Numerical simulation of polydisperse gas-particle flow in a vertical riser using a size-velocity quadrature-based moment method

Bo Kong\textsuperscript{1,2} and Rodney O. Fox\textsuperscript{1,2}

\textsuperscript{1}Department of Chemical and Biological Engineering
Iowa State University, Ames, IA, USA

\textsuperscript{2}Ames Laboratory – U.S. DOE, Ames, IA, USA

2015 Crosscutting Technology Research Review Meeting
Completed Tasks in FY15

MFIX-QBMM

*Created collection of gas-particle solvers using quadrature-based moment methods*

- Migrated from MFIX-2013 to current MFIX version, using MFIX git development repository
- Developed comprehensive post-processing capabilities using Python and VTK package
- Prepared documentation and tutorials for code
- Enabled code to run in both DMP and SMP mode
- Developed capability of handling non-uniform grid
- Provided users with a full range of drag models
- Developed realistic wall boundary condition
- Validated code against Euler-Lagrangian simulations
Outline

1. Introduction
2. Governing Equations for Polydisperse Gas Particle Flows
3. Numerical Methods
   - Moment inversion
   - Kinetic flux and forces
   - Polydisperse collision model
4. Wall-bounded Vertical Riser Test Case
5. Cluster-Induced Turbulence: Comparison with DPM Simulation
6. Summary and Future Work
Motivation

Problem:

In many commonly encountered engineering applications

1. polydispersity (e.g., size, density, shape) is present
2. “size” and velocity of disperse phase are closely coupled

Proposed solution:

Joint number density function of “size” and velocity of disperse phase can be solved using quadrature-based moment methods (QBMM)
Existing models for polydisperse gas-particle flows

**Euler-Lagrange Models**
- Discrete Element Method (DEM)
  
  Limitation: Computationally expensive for industrial applications

**Euler-Euler Models**
- Population Balance Equation (PBE) carried by fluid velocity
  
  Limitation: Spatial fluxes do not depend on size

- Class method with separate class velocities
  
  Limitation: Computationally expensive for continuous size distribution

- Direct Quadrature Method of Moments (DQMOM) with a multi-fluid model
  
  Limitation: Weights and abscissas are not conserved quantities

**Objective**

*Develop a robust and accurate moment-based polydisperse flow solver that incorporates microscale physics at reasonable computation cost*
Governing equations for polydisperse gas-particle flow

Gas phase: Continuity and momentum transport equations

\[
\frac{\partial}{\partial t} \rho_g \varepsilon_g + \nabla \cdot \rho_g \varepsilon_g U_g = 0
\]

\[
\frac{\partial}{\partial t} \rho_g \varepsilon_g U_g + \nabla \cdot \rho_g \varepsilon_g U_g \otimes U_g = \nabla \cdot \varepsilon_g \tau_g - \nabla p + \rho_g \varepsilon_g g + M_{lb}
\]

Particle phase: Kinetic equation for joint size-velocity NDF \(f(\xi, v)\)

\[
\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + \frac{\partial}{\partial v} \cdot fA = S
\]

where \(A\) represents acceleration due to forces acting on each particle, \(S\) represents other possible source terms (e.g., collisions, aggregation, break up, and chemical reaction in particles)
Moments method for solving Kinetic Equation

Moments for joint size-velocity NDF

\[ m_{p,i,j,k} = \int \xi^p v_x^i v_y^j v_z^k f (\xi, \mathbf{v}) \, d\xi d\mathbf{v} \]

Lower-order moments have particular physical significance:

\[ m_{1,0,0,0} = \rho_p \varepsilon_p, \quad m_{1,1,0,0} = \rho_p \varepsilon_p U_{bx}, \quad m_{1,0,1,0} = \rho_p \varepsilon_p U_{by}, \quad m_{1,0,0,1} = \rho_p \varepsilon_p U_{bz} \]

Moments transport equation:

\[ \frac{\partial m_{p,i,j,k}}{\partial t} + \frac{\partial m_{p,i+1,j,k}}{\partial x} + \frac{\partial m_{p,i,j+1,k}}{\partial y} + \frac{\partial m_{p,i,j,k+1}}{\partial z} = F_{p,i,j,k} \]

\[ F_{p,i,j,k} = \int \xi^p v_x^i v_y^j v_z^k \left[ iv_x^{-1}(A_x) + jv_y^{-1}(A_y) + kv_z^{-1}(A_z) \right] f (\xi, \mathbf{v}) \, d\xi d\mathbf{v} \]

