Enhancing the Physical Modeling Capability of Open-Source MFIx-DEM Software for Handling Particle Size Polydispersity: Implementation and Validation

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Abstract

Multiphase flows are ubiquitous in many industrial processes. The inherent coupling of different phases poses many unique challenges in predicting and effectively controlling these processes. Hence, computational modeling and simulation offers a viable approach to overcome these challenges. In this study, we present recent development efforts for enhancing the physical modeling capabilities of an open-source computational modeling tool for real life industrial multiphase processes by enabling particle-size polydispersity and demonstrating with an associated validation study. The proposed implementation was performed in MFIx open-source framework due to its unique feature of tightly integrated computational fluid dynamics and discrete element method solvers for simulating coupled continuum fluid and granular flows. We have implemented the polydispersity feature in a minimally invasive way and provided means to allow easy specification of an arbitrary particle size distribution function, which also enables the user to easily handle an arbitrary number of solid phases, each possessing a distinct arbitrary particle-size distribution. To establish the credibility

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of improvements, we have carried out a preliminary verification and validation (V&V) study for the polydispersity feature by employing a hopper bin discharge problem, which is frequently encountered in industrial applications. Specifically, two types of micro glass beads with distinct size distributions are used to fill the hopper in two possible packing arrangements, i.e., well-mixed and layered configurations, with varying mass (particle number) ratios. The experimentally obtained discharge dynamics (e.g., normalized discharge mass fraction for one of the phases versus the overall discharge mass fraction) for different systems is found to be in excellent agreement with the corresponding simulation results.

Keywords: Granular flow, polydisperse particles, discharge hopper, open-source modeling and simulation, discrete element method (DEM), MFIX-DEM

1. Introduction

2 Multiphase flows are ubiquitous in many industrial processes. Common ex-
 3 amples include wet granulation, coating, spray drying, pneumatic conveying,
 4 and fluidization. The inherent coupling of these different phases poses many
 5 unique problems in predicting, and effectively controlling these processes. Com-
 6 putational simulations are often employed for this purpose. Typically, separate
 7 scientific computational modeling software for discrete element method (DEM)
 8 to solve the solid phase, such as LIGGGHTS [1, 2, 3, 4], and computational
 9 fluid dynamics (CFD) to solve the continuum fluid phase, such as OpenFOAM
 10 [5, 6, 7], are externally coupled to model the governing physics in such flows.

11 Here, we present our recent developments for enhancing MFIX [8, 9, 10],
 12 a suite of open-source software for multiphase flow simulations including both
 13 the two-fluid model (TFM) and the coupled CFD-DEM model, developed and
 14 maintained by the National Energy Technology Laboratory (NETL) of the U.S.
 15 Department of Energy. For the TFM model, both the carrier fluid and the solid
 16 particle phases are treated as a continuum, and the Eulerian-Eulerian framework
 solver is utilized to solve the associated conservation equations for both phases.

18 For the coupled CFD-DEM model, MFIX is a unique tool that provides a unified
framework for a single user interface and code base to simulate a diverse range
20 of multiphase flow problems [11, 12]. Hence, MFIX eliminates the need to
externally couple two separate modeling software. Instead, MFIX utilizes the
22 TFM solver (i.e., Two-Fluid Model-based Eulerian-Eulerian framework solver)
for performing the computations of the carrier fluid and the DEM solver (which
24 is the Lagrangian framework based solution process) for handling particles.

Since its initial release, MFIX has been successfully employed to model a
26 variety of multiphase flow problems relevant to industrial and energy-related
applications [13, 14, 15, 16, 17, 18, 19, 20, 21]. Due to the inherent complexity
28 and diverse range of spatial/temporal scales involved in multiphase flow simula-
tions, several initiatives were carried out to reduce the time-to-solution through
30 performance improvements [22, 23, 24, 25, 26, 27, 28, 29, 30]. Also, a number
of studies have been carried out to systematically perform uncertainty quan-
32 tification analysis in multiphase flow simulations with MFIX [31, 32, 33, 34] to
improve the credibility of the prediction capability.

34 Despite these enhancements and improvements, the lack of computationally
efficient methods to simulate polydisperse systems (heterogeneity of sizes) has
36 posed some problems when modeling industrial applications. For example, even
with the recent 2016-1 release version of MFIX-DEM, each distinct solid phase
38 is only allowed to possess a unique particle size, making it extremely difficult to
simulate a true polydisperse system, in which each particle possesses a unique
40 size (e.g., particle diameter). Accurately capturing the particle size distribu-
tion is crucial to processes involving denser granular flows and jammed granular
42 packings [35, 36]. More importantly, the capability to handle polydisperse sys-
tems easily is often available in other open-source and commercial DEM software
44 (e.g., LIGGGHTS [37] and EDEM [38]), and also in other particle-based simu-
lation techniques, such as event-driven molecular dynamics [39, 40] and Monte
46 Carlo simulations [41].

