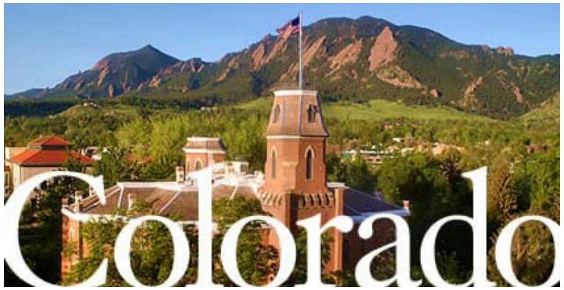
Experiments and Model Development for Polydisperse, Gas-fluidized Systems



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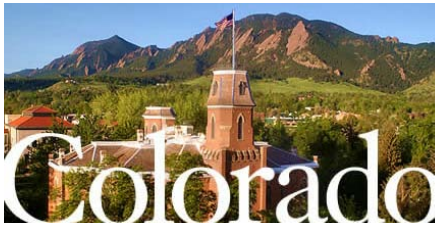
NETL 2010 Workshop on Multiphase Flow Science
4 May 2010
Pittsburgh, PA

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



Iowa State

PRINCETON UNIVERSITY

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NATIONAL ENERGY TECHNOLOGY LABORATORY

Particulate Solid Research Inc.

Univ. Colorado Tasks for Year 3

Validation data

1) **Bubbling-bed experiments (Colorado)**

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   Ray Cocco (PSRI) – Thursday

Theory

4) **Application of polydisperse kinetic theory to clustering (Princeton & NETL & Colorado)**

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5) **Kinetic Theory Extension to Gas-Solid Flows (Colorado & Iowa State)**

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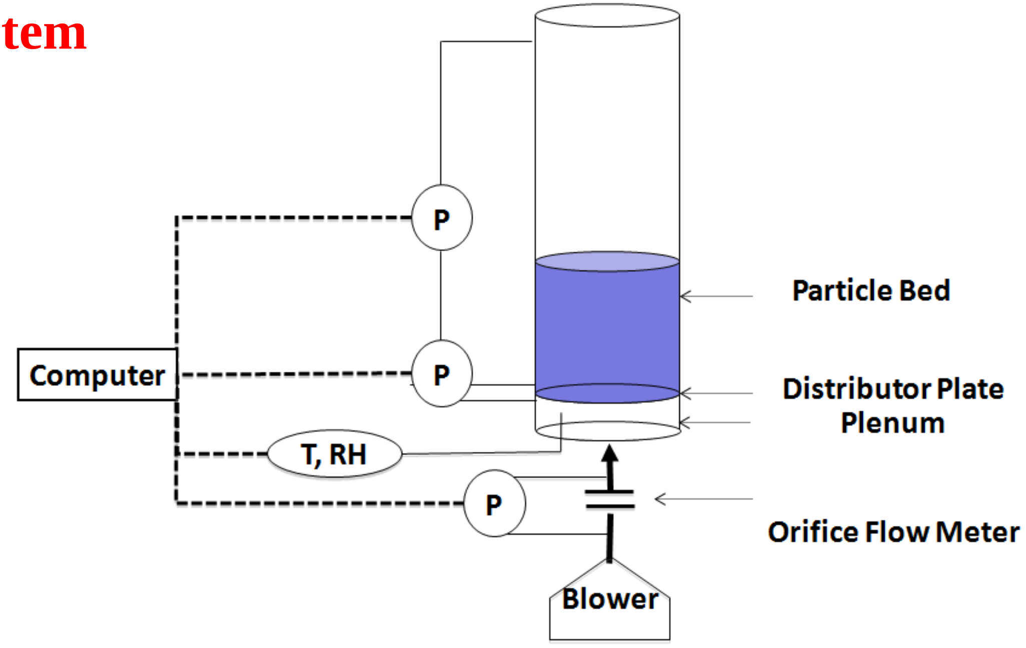
Overview: Bubbling Bed Experiments

Objective

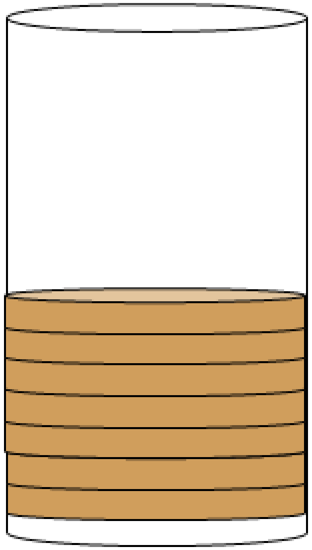
To characterize segregation and bubbling behavior of bubbling beds with continuous size distributions