Quadrature-Based Moment Methods (QBMM) are introduced to attain closure of higher-order moments (spatial fluxes) and \( F_{p,i,j,k} \)
Representation of joint size-velocity NDF

**Joint size-velocity NDF**

\[ n(\xi, \mathbf{v}) = f(\xi) \ g(\mathbf{v}|\xi) \]

**Comparison with traditional particle size population transport method**

Kinetic equation for particle size number density (with $S = 0$) can be rewritten

\[
\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{U}n = 0
\]

\[
\frac{\partial n\mathbf{U}}{\partial t} + \nabla \cdot \mathbf{U} \otimes \mathbf{U}n = ng + A(U)n
\]

$\mathbf{U}$ is often assumed to be independent of size $\xi$, however, a model with a continuous particle velocity conditioned on size $\mathbf{U}(\xi)$ needed for polydisperse particles.
Reconstructed size NDF

\[ n(\xi) = \sum_{\alpha=1}^{N} w_\alpha \delta_\sigma(\xi, \xi_\alpha) \]

with parameters found from size moments:

- Gamma \((0 < \xi < \infty)\)
  \[ \delta_\sigma(\xi, \xi_\alpha) \equiv \frac{\xi^{\lambda_\alpha - 1} e^{-\xi/\sigma}}{\Gamma(\lambda_\alpha) \sigma^{\lambda_\alpha}} \]
  with \(\lambda_\alpha = \xi_\alpha / \sigma\)

- Beta \((0 < \xi < 1)\)
  \[ \delta_\sigma(\xi, \xi_\alpha) \equiv \frac{\xi^{\lambda_\alpha - 1} (1 - \xi)^{\mu_\alpha - 1}}{B(\lambda_\alpha, \mu_\alpha)} \]
  with \(\lambda_\alpha = \xi_\alpha / \sigma\) and \(\mu_\alpha = (1 - \xi_\alpha) / \sigma\)

First \(2N\) moments always exact

Converges to exact NDF as \(N \to \infty\)

Dual-quadrature form

\[ \delta_\sigma(\xi, \xi_\alpha) \approx \sum_{\beta=1}^{M} w_{\alpha\beta} \delta(\xi - \xi_{\alpha\beta}) \]

with known weights \(w_{\alpha\beta}\) and abscissas \(\xi_{\alpha\beta}\)

2-node beta-EQMOM

First 2N moments always exact

Converges to exact NDF as \(N \to \infty\)
Size-conditioned particle velocity distribution $g(v|\xi)$

### Anisotropic Gaussian velocity distribution

$$g(u - \mu(\xi), \sigma^2(\xi)R) = \frac{1}{(2\pi)^{3/2} \sqrt{\sigma^2(\xi) R}} \exp \left[ -\frac{1}{2\sigma^2(\xi)} (u - \mathbf{U}(\xi))^T R^{-1} (u - \mathbf{U}(\xi)) \right]$$

### Approximation method

$\mathbf{U}(\xi)$ and $\sigma^2(\xi)$ can be approximated as

$$\mathbf{U}(\xi) = \sum_{n=0}^{2N_s} u_n g_n(\xi)$$

$$\sigma^2(\xi) = \sum_{n=0}^{2N_s} \sigma_n g_n(\xi)$$

where $u_n(\xi)$ and $\sigma_n$ are constant coefficients, and $g_n(\xi)$ are basis functions, which can be defined using various kinds of **orthogonal polynomial functions** and **piecewise functions**

