DOE Annual Review Meeting: Development, Verification and Validation of Multiphase Models for Polydisperse Flows

PI: Prof. Christine Hrenya (Colorado)

co-PIs: Dr. Ray Cocco (PSRI)

Prof. Rodney Fox (Iowa State)

Prof. Shankar Subramaniam (Iowa State)

Prof. Sankaran Sundaresan (Princeton)

22 April 2009

Morgantown, WV

Project Goals & 2006 Technology Roadmap

Theme: Particle Size Distribution (PSD)

Relevant Tracks in 2006 Technology Roadmap

1. **Continuum Theory for the Solid Phase**
2. **Improved Gas-Particle Drag Laws**
3. **Gas-Phase Instabilities: Turbulence Models**

Theory and Model Development

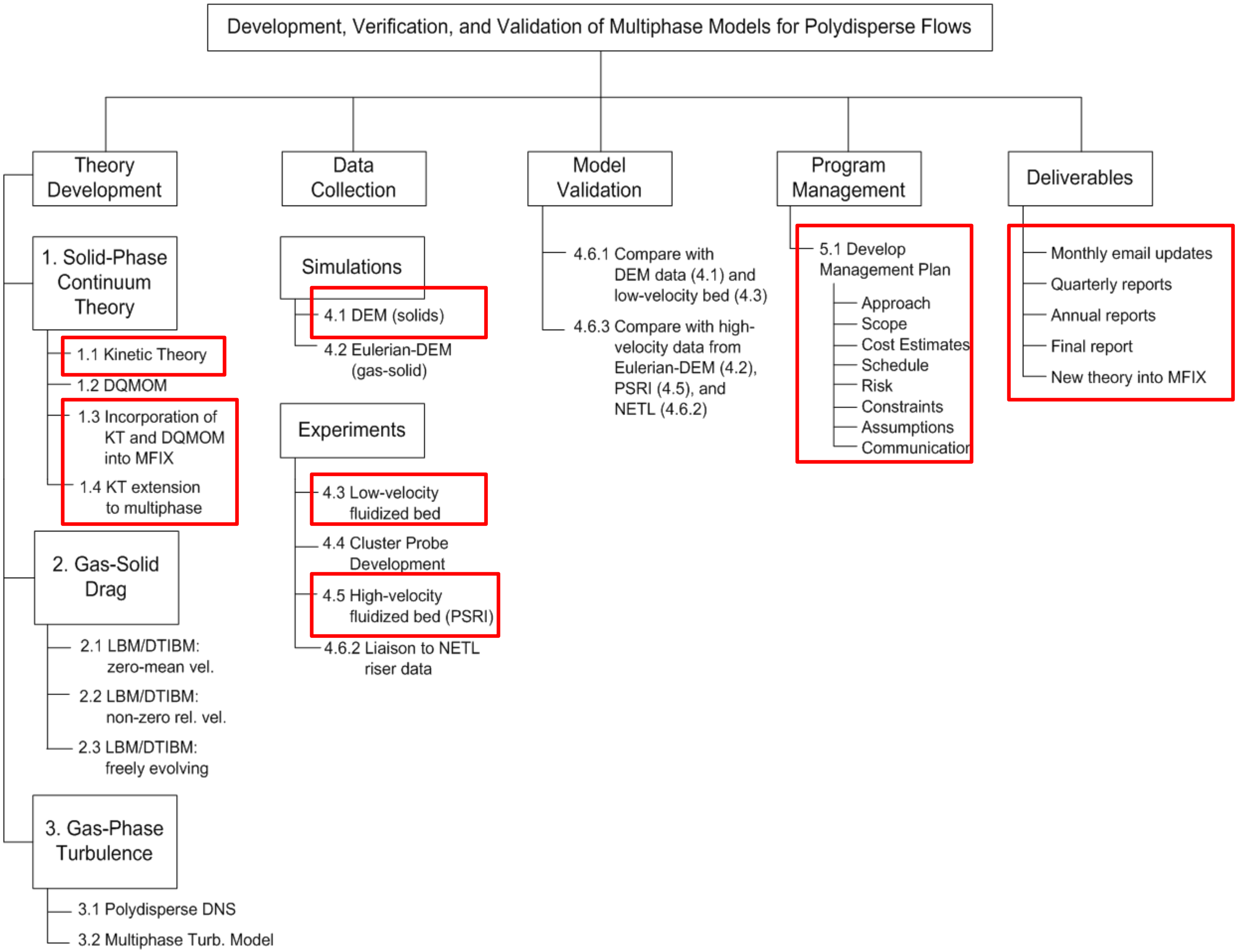
4. **Data Collection and Model Validation**