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

System

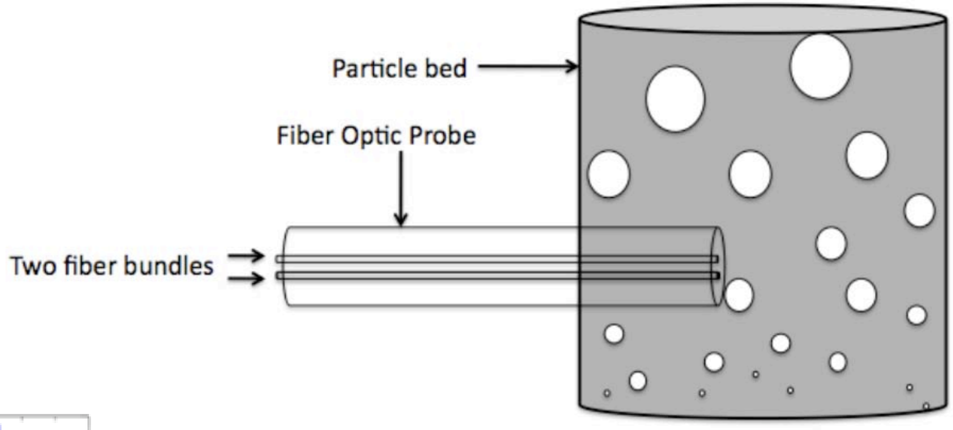


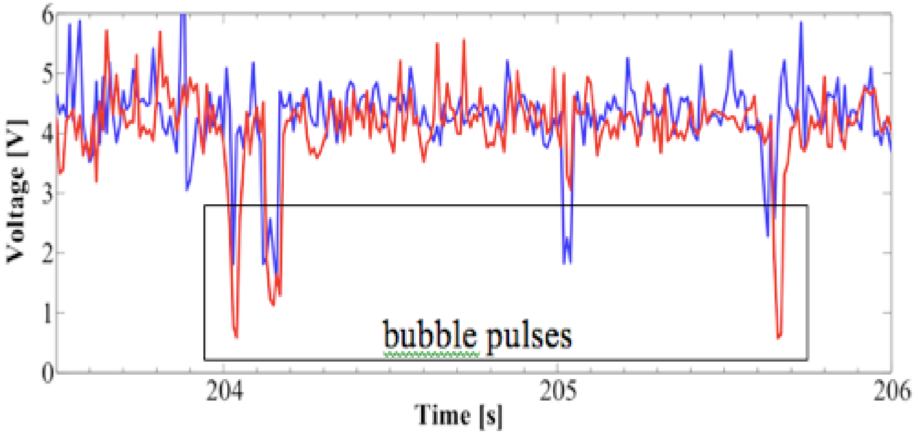
Measurements: Segregation and Bubbling



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



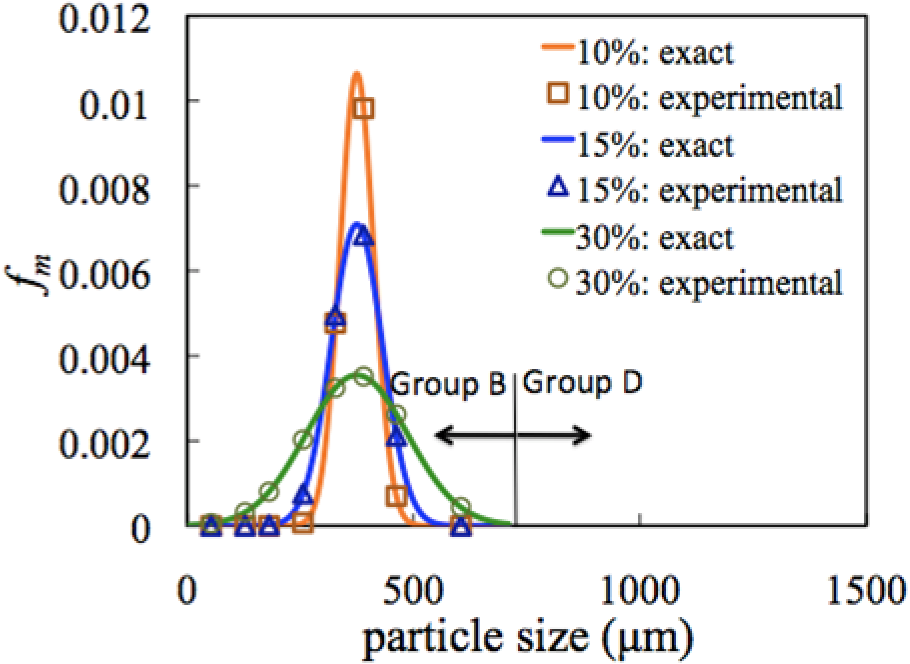


Bubbling: fiber optic probe

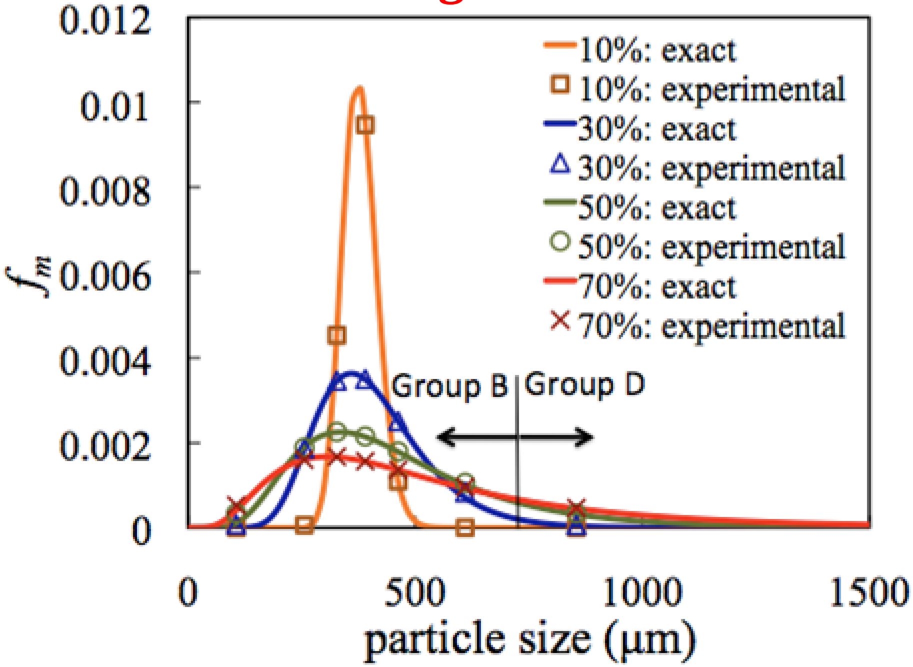
1. 7 axial x 9 radial positions
2. Bubble frequency, velocity & size