### Conditional mean velocity

Vector function $\mathbf{U}(\xi)$ is defined to have following properties, which can be used to solve for $u_n(\xi)$

$$\sum_{\alpha=1}^{N_s} \rho_\alpha \int_{\Omega} \xi^s \mathbf{U}(\xi) K(\xi; \xi_\alpha, \sigma_s) d\xi = \begin{bmatrix} M_{s,1,0,0} \\ M_{s,0,1,0} \\ M_{s,0,0,1} \end{bmatrix}$$

$$M_{s,i,j,k} = \int_{\Omega} \int_{\mathbb{R}^3} \xi^s u^i v^j w^k n(\xi, \mathbf{u}) d\xi d\mathbf{u}$$

for $s = 0, \ldots, d_s$ with $d_s \leq 2N_s$
Solving size-conditioned velocity

**Conditional granular temperature**

Similarly, the conditional granular temperature $\sigma^2(\xi)$ has the following properties, which are used to solve for $\sigma_n$:

$$\sum_{\alpha=1}^{N_s} \rho_{\alpha} \int_{\Omega} \xi^s \left( \mathbf{U}(\xi) \cdot \mathbf{U}(\xi) + 3\sigma^2(\xi) \right) K(\xi; \xi_\alpha, \sigma_s) d\xi = M_{s,2,0,0} + M_{s,0,2,0} + M_{s,0,0,2}$$

for $s = 0, \ldots, d_s$ with $d_s \leq 2N_s$

**Normalized velocity covariance tensor**

Finally, normalized velocity covariance tensor (size-independent) is found using its definition:

$$\sum_{\alpha=1}^{N_s} \rho_{\alpha} \int_{\Omega} \xi^s \left[ \mathbf{U}(\xi) \otimes \mathbf{U}(\xi) + \sigma^2(\xi)\mathbf{R} \right] K(\xi; \xi_\alpha, \sigma_s) d\xi = \begin{bmatrix} M_{s,2,0,0} & M_{s,1,1,0} & M_{s,1,0,1} \\ M_{s,1,1,0} & M_{s,0,2,0} & M_{s,0,1,1} \\ M_{s,1,0,1} & M_{s,0,1,1} & M_{s,0,0,2} \end{bmatrix}$$
Sample size and sample velocity

Sample size: Jacobi quadrature for Beta kernel function

\[ K(\xi; \xi_\alpha, \sigma_s) = \sum_{\beta=1}^{N_{jq}} \tilde{\rho}_{\alpha\beta} \delta(\xi, \tilde{\xi}_{\alpha, \beta}) \]

Sample velocity: 3-D Hermite quadrature for anisotropic Gaussian kernel function

\[
g(u - U(\xi), \sigma^2(\xi)R) = \sum_{\gamma=1}^{N_{hq}} \tilde{\rho}_\gamma \delta(u, \tilde{u}_\gamma) = \sum_{\gamma=1}^{N_{hq}} \tilde{\rho}_\gamma \delta \left( u, \begin{bmatrix} \tilde{u}_\gamma \\ \tilde{v}_\gamma \\ \tilde{w}_\gamma \end{bmatrix} \right)\]

Using spectral decomposition scheme with triple 1-D Hermite quadratures

Moments calculation using sample size and velocity

Now moments can be calculated as

\[
M_{s, i, j, k} = \sum_{\alpha=1}^{N_s} \rho_\alpha \xi^s_\alpha u^i v^j w^k K(\xi; \xi_\alpha, \sigma_s) g(u - U(\xi), \sigma^2(\xi)R)
\]

\[
= \sum_{\alpha=1}^{N_s} \rho_\alpha \sum_{\beta=1}^{N_{jq}} \tilde{\rho}_{\alpha\beta} \tilde{\xi}^s_{\alpha, \beta} \sum_{\gamma=1}^{N_{hq}} \tilde{\rho}_{\alpha\beta\gamma} \tilde{u}_{\alpha\beta\gamma}^i \tilde{v}_{\alpha\beta\gamma}^j \tilde{w}_{\alpha\beta\gamma}^k
\]
Spatial moment fluxes are decomposed into two contributions corresponding to positive and negative velocity in each spatial direction:

\[ F_{s,i,j,k}^x = Q_{s,i,j,k}^{x,+} + Q_{s,i,j,k}^{x,-} \]

\[ Q_{s,i,j,k}^{x,+} = \int_{\mathbb{R}} \left( \int_0^\infty \xi^i u^{i+1} v^j w^k f_{sv}(\xi, u) \, du \right) d\xi \]