In the current paper, we present our recent work on enhancing MFIX-DEM's
48 physical modeling capability for handling particle-size polydispersity for the

pure DEM mode. Specifically, we have modified the data structure and created
50 new subroutines to separately handle geometrical and physical parameters of the
solid phase particles. This approach has enabled MFIX-DEM to easily handle
52 an arbitrary number of solid (particle) phases where the particles in each phase
are allowed to possess a distinct arbitrary particle-size distribution. Several new
54 input keywords have been introduced to allow easy specification of the particle-
size distribution function for each phase. The user can select either one of the
56 built-in distributions (e.g., normal, log-normal, and uniform) or user-defined dis-
tributions (that can be specified via the restart files). To establish the credibility
58 of the new improvements implemented, a preliminary verification and validation
(V&V) study is performed using hopper bin discharge experiments, which is a
60 commonly used configuration with many industrially relevant applications. In
particular, we use two types of micro glass beads with distinct size distributions
62 to fill the hopper in two possible packing arrangements, i.e., well-mixed and
layered configurations, with varying mass (particle number) ratios. The experi-
64 mentally obtained discharge dynamics (e.g., normalized discharge mass fraction
for one of the phases vs. the overall discharge mass fraction) for different sys-
66 tems is found to be in excellent agreement with the corresponding simulation
results, which clearly validates the newly implemented polydispersity features.
68 The new features for handling polydispersity will be available in a future version
of MFIX.

70 The rest of the paper is organized as follows. In Sec. 2, a brief overview of the
implementation for polydispersity is presented, followed by a verification study
72 using a discharge hopper. In Sec. 3, we present the details of our hopper bin
discharge experiments using micro glass beads, which were designed for the val-
74 idation study as discussed in the following section. In Sec. 4, we systematically
validate the newly implemented polydispersity feature using the experimental
76 data. Both our hopper discharge experimental results and MFIX-DEM simula-
tion results are reported and are observed to be in excellent agreement. In Sec.
78 5, we provide concluding remarks.

2. Implementation

80 2.1. Brief background on MFIX-DEM

Before discussing our implementation for polydispersity, a brief background
82 on MFIX-DEM is provided in this section. As mentioned in Sec. 1, MFIX
(<https://mfix.netl.doe.gov>) is a unique open-source computational fluid
84 dynamics (CFD) software for modeling multiphase flows, developed and main-
tained by the U.S. Department of Energy over several decades. It offers a
86 unified framework for CFD and discrete element method (DEM) and is exten-
sively used in diverse areas, from coal gasification to volcano explosion modeling
88 [13, 14, 25, 42, 43, 44, 45, 46, 47].

Fig. 1 illustrates the overall workflow of MFIX when the CFD and DEM so-
90 lution processes are invoked for solving granular flows coupled with a continuum
fluid [48, 49]. As seen from the flowchart in Fig. 1, once the coupling is enabled,
92 at a particular CFD time step, the conservation equations are solved iteratively
by the CFD solver, and the resulting drag forces and fluid-solid momentum
94 transfer are subsequently computed and passed to the DEM solvers. Within a
single CFD time step, multiple DEM time steps are carried out to integrate the
96 equations of motion associated with the particles for the given contact and drag
forces.

Figure 1: Schematic illustration of MFIX-DEM’s unified framework coupling both the CFD solver and DEM solver under a single user interface with the major subroutines being called. The subroutines modified for implementing the polydispersity feature are highlighted in the red boxes. Adapted from Fig. 1 in Ref. [27].

98 2.2. Modification of data structure and subroutines

Our implementation for polydispersity aimed to minimize the invasive struc-
100 tural changes in the algorithm and the original MFIX-DEM code. In the latest
release of MFIX-DEM (i.e., 2016-1), each distinct solid phase is only allowed to
102 possess a unique particle size, which is saved in the array `D_P0`, whose size is the
maximum number of solid phases in the system. Each solid particle is assigned a

104 unique phase index based on its diameter, which helps in phase-specific physical
properties of the particles (e.g., material density, Young’s modulus, coefficient
106 of friction, coefficient of restitution, etc.) to be retrieved and employed in the
subsequent computation of particle contact forces.

108 The basic idea of our new implementation is to separately save the parti-
cle geometrical parameters (i.e., diameters), which are particle-specific and the
110 phase-specific physical parameters. In particular, we modified the array `D_PO`
such that it saves the diameter of each particle in the system, thus possessing a
112 size of the total particle number N . For example, `D_PO(i)` now gives the diame-
ter of particle i , instead of the diameter of particles for phase i . Accordingly, the
114 phase index of each particle is not assigned according to its diameter, but as-
signed based on its physical properties, e.g., material density. The change of data
116 structure for saving and retrieving an individual particle diameter (or radius)
affects a number of subroutines which utilize `D_PO(i)` as input for subsequent
118 calculations. As summarized in Fig. 1, the modified subroutines include those
for particle force/torque calculation (`calc_force_dem.f`), solid-gas momentum
120 transfer calculation (`calc_drag_des.f`), grid cell locator (`desgrid_mod.f`) and
neighbor locator (`neighbour.f`). We note the modifications do not affect any
122 of the underlying governing equations for the system nor specific contact force
models to be utilized.

124 The new implementation offers three types of built-in probability distribu-
tion functions (PDF) for size, including normal, log-normal and uniform distri-
126 butions. However, the addition of new distributions can easily be done through
the `DES/RANDOMNO_mode.F` subroutine. For a user-specified distribution, the
128 particle diameter information is provided in the restart files (*.RES) and is read
in during the initialization stage. In addition, users can specify the particle size
130 distribution for both the initial condition (IC) and mass-in-flow (MIF) bound-
ary conditions (BC). This allows the simulation of complex multiphase flow
132 processes during which additional solids are injected into the system. This im-
plementation is achieved by introducing two sets of new keywords, respectively,
134 for ICs and MIF BCs. The new polydispersity feature will be available in the

next release version of MFIX with detailed documentation and tutorial cases.