Physical and Computational Experiments

5. **Project Management**

Communication, Collaboration, and Education

Project Scope: Work Breakdown Structure



Task 1.1 Kinetic Theory

Mass Balance (s balances)

$$\frac{Dn_i}{Dt} + n_i \nabla \cdot \mathbf{U} + \frac{1}{m_i} \nabla \cdot \mathbf{j}_{0i} = 0$$

Momentum Balance (1 balance)

$$\rho \frac{D\mathbf{U}}{Dt} + \nabla \cdot \boldsymbol{\sigma} = \sum_{i=1}^{s} n_i \mathbf{F}_\mathbf{i}$$

Granular Energy Balance (1 balance)

$$\frac{3}{2} n \frac{DT}{Dt} - \frac{3}{2} T \sum_{i=1}^{s} \frac{1}{m_i} \nabla \cdot \mathbf{j}_{0i} = -\nabla \cdot \mathbf{q} + \boldsymbol{\sigma} : \nabla \mathbf{U} - \frac{3}{2} n T \zeta + \sum_{i=1}^{s} \frac{1}{m_i} \mathbf{F}_i \cdot \mathbf{j}_{0i}$$

Garzó, Dufty & Hrenya (PRE, 2007)
Garzó, Hrenya & Dufty (PRE, 2007)

Constitutive Relations

Mass flux

$$\mathbf{j}_{0i} = -\sum_{j=1}^{N} \frac{m_i m_j n_j}{\rho} D_{ij} \nabla \ln n_j - \rho D_i^T \nabla \ln T - \sum_{j=1}^{s} D_{ij}^F \mathbf{F}_j$$

Stress tensor

$$\sigma_{\alpha\beta} = p\delta_{\alpha\beta} - \eta \left(\frac{\partial U_\beta}{\partial r_\alpha} + \frac{\partial U_\alpha}{\partial r_\beta} - \frac{2}{3} \delta_{\alpha\beta} \nabla \cdot \mathbf{U} \right) - \kappa \delta_{\alpha\beta} \nabla \cdot \mathbf{U}$$

Heat flux

$$\mathbf{q} = -\sum_{i=1}^{s} \sum_{j=1}^{s} T^2 D_{q,ij} \nabla \ln n_j + L_{ij} \mathbf{F}_j - T\lambda \nabla \ln T$$

Cooling Rate

$$\zeta = \zeta^{(0)} + \zeta_U \nabla \cdot \mathbf{U}$$

Garzó, Dufty & Hrenya (PRE, 2007)
Garzó, Hrenya & Dufty (PRE, 2007)

Summary of New Theory

1) **<u>No limiting assumptions: non-equipartition & non-Maxwellian</u>**

2) **<u>Fewer hydrodynamic variables</u>**

- Current Theory: n_i, **U**, and T (s + 2 governing equations)
- Previous Theories: n_i, $\mathbf{U}_\mathrm{i}$, and T_i (3s governing equations)

