Meso-scale structures in bidisperse fluidized suspensions

William Holloway, Sofiane Benyahia, Christine Hrenya, and Sankaran Sundaresan

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Outline

• Project objective
• Current status of GHD theory in MFIX
• Connection to Roadmap
• Model framework
• Test cases
• Model predictions
• Grid resolution effects
• Range of validity of kinetic theory formulation
• Summary
Project objective

Goal:

Study the segregation behavior of binary gas-solid flows in risers predicted by the kinetic theory model framework of Garzó, Hrenya, and Dufty\(^1\) (GHD theory) with the fluid-particle drag model developed by Holloway, Yin and Sundaresan (HYS).\(^2,3,4\)

\(^1\)Garzó, Hrenya, and Dufty, *Phys. Rev. E*, 2007
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Necessitates the robust operation of HYS drag model and GHD theory in MFIX.

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Demonstrated

Necessitates the robust operation of HYS drag model and GHD theory in MFIX.

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Current focus

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- Currently GHD theory implementation is only compatible with binary mixtures.
Current status of GHD theory in MFIX

• GHD theory has been successfully incorporated within the MFIX framework and has been tested extensively.

• The GHD theory implementation has operated robustly for both homogeneous and inhomogeneous gas-solid flows with binary particle size distributions (PSD).

• Currently GHD theory implementation is only compatible with binary mixtures.

• Only two drag relations have been implemented with GHD theory at this point (namely, HYS and Wen-Yu).
1. Fundamental aspects of stress and flow fields in dense particulate systems.

2. Definition of material properties on relevant scales, along with efficient ways to represent properties in models and establish standards for material property measurements.

3. Given the practical need for continuum modeling capability, identify the inherent limitations and how to proceed forward, e.g., hybrid models that connect with finer scale models (DNS, DEM, finite element, stochastic, etc.) for finer resolution.

4. Size-scaling and process control (particle/unit-op/processing system) is critical to industrial applications.
Princeton Tasks

Task 4.6:

The MFIX framework, modified to account for the new physical models will be developed as part of this work and compared to experimental data obtained from high-velocity systems.
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Near Term:
- Perform high-fidelity, transient 3-D multiphase flow computations with PSD (particle size distribution).
- Identify deficiencies of current models developed for gas-solid flows.
Continuum models for polydisperse flows

\(^1\) Garzó, Hrenya, and Dufty, *Phys. Rev. E*, 2007
Continuum models for polydisperse flows

Continuity

\[
\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{V}) = -\frac{1}{m_i} \nabla \cdot \mathbf{j}_{0i}
\]

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Continuum models for polydisperse flows

Continuity

\[ \frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{V}) = -\frac{1}{m_i} \nabla \cdot \mathbf{j}_{0i} \]

Momentum

\[ \rho_s \phi \left( \frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} \right) = -\nabla \cdot \sigma_s + \sum_{i=1}^{s} n_i \mathbf{F}_i \]

\[ \mathbf{j}_{0i} = -\sum_{j=1}^{s} \frac{m_i m_j n_j}{\rho} D_{ij} \nabla \ln(n_j) - \rho D_{i}^{T} \nabla \ln(T) - \sum_{j=1}^{s} D_{ij}^{F} \mathbf{F}_j \]

Continuum models for polydisperse flows

**Continuity**

\[
\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i V) = - \frac{1}{m_i} \nabla \cdot j_{0i}
\]

**Momentum**

\[
\rho_s \phi \left( \frac{\partial V}{\partial t} + V \cdot \nabla V \right) = -\nabla \cdot \sigma_s + \sum_{i=1}^{s} n_i F_i
\]

\[
j_{0i} = -\sum_{j=1}^{s} \frac{m_i m_j n_j}{\rho} D_{ij} \nabla \ln(n_j) - \rho D_i^T \nabla \ln(T) - \sum_{j=1}^{s} D_{ij}^F F_j
\]