Continuous PSD’s Investigated

Gaussian



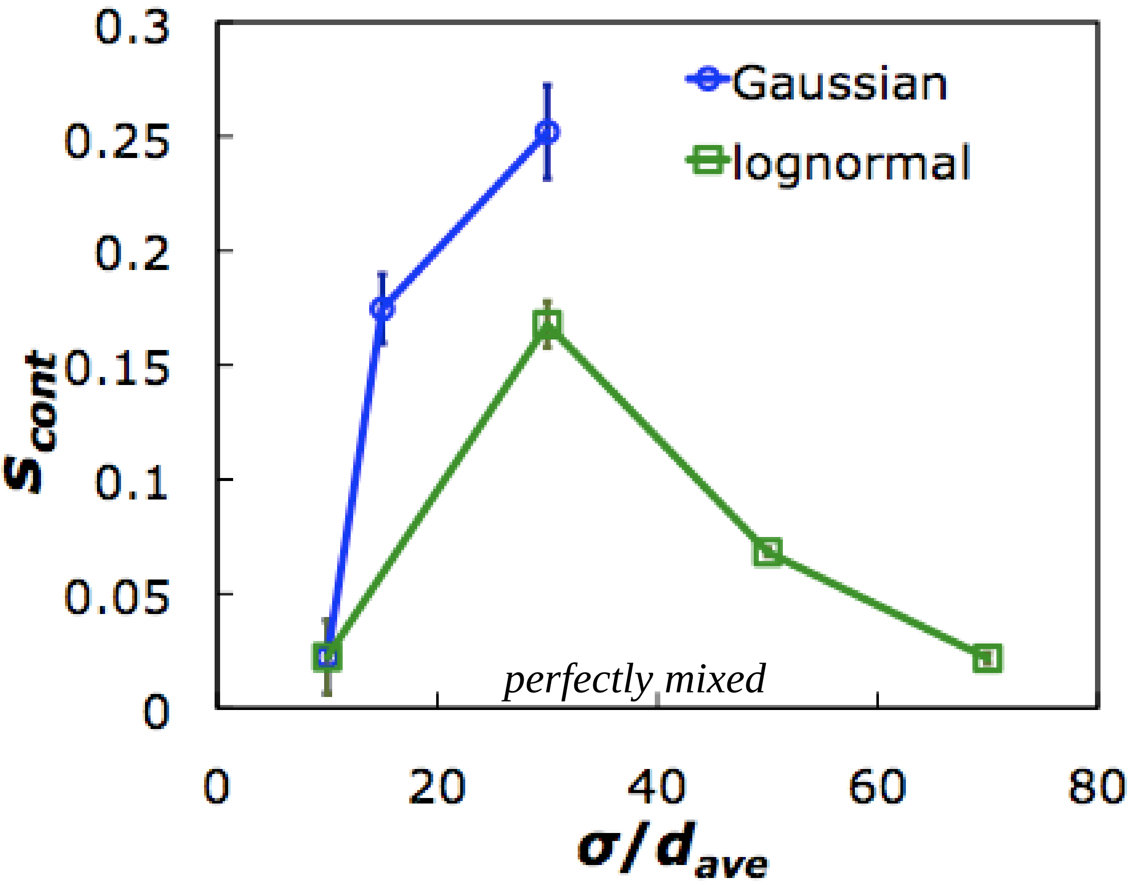
lognormal



Width of distribution: $\boldsymbol{\sigma}/\mathbf{d}_{\mathbf{ave}}$ (%)

Material: sand

Results: Segregation



$$s_{cont} = \frac{S-1}{S_{\max}-1}$$

$$S = \frac{<h_{small}>}{<h_{large}>} \qquad S_{\max} = \frac{2x_{large}+x_{small}}{x_{large}}$$

$s_{cont} = 0$ ➔ perfect mixing

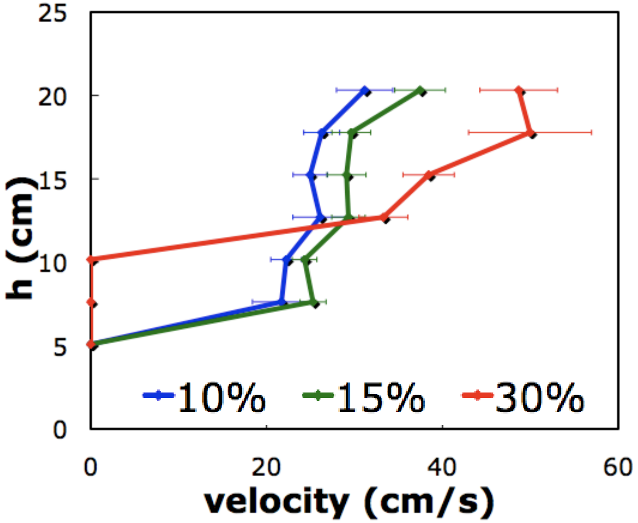
$s_{cont} = 1$ ➔ perfect segregation

Gaussian: as PSD width increases ↑, segregation ↑

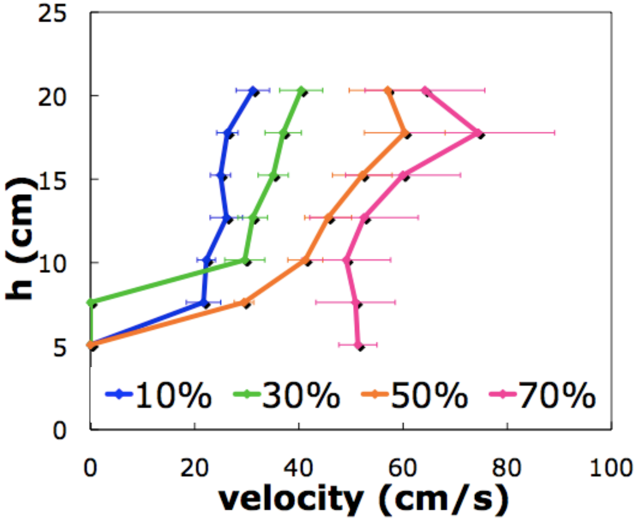
lognormal: *non-monotonic* variation of segregation with PSD width

Chew, Wolz & Hrenya, *AIChE J* (in press)

Results: Bubbling



Gaussian



lognormal

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

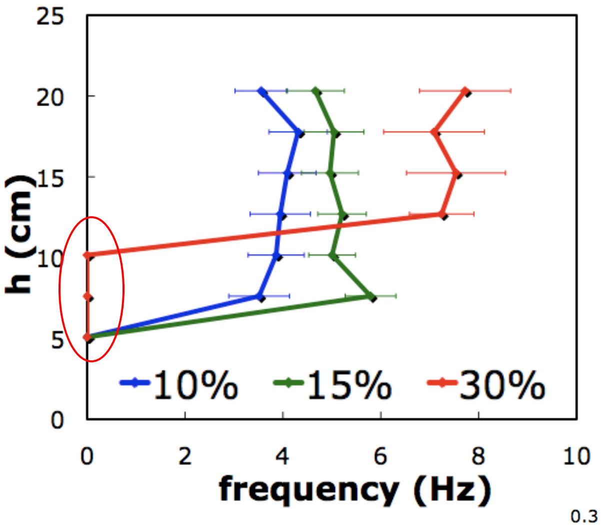
Chew & Hrenya, *I&ECR* (submitted)

Reconciliation: Segregation and Bubbling Measurements

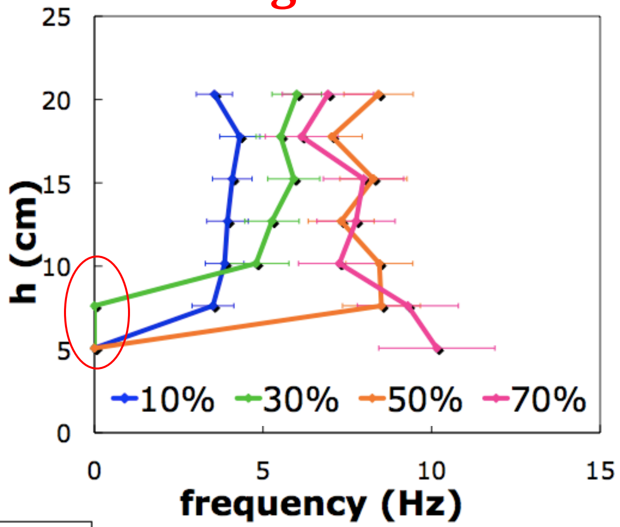
Explanation

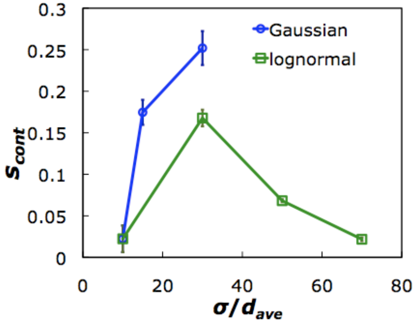
- presence of *bubble-less layer* in some systems
- size of bubble-less layer correlates with degree of segregation

