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-DOE, Ames, IA, USA

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Tasks accomplished in FY14:

**Quadrature-based moment method (QBMM)**
- Advanced library to manage moments in CFD context, based on Hash-Table method
- Comprehensive moment inversion library (univariate/multivariate), including QMOM, EQMOM, TP, CQMOM, ECQMOM
- New explicit disperse-phase volume fraction limit scheme used in general QBMM
- New high-order moment kinetic flux algorithm to improve accuracy of continuous QBMM (EQMOM)

**Polydisperse gas-particle flow**
- Variable-particle-size model with size-conditioned particle velocity, based on EQMOM
- Polydisperse particle collision model, including granular pressure term
1. Introduction

2. Governing Equations for Polydisperse Gas Particle Flows

3. Numerical Methods
   - Moment inversion
   - Kinetic flux and forces
   - Polydisperse collision model

4. Test Case: Wall-bounded Vertical Riser

5. Summery
Motivation

Polydisperse multiphase flows: continuous phase and disperse phase

In many commonly encountered applications

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

Thus, to accurately model polydisperse multiphase flows, joint number density function of “size” and velocity has to be properly described
## Existing models for polydisperse bubbly 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 with reasonable computation cost

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Governing equations for polydisperse gas-particle flow

Gas phase: Continuity and momentum transport equations

\[
\frac{\partial}{\partial t} \rho_g \varepsilon_g + \nabla \cdot \rho_g \varepsilon_g \mathbf{U}_g = 0
\]

\[
\frac{\partial}{\partial t} \rho_g \varepsilon_g \mathbf{U}_g + \nabla \cdot \rho_g \varepsilon_g \mathbf{U}_g \otimes \mathbf{U}_g = \nabla \cdot \varepsilon_g \tau_g - \nabla p + \rho_g \varepsilon_g \mathbf{g} + \mathbf{M}_{lb}
\]

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

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot f \mathbf{A} = \mathcal{S}
\]

where \( \mathbf{A} \) represents acceleration due to forces acting on each particle, \( \mathcal{S} \) 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

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

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:

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

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

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**

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

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

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

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

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

$U$ is often assumed to be independent of size $\xi$, however, a model with a continuous particle velocity conditioned on size $U(\xi)$ needed for polydisperse particles
Particle size distribution $f(\xi)$: Extended quadrature method of moments (EQMOM)

**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**

<table>
<thead>
<tr>
<th>Mass (x 10^-7)</th>
<th>NDF</th>
<th>EQMOM first quadrature nodes</th>
<th>NDF corresponding first node of first quadrature</th>
<th>second quadrature nodes corresponding to first node of first quadrature</th>
<th>NDF corresponding second node of first quadrature</th>
<th>second quadrature nodes corresponding to second node of first quadrature</th>
</tr>
</thead>
</table>
Size-conditioned particle velocity distribution $g(v|\xi)$

**Monokinetic:** *PTC effect and Brownian fluctuation are both negligible*

$$n(\xi, u) = \sum_{\alpha=1}^{N_s} \rho_\alpha K(\xi; \xi_\alpha, \sigma_s) \delta(u - U(\xi))$$

$U(\xi)$ is size-conditioned particle mean velocity

**Anisotropic Gaussian:** *PTC small but Brownian fluctuation non-negligible*

$$n(\xi, u) = \sum_{\alpha=1}^{N_s} \rho_\alpha K(\xi; \xi_\alpha, \sigma_s) g(u - U(\xi); \sigma^2(\xi) R)$$

$\sigma^2(\xi)$ is size-conditioned granular temperature, $R$ is normalized velocity covariance tensor

**ECQMOM method:** *PTC significant and Brownian fluctuation non-negligible*

$$n(\xi, u, v, w) = \sum_{\alpha=1}^{N_s} \rho_\alpha K(\xi; \xi_\alpha, \sigma_s) \left\{ \sum_{\beta=1}^{N_1} \rho_{\alpha\beta} g(u - U(\xi); u_{\alpha\beta}, \sigma_{1\alpha}) \right. $$

$$\left. \left[ \sum_{\gamma=1}^{N_2} \rho_{\alpha\beta\gamma} g(v - V(\xi, u); v_{\alpha\beta\gamma}, \sigma_{2\alpha\beta}) \right. \right. $$

$$\left. \left. \left( \sum_{\kappa=1}^{N_3} \rho_{\alpha\beta\gamma\kappa} g(w - W(\xi, u, v); w_{\alpha\beta\gamma\kappa}, \sigma_{3\alpha\beta\gamma}) \right) \right] \right\}$$
Solving size-conditioned velocity