but…new theory has implicit form of constitutive relations

3) **<u>No restrictions on dissipation levels</u>**

- Previous theories: expansion about e ~ 1
- Current theory: expansion about HCS

Representation of Continuous PSD

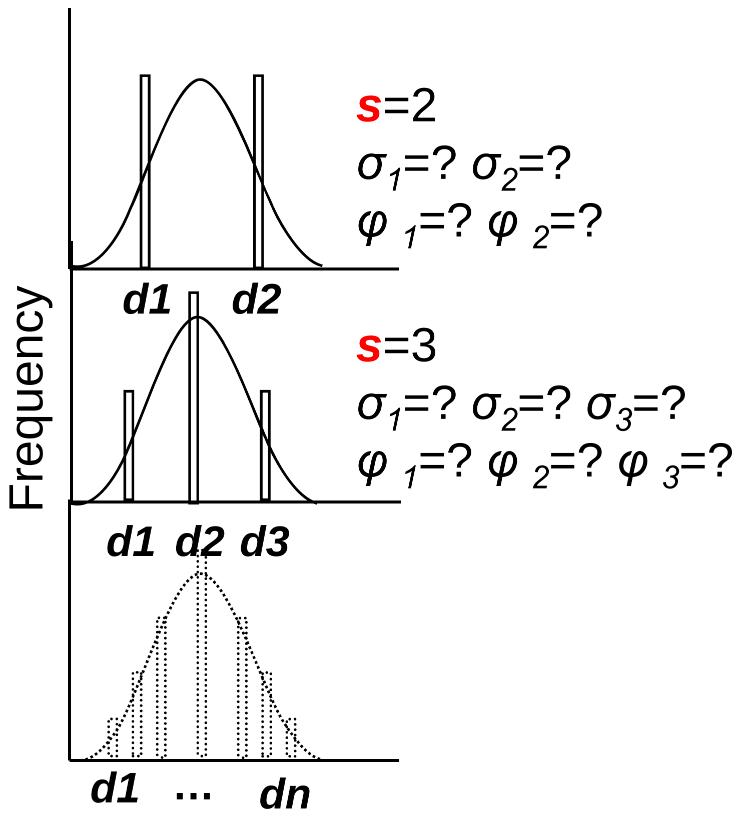
Basic Idea: **How to accurately represent a continuous PSD using the transport coefficients for '*s*' discrete species.**

Q1: What ***method*** do we choose to find σ's and φ_i's for given φ?