\[ = \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_{jq}} \sum_{\gamma=1}^{N_{hq}} \max(\tilde{u}_{\alpha\beta\gamma}, 0) \rho_\alpha \tilde{\rho}_{\alpha\beta} \tilde{\rho}_{\alpha\beta\gamma} \tilde{\xi}_s^i \tilde{u}_{\alpha\beta\gamma}^j \tilde{v}^j \tilde{w}^k \]

\[ Q_{s,i,j,k}^{x,-} = \int_{\mathbb{R}} \left( \int_{-\infty}^0 \xi^i u^{i+1} v^j w^k f_{sv}(\xi, u) \, du \right) d\xi \]

\[ = \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_{jq}} \sum_{\gamma=1}^{N_{hq}} \min(\tilde{u}_{\alpha\beta\gamma}, 0) \rho_\alpha \tilde{\rho}_{\alpha\beta} \tilde{\rho}_{\alpha\beta\gamma} \tilde{\xi}_s^i \tilde{u}_{\alpha\beta\gamma}^j \tilde{v}^j \tilde{w}^k \]

Realizability condition:

\[ \Delta t = CFL_{\min} \frac{\Delta x}{|\tilde{u}_{\alpha\beta\gamma}|} , \frac{\Delta y}{|\tilde{v}_{\alpha\beta\gamma}|} , \frac{\Delta z}{|\tilde{w}_{\alpha\beta\gamma}|} \]
Forces: drag and gravity

Contributions to evolution of moments due to drag force acting on each particle are directly computed, operating on sample velocities $\tilde{u}$ from quadrature approximation by solving an ODE:

$$\frac{d\tilde{u}}{dt} = A_d + g = K_D (u_g - \tilde{u}) + g$$

The sample velocity at next time step is

$$\tilde{u}^* = \tilde{u} e^{-K_D \Delta t} + \left(1 - e^{-K_D \Delta t} \right) \left( u_g + \frac{g}{K_D} \right)$$

And overall drag force received by entire particle phase is

$$F_{D,pg} = \sum m_p \cdot A_d = \frac{\rho_p \pi}{6} \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_{jg}} \rho_\alpha \tilde{\rho}_\alpha \beta \xi_{\alpha \beta}^3 \sum_{\gamma=1}^{N_{hq}} \tilde{\rho}_\alpha \beta \gamma K_{D,\alpha \beta \gamma} (u_g - \tilde{u}_\alpha \beta \gamma)$$

So using Newton’s first law, drag force received by gas phase is

$$F_{D,gp} = -F_{D,pg}$$
Polydisperse collision model

Moment transport equation

\[
\frac{\partial M_{s,i,j,k}}{\partial t} + \frac{\partial M_{s,i+1,j,k}}{\partial x} + \frac{\partial M_{s,i,j+1,k}}{\partial y} + \frac{\partial M_{s,i,j,k+1}}{\partial z} = A_{s,i,j,k} + \boxed{C_{s,i,j,k}}
\]

Using operator splitting, collision term can be conveniently updated by solving

\[
\frac{\partial M_{s,i,j,k}}{\partial t} = \boxed{C_{s,i,j,k}}
\]

\[
M_{s,i,j,k} = \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_{jq}} \rho_\alpha \tilde{\rho}_\alpha \beta \tilde{\xi}_s^{\alpha \beta} \sum_{\gamma=1}^{N_{hq}} \tilde{\rho}_\alpha \beta \gamma \tilde{u}^i_{\alpha \beta \gamma} \tilde{v}^j_{\alpha \beta \gamma} \tilde{w}^k_{\alpha \beta \gamma} = \sum_{a=1}^{N_t} w_a \xi_a^s G_{ijk}(\xi_a)
\]

Since we can assume that size does not change due to collisions, and also that collisions are binary

\[
\boxed{C_{s,i,j,k}} = \frac{\partial}{\partial t} \sum_{a=1}^{N_t} w_a \xi_a^s G_{ijk}(\xi_a) = \sum_{a=1}^{N_t} w_a \xi_a^s \frac{\partial G_{ijk}(\xi_a)}{\partial t} = \sum_{a=1}^{N_t} w_a \xi_a^s \sum_{b=1}^{N_t} C_{i,j,k}(\xi_a, \xi_b)
\]

\[
C_{i,j,k}(\xi_a, \xi_b) = C_{i,j,k}(\xi_a, \xi_b) + \nabla \cdot G_{i,j,k}(\xi_a, \xi_b)
\]
Collision source term