136 2.3. Verification of the polydispersity implementation

As part of our preliminary V&V effort, we first verified the new implementation by simulating particle discharge from a 3D hopper with equal-sized spherical beads. The 2016-1 release version of MFIX is also used to simulate the same system for comparison. The hopper contains a cylinder part of height 5 cm and diameter 6 cm, connected to a cone part with height 5 cm and angle of 30 degrees. The bottom of the hopper cone is further connected to a short cylinder tube of height 0.2 cm and diameter 0.5 cm. The monodisperse beads possess a diameter of 0.068 cm, spring constant of $2.5 \times 10^5 g/s^2$, friction coefficient of 0.01 and coefficient of restitution of 0.5.

146 The initial configuration for the discharge simulation is obtained by first filling the hopper with 15540 beads from the top (through the mass-in-flow boundary condition), while the bottom is kept closed (through the no-flow boundary condition). The resulting packing is allowed to settle completely, to dissipate the kinetic energy. The stable packing at the end of settling is used as the initial configuration for the discharge simulation until the hopper is fully discharged.

Table 1: Verification simulation details for the discharge hopper with monodisperse spherical beads.

Figure 2: Discharge dynamics for a 3D hopper with equal-sized spherical beads. The discharged mass vs. discharge time curves obtained from both the 2016-1 MFIX and our new implementation agree well with one another.

152 Tab. 1 summarizes the simulation details, including the number of particles, domain decomposition configuration and total CPU hours required for full discharge. Fig. 2 shows the discharged mass vs. time for the monodisperse system, obtained using the 2016-1 MFIX-DEM release and our new polydisperse implementation derived from the 2016-1 release. It can be seen that in both cases, 156 the initial discharge rates are relatively small and stabilize ~ 2 seconds after

158 discharge starts. The discharged mass fractions for the two cases slightly deviate
 from one another due to uncertainty in the initial packing configurations. The
 160 overall discharge dynamics agree very well with one another. Also, the total
 computational cost in terms of wall-clock CPU hours for the simulations are
 162 also comparable in the two cases. Hence, these results verify the correctness of
 our new implementation.

164 3. Hopper Discharge Experiment

In the next step of our V&V effort, to validate our polydispersity imple-
 166 mentation, hopper discharge experiments were carried out using two types of
 polydisperse particles with varying initial packing configurations. Detailed dis-
 168 charge dynamics were obtained for both types of particles for comparison with
 simulation results. The hopper used in the experiments (shown in Fig. 3) is 3D
 170 printed using a Stratasys Dimension 1200es SST (Stratasys Ltd. MN, USA),
 with ABSplus thermoplastic. It contains a cylinder of 12.5 cm height and 12.5
 172 cm diameter, connected to a cone with a height of 3.5 cm and 55° cone angle.
 The bottom of the hopper cone is further connected to a short cylinder of height
 174 1.3 cm and diameter 2.5 cm. The hopper is leveled and clamped to a support
 stand. A glass slide gate is used to close and open the hopper outlet, to fill and
 176 discharge, respectively.

Figure 3: Experimental setup of hopper: Clamped 3D printed hopper with a beaker, for col-
 lecting discharged particles, placed on an analytical balance to measure the mass of discharged
 particles for sampling.

The granular materials used in the experiments are silica beads (soda-lime
 178 silica glass). The silica beads are purchased from Potters Industries, PA, USA;
 with particle density 2.5 g/cm^3 in different sizes. The particles are further
 180 sieved to narrow the particle size distribution (PSD). The sieved particles are
 analyzed using a Malvern Morphologi G3SE (Malvern Instruments Ltd, UK),
 182 and two distinct sized polydisperse silica beads with a bi-modal size distribution

Figure 4: A bi-modal particle size distribution (i.e., number frequency vs. particle sizes) was employed, which includes two normal distributions for fine and coarse silica bead particles.

(shown in Fig. 4) are used for the experiments. Specifically, the system can be
184 considered to contain two phases of solid particles, each possessing a distinct
normal size distribution, with the same physical properties. The fine particles
186 possess a normal distribution with a mean of 1.5 mm and standard deviation of
0.3 mm, and the coarse particles possess a normal distribution with a mean of
188 2.9 mm and standard deviation of 0.1 mm (see Fig. 5).

While the particles discharge through the hopper, they become tribocharged
190 and tend to stick to the walls of the hopper. To remove any charging of the
particles during discharge, the particles are treated with an anti-static solution.
192 The anti-static solution is prepared by dissolving 1 ml of ASA antistatic agent
(Electrolube, UK) into 100 ml of ethanol. No change in the discharge dynamics
194 and segregation is observed before and after the particles are coated with the
anti-static solution.

Figure 5: Silica beads: Normal distribution of the fine particles with mean of 1.5 mm and standard deviation of 0.3 mm, colored in red; and the coarse particles with a mean of 2.9 mm and standard deviation of 0.1 mm, colored in green.