Gaussian



lognormal





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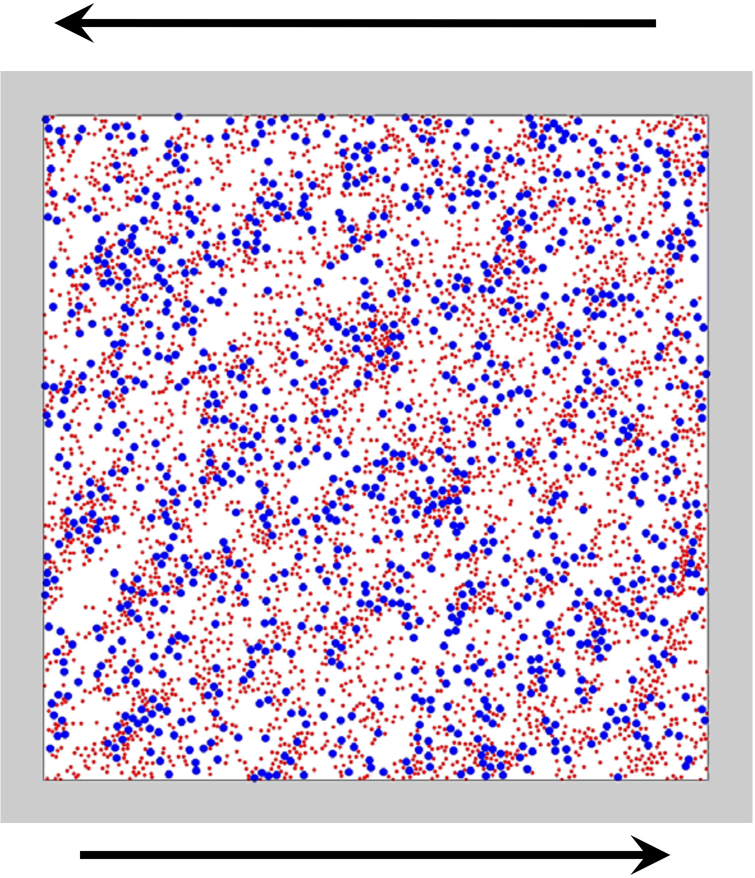
Objective