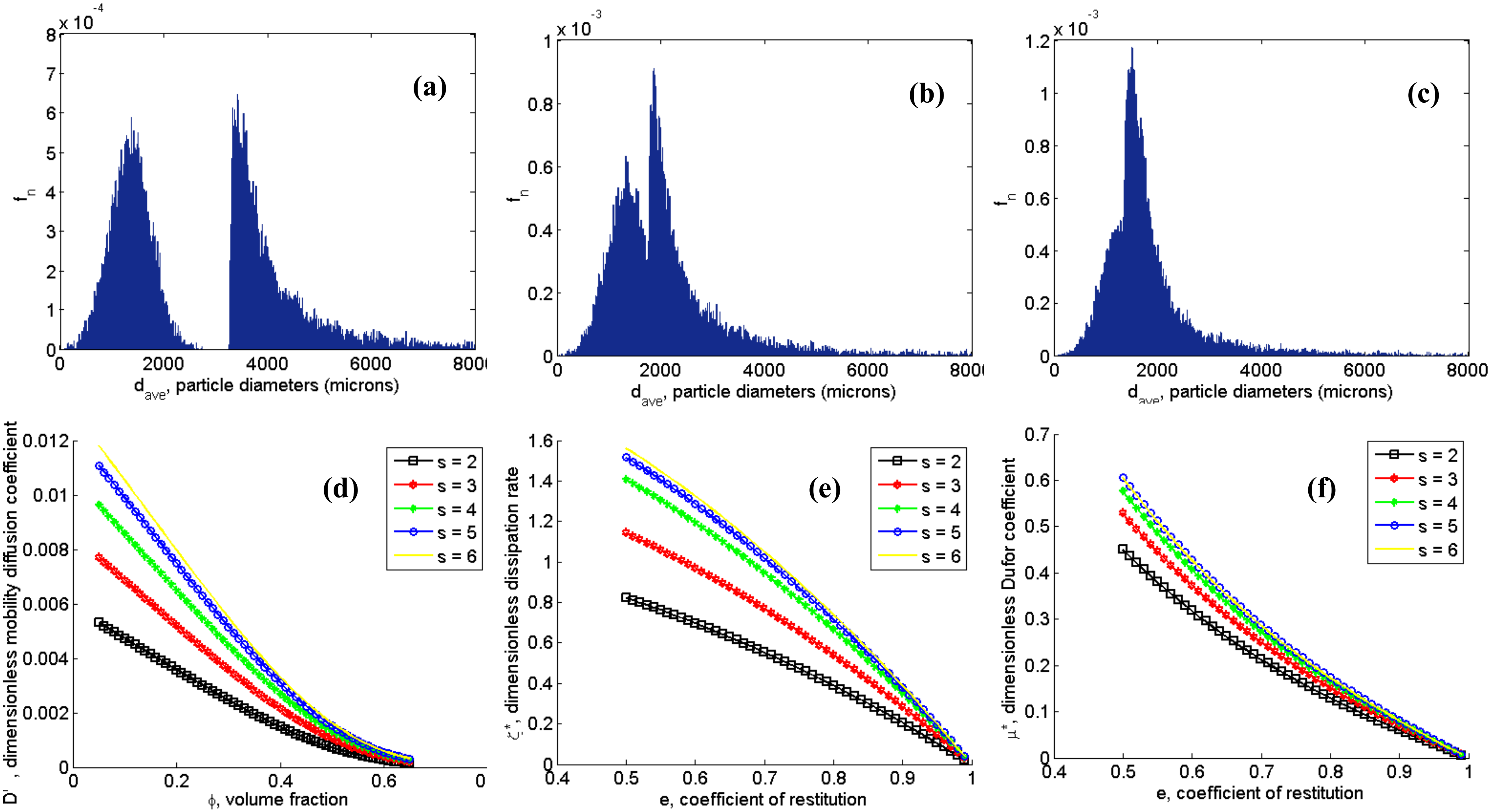
A1: moment-based method

Q2: What ***value*** of '***s***' is required for '*accurate*' representation of continuous PSD?

A2: "collapsing" of transport coefficients from new KTGF



Representation of Continuous PSD's with discrete approximations: Mixed distributions (Gaussian-lognormal)