196 The masses of the fine and coarse particles used in the experiments are
580 g and 420 g, respectively. Two initial packing configurations are prepared
198 using the fine and coarse particles. In the first configuration, the fine and
coarse particles are well mixed. For this, both the fine and coarse particles are
200 divided into 10 equal portions. One portion of fine particles is mixed with one
portion of coarse particles using a Turbula T2F Shaker-Mixer (Glen Mills Inc.,
202 NJ, USA). The same procedure is repeated with the remaining 9 portions to
produce 10 equal portions of well-mixed fine and coarse particles. The hopper
204 outlet is closed, and each portion is loaded slowly into the hopper, to minimize
segregation due to free fall. The particle bed is leveled after each portion is
206 loaded. In the second configuration, the coarse particles are first packed at the

bottom of the hopper (with the outlet closed). Then the fine particles are loaded
 208 on top of the coarse particles to form a layered packing. Each layer is leveled
 after loading into the hopper. We note that these configurations were also used
 210 by Ketterhagen et al., (2007) [50].

Figure 6: Particle arrangement: (a) First discharged sample from the well-mixed configuration. An approximately equal number of fine and coarse particles are discharged. (b) Last discharged sample from the well-mixed configuration. A majority of fine particles are discharged. (c) First discharged sample from the layered configuration. Only coarse particles are discharged. (d) Last discharged sample from the layered configuration. A mixture of both fine and coarse particles are discharged.

The discharge experiment is carried out using a discontinuous sampling
 212 method [51]. The outlet of the hopper is opened, and samples of equal mass
 are collected using the discontinuous sampling method. The initial and final
 214 arrangement of particles, for both mixed and layered configurations, are shown
 in Fig. 6. The collected samples are sieved and weighed to determine the mass
 216 of fine and coarse particles. Then the discharged mass fractions of both the fine
 and the coarse particles are determined, and the segregation data is plotted as
 218 the normalized mass fraction of fines (γ_f^N) and the overall discharged fractional
 mass ($\bar{\gamma}$), using Equations [1 and 2].

$$\gamma_f^N = \gamma_f^{discharge} / \gamma_f^0 \quad (1)$$

$$\bar{\gamma} = m^{discharge} / m^0 \quad (2)$$

220 where, γ_f^N is the normalized fine mass fraction of the discharged particles,
 $\gamma_f^{discharge}$ is the fine mass fraction of the discharged particles, γ_f^0 is the fine
 222 mass fraction in the initial packing configuration, $\bar{\gamma}$ is the overall discharged
 mass fraction, $m^{discharge}$ is the total discharged mass and m^0 is the mass of the
 224 initial particle packing. During the experiments with the well-mixed configuration,
 segregation occurs while loading. Therefore, each experiment is replicated
 226 five times to minimize the effects of any non-homogeneous regions on

discharge segregation results, for both well mixed and layered configurations.

228 The experimental results are reported in the subsequent section to validate our
polydispersity implementation.

230 4. Comparison of Experiment and Simulation Results

In this section, we present the validation of our newly implemented poly-
232 dispersity feature by replicating the experimental setup in Sec. 3. For the
simulations, we consider that the glass beads possess model properties consis-
234 tent with the previous studies [50]. As discussed in Sec. 2, in order to handle
size distribution more efficiently in the simulation, a maximum value and a min-
236 imum value are specified for each size distribution. The fine-to-coarse particle
mass ratio is 0.58:0.42, corresponding to a fine-to-coarse number ratio of 8:1.
238 The parameters for the particle phases used in our simulations are summarized
in Tab. 2. We note that for both solid phases, we specify an upper and lower
240 bound for the particle size PDF, to avoid generating non-realistic large/small
particles. In our subsequent simulations, the initial packings are generated us-
242 ing the mass-in-flow (MIF) boundary condition (i.e., the particles are filled into
the hopper from the top). In the current implementation, the MIF boundary
244 condition does not allow one to precisely control the number of particles for
each solid phase to be filled in the hopper. Therefore, the mass ratio is first
246 determined in the hopper discharge simulation and then reproduced in the ex-
periments, in which the mass for each phase can be controlled more precisely.
248 The simulations are carried out on Stampede at the Texas Advanced Comput-
ing Center (TACC), which consists of 64-bit Xeon E5-2680 2.7GHz (turbo, 3.5)
250 cores. The code is compiled with mvapich2/2.1.

Table 2: Geometrical parameters, masses of the two solid particle phases and global parameters used in validation simulations.

Figure 7: Initial configuration of the discharge hopper containing a well-mixed packing of spherical beads with a bi-modal size distribution. The unit of the particle diameter is centimeter.

4.1. Discharge hopper with polydisperse particles in well-mixed configuration

252 We first consider the well-mixed configuration (see Fig. 7). The initial con-
 254 figuration for the discharge simulation is obtained by filling the hopper with both
 256 fine and coarse beads together from the top through the mass-in-flow boundary
 condition, while keeping the bottom closed with a no-flow boundary condition.
 258 The injection velocities of the fine and coarse beads through the top are 16 cm/s,
 with a volume fraction of 0.0145 for coarse beads and 0.0165 for fine beads. The
 260 resulting packing is allowed to settle to completely dissipate the kinetic energy,
 and the resulting well-mixed stable packing is used as the initial configuration
 262 for the discharge simulation until the hopper is fully discharged. The number
 of computational grids used in this simulation is 30 by 30 by 40, along the
 264 two lateral directions and the axial direction of the hopper, respectively. We
 note that although the grid resolution needs to be specified for MFIX logistics,
 the actual fidelity is determined by the number of particles employed for the
 simulation when running MFIX-DEM in granular-flow-only mode. **The domain
 266 decomposition configuration is 4 by 4 by 4 with 64 cores, and the total CPU
 hours for the discharge simulation are 6.73 hours.**

Figure 8: 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.