**BGK model (valid to second order)**

\[
C_{ijk}(\xi_a, \xi_b) = \kappa_{ab} \left( G_{ijk,ab}^* - G_{ijk,a} \right) = \frac{24 g_{0,ab} \alpha_b \chi_{ab}^3 \sqrt{\sigma_{ab}^2}}{\sqrt{\pi} d_{ab}} \left( G_{ijk,ab}^* - G_{ijk,a} \right)
\]

- **Zero-order moments**
  \[C_{i+j+k=0}(\xi_a, \xi_b) = 0\]
- **First-order moments**
  \[C_{i+j+k=1}(\xi_a, \xi_b) = \kappa_{ab} \left( U_{ab} - U_a \right)\]
- **Second-order moments**
  \[C_{i+j+k=2}(\xi_a, \xi_b) = \kappa_{ab} \left( U_{ab} \otimes U_{ab} + \Sigma_{ab} - U_a \otimes U_a - \Sigma_a \right)\]

For equilibrium Gaussian distribution

**Mean velocity**

\[U_{ab} = U_a + \frac{1}{4} (1 + e_{ab}) \mu_{ab} (U_b - U_a)\]

**Covariance tensor**

\[\Sigma_{ab} = \Sigma_a + \frac{1}{2} (1 + e_{ab}) \mu_{ab} \left[ \frac{1}{4} (1 + e_{ab}) \mu_{ab} \mathbf{S}_{ab} - \Sigma_a \right]\]

where \(\mathbf{S}_{ab} = 1/2(\Sigma_a + \Sigma_b + \sigma_{ab}^2 \mathbf{I}), \quad \Sigma_a = \sigma_a^2 R, \quad \Sigma_b = \sigma_b^2 R\)
Component of collisional-flux term caused by collisions between particles of size $\xi_a$ and $\xi_b$ can be calculated as

$$G_{m,ijk}(\xi_a, \xi_b) = G_{m,ijk}^{(0)}(\xi_a, \xi_b) + G_{m,ijk}^{(1)}(\xi_a, \xi_b)$$

$$G_{m,ijk}^{(0)}(\xi_a, \xi_b) = \frac{3\chi^2_{ab}\xi_a g_{0,ab}}{\xi_b} \int_{\mathbb{R}^6} I_{ijk}^{(m)}(\omega_{ab}, \mathbf{v}_a, \mathbf{v}_a - \mathbf{v}_b) f(\mathbf{v}_a)f(\mathbf{v}_b) d\mathbf{v}_a d\mathbf{v}_b$$

If let $M_{s,1} = [M_{s,1,0,0}, M_{s,0,1,0}, M_{s,0,0,1}]^T$, the collisional fluxes for this vector can thus be written as a tensor

$$P_{s,1} = \sum_{a=1}^{N_t} w_a \xi_s^a \left\{ \rho_p \alpha_a \sum a + \rho_p \alpha_a \sum a \cdot \frac{2\chi^3_{ab} \mu_{ab}(1 + e_{ab}) g_{0,ab}}{5 \chi_{ba}} \left[ \frac{1}{2} E_{ab} \mathbf{I} + \sum a + \sum b + (U_a - U_b) \otimes (U_a - U_b) \right] \right\}$$

where $E_{ab} = 3\sigma^2_a + 3\sigma^2_b + |U_a - U_b|^2$, which is defined as the energy scaling factor.
Test case: Wall-bounded vertical riser

Geometry and mesh (2D)

Gas phase is statistically stationary with zero volume flow rate

- gas density \( (\rho_p) \) 1 kg/m³
- gas viscosity \( (\nu_g) \) 1.84e-5 m²/s
- particle density \( (\rho_g) \) 2000 kg/m³
- mean diameter \( (d_p) \) 0.0002 m
- restitution coeff \( (e) \) 0.9
Animation: velocity fields, 2–5 second

Particle-phase velocity, gas-phase velocity, and granular temperature
Animation, scalar fields, 2–5 second