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

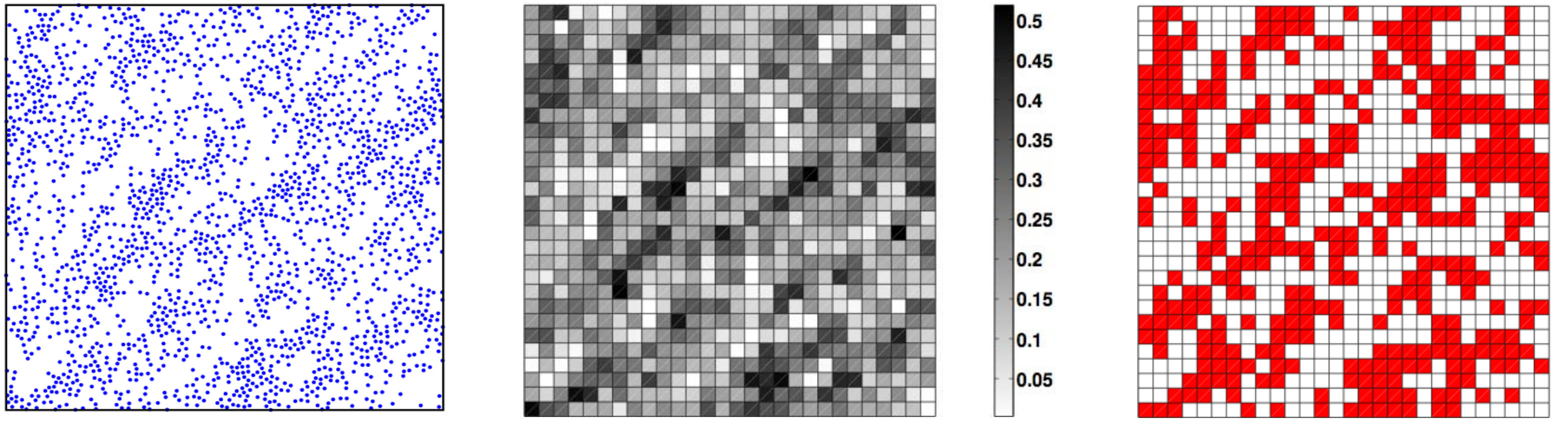


MD Simulations

Simulation Description

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

Concentration mapping



$\nu_{avg} = 0.2$

Cluster Region: $\nu > \nu_{avg}$

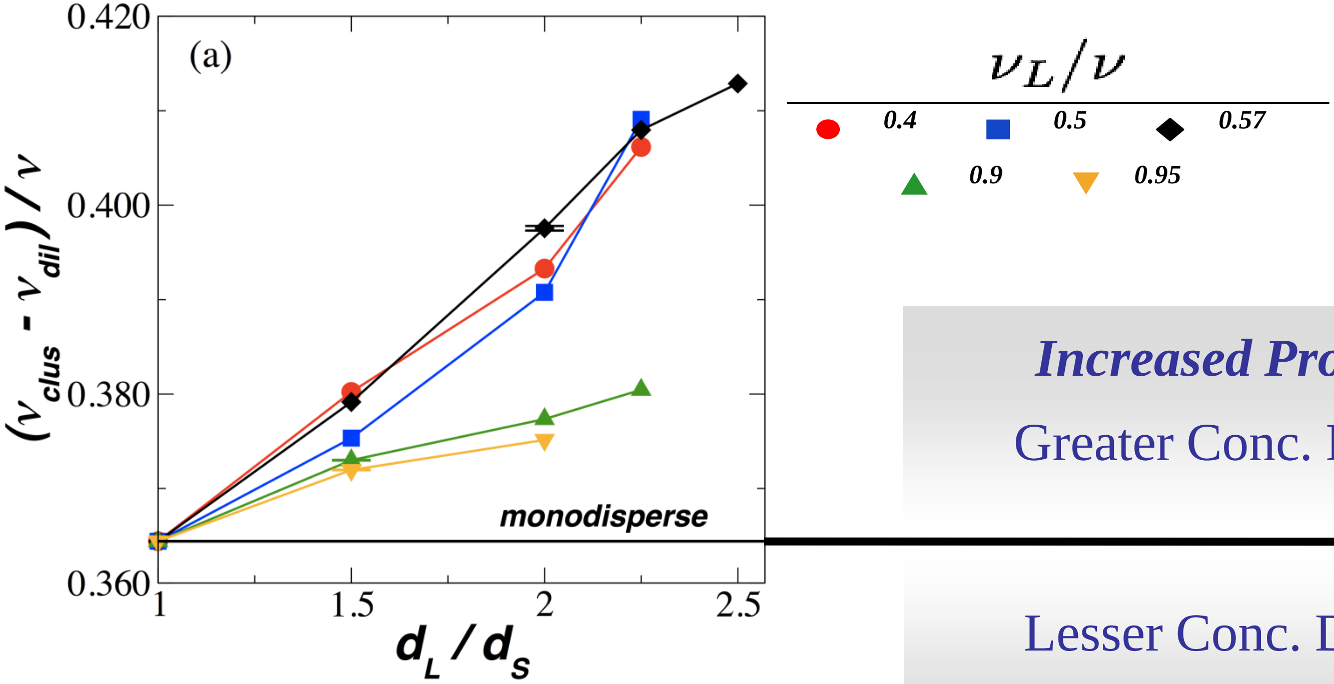
Dilute Region: $\nu > \nu_{avg}$

Resulting Quantities: ν_{clus} ν_{dil} T_{clus} T_{dil}

$\nu_{L,clus}$ $\nu_{L,dil}$ $T_{L,clus}$ $T_{L,dil}$

Results: Cluster Prominence

binary



Increased Prominence

Greater Conc. Difference

Lesser Conc. Difference

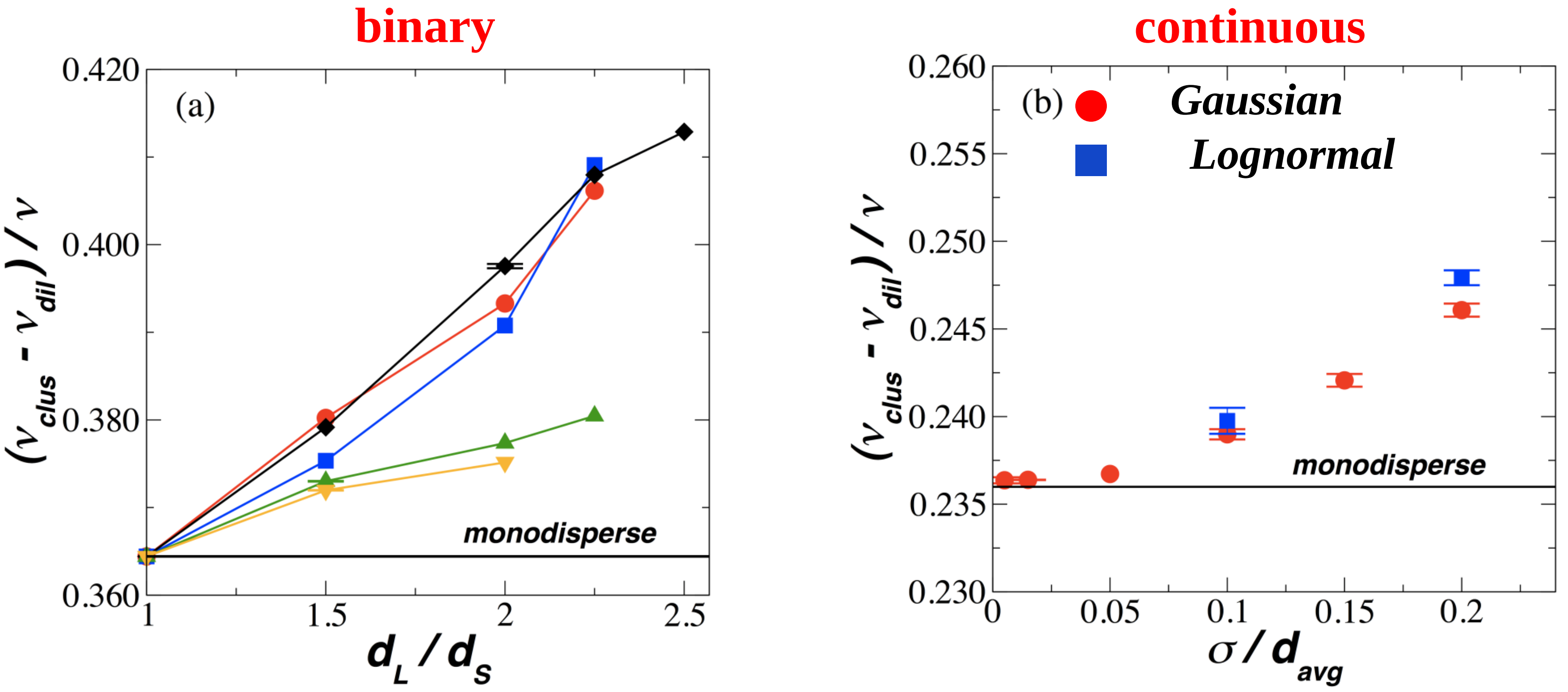
Decreased Prominence

Cluster prominence greater for systems with more than one species

→

Tendency increases with deviation from monodisperse limit

Results: Cluster Prominence



Cluster prominence greater for systems with more than one species

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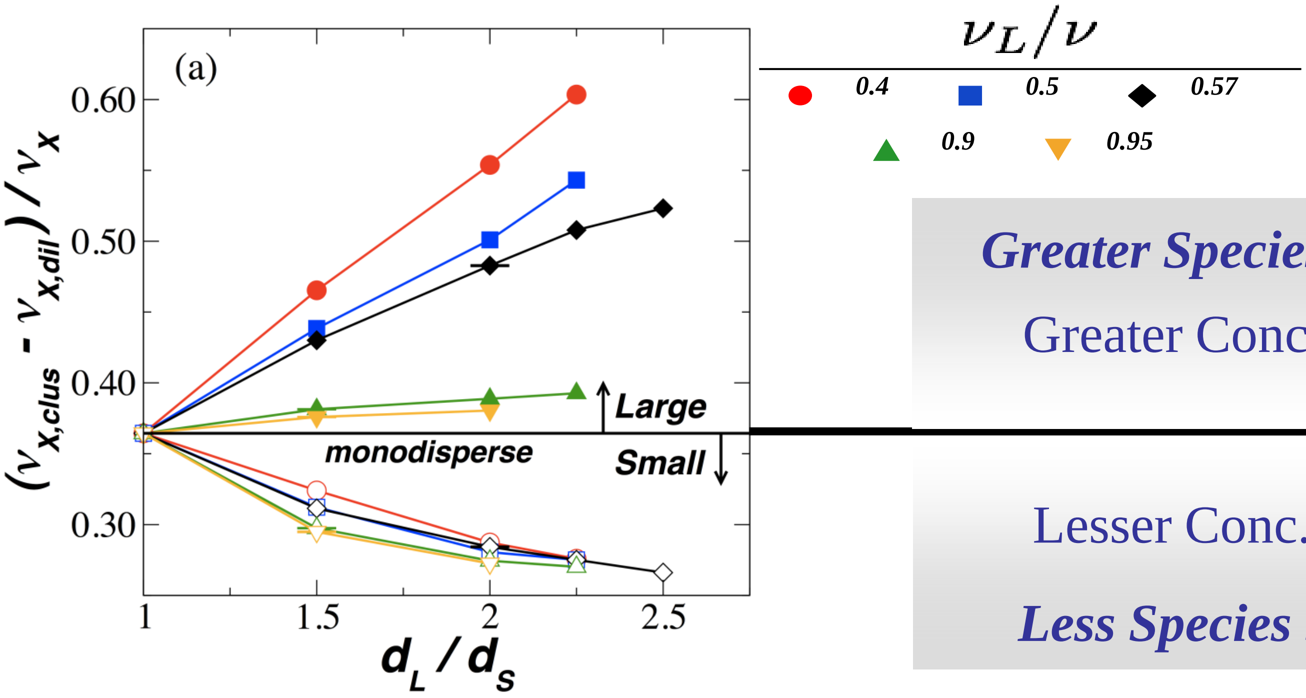
Tendency increases with deviation from monodisperse limit

Rice & Hrenya *Phys. Rev. E* (2010)

Results: Species Segregation