Figure 9: Discharge dynamics are quantified using the normalized fine mass fraction γ_f^N of the discharged particles vs. the overall discharged mass fraction $\bar{\gamma}$ for the well-mixed configuration. The experimental results are represented as a box plot.

268 Fig. 8 shows the snapshots of the discharge simulations at several different
 times. The discharge dynamics are quantified using the normalized fine mass

270 fraction, γ_f^N , of the discharged particles vs. the overall discharged mass fraction, $\bar{\gamma}$, which are calculated by using Equations [1 and 2].

272 In the ideal case that during the entire discharge process, the packing configuration stays well mixed, the resulting $\gamma_f^N - \bar{\gamma}$ curve would be a simple constant
274 function with value 1. However, due to segregation effects, the fine particles cluster at the hopper bottom towards the end of the discharge, leading to an
276 increase of γ_f^N towards the end of discharge (see Fig. 9). As can be seen from the figure, our simulated $\gamma_f^N - \bar{\gamma}$ curve agrees very well quantitatively with our
278 experimental data.

Nonetheless, it can be seen that the experimental data tends to deviate more
280 from the ideally mixed case (i.e., the constant function), indicating a stronger segregation effect during the discharge. We note that in an “ideally mixed
282 case”, there will be no aggregation of particles of similar sizes during the entire discharge process. This situation is not possible in practice, as the particles
284 during a discharge process always gain kinetic energy and thus, inevitably form aggregations of different sizes. The observed discrepancy is possibly because of
286 the existence of locally segregated regions in the experimentally prepared initial packing configuration due to particle size dispersity, which is inevitable even
288 though very careful mixing was conducted in the experiment. On the other hand, the particle mixing in the initial configuration can be much better controlled in the simulation through mass-in-flow boundary conditions. Therefore,
290 the segregation in the simulated system is mainly due to discharge and becomes
292 significant toward the end of the discharge process.

4.2. Discharge hopper with polydisperse particles in a layered configuration

Figure 10: Initial configuration of the hopper discharge containing a layered packing of spherical beads with a bi-modal size distribution. The unit of the particle diameter is centimeter.

294 For the second validation case, we consider the discharge hopper with a layered configuration (see Fig. 10). The initial configuration for the discharge
296 simulation is obtained by first filling the hopper with coarse beads from the top

through the mass-in-flow boundary condition, while the bottom is kept closed
 298 through the no-flow boundary condition, and then continuing to fill the hopper
 with fine beads, which pack on top of the coarse beads (see Fig. 10). The
 300 injection velocities of the fine and coarse beads through the top are 16 cm/s,
 with a volume fraction of 0.02 for each layer. The resulting packing is allowed to
 302 settle to completely dissipate the kinetic energy, and the resulting layered stable
 packing is used as the initial start for the discharge simulation until the hopper
 304 is fully discharged. The number of computational grids used in this simulation
 is 30 by 30 by 40, along the two lateral directions and the axial direction of
 306 the hopper, respectively. The domain decomposition configuration is 4 by 4 by
 4 with 64 cores and the total CPU hours for the discharge simulation are 6.81
 308 hours.

Figure 11: 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.

Figure 12: Discharge dynamics are quantified using the normalized fine mass fraction γ_f^N of the discharged particles vs. the overall discharged mass fraction $\bar{\gamma}$ for the layered configuration. The experimental results are represented as a box plot.

Fig. 11 shows the snapshots of the discharge simulations. The discharge
 310 dynamics as quantified via $\gamma_f^N - \bar{\gamma}$ are shown in Fig. 12. As seen in Fig. 11, in
 this case, the coarse particles packed at the hopper bottom discharge first, which
 312 opens up a channel for the fine particles on the top. Therefore, the resulting γ_f^N
 remains zero for a while (before a channel is opened up), and is monotonically
 314 increasing as the discharge proceeds after the channel is open. Towards the end
 of discharge, since most of the fine particles in the hopper are gone, γ_f^N begins
 316 to decrease and finally starts to fluctuate due to a very small number of fine
 particles remaining in the hopper. Again, our simulated $\gamma_f^N - \bar{\gamma}$ curve agrees
 318 very well quantitatively with the experimental data, as shown in Fig. 12.

Our simulation also reveals how the channel for fine particles is opened up

320 during the discharge. Due to the geometry of the hopper, the particles in the
 central region corresponding to a virtual extension of the cylinder-shaped outlet
 322 at the hopper bottom always discharge first, regardless of the initial packing
 configurations in the hopper. The fast flow of discharging particles in this
 324 central region generates a pressure on the remaining particles and pushes them
 against the container wall. In the layered configuration, the coarse particles
 326 are packed at the bottom of the hopper and fine particles are then stacked on
 top. Thus, once the discharge process starts, the coarse particles in the central
 328 region discharge first, which efficiently open up a channel for the fine particles
 that were originally packed on top of the coarse ones.