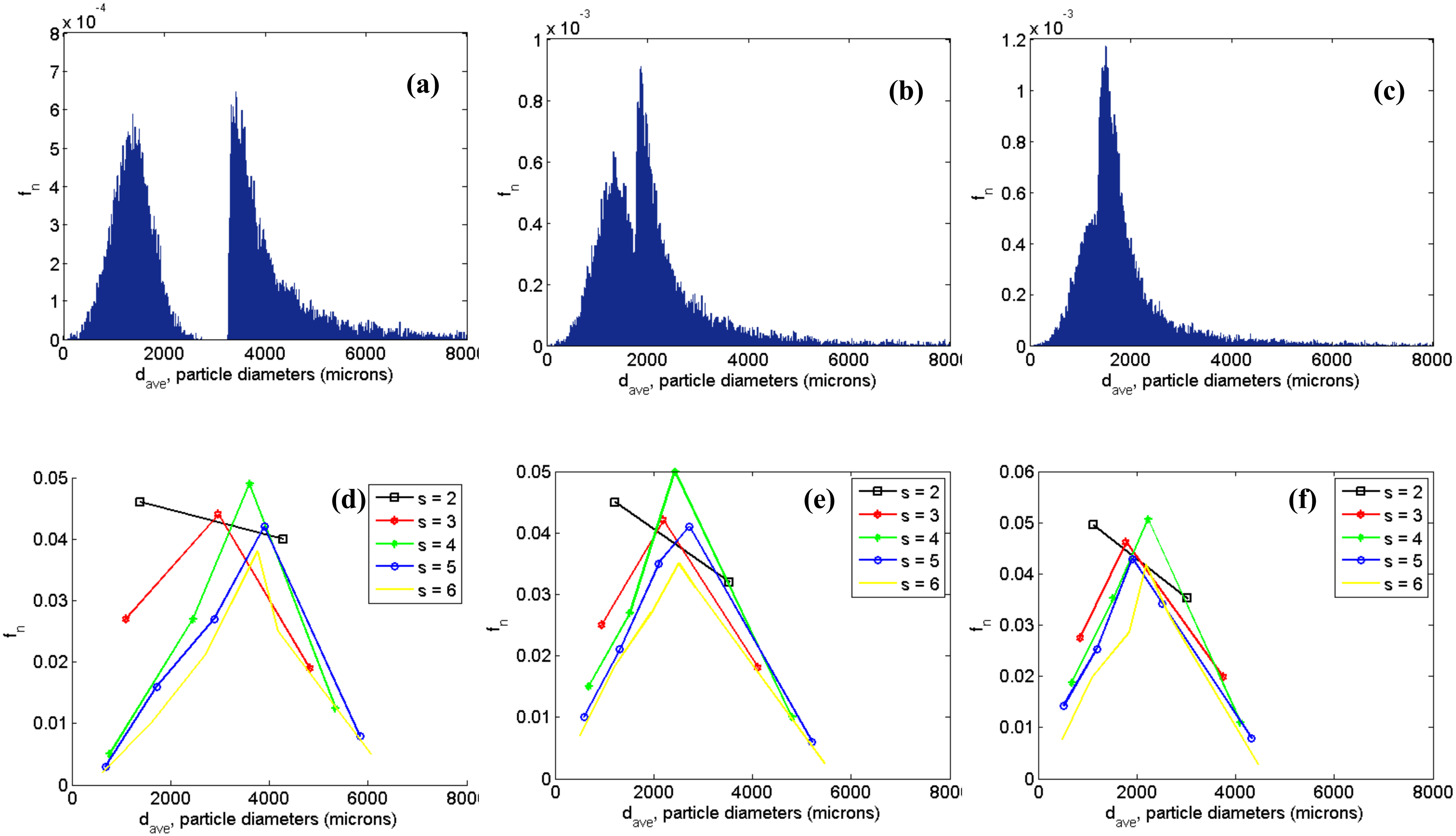


s =6 most accurate

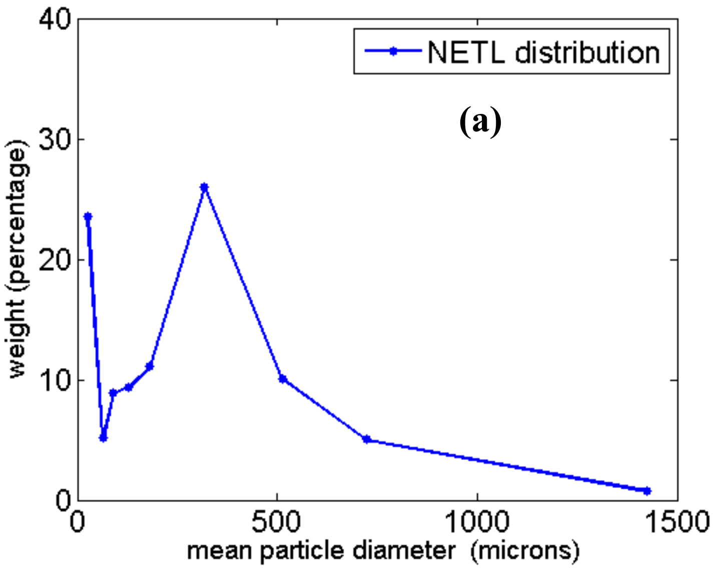
s =5 ~ *s* =6

s =5 & *s* =6 indistinguishable; *s* = 4 approaching *s*=5

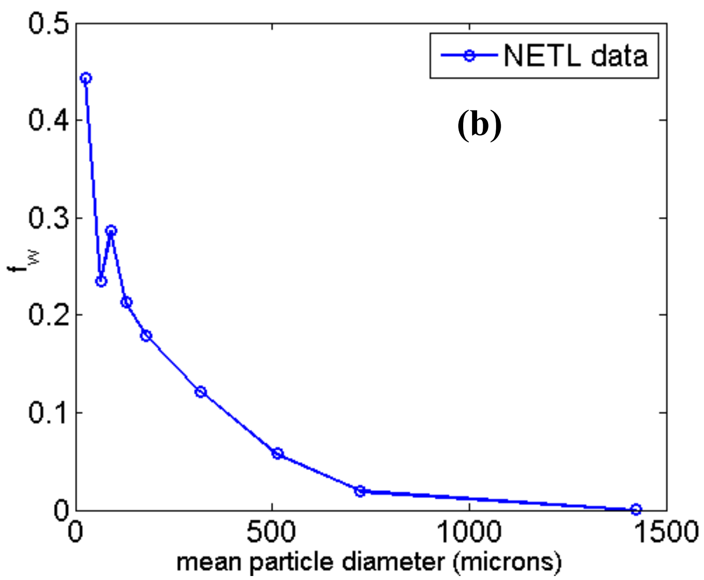
