Experiments and Model Development for Polydisperse, Gas-fluidized Systems

Jia-Wei Chew
R. Brent Rice
Christine M. Hrenya

S. Tenneti
R. Garg
Shankar Subramaniam

Vicente Garzó

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Project Scope: Work Breakdown Structure

Development, Verification, and Validation of Multiphase Models for Polydisperse Flows

Theory Development

1. Solid-Phase Continuum Theory
   - 1.1 Kinetic Theory
   - 1.2 DQMOM
   - 1.3 Incorporation of KT and DQMOM into MFIX
   - 1.4 KT extension to multiphase

2. Gas-Solid Drag
   - 2.1 LBM/DTIBM: zero-mean vel.
   - 2.2 LBM/DTIBM: non-zero rel. vel.
   - 2.3 LBM/DTIBM: freely evolving

3. Gas-Phase Turbulence
   - 3.1 Polydisperse DNS
   - 3.2 Multiphase Turb. Model

Data Collection

Simulations
   - 4.1 DEM (solids)
   - 4.2 Eulerian-DEM (gas-solid)

Experiments
   - 4.3 Low-velocity fluidized bed
   - 4.4 Cluster Probe Development
   - 4.5 High-velocity fluidized bed (PSRI)
   - 4.6.2 Liaison to NETL riser data

Model Validation

- 4.6.1 Compare with DEM data (4.1) and low-velocity bed (4.3)
- 4.6.3 Compare with high-velocity data from Eulerian-DEM (4.2), PSRI (4.5), and NETL (4.6.2)

Program Management

- 5.1 Develop Management Plan
  - Approach
  - Scope
  - Cost Estimates
  - Schedule
  - Risk
  - Constraints
  - Assumptions
  - Communication

Deliverables

- Monthly email updates
- Quarterly reports
- Annual reports
- Final report
- New theory into MFIX
Univ. Colorado Tasks for Year 3

Validation data
1) Bubbling-bed experiments (Colorado)
2) DEM simulations of simple shear (Colorado)
3) Riser experiments (Colorado & PSRI)
   Ray Cocco (PSRI) – Thursday

Theory
4) Application of polydisperse kinetic theory to clustering
   (Princeton & NETL & Colorado)
   Bill Holloway (Princeton) - Tuesday

5) Kinetic Theory Extension to Gas-Solid Flows (Colorado & Iowa State)
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Overview: Bubbling Bed Experiments

Objective

To characterize segregation and bubbling behavior of bubbling beds with continuous size distributions

• Do continuous PSD’s behave like binary mixtures?
• Is there a direct link between the segregation and bubbling levels?

System
Measurements: Segregation and Bubbling

Segregation: sieving of thin vertical sections
1. High velocity \( (3 \ U_{cf}) \) to mix bed
2. Low velocity \( (1.2 \ U_{cf}) \) for segregation
3. Shut down, vacuum sections, sieve

Bubbling: fiber optic probe
1. 7 axial x 9 radial positions
2. Bubble frequency, velocity & size
Continuous PSD’s Investigated

Width of distribution: $\sigma/d_{ave}$ (%)

Material: sand
Results: Segregation

\[ S_{\text{cont}} = \frac{S - 1}{S_{\text{max}} - 1} \]

\[ S = \frac{< h_{\text{small}} >}{< h_{\text{large}} >} \quad S_{\text{max}} = \frac{2x_{\text{large}} + x_{\text{small}}}{x_{\text{large}}} \]

\[ s_{\text{cont}} = 0 \rightarrow \text{perfect mixing} \]
\[ s_{\text{cont}} = 1 \rightarrow \text{perfect segregation} \]

**Gaussian:** as PSD width increases \( \uparrow \), segregation \( \uparrow \)

**lognormal:** non-monotonic variation of segregation with PSD width

Results: Bubbling

**Gaussian**: as PSD width increases ↑, all bubble parameters ↑ (some not shown)
**lognormal**: same as Gaussian (*monotonic* variation)

Chew & Hrenya, *I&ECR* (submitted)
Reconciliation: Segregation and Bubbling Measurements

Explanation

- presence of *bubble-less layer* in some systems
- size of bubble-less layer correlates with degree of segregation

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**Gaussian**

![Gaussian graph]

**lognormal**

![lognormal graph]

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**S_{cont} vs \( \sigma/d_{ave} \)**

![S_cont vs \( \sigma/d_{ave} \) graph]
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Objective

Assess the impact of *polydispersity* on *clustering* in *granular* flows

- How does polydispersity affect the prominence of clusters?
- Does species segregation occur in a *transient* cluster?