**Fluctuating energy**

\[
\frac{3n}{2} \left( \frac{\partial T}{\partial t} + V \cdot \nabla T \right) = -\nabla \cdot q - \sigma_s : \nabla V - \frac{3n \zeta T}{2} + \frac{3T}{2} \sum_{i=1}^{s} \frac{1}{m_i} \nabla \cdot j_{0i} + \sum_{i=1}^{s} \frac{F_i \cdot j_{0i}}{m_i}
\]

\[
q = -\lambda \nabla T - \left( \sum_{i=1}^{s} \sum_{j=1}^{s} T^2 D_{q,ij} \nabla \ln(n_j) + L_{ij} F_j \right)
\]

\(^1\)Garzó, Hrenya, and Dufty, *Phys. Rev. E*, 2007
External forces in polydisperse systems

\[ \mathbf{j}_0 = - \sum_{j=1}^{s} \frac{m_i m_j n_j}{\rho} D_{ij} \nabla \ln(n_j) - \rho D_i^T \nabla \ln(T) - \sum_{j=1}^{s} D_{ij}^F \mathbf{F}_j \]
External forces in polydisperse systems

\[ \mathbf{j}_0 = - \sum_{j=1}^{s} \frac{m_i m_j n_j}{\rho} D_{ij} \nabla \ln(n_j) - \rho D_i^T \nabla \ln(T) - \sum_{j=1}^{s} D_{ij} F_j \]

\[ F_j = m_j g + V_j \nabla P_g + F_{Dj} \]
External forces in polydisperse systems

\[ j_{0i} = - \sum_{j=1}^{s} \frac{m_i m_j n_j}{\rho} D_{ij} \nabla \ln(n_j) - \rho D_{i}^{T} \nabla \ln(T) - \sum_{j=1}^{s} D_{ij}^{F} F_{j} \]

\[ F_{j} = m_j g + V_j \nabla P_g + F_{Dj} \]

Fluid-particle drag model (HYS):\(^2,^3,^4\)

\[ F_{Dj} = -\frac{\beta_j}{n_j} (V_j - V_g) \]

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External forces in polydisperse systems

\[ \mathbf{j}_0 = -\sum_{j=1}^{s} \frac{m_i m_j n_j}{\rho} \mathbf{D}_{ij} \nabla \ln(n_j) - \rho \mathbf{D}_i^T \nabla \ln(T) - \sum_{j=1}^{s} \mathbf{D}_{ij}^F \mathbf{F}_j \]

\[ \mathbf{F}_j = m_j \mathbf{g} + V_j \nabla P_g + \mathbf{F}_{Dj} \]

Fluid-particle drag model (HYS):\(^2,3,4\)

\[ \mathbf{F}_{Dj} = -\frac{\beta_j}{n_j} (\mathbf{V}_j - \mathbf{V}_g) - \sum_{i\neq j}^{s} \frac{\beta_{ji}}{n_j} (\mathbf{V}_i - \mathbf{V}_j) \]

\[ \beta_{ji} = -\frac{2\alpha \phi_i \phi_j}{\phi_i/\beta_i + \phi_j/\beta_j} \]

Off-diagonal friction coefficient

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\(^2\)Holloway, Yin, and Sundaresan, *AIChE J.*, 2010
\(^3\)Yin and Sundaresan, *AIChE J.*, 2009
Test cases

Broad PSD
Test cases

Broad PSD

- Binary approximation
  - $d_1 = 212.5 \, \mu m$, $d_2 = 127.5 \, \mu m$
  - $\phi = 0.15$
Test cases

Broad PSD

- Binary approximation
  - $d_1 = 212.5 \mu m$, $d_2 = 127.5 \mu m$
  - $\phi = 0.15$

- Monodisperse approximation
  - $d = 170 \mu m$
  - $\phi = 0.15$
Test cases

Broad PSD

- Binary approximation
  - $d_1 = 212.5 \, \mu m, \ d_2 = 127.5 \, \mu m$
  - $\phi = 0.15$
- Monodisperse approximation
  - $d = 170 \, \mu m$
  - $\phi = 0.15$