Gaussian-lognormal distributions (cont…)

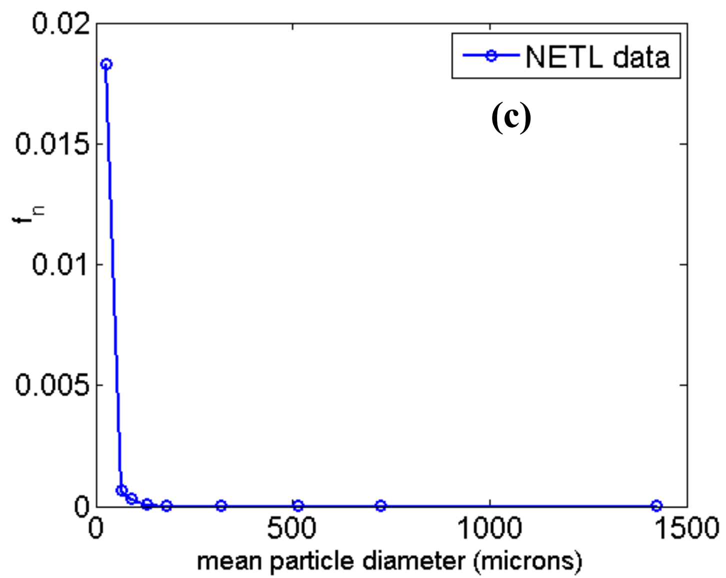


Representation of Continuous PSD's with discrete approximations: Experimental distribution (NETL)