binary



Greater Species Segregation

Greater Conc. Difference

Lesser Conc. Difference

Less Species Segregation

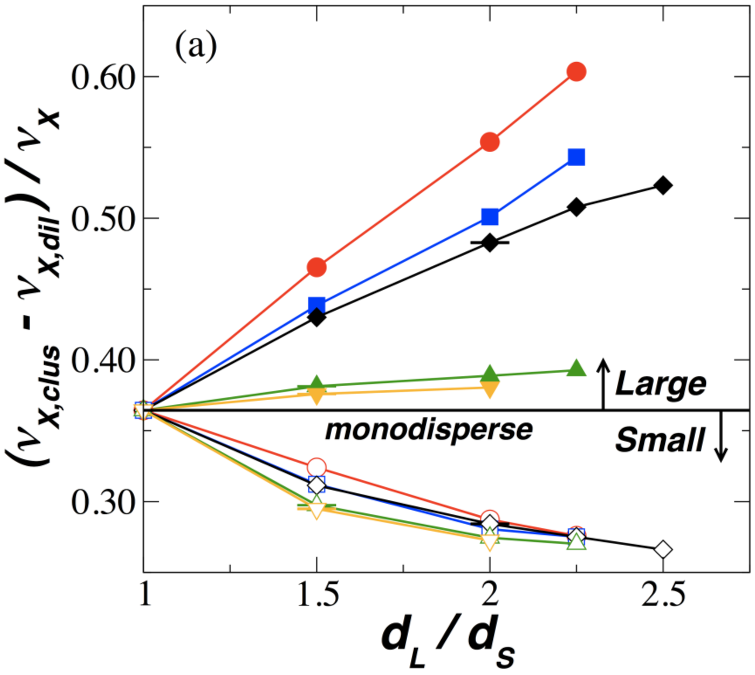
Large Particles **segregate preferentially toward the *clustered regions***

Tendency increases with increasing size disparity

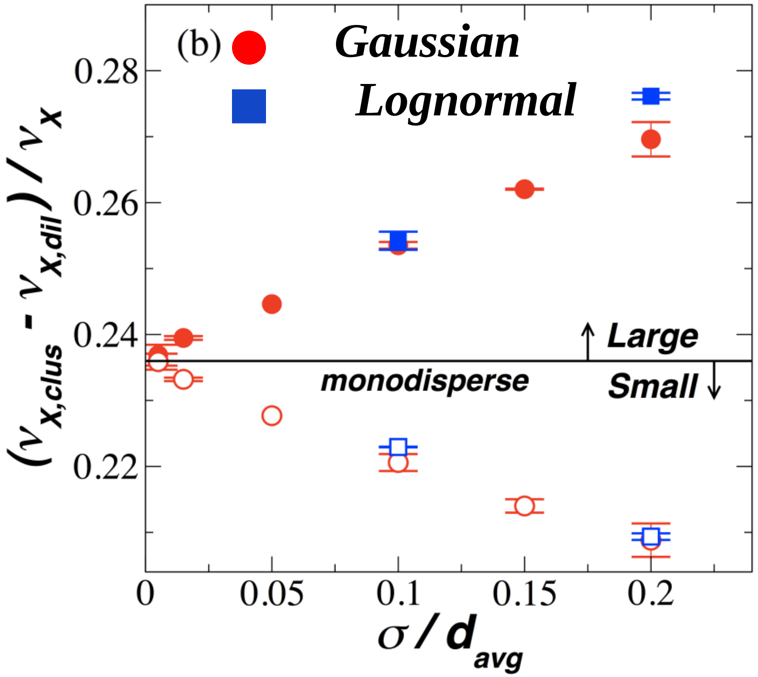
Rice & Hrenya *Phys. Rev. E* (2010)

Results: Species Segregation

binary



continuous



Large Particles segregate preferentially toward the *clustered regions*

Tendency increases with increasing size disparity

Rice & Hrenya *Phys. Rev. E* (2010)

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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

modifications to
kinetic-theory closures

new terms

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)

$$F_{fluid} = F_n + F_t = \int_0^{2\pi}\int_0^{\pi} \left(\boxed{-p\big|_{r=R}}\ \cos\theta\right) R^2 \sin\theta\ d\theta d\phi + \int_0^{2\pi}\int_0^{\pi} \left(\boxed{\tau_{r\theta}\big|_{r=R}}\ \sin\theta\right) R^2 \sin\theta\ d\theta d\phi$$

= *f* (velocity & pressure at surface)