Volume fraction, mean particle diameter, and standard deviation
Statistical results (time averaged)

Particle volume fraction and mean diameter

Particle velocity, gas-phase velocity, and granular temperature
Influence of domain size on CIT statistics

In gravity-driven gas solids flows, slip velocity between clusters and gas drive turbulence, referred to as cluster-induced turbulence (CIT)

\[ \mathcal{L} = \tau_p^2 g \]

<table>
<thead>
<tr>
<th>Domain size</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
<th>Case 5</th>
<th>Case 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_1/\mathcal{L}$</td>
<td>4.03</td>
<td>8.06</td>
<td>16.13</td>
<td>32.26</td>
<td>64.51</td>
<td>129.01</td>
</tr>
<tr>
<td>$L_2/\mathcal{L}$</td>
<td>1.01</td>
<td>2.02</td>
<td>4.03</td>
<td>8.06</td>
<td>16.13</td>
<td>32.25</td>
</tr>
<tr>
<td>$L_3/\mathcal{L}$</td>
<td>1.01</td>
<td>2.02</td>
<td>4.03</td>
<td>8.06</td>
<td>16.13</td>
<td>32.25</td>
</tr>
<tr>
<td>$N_1$</td>
<td>64</td>
<td>128</td>
<td>256</td>
<td>512</td>
<td>1024</td>
<td>2048</td>
</tr>
<tr>
<td>$N_2$</td>
<td>16</td>
<td>32</td>
<td>64</td>
<td>128</td>
<td>256</td>
<td>512</td>
</tr>
<tr>
<td>$N_3$</td>
<td>16</td>
<td>32</td>
<td>64</td>
<td>128</td>
<td>256</td>
<td>512</td>
</tr>
<tr>
<td>$N_p$</td>
<td>1,678</td>
<td>13,417</td>
<td>107,329</td>
<td>858,629</td>
<td>6,869,032</td>
<td>54,952,240</td>
</tr>
</tbody>
</table>
Instantaneous particle volume fraction field

Case 2: $32 \times 32 \times 128$

Case 4: $128 \times 128 \times 512$
Comparison between DPM and EE-AG simulation results

Particle average settling velocity, $\langle u_{p,1} \rangle_p / \nu$

Particle total fluctuation energy, $K_p / \nu^2$

Deviation of volume fraction fluctuations

Fluid total fluctuation energy, $K_f / \nu^2$
Summary

Conclusions

- Novel approach to model polydisperse gas-particle flows with quadrature-based moment methods using kinetic equation for joint size-velocity number density function.

- Quasi-2D wall-bounded vertical riser simulated with continuous particle size distribution initial condition.

- Solver includes explicit representation of joint NDF using EQMOM that directly incorporates effects of polydispersity.

- Size segregation is captured in simulations, and results demonstrate our approach is effective way to model complicated polydisperse gas-particle flows.

- Comparison between CIT simulations using anisotropic Gaussian model and DPM method has demonstrated assumption for particle velocity is valid and this novel method can be used to perform mesoscale DNS for gas-particle flows.
Summary

Plans for future work

- Detailed validation with high resolution Euler-Lagrange simulation data for polydisperse gas-particle flows
- Implement realizable high-order numerical schemes for moment transport equations in MFIX
- Replace and update all previous implemented QBMM methods in MFIX, and implement newly developed QBMM methods in MFIX
- **Extend QBMM models to dense regime**
- Perform mesoscale DNS of CIT and wall-bounded channel flow to study gas-particle turbulence, such as effect of size distribution on cluster size
- Implement a new multiphase turbulence model, and validate against Euler-Lagrange simulations
Acknowledgment

Financial support from DOE - National Energy Technology Laboratory (Contract Number: DE-AC02-07CH11358)

Tasks completed in FY15

- Migrated from MFIX-2013 to current MFIX version, using MFIX git development repository
- Developed comprehensive post-processing capabilities using Python and VTK package
- Prepared documentation and tutorials for the code
- Enabled code to run in both DMP and SMP mode
- Developed the capability of handling non-uniform grid
- Provided a range of drag models
- Developed more realistic wall boundary condition
- Validated code against Lagrangian particle simulations