330 Again, it can be seen that the experimental data tends to deviate more
 from the ideally mixed case (i.e., unity) compared to the simulation results. Al-
 332 though, in this layered configuration, the coarse and fine particles are separately
 packed in their own layers, within each layer the locally segregated regions still
 334 exist (due to the polydispersity of particles within the same solid phase) in
 the experimentally prepared initial configurations. This leads to the observed
 336 stronger segregation effects during the discharge process. For better controlled
 initial configurations in the simulations, the segregation is better suppressed
 338 and thus, the deviation of the simulated results from the ideally mixed case is
 less significant.

340 **5. Summary and Concluding Remarks**

In this paper, we presented our recent developments for enhancing MFI-
 342 DEM's capability for handling particle size polydispersity for the pure DEM
 mode flow simulations. We have modified the data structure and created new
 344 subroutines to separately handle geometrical and physical parameters of the
 solid phase particles. This allows MFI-DEM to easily handle an arbitrary
 346 number of solid phases, each possessing a distinct arbitrary particle-size distri-
 bution. New keywords have been introduced to allow easy specification of a
 348 variety of built-in and user-defined distributions, for both the initial condition

and mass-in-flow boundary condition. The new implementation is systematically validated using discharge hopper experiments, a commonly encountered set-up with many industrial applications, with polydisperse particles. The simulated discharge dynamics, including the normalized fine-mass-fraction vs. the overall discharged mass fraction, are found to be in reasonably good agreement with the corresponding experimental data, for the purposes of the preliminary V&V study. To better understand discrepancy observed and assess the potential sources, based on the insight gained from the current work, a follow-up uncertainty quantification study is being employed by utilizing global sensitivity analysis to determine which set of factors have the most influence on the normalized fine-mass-fraction vs. the overall discharged mass fraction ratio. For this purpose, an ensemble simulation matrix based on statistical design of experiments is being carried out to explore the parameter space (e.g., spring coefficient variables range which is used in contact models) and assess the sensitivities of the quantity of interest. The findings of the sensitivity study will pave the way for our future efforts on reducing the uncertainty in modeling parameters by employing techniques like Bayesian calibration.

The current implementation can easily handle particle size dispersity as large as 10:1. To efficiently handle larger dispersity (e.g., $> 20 : 1$), additional modifications of the codes (e.g., by implementing adaptive near-neighbor list [39]) are required. Nonetheless, the new polydispersity feature added to MFIX-DEM enables users to better capture the actual particle geometry of the solid phases, and thus, would lead to more accurate simulations of multiphase flows involving particle phases, especially in the dense flow regime. The current implementation will also pave the way for the non-spherical and reacting flow related revisions, as the data structures for handling individual particle sizes can be readily generalized to handle other particle geometry parameters and chemical reaction related parameters. This will allow the users to specify individual particle-based physical properties. We will explore these additional enhancements to the physical modeling capability of MFIX-DEM in our future work.

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References

- [1] M. Jahani, A. Farzanegan, M. Noaparast, Investigation of screening performance of banana screens using liggghts dem solver, Powder Technology 283 (2015) 32–47.
- [2] Y. Gu, A. Ozel, S. Sundaresan, A modified cohesion model for cfd–dem simulations of fluidization, Powder Technology 296 (2016) 17–28.
- [3] J. C. Loh, W. R. Ketterhagen, J. A. Elliott, A hybrid tabulation-scaling implementation of thornton and ning’s plastic–adhesive particle contact theory, Powder Technology 264 (2014) 599–607.
- [4] P. L. Falkingham, S. M. Gatesy, The birth of a dinosaur footprint: Subsurface 3d motion reconstruction and discrete element simulation reveal track ontogeny, Proceedings of the National Academy of Sciences 111 (51) (2014) 18279–18284.

- [5] T. Kopsch, D. Murnane, D. Symons, Optimizing the entrainment geometry of a dry powder inhaler: Methodology and preliminary results, *Pharmaceutical Research* (2016) 1–12.
- [6] H. S. Rabbani, V. Joekar-Niasar, N. Shokri, Effects of intermediate wettability on entry capillary pressure in angular pores, *Journal of colloid and interface science* 473 (2016) 34–43.
- [7] A. Sharifi, H. Niazmand, Analysis of flow and ldl concentration polarization in siphon of internal carotid artery: Non-newtonian effects, *Computers in biology and medicine* 65 (2015) 93–102.
- [8] MFIX-GUI, url = <https://mfix.netl.doe.gov/mfix/mfix-gui-2/>.
- [9] R. Garg, J. Galvin, T. Li, S. Pannala, Documentation of open-source MFIX-DEM software for gas-solids flows.
URL https://mfix.netl.doe.gov/documentation/dem_doc_2012-1.pdf
- [10] M. Syamlal, W. Rogers, T. J. O’Brien, MFIX documentation theory guide.
URL <https://mfix.netl.doe.gov/documentation/Theory.pdf>
- [11] T. Li, W. A. Rogers, M. Syamlal, J.-F. Dietiker, J. Musser, M. Shahnam, S. Rabha, The NETL MFIX Suite Of Multiphase Flow Models: A Brief Review And Recent Applications Of MFIX-TFM To Fossil Energy Technologies, *Chemical Engineering Science* doi:10.1016/j.ces.2016.07.043.
- [12] W. Rogers, NETL Multiphase Flow Research Overview, in: Presented as part of the NETL Workshop on Multiphase Flow Science, National Energy Technology Laboratory, 2016.
- [13] M. Syamlal, C. Guenther, A. Gel, S. Pannala, Advanced coal gasifier designs using large-scale simulations, in: *Journal of Physics: Conference Series*, Vol. 180, IOP Publishing, 2009, p. 012034.