***Mean* fluid force on *single* particle**

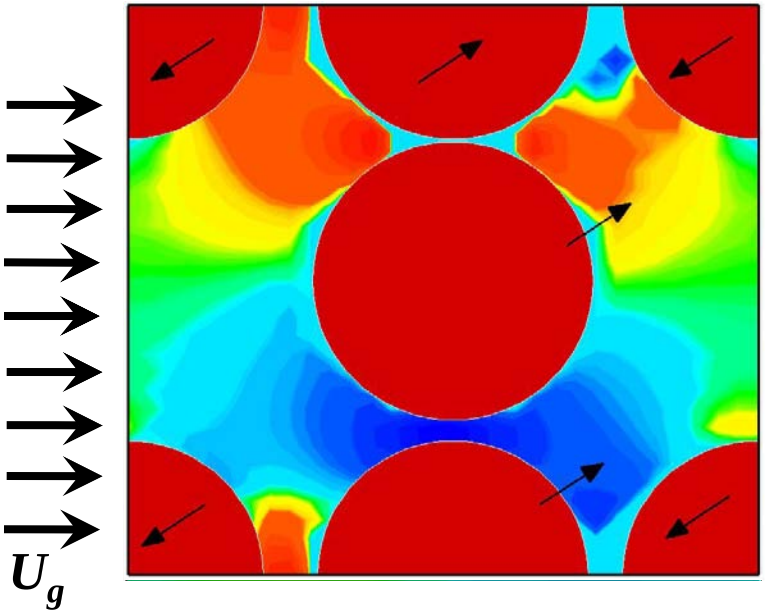
$$F_{fluid} = f\left(U_g - U\right)$$

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

- Fluctuations in particle velocity
- Fluctuations in gas velocity

➡ ***Mean* vs. *Instantaneous* Fluid Force**

pressure field

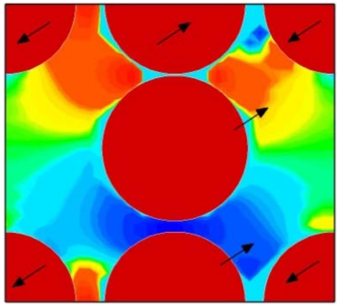


Incorporation of Instantaneous Fluid Force

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 ($\mathbf{P}$, $\mathbf{q}$, ζ)?

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

More details…

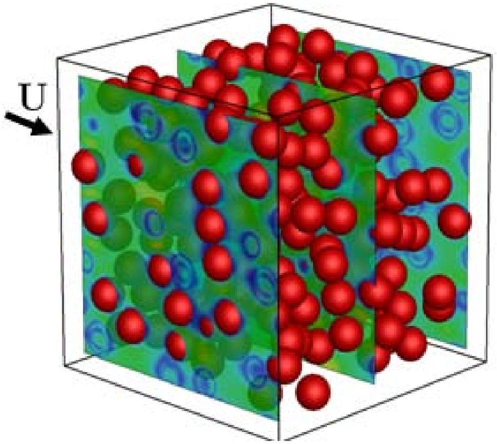
Basic Idea: Incorporation of fluid force into Enskog kinetic equation

$$\overset{\textit{transient}}{\frac{\partial}{\partial t} f} + \overset{\textit{convective}}{v_i \frac{\partial f}{\partial x_i}} + \boxed{\frac{\partial}{\partial v_i}\left(\frac{F_{fluid,i}}{m}\right)} + \overset{\textit{gravity}}{g_i \frac{\partial}{\partial v_i} f} = \overset{\textit{collisions}}{J}$$

instantaneous *fluid force*
on single particle

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

- Hydrodynamic variables: ϕ, U_i, T, U_{gi}
- Physical parameters: m, d, α, μ_g , ρ_g



IBM-based model for acceleration

coefficients extracted from IBM simulations

$$\frac{F_{fluid,i}}{m} = A_i = -\frac{\beta_{IBM}}{m}\left(U_i - U_{gi}\right) - \frac{1}{m}\gamma_{ij}V_j - B_{ij}dW_j$$

instantaneous particle acceleration

mean particle velocity

mean gas velocity

fluctuating particle velocity

Wiener process increment (stochastic model for fluctuating fluid velocity)

Use IBM simulations to find β^*, γ_{ij}^*, and B_{ij}^* as functions of

• ϕ	solids volume fraction
• ρ_s/ρ_f	density ratio
• $Re_m = \frac{(1-\phi)\rho_g d \left\lvert \mathbf{U} - \mathbf{U_g} \right\rvert}{\mu_g}$	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)

$$D_t \mathbf{U} + \frac{1}{mn}\nabla \mathbf{P} = \underbrace{\boxed{-\frac{\beta_{IBM}}{m}\left(\mathbf{U}-\mathbf{U}_g\right)}}_{\textit{mean drag}} + \mathbf{g}$$

$$D_t T + \frac{2}{3n}\left(\nabla\cdot\mathbf{q} + P_{ij}\nabla_j U_i\right) = -\zeta T \underbrace{\boxed{-\frac{2}{3\rho}\gamma_{ij}P_{ij}^{\;k}}}_{\substack{\textit{sink due to}\\ \textit{viscous drag}}} \underbrace{\boxed{+\frac{\rho}{3n}B_{ij}B_{ij}}}_{\substack{\textit{source due to}\\ \textit{fluid-particle}\\ \textit{fluctuations}}}$$

Explicit Constitutive relations obtained for ζ, 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)

