaussian), Log Normal

- New subroutines have been written to generate initial particle configurations with arbitrary user-defined particle size distributions.

Added commands for ICs:
IC_PSD_TYPE(ICV, Phase)
IC_PSD_MEAN_DP(ICV, Phase)
IC_PSD_STDEV(ICV, Phase)
IC_PSD_MAX_DP(ICV, Phase)
IC_PSD_MIN_DP(ICV, Phase)

- Subroutines using particle radii as parameters have been modified accordingly.

- The implementations have been tested in a discharging hopper case provided by our collaborator.