Bimodal PSD with disparate size ratio
Test cases

Broad PSD

- Binary approximation
  - \( d_1 = 212.5 \, \mu m, \, d_2 = 127.5 \, \mu m \)
  - \( \phi = 0.15 \)
- Monodisperse approximation
  - \( d = 170 \, \mu m \)
  - \( \phi = 0.15 \)

Bimodal PSD with disparate size ratio

- Binary approximation
  - \( d_1 = 650 \, \mu m, \, d_2 = 170 \, \mu m \)
  - \( \phi = 0.15 \)
Test cases

Broad PSD

- Binary approximation
  - \(d_1 = 212.5 \, \mu m, \; d_2 = 127.5 \, \mu m\)
  - \(\phi = 0.15\)
- Monodisperse approximation
  - \(d = 170 \, \mu m\)
  - \(\phi = 0.15\)

Bimodal PSD with disparate size ratio

- Binary approximation
  - \(d_1 = 650 \, \mu m, \; d_2 = 170 \, \mu m\)
  - \(\phi = 0.15\)
- Monodisperse approximation
  - \(d = 270 \, \mu m\)
  - \(\phi = 0.15\)
Model predictions

Broad PSD \((e = 0.95)\)
Model predictions

Broad PSD ($e = 0.95$)

Bidisperse

Monodisperse

MFIX simulations:
- $d_1 = 212.5 \, \mu m$, $d_2 = 127.5 \, \mu m$
- $\langle \phi_1 \rangle = 0.125$, $\langle \phi_2 \rangle = 0.025$
- Doubly periodic
- 16 cm x 64 cm
- 0.25 cm grids
Model predictions

Broad PSD \((e = 0.95)\)

**Bidisperse**

**Monodisperse**

\[
\langle V_{\text{slip}} \rangle = \frac{\langle (1 - \phi) V_g \rangle}{\langle 1 - \phi \rangle} - \frac{\phi \langle V_{\text{mix}} \rangle}{\langle \phi \rangle}
\]

**MFIX simulations:**
- \(d_1 = 212.5 \mu m, \ d_2 = 127.5 \mu m\)
- \(\langle \phi_1 \rangle = 0.125, \ \langle \phi_2 \rangle = 0.025\)
- Doubly periodic
- 16 cm x 64 cm
- 0.25 cm grids

\[
\tau = t \frac{g}{V_t}
\]
Model predictions

Broad PSD \((e = 0.99)\)
Model predictions

Broad PSD ($e = 0.99$)

Bidisperse

Monodisperse

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Model predictions

Broad PSD ($e = 0.99$)

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Monodisperse

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- 16 cm x 64 cm
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\[
\tau = t \frac{g}{V_t}
\]

\[
\langle V_{\text{slip}}^* \rangle = \frac{\langle V_{\text{slip}} \rangle}{V_t}
\]
Model prediction: Volume fraction ratios

Broad PSD
Model prediction: Volume fraction ratios

Broad PSD

\[ e = 0.99 \quad \text{and} \quad e = 0.95 \]

MFIX simulations:
- GHD theory
- HYS drag model
- \( \frac{d_1}{d_2} = 212.5 \, \mu m, \frac{d_2}{d_1} = 127.5 \, \mu m \)
- \( \langle \phi_1 \rangle = 0.125, \langle \phi_2 \rangle = 0.025 \)
- Doubly periodic
- 16 cm x 64 cm
Model prediction: Volume fraction ratios

Broad PSD

$e = 0.99$

$e = 0.95$

$\phi_1 / \phi$

MFIX simulations:
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- HYS drag model
- $d_1 = 212.5 \mu m$, $d_2 = 127.5 \mu m$
- $\langle \phi_1 \rangle = 0.125$, $\langle \phi_2 \rangle = 0.025$
- Doubly periodic
- 16 cm x 64 cm

Broad PSD maintains a very tight distribution of volume fraction ratio throughout the flow domain for both coefficients of restitution.
Model predictions

Bimodal PSD \((e = 0.95)\)
Model predictions

Bimodal PSD \((e = 0.95)\)