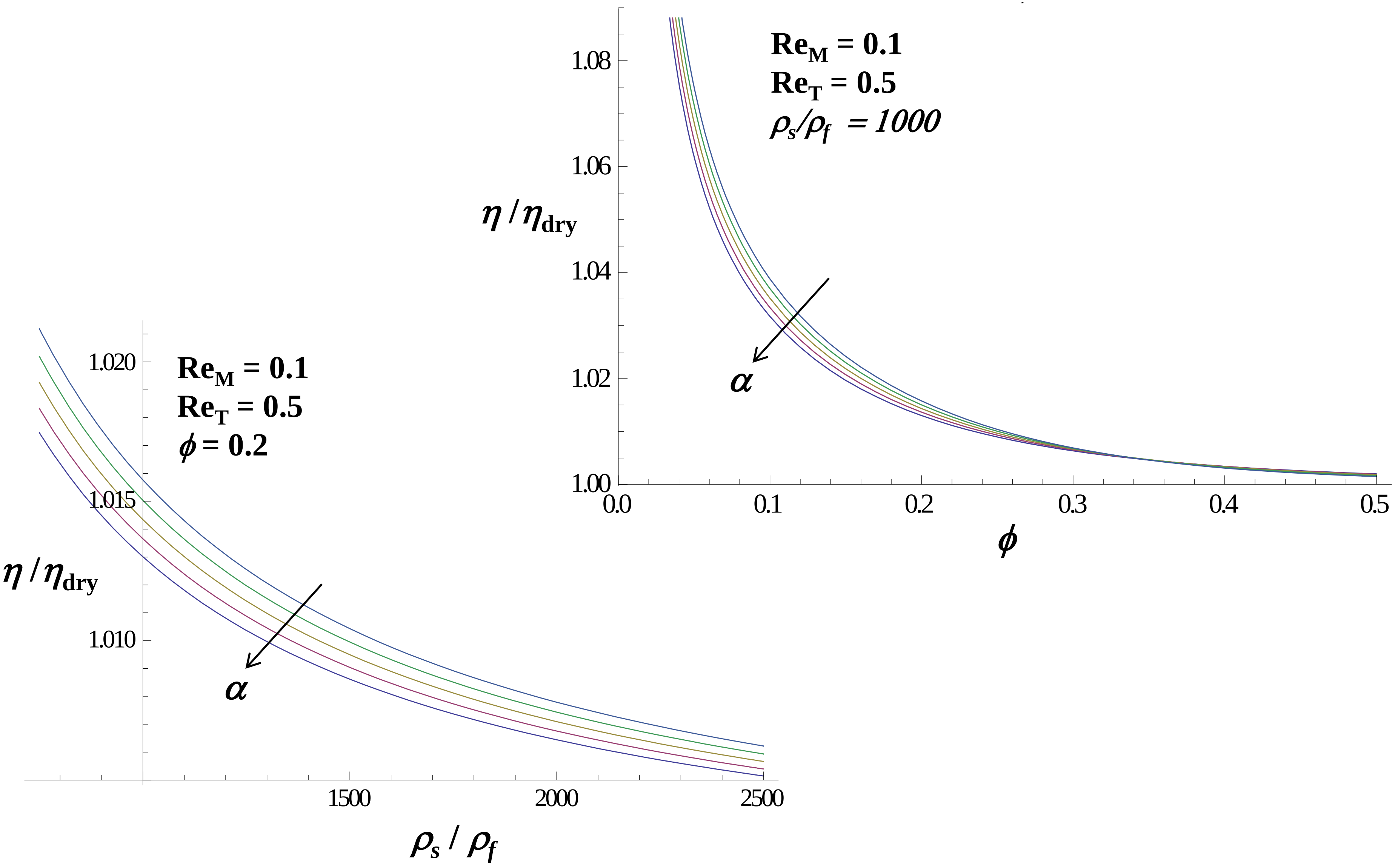
Typical Ranges in CFB (Circulating Fluidized Bed) riser

- ϕ 0.01 – 0.5
- ρ_s/ρ_f 800 – 250 ⟶ *high St*
- Re_m 0.1 – 50 ⟶ *low – moderate Re* ➡ *only low* Re_m *= 0.1 – 1 considered here*
- Re_T 0.5 – 5

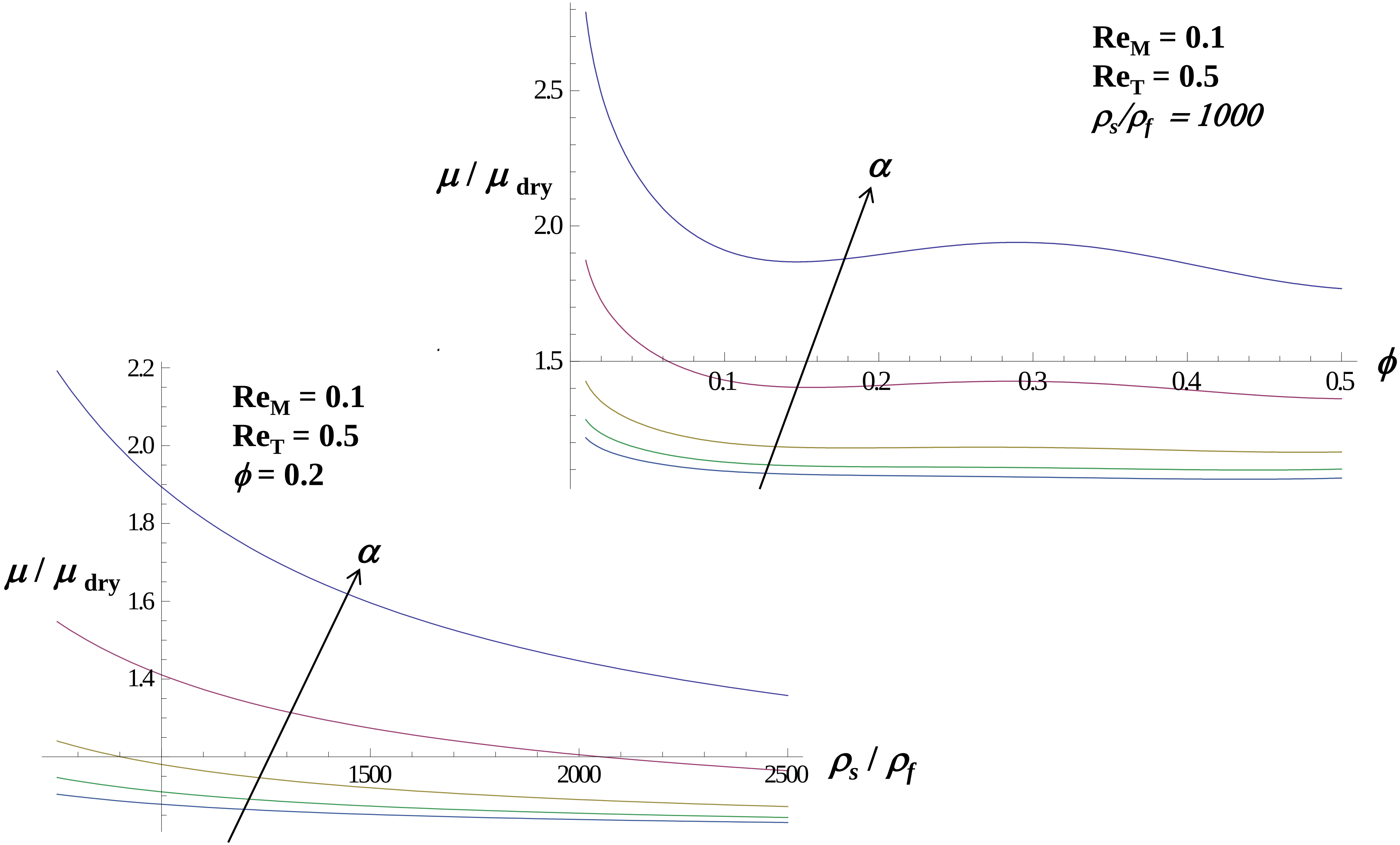
Summary of Results

- *Negligible* gas-phase influence
  - Cooling rate ($\zeta_{(0)}$, ζ_U)
  - Bulk viscosity (λ)
  - Conductivity (κ)
- *Non-negligible* gas-phase influence
  - Shear viscosity (η)
  - Dufour coefficient (μ)

Shear Viscosity



Dufour Coefficient



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…)