**Anisotropic Gaussian velocity distribution**

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

**Approximation method**

\(U(\xi)\) and \(\sigma^2(\xi)\) can be approximated as

\[
U(\xi) = \sum_{n=0}^{2N_s} u_n g_n(\xi) \quad \sigma^2(\xi) = \sum_{n=0}^{2N_s} \sigma_n g_n(\xi)
\]

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 \(U(\xi)\) is defined to have following properties, which can be used to solve for \(u_n(\xi)\)

\[
\sum_{\alpha=1}^{N_s} \rho_\alpha \int_{\Omega} \xi^s U(\xi) K(\xi; \xi_\alpha, \sigma_s) d\xi = \begin{bmatrix} M_{s,1,0,0} \\ M_{s,0,1,0} \\ M_{s,0,0,1} \end{bmatrix} \quad M_{s,i,j,k} = \int_{\Omega} \int_{\mathbb{R}^3} \xi^s u^i v^j w^k n(\xi, u) \, d\xi \, du
\]

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 is 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

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

\[
= \sum_{\alpha=1}^{N_s} \rho_{\alpha} \sum_{\beta=1}^{N_{jq}} \tilde{\rho}_{\alpha\beta} \tilde{\xi}_{\alpha,\beta}^s \sum_{\gamma=1}^{N_{hq}} \tilde{\rho}_{\alpha\beta\gamma} \tilde{u}_{\alpha\beta\gamma}^i \tilde{v}_{\alpha\beta\gamma}^j \tilde{w}_{\alpha\beta\gamma}^k
\]
Kinetics-based finite-volume method: spatial fluxes

Spatial moment fluxes are decomposed into two contributions corresponding to positive and negative velocity in each spatial direction:

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

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

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

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

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

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

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

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**

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

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

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

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

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

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

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

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

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

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

\[C_{i+j+k=2}(\xi_a, \xi_b) = \kappa_{ab} \left( U_{ab} \otimes U_{ab} + \sum_{ab} - U_a \otimes U_a - \sum_a \right)\]

For equilibrium Gaussian distribution

Mean velocity

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

Covariance tensor

\[\sum_{ab} = \sum_a + \frac{1}{2} \left( 1 + e_{ab} \right) \mu_{ab} \left[ \frac{1}{4} \left( 1 + e_{ab} \right) \mu_{ab} S_{ab} - \sum_a \right]\]

where \( S_{ab} = 1/2 \left( \sum_a + \sum_b + \sigma_{ab}^2 I \right) \), \( \sum_a = \sigma_a^2 R \), \( \sum_b = \sigma_b^2 R \)
Collisional flux and Granular pressure

Collisional flux

$m^{th}$ component of collisional-flux term caused by collisions between particles of size $\xi_a$ and $\xi_b$ can be calculated as

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

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

This term can be explicitly closed by using sample size and sample velocity, which can make system unstable in simulations.

Granular pressure

For first-order velocity moments $M_{s,i+j+k=1}$, collisional flux can be treated as part of solid stress tensor $T_s$ in particle-phase momentum equation, which can be decomposed as

\[ T_{s,k} = p_{s,k} \mathbf{I} + \tau_{s,k} \]

Granular pressure due to particle collisions for particle phase can be calculated as

\[ p_{s,k} = \rho_s \sum_{a=1}^{N_t} w_a \left[ \sigma_a^2 + \sum_{b=1}^{N_t} w_b \frac{\chi_{ab}^3 \mu_{ab}(1 + e_{ab}) g_{0,ab} E_{ab}}{3\chi_{ba}} \right] \]
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/m$^3$
- Gas viscosity ($\nu_g$) 1.84e-5 m$^2$/s
- Particle density ($\rho_g$) 2000 kg/m$^3$
- Mean diameter ($d_p$) 0.0002 m
- Restitution coeff (e) 0.9

Periodic in X-direction

Initial particle size distribution
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

![Graphs showing particle volume fraction and mean diameter for polydisperse and monodisperse systems.]

Particle velocity, gas-phase velocity, and granular temperature

![Graphs showing particle velocity, gas-phase velocity, and granular temperature for polydisperse and monodisperse systems.]

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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

Plans for future work in FY15

- Detailed validation with 3-D experimental/Lagrangian simulation data for polydisperse gas-particle flows
- Implementation of new multiphase turbulence model, and validation with Lagrangian simulation of Capecelatro et al.
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Thanks for your attention!

Questions?