- [14] A. Gel, R. Sankaran, S. Pannala, C. Guenther, Accelerating clean coal
 432 gasifier designs with hybrid MPI/OpenMP high performance computing,
 Parallel Computational Fluid Dynamics: Recent Advances and Future Di-
 434 rections (2010) 372.
- [15] E. F. D’Azevedo, S. Pannala, M. Syamlal, A. Gel, M. Prinkey, T. J.
 436 O’Brien, Parallelization of MFIX: A multiphase cfd code for modeling flu-
 idized beds, in: Tenth SIAM Conference on Parallel Processing for Scientific
 438 Community (PPSC), 2001.
- [16] M. Syamlal, T. J. O’Brien, Fluid dynamic simulation of o_3 decomposition
 440 in a bubbling fluidized bed, *AIChE Journal* 49 (2003) 2793–2801.
- [17] T. Li, C. Guenther, MFIX-DEM simulations of change of volumetric flow
 442 in fluidized beds due to chemical reactions, *Powder Technology* 220 (2012)
 70–78.
- [18] R. Garg, J. Galvin, T. Li, S. Pannala, Open-source MFIX-DEM software
 444 for gas-solids flows: Part i. verification studies, *Powder Technology* 220
 446 (2012) 122–137.
- [19] T. Li, R. Garg, J. Galvin, S. Pannala, Open-source MFIX-DEM software
 448 for gas-solids flows: Part ii. validation studies, *Powder Technology* 220
 (2012) 138–150.
- [20] P. Liu, C. M. Hrenya, Challenges of DEM: I. competing bottlenecks in
 450 parallelization of gas-solid flows, *Powder Technology* 264 (2014) 620–626.
- [21] J. Musser, Modeling of heat transfer and reactive chemistry for particles
 452 in gas-solid flow utilizing continuum-discrete methodology (cdm), Ph.D.
 454 thesis, West Virginia University Libraries (2011).
- [22] A. Gel, J. Hu, Scaling an open source cfd code by leveraging parallel open
 456 source solvers within the Trilinos framework-preliminary results, in: Pro-
 ceedings of the 2011 Parallel CFD Conference, Barcelona, Spain, 2011.

- 458 [23] A. Gel, E. Ould-Ahmed-Vall, A. Kalinkin, Optimization Of A Legacy Open
Source CFD Code For The New High Performance Computing Archi-
460 tectures: Preliminary Results, 27th International Conference on Parallel
Computational Fluid Dynamics Conference (ParallelCFD 2015), Montreal,
462 Canada, 2015.
- [24] A. Gel, J. Hu, Modernizing A Legacy Open Source CFD Code By Lever-
464 aging Scalable Parallel Preconditioners And Linear Equation Solvers, 27th
International Conference on Parallel Computational Fluid Dynamics Con-
466 ference (ParallelCFD 2015), Montreal, Canada, 2015.
- [25] A. Gel, R. Sankaran, S. Pannala, C. Guenther, Accelerating clean coal gasi-
468 fier designs with hybrid mpi/openmp high performance computing, Parallel
Computational Fluid Dynamics: Recent Advances and Future Directions
470 (2010) 372.
- [26] S. Pannala, E. D’Azevedo, M. Syamlal, Hybrid (OpenMP and MPI) paral-
472 lelization of MFIx: a multiphase cfd code for modeling fluidized beds, in:
Proceedings of the 2003 ACM symposium on Applied computing, ACM,
474 2003, pp. 199–206.
- [27] H. Liu, D. K. Tafti, T. Li, Hybrid parallelism in MFIx cfd-dem using
476 openmp, Powder Technology 259 (2014) 22–29.
- [28] P. Gopalakrishnan, D. Tafti, Development of parallel dem for the open
478 source code MFIx, Powder Technology 235 (2013) 33–41.
- [29] P. Gopalakrishnan, D. Tafti, Development of parallel dem for the open
480 source code MFIx, Powder Technology 235 (2013) 33–41.
- [30] H. Liu, D. Tafti, T. Li, Hybrid parallelism in MFIx CFD-DEM using
482 OpenMP, Powder Technology 259 (2014) 22–29.
- [31] A. Gel, M. Shahn timer, J. Musser, A. K. Subramaniyan, J.-F. Dietiker, Non-
484 intrusive uncertainty quantification of computational fluid dynamics sim-