Bidisperse

Monodisperse

MFIX simulations:
- \(d_1 = 650 \mu m, d_2 = 170 \mu m\)
- \(\langle \phi_1 \rangle = \langle \phi_2 \rangle = 0.075\)
- Doubly periodic
- 16 cm x 64 cm
- 0.25 cm grids
Model predictions

Bimodal PSD ($e = 0.95$)

Bidisperse

Monodisperse

\[ \langle V_{\text{slip}} \rangle = \frac{\langle (1 - \phi)V_g \rangle}{\langle 1 - \phi \rangle} - \frac{\phi V_{s_{\text{mix}}}}{\langle \phi \rangle} \]

MFIX simulations:
- \(d_1=650 \, \mu m, d_2=170 \, \mu m\)
- \(\langle \phi_1 \rangle = \langle \phi_2 \rangle = 0.075\)
- Doubly periodic
- 16 cm x 64 cm
- 0.25 cm grids

\[ \tau = t \frac{g}{V_t} \]

\[ \langle V_{\text{slip}}^* \rangle = \frac{\langle V_{\text{slip}} \rangle}{V_t} \]
Model predictions

Bimodal PSD \( (e = 0.99) \)
Model predictions

Bimodal PSD ($e = 0.99$)

Bidisperse | Monodisperse

- $d_1 = 650 \mu m$, $d_2 = 170 \mu m$
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MFIX simulations:
Model predictions

**Bimodal PSD \((e = 0.99)\)**

Bidisperse

Monodisperse

\[
\langle V_{\text{slip}} \rangle = \frac{\langle (1 - \phi) V_g \rangle}{\langle 1 - \phi \rangle} - \frac{\langle \phi V_{s_{\text{mix}}} \rangle}{\langle \phi \rangle}
\]

**MFIX simulations:**
- \(d_1 = 650 \mu m, d_2 = 170 \mu m\)
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- 0.25 cm grids

\[
\tau = t \frac{g}{V_t}
\]
Model prediction: Volume fraction ratios

Bimodal PSD
Model prediction: Volume fraction ratios

**Bimodal PSD**

$e = 0.99$

$e = 0.95$

\[ \frac{\phi_1}{\phi} \]

**MFIX simulations:**

- GHD theory
- HYS drag model
- $d_1 = 650 \, \mu m$, $d_2 = 170 \, \mu m$
- $\langle \phi_1 \rangle = 0.075$, $\langle \phi_2 \rangle = 0.075$
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Model prediction: Volume fraction ratios

Bimodal PSD

$e = 0.99$

$e = 0.95$

$\phi_1 / \phi$

MFIX simulations:

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- HYS drag model
- $d_1 = 650 \, \mu m$, $d_2 = 170 \, \mu m$
- $\langle \phi_1 \rangle = 0.075$, $\langle \phi_2 \rangle = 0.075$
- Doubly periodic
- 16 cm x 64 cm

Bimodal PSD has a much broader distribution of particle volume fraction ratio than the Broad PSD case.
Grid resolution effects

Broad PSD \((e = 0.99)\)
Broad PSD \((e = 0.99)\)

1 cm grids

MFIX simulations:
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- HYS drag model
- \(d_1=212.5 \mu m, d_2=127.5 \mu m\)
- \(\langle \phi_1 \rangle = 0.125, \langle \phi_2 \rangle = 0.025\)
- Doubly periodic
- 16 cm x 64 cm
Grid resolution effects

Broad PSD \((e = 0.99)\)

- 1 cm grids
- 0.5 cm grids

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- Doubly periodic
- 16 cm x 64 cm
Grid resolution effects

**Broad PSD** \((e = 0.99)\)

1 cm grids | 0.5 cm grids | 0.25 cm grids

- **MFIX simulations:**
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Grid resolution effects

**Broad PSD** ($e = 0.99$)

- 1 cm grids
- 0.5 cm grids
- 0.25 cm grids

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- 16 cm x 64 cm

As grid resolution is increased, finer structures begin to appear in the flow domain.
Grid resolution effects

Bimodal PSD \((e = 0.99)\)
Grid resolution effects

Bimodal PSD \((e = 0.99)\)

