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

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A. Gel, S. Chen, Y. Jiao, H. Emady, C. Tong and J. Hu

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Team members

Potential Significance of The Results of The Work

Physical Modeling Enhancements

Results and Discussion

Acknowledgements
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

PI: Aytekin Gel
- 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

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: **Multiphase Flow with Interphase eXchanges**

*A suite of multiphase flow models & solvers*

- **PIC**:
  - Trade-off between simulation fidelity and time-to-solution

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

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

Time-to-Solution

→ Shows the proposed targeted change in MFIX suite of solver features.
Task 1 Aim:
Demonstrate usability for industrial scale problems and collaboration for industrial adoption.

Task 2 Aim:
Increase the speed to reduce time-to-solution by optimizing modern computing platforms.

Task 3 Aim:
Develop physics w.r.t. the targeted application.

Task 4 Aims:
Ensure the results of the code are accurate.
Increase usability by reducing complexity.
Achievements in Physical Modeling Enhancements

Particle Size Distributions
- Implementation of particle size polydispersity
  - Verification
    - Hopper discharge & Rotary drum
  - Validation
    - Multilayer hopper discharge
Heat Transfer models
- Testing existing heat transfer models with rotary drum
  - Validation
    - Local experimental setup
    - Experiments from Literature

COND CONV RAD COND
Hopper with mass inflow BC

Three solid phases:

phase 1, $\mu=5.3$ $\sigma=0.05$ (MI)
phase 2, $\mu=5.5$ $\sigma=0.05$
phase 3, $\mu=5.8$ $\sigma=0.05$
Enhance the Capability for Handling Particle Size Distributions

Testing polydispersity implementation with conduction heat transfer

Particle distribution under initial condition

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>IC_PSD_TYPE</td>
<td>NORMAL</td>
</tr>
<tr>
<td>IC_PSD_MEAN_DP</td>
<td>4 mm</td>
</tr>
<tr>
<td>IC_PSD_STDEV</td>
<td>0.9</td>
</tr>
<tr>
<td>IC_PSD_MIN_DP</td>
<td>3.1 mm</td>
</tr>
<tr>
<td>IC_PSD_MAX_DP</td>
<td>4.9 mm</td>
</tr>
</tbody>
</table>

Parameter used for studying HT

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

Temperature profile
Enhance the Capability for Handling Particle Size Distributions

Testing polydispersity implementation with conduction heat transfer

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

Initialization 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)
Enhance the Capability for Handling Particle Size Distributions

Validation of Polydispersity Implementation

<table>
<thead>
<tr>
<th>Sample</th>
<th>mean diameter (m)</th>
<th>max diameter (m)</th>
<th>min diameter (m)</th>
<th>STDV (m)</th>
<th>total mass (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine</td>
<td>0.0015</td>
<td>0.0017</td>
<td>0.0013</td>
<td>0.0003</td>
<td>580</td>
</tr>
<tr>
<td>Coarse</td>
<td>0.0029</td>
<td>0.0031</td>
<td>0.0027</td>
<td>0.0001</td>
<td>420</td>
</tr>
</tbody>
</table>

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)
Snapshots of the discharge simulation of the well-mixed 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.

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)
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.

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

Multilayer Discharge Segregation result: MFIX Vs Experiments
Enhance the Capability for Handling Heat Transfer

Wall heat transfer in a rotary drum

- Conduction, convection, and radiation occur in many multiphase processes. Particle-particle conduction is now commonly used in DEM codes, but more complex heat transfer models 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/
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 298 K.

Simulations demonstrates:
1. particle-wall and particle-fluid-wall heat transfer
2. Radiation heat transfer

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

Parameters employed for the simulations

Settled particles: Used as the initial setup
## Enhance the Capability for Handling Heat Transfer

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

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Conduction in vacuum</th>
<th>Conduction in stagnant air</th>
<th>Convection &amp; Conduction</th>
<th>Conduction, convection and radiation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solid Phase</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Specific heat [J/KgK]</td>
<td>840</td>
<td>840</td>
<td>840</td>
<td>840</td>
</tr>
<tr>
<td>Thermal conductivity [W/mK]</td>
<td>1.05</td>
<td>1.05</td>
<td>1.05</td>
<td>1.05</td>
</tr>
<tr>
<td>Thermal emissivity</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.8</td>
</tr>
<tr>
<td><strong>Coupling</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Drag model</td>
<td>-</td>
<td>-</td>
<td>SYAM_OBRIEN</td>
<td>SYAM_OBRIEN</td>
</tr>
<tr>
<td><strong>Gas phase</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Specific heat [J/Kg-K]</td>
<td>0</td>
<td>1000.7</td>
<td>1000.7</td>
<td>1000.7</td>
</tr>
<tr>
<td>Thermal conductivity [W/mK]</td>
<td>0</td>
<td>0.0261</td>
<td>0.0261</td>
<td>0.0261</td>
</tr>
</tbody>
</table>
Validation of conduction heat transfer


- 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.
Enhance the Capability for Handling Heat Transfer

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.