System: Simple Shear Flow

Approach: MD simulations
MD Simulations

Simulation Description

- 2D, event-driven
- Inelastic, frictionless, hard disks
- Size distributions: binary, Gaussian, lognormal

Concentration mapping

Resulting Quantities: \( \nu_{clus} \), \( \nu_{dil} \), \( T_{clus} \), \( T_{dil} \), \( \nu_{L,clus} \), \( \nu_{L,dil} \), \( T_{L,clus} \), \( T_{L,dil} \)

\( \nu_{avg} = 0.2 \)

Cluster Region: \( \nu > \nu_{avg} \)
Dilute Region: \( \nu > \nu_{avg} \)
Results: Cluster Prominence

Cluster prominence greater for systems with more than one species

Tendency increases with deviation from monodisperse limit

Increased Prominence
Greater Conc. Difference

Lesser Conc. Difference
Decreased Prominence
Results: Cluster Prominence

Cluster prominence greater for systems with more than one species

Tendency increases with deviation from monodisperse limit

Results: Species Segregation

Large Particles segregate preferentially toward the clustered regions.

Tendency increases with increasing size disparity.
Results: Species Segregation

Large Particles segregate preferentially toward the clustered regions. Tendency increases with increasing size disparity.

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Modeling of Gas-solid Flows

Continuum (“Two-fluid”) Description

- Gas phase: Navier-Stokes + turbulence + drag force
- Solids phase: Kinetic-theory-based models + fluid-phase interactions

Current Objective: Incorporation of gas-phase (drag) effects into kinetic-theory-based models for solid phase
Physical Picture

Recall fluid-solid interaction force (drag force)

\[
F_{\text{fluid}} = F_n + F_t = \int_0^{2\pi} \int_0^{2\pi} \left( -p \bigg|_{r=R} \right) R^2 \sin \theta \, d\theta \, d\phi \\
+ \int_0^{2\pi} \int_0^{2\pi} \left( \tau_{r\theta} \bigg|_{r=R} \right) R^2 \sin \theta \, d\theta \, d\phi
\]

Mean fluid force on single particle

\[
F_{\text{fluid}} = f \left( U_g - U \right)
\]

Velocity & pressure fields (& thus fluid force) change with:

- Fluctuations in particle velocity
- Fluctuations in gas velocity

Mean vs. Instantaneous Fluid Force
Incorporation of Instantaneous Fluid Force

**Alternative 1:** DEM (solids) / DNS (fluid) – resolve flow field around particles

+ fluid force is “output”
- too computationally expensive
  (no-slip BC at each moving particle surface)

**Alternative 2:** Two-fluid model – “averaged” flow field over several particles

+ computationally feasible (single equation of motion for each phase)
- fluid effects are “input” – model is needed to subsume *instantaneous* effects

Q1: Impact on governing equations (additional terms)?
Q2: Impact on constitutive relations for solid phase \((P, q, \zeta)\)?

**Current Approach**

(i) use DEM/DNS simulations to develop model for instantaneous force
(ii) incorporate this force model into starting kinetic equation & derive hydrodynamic description
Basic Idea: Incorporation of fluid force into Enskog kinetic equation

\[
\frac{\partial}{\partial t} f + \nu_i \frac{\partial f}{\partial x_i} + \frac{\partial}{\partial v_i} \left( \frac{F_{\text{fluid},i}}{m} \right) + g_i \frac{\partial}{\partial v_i} f = J
\]

instantaneous fluid force on single particle

DEM/DNS technique for closure: IBM (Immersed Boundary Method) based model of \(F_{\text{fluid},i}\) as function of:

- Hydrodynamic variables: \(\phi, U_i, T, U_{gi}\)
- Physical parameters: \(m, d, \alpha, \mu_g, \rho_g\)
Use IBM simulations to find $\beta^*$, $\gamma_{ij}^*$, and $B_{ij}^*$ as functions of

- $\phi$ solids volume fraction
- $\rho_s/\rho_f$ density ratio
- $Re_m = \frac{(1 - \phi) \rho_d d |U - U_g|}{\mu_g}$ particle $Re$ based on mean flow
- $Re_T = \frac{\rho_g d}{\mu_g} \sqrt{\frac{T}{m}}$ particle $Re$ based on particle velocity fluctuations
Resulting Hydrodynamic Description

Balance Equations (Solid-Phase Momentum & Granular Energy)

\[
D_t U + \frac{1}{mn} \nabla P = -\frac{\beta_{IBM}}{m} \left( U - U_g \right) + g
\]

(mean drag)

\[
D_t T + \frac{2}{3n} \left( \nabla \cdot q + P_{ij} \nabla_j U_i \right) = -\zeta T \left( 2 \frac{\gamma_{ij} P_{ij}^k}{3\rho} + \frac{\rho}{3n} B_{ij} B_{ij} \right)
\]

(sink due to viscous drag
source due to fluid-particle fluctuations)

Explicit Constitutive relations obtained for \( \zeta, P, \) and \( q \):

- Cooling rate \( \zeta^{(0)} = \zeta^{(0)} \left( B_{ij} \right) \)
- Cooling rate TC \( \zeta_U = \zeta_U \left( \gamma_{ij}, B_{ij} \right) \)
- Shear viscosity \( \eta = \eta \left( \gamma_{ij}, B_{ij} \right) \)
- Bulk viscosity \( \lambda = \lambda \left( B_{ij} \right) \)
- Conductivity \( \kappa = \kappa \left( \gamma_{ij}, B_{ij} \right) \)
- Dufour coefficient \( \mu = \mu \left( \gamma_{ij}, B_{ij} \right) \)
Base Case: Massive Particles ($St >> 1$) and Stokes flow ($Re_m << 1$)

Typical Ranges in CFB (Circulating Fluidized Bed) riser

- $\phi$  $0.01 – 0.5$
- $\rho_s/\rho_f$  $800 – 250$  $\rightarrow$  high $St$
- $Re_m$  $0.1 – 50$  $\rightarrow$  low – moderate $Re$
- $Re_T$  $0.5 – 5$

Summary of Results

- **Negligible** gas-phase influence
  - Cooling rate ($\zeta(0)$, $\zeta_U$)
  - Bulk viscosity ($\lambda$)
  - Conductivity ($\kappa$)
- **Non-negligible** gas-phase influence
  - Shear viscosity ($\eta$)
  - Dufour coefficient ($\mu$)

only low $Re_m = 0.1 – 1$ considered here
Shear Viscosity

\[ \frac{\eta}{\eta_{dry}} \]

- \( \text{Re}_M = 0.1 \)
- \( \text{Re}_T = 0.5 \)
- \( \phi = 0.2 \)
- \( \frac{\rho_s}{\rho_f} = 1000 \)
Dufour Coefficient

\[ \frac{\mu}{\mu_{\text{dry}}} \]

\( \text{Re}_M = 0.1 \)
\( \text{Re}_T = 0.5 \)
\( \frac{\rho_s}{\rho_f} = 1000 \)

\( \alpha \)

\( \mu / \mu_{\text{dry}} \)

\( \phi = 0.2 \)

\( \rho_s / \rho_f \)
Summary

IBM-based model for instantaneous fluid acceleration has been incorporated into Enskog equation, and corresponding hydrodynamic description derived

• Additional source/sink in momentum and granular energy balances

• Modification of constitutive closures
  - *For limiting case of $Re_m << 1$ and $St > 1$*: non-negligible gas-phase influence on shear viscosity and Dufour coefficient

• Framework extendible to non-limiting cases once IBM coefficients are extracted (coming soon...)