1 cm grids

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Grid resolution effects

**Bimodal PSD \((e = 0.99)\)**

1 cm grids

0.5 cm grids

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Grid resolution effects

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Grid resolution effects

Bimodal PSD ($e = 0.99$)

1 cm grids  0.5 cm grids  0.25 cm grids

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- GHD theory
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- Doubly periodic
- 16 cm x 64 cm

The emergence of fine structure with grid resolution indicates that equations used to model binary gas-solid flows must be coarse grained.
Range of validity of kinetic theory formulation

Bimodal PSD ($e = 0.95$)

**Assumption:**

$$Kn \ll 1$$

$$Kn = \frac{l_{mf}}{l_{grad}}$$

$$l_{mf} \approx \frac{d}{6\sqrt{2}\phi}$$

$$l_{grad} = \left| \frac{\bar{\chi}}{\nabla \chi} \right|$$
Range of validity of kinetic theory formulation

Bimodal PSD \((e = 0.95)\)

Assumption:  
\(Kn << 1\)

\[Kn = \frac{l_{mf}}{l_{\text{grad}}}\]

\[l_{mf} \approx \frac{d}{6\sqrt{2}\phi}\]

\[l_{\text{grad}} = \left| \frac{\bar{\chi}}{\nabla \chi} \right|\]
Range of validity of kinetic theory formulation

**Bimodal PSD** $(e = 0.95)$

**Assumption:**

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\[ l_{grad} = \left| \overline{\nabla \chi} \right| \]

\[ Kn\phi \]
Range of validity of kinetic theory formulation

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Range of validity of kinetic theory formulation

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\]
Range of validity of kinetic theory formulation

**Bimodal PSD \((e = 0.95)\)**

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\(l_{grad} = \left| \frac{\bar{\chi}}{\nabla \chi} \right|\)
Assumption: $Kn << 1$

$Kn = \frac{l_{mf}}{l_{grad}}$

$l_{mf} \approx \frac{d}{6\sqrt{2}\phi}$

$l_{grad} = \left| \frac{\vec{\nabla} \chi}{\nabla \chi} \right|$
Range of validity of kinetic theory formulation

Bimodal PSD ($e = 0.95$)

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$Kn = \frac{l_{mf}}{l_{grad}}$

$l_{mf} \approx \frac{d}{6\sqrt{2\phi}}$

$l_{grad} = \left| \frac{\bar{\chi}}{\nabla \chi} \right|$
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- HYS drag model has been implemented within new CVS version of MFIX.
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• GHD theory has been implemented within MFIX and operates robustly, even in very inhomogeneous gas-solid flows.
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- GHD theory has been implemented within MFIX and operates robustly, even in very inhomogeneous gas-solid flows.

- Binary fluidized gas-solid suspensions manifest inhomogeneous structures similar to monodisperse systems.

- Volume averaged slip velocities in both monodisperse and bidisperse gas-solid flows are qualitatively similar when both PSDs have the same Sauter mean diameter.
Summary

• HYS drag model has been implemented within new CVS version of MFIX.

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• Binary fluidized gas-solid suspensions manifest inhomogeneous structures similar to monodisperse systems.

• Volume averaged slip velocities in both monodisperse and bidisperse gas-solid flows are qualitatively similar when both PSDs have the same Sauter mean diameter.

• The scale of structures in binary gas-solid flows depends on grid resolution, similar to monodisperse suspensions.
Summary

- HYS drag model has been implemented within new CVS version of MFIX.
- GHD theory has been implemented within MFIX and operates robustly, even in very inhomogeneous gas-solid flows.
- Binary fluidized gas-solid suspensions manifest inhomogeneous structures similar to monodisperse systems.
- Volume averaged slip velocities in both monodisperse and bidisperse gas-solid flows are qualitatively similar when both PSDs have the same Sauter mean diameter.
- The scale of structures in binary gas-solid flows depends on grid resolution, similar to monodisperse suspensions.
- Knudsen number was found to be $O(1)$ or less throughout simulation domain.
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• Yesim Igci
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