- ulations of a bench-scale fluidized-bed gasifier, *Industrial & Engineering Chemistry Research* 55 (2016) 12477–12490.
- [32] A. Gel, R. Garg, C. Tong, M. Shahnam, C. Guenther, Applying uncertainty quantification to multiphase flow computational fluid dynamics, *Powder Technology* 242 (2013) 27–39.
- [33] D. C. Miller, B. Ng, J. Eslick, Advanced computational tools for optimization and uncertainty quantification of carbon capture processes, Tech. rep., National Energy Technology Laboratory-In-house Research; National Energy Technology Laboratory (NETL), Pittsburgh, PA, and Morgantown, WV (United States) (2014).
- [34] J. C. Eslick, B. Ng, Q. Gao, C. H. Tong, N. V. Sahinidis, D. C. Miller, A framework for optimization and quantification of uncertainty and sensitivity for developing carbon capture systems, *Energy Procedia* 63 (2014) 1055–1063.
- [35] K. J. Berger, C. M. Hrenya, Challenges of dem: Ii. wide particle size distributions, *Powder Technology* 264 (2014) 627–633.
- [36] Y. Jiao, F. H. Stillinger, S. Torquato, Distinctive features arising in maximally random jammed packings of superballs, *Physical Review E* 81 (2010) 041304.
- [37] C. Kloss, C. Goniva, A. Hager, S. Amberger, S. Pirker, Models, algorithms and validation for opensource dem and cfd–dem, *Progress in Computational Fluid Dynamics, an International Journal* 12 (2-3) (2012) 140–152.
- [38] H. N. Emady, K. V. Anderson, W. G. Borghard, F. J. Muzzio, B. J. Glasser, A. Cuitino, Prediction of conductive heating time scales of particles in a rotary drum, *Chemical Engineering Science* 152 (2016) 45–54.
- [39] A. Donev, S. Torquato, F. H. Stillinger, Neighbor list collision-driven molecular dynamics for nonspherical hard particles: Ii. applications to ellipses and ellipsoids, *Journal of Computational Physics* 202 (2005) 765.

- [40] Y. Jiao, F. H. Stillinger, S. Torquato, Dense packings of superballs, Physical
Review E 79 (2009) 041309.
- [41] Y. Jiao, S. Torquato, Dense packings of platonic and archimedean solids,
Nature 460 (2009) 876.
- [42] P. Von Zedtwitz, W. Lipiński, A. Steinfeld, Numerical and experimental
study of gas-particle radiative heat exchange in a fluidized-bed reactor for
steam-gasification of coal, Chemical engineering science 62 (1) (2007) 599–
607.
- [43] J. Dufek, G. Bergantz, Transient two-dimensional dynamics in the upper
conduit of a rhyolitic eruption: A comparison of closure models for the
granular stress, Journal of Volcanology and Geothermal Research 143 (1)
(2005) 113–132.
- [44] M. R. Sweeney, G. A. Valentine, Transport and mixing dynamics from
explosions in debris-filled volcanic conduits: numerical results and impli-
cations for maar-diatreme volcanoes, Earth and Planetary Science Letters
425 (2015) 64–76.
- [45] J. Estep, J. Dufek, Discrete element simulations of bed force anomalies
due to force chains in dense granular flows, Journal of Volcanology and
Geothermal Research 254 (2013) 108–117.
- [46] S. Darteville, From model conception to verification and validation, a
global approach to multiphase navier-stoke models with an emphasis on
volcanic explosive phenomenology, Tech. rep., Los Alamos National Labo-
ratory (LANL), Los Alamos, NM (2007).
- [47] S. Darteville, G. Valentine, Transient multiphase processes during the ex-
plosive eruption of basalt through a geothermal borehole (námafjall, ice-
land, 1977) and implications for natural volcanic flows, Earth and Planetary
Science Letters 262 (3) (2007) 363–384.

- 540 [48] M. D. Team, Multiphase Flow with Interphase eXchanges (MFIx) user
guide, National Energy Technology Laboratory, Morgantown, WV.
- 542 [49] J. F. Dietiker, Multiphase flow with interphase exchanges cartesian grid
user guide, National Energy Technology Laboratory, Morgantown, WV.
- 544 [50] W. R. Ketterhagen, J. S. Curtis, C. R. Wassgren, A. Kong, P. J. Narayan,
B. C. Hancock, Chemical Engineering Science.
- 546 [51] N. Standish, A. Kilic, Comparison of stop, start and continuous sampling
methods of studying segregation of materials discharging from a hopper,
548 Chemical engineering science 40 (11) (1985) 2152–2153.

Well-Mixed Configuration

Layered Configuration

Top View

$t = 6 \text{ s}$

$t = 9 \text{ s}$

$t = 11 \text{ s}$

$t = 12 \text{ s}$

Front View

$t = 6 \text{ s}$

$t = 9 \text{ s}$

$t = 11 \text{ s}$

$t = 12 \text{ s}$

Top View

t = 6 s

t = 9 s

t = 11 s

t = 12 s

Front View

t = 6 s

t = 9 s

t = 11 s

t = 12 s

	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

Sample	Fine	Coarse
Mean Dia.	0.15 cm	0.29 cm
Max Dia.	0.17 cm	0.31 cm
Min Dia.	0.13 cm	0.27 cm
Std. Dev.	0.03 cm	0.01 cm
Total Mass	580 g	420 g
Spring Constant	$2.5 \times 10^5 g/s^2$	$2.5 \times 10^5 g/s^2$
Friction Coefficient	0.5	0.5
Coefficient of Restitution	0.9	0.9

Hopper Bin Discharge Experiment

MFIX-DEM-Phi Simulations