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:

\[ M_s C_{ps} \frac{d}{dt} (T_s) = \alpha e A_v L (T_w - T_s) \]

\[ \ln \left( \frac{T_w - T_s}{T_w - T_s^0} \right) = -\frac{\alpha e A_v L}{M_s C_{ps}} t = -\frac{t}{\tau} \]

From the graph, slope = \(-1/\tau = -0.0057\) (paper experiments)

slope = \(-1/\tau = -0.0054\) (MFIX simulations)

- The thermal time constant is estimated,

\( \tau \text{ (experiments)} = 175 \text{ s} \)

\( \tau \text{ (MFIX)} = 185 \text{ s} \)

- A discrepancy of 5.6% is observed.


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
Enhance the Capability for Handling Heat Transfer

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

Capacity to capture heat transfer profile using an IR camera.
Enhance the Capability for Handling Heat Transfer

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

MFIIX 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

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

- This research effort is funded by the U.S. Department of Energy’s National Energy Technology Laboratory (NETL) Crosscutting Research Program’s Transitional Technology Development to Enable Highly Efficient Power Systems with Carbon Management initiative under award DE-FE0026393, titled “MFIX-DEM Phi: Performance and Capability Improvements Towards Industrial Grade Open-source DEM Framework with Integrated Uncertainty Quantification”.

- 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: **Multiphase Flow with Interphase eXchanges**

(1) MFIX-TFM (Eulerian-Eulerian)

<table>
<thead>
<tr>
<th>Serial</th>
<th>1DMP</th>
<th>2SMP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Momentum Equations</td>
<td>●</td>
<td>●</td>
</tr>
<tr>
<td>Energy Equations</td>
<td>●</td>
<td>●</td>
</tr>
<tr>
<td>Species Equations</td>
<td>●</td>
<td>●</td>
</tr>
<tr>
<td>Chemical Reactions</td>
<td>●</td>
<td>●</td>
</tr>
<tr>
<td>Cartesian cut-cell</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Serial</th>
<th>1DMP</th>
<th>2SMP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Momentum Equations</td>
<td>●</td>
<td>●</td>
</tr>
<tr>
<td>Energy Equations</td>
<td>●</td>
<td>?</td>
</tr>
<tr>
<td>Species Equations</td>
<td>●</td>
<td>?</td>
</tr>
<tr>
<td>Chemical Reactions</td>
<td>●</td>
<td>?</td>
</tr>
<tr>
<td>Cartesian cut-cell</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Serial</th>
<th>1DMP</th>
<th>2SMP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Momentum Equations</td>
<td>●</td>
<td>?</td>
</tr>
<tr>
<td>Energy Equations</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Species Equations</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chemical Reactions</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cartesian cut-cell</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>

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

- ● – implemented and fully tested
- ○ – implemented with limited testing
- □ – not tested or status unknown
MFIX Two-Fluid Model (TFM) Equations Solved:

Mass conservation for phase m (m=g for gas and s for solids)
\[ \frac{\partial}{\partial t} (\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \mathbf{\dot{v}}_m) = \sum_{i=1}^{N_m} R_{ml} \]

Momentum conservation
\[ \frac{\partial}{\partial t} (\varepsilon_m \rho_m \mathbf{\dot{v}}_m) + \nabla \cdot (\varepsilon_m \rho_m \mathbf{\dot{v}}_m \mathbf{\dot{v}}_m) = \nabla \cdot \mathbf{\overline{S}}_m + \varepsilon_m \rho_m \mathbf{\ddot{g}} + \sum_n \mathbf{I}_{mn} \]

Granular energy conservation (m \neq g)
\[ \frac{3}{2} \varepsilon_m \rho_m \left( \frac{\partial \Theta_m}{\partial t} + \mathbf{\dot{v}}_m \cdot \nabla \Theta_m \right) = \nabla \cdot \mathbf{\overline{q}}_m + \mathbf{\overline{S}}_m : \nabla \mathbf{\dot{v}}_m - \varepsilon_m \rho_m J_m + \Pi_{\Theta_m} \]

Energy conservation
\[ \varepsilon_m \rho_m C_{pm} \left( \frac{\partial T_m}{\partial t} + \mathbf{\dot{v}}_m \cdot \nabla T_m \right) = -\nabla \cdot \mathbf{\overline{q}}_m + \sum_n \gamma_{mn} (T_n - T_m) - \Delta H_{rm} \]

Species mass conservation
\[ \frac{\partial}{\partial t} (\varepsilon_m \rho_m X_{ml}) + \nabla \cdot (\varepsilon_m \rho_m X_{ml} \mathbf{\dot{v}}_m) = R_{ml} \]

Sources:
* MFIX: Multiphase Flow with Interphase eXchanges
MFIX* Open Source Multiphase Flow Solver Suite

MFIX Discrete Element Method (DEM) Equations:

Newtonian Equations for Particles
\[
\frac{d\mathbf{X}^{(i)}(t)}{dt} = \mathbf{v}^{(i)}(t),
\]
\[
m^{(i)} \frac{d\mathbf{v}^{(i)}(t)}{dt} = \mathbf{F}^{(i)} = m^{(i)} g + \mathbf{F}_{d}^{(i \in k,m)}(t) + \mathbf{F}^{(i)}(t),
\]
\[
I^{(i)} \frac{d\omega^{(i)}(t)}{dt} = \mathbf{T}^{(i)}
\]

Particle Contact Force Models
\[
\mathbf{F}_{nij}(t) = \mathbf{F}_{nij}^S(t) + \mathbf{F}_{nij}^D(t)
\]
\[
\mathbf{F}_{tij}(t) = \mathbf{F}_{tij}^S(t) + \mathbf{F}_{tij}^D(t)
\]

Drag Forces on Particles
\[
\mathbf{F}_{d}^{(i \in k,m)} = -\nabla P_g(x_k) v_m + \beta_m^{(k)} v_m \left( v_g(x_k) - v_{sm}(x_k) \right)
\]

Solid-Fluid Momentum Transfer
\[
\mathbf{I}_{gm}^k = -\varepsilon_{sm} \nabla P_g(x_k) + \beta_m^{(k)} \left( v_g(x_k) - v_{sm}(x_k) \right)
\]

Sources:
A suite of multiphase flow models & solvers

PIC
Track parcels of particles and approximate collisions

Two-Fluid Model:
Gas and solids form an interpenetrating continuum

TFM

Continuum and discrete solids coexist

Hybrid

Discrete Element Method: Track individual particles and resolve collisions

Trade-off between simulation fidelity and time-to-solution

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

- CFD solver $t^n$
  - Compute fluid velocity and pressure etc.
  - Compute the momentum exchange term using current particle location

- DEM solver $t^{n+1}$
  - Compute the contact force and torque
  - Compute the drag force and pressure
  - Update the particle position and velocity to $t + dt_{solid}$
  - Mark the particles
  - Build neighbor list

- Governing Equations Solved
  - Spring-dashpot & Hertzian contact models are implemented
  - First-order integration scheme
  - Adams-Bashforth second-order integration scheme

- No need for external coupling of multiple software
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

Conduction in vacuum

Conduction in stagnant air

Convection and Conduction

Conduction, convection and radiation
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)
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Verification of Polydispersity Implementation

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

<table>
<thead>
<tr>
<th>Domain Decomposition</th>
<th>Total Number of Particles</th>
<th>CPU hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>MFIX-DEM 2016-1</td>
<td>2 x 2 x 2</td>
<td>15544</td>
</tr>
<tr>
<td>Our implementation</td>
<td>2 x 2 x 2</td>
<td>15540</td>
</tr>
</tbody>
</table>

- 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.
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Validation of Polydispersity Implementation

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

**Monodispersed**
- 1st layer: 0.10 cm
- 2nd layer: 0.15 cm
- 3rd layer: 0.21 cm
- 4th layer: 0.38 cm
- 199442 particles

**Polydispersed distributed**
- 1st layer: $\mu = 0.10 \text{ cm}; \sigma = 0.02 \text{ cm}$
- 2nd layer: $\mu = 0.15 \text{ cm}; \sigma = 0.02 \text{ cm}$
- 3rd layer: $\mu = 0.21 \text{ cm}; \sigma = 0.02 \text{ cm}$
- 4th layer: $\mu = 0.38 \text{ cm}; \sigma = 0.02 \text{ cm}$
- 199442 particles

**Uniform distributed**
- 1st layer: 0.1~0.118 cm
- 2nd layer: 0.14~0.17 cm
- 3rd layer: 0.20~0.22 cm
- 4th layer: 0.37~0.40 cm
- 199442 particles
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Multilayer Discharge Simulation

Graphs showing the remaining mass in grams over time in seconds for different layers and distributions.
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.