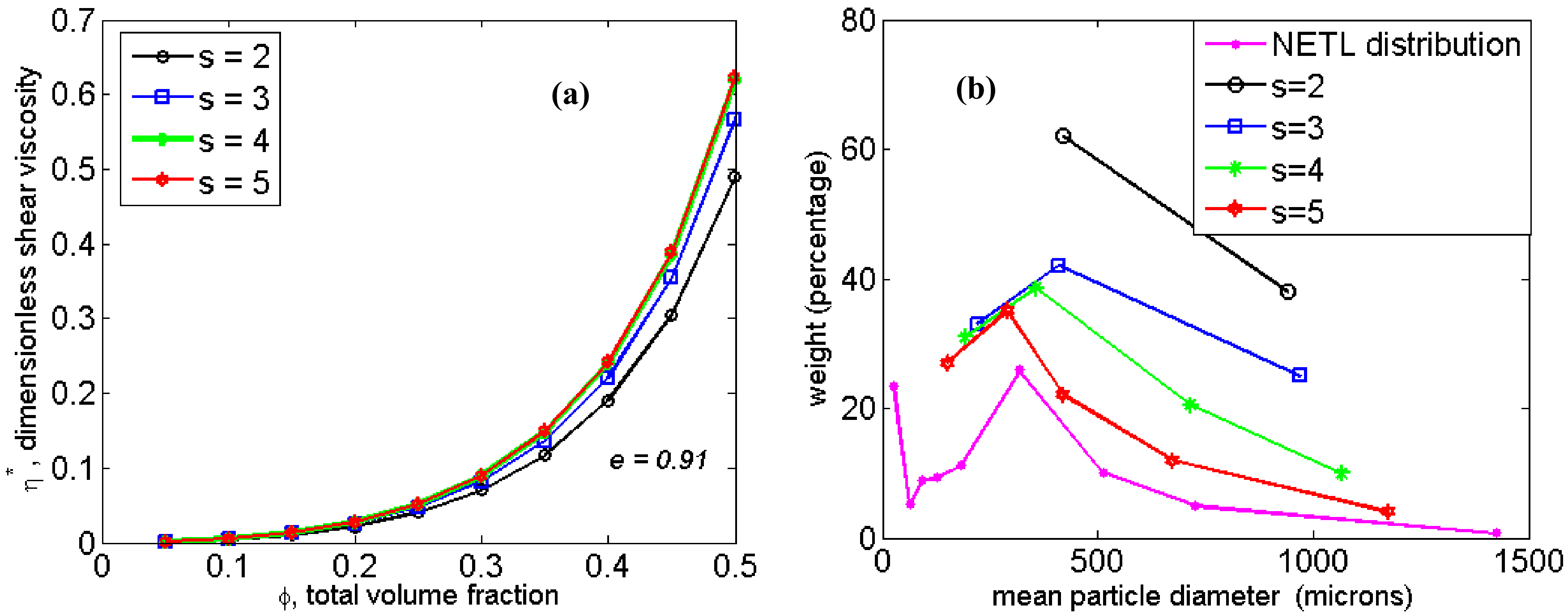


- Weight based distribution is bidisperse in nature.
- The number based frequency (f_n) is obtained using the weight based frequency distribution (f_w).
- f_n is used as the (i) basis for kinetic theory, and (ii) used for matching moments of discrete with continuous distribution.





NETL distribution (cont..)



s =4 needed for accurate representation, found to be true with all transport coefficients.

As *s* increases, the discrete approximations are close to NETL data (figure(b)).

Task 1.3: Incorporation of KTGF into MFIX

NETL Collaborators
Sofiane Benyahia
Janine Galvin

Verification of 11 transport coefficients

- Coded in Matlab
  - » System of linear & nonlinear algebraics
  - » Analytical derivatives: Mathematica
  - » Numerical derivatives
- Verification tests
  - » monodisperse limit (s=1 & 2)
  - » non-dimensionalization testing
  - » switching of indices

MFIX implementation of 11 transport coefficients

- Conversion to stand-alone Fortran subroutines for each coefficient; called as-is by MFIX (*key "finding"!*)
  - » New linear & nonlinear equation solvers added
- Independent check of hand-generated notes & Fortran code
- Verification test cases: simple shear flow & bounded conduction

Task 1.4: Extension of KTGF to Multiphase Systems

Basic Idea: Incorporation of fluid force into kinetic equation

Monodisperse:
(for illustration)

gravity *collisions*

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

instantaneous *fluid force*
on single particle

- Starting equation for KTGF & DQMOM
- Previous efforts: Koch and coworkers (e.g., *Phys. Fluids* 1990)
  - Limited to low Re (Stokes flow)
  - Uses concept of "fluid velocity at particle location"
    - » will lead to unphysical statistics like single-point fluid-particle velocity correlation

Alternative: IBM-based model of instantaneous particle acceleration

Collaborators
Rodney Fox (ISU)
Vicente Garzo (Extremadura)
Shankar Subramaniam (ISU)

Idealized First Case: Stokes-flow-based acceleration

Stokes drag coefficient (=6πμd)

$$\frac{F_{fluid,i}}{m} = A_i = -\frac{\beta_{St}}{m}\left(v_i - U_{gi}\right)$$

instantaneous particle acceleration

instantaneous particle velocity

mean gas velocity

Idea: Gain experience with Idealized Case

- *Does not account for*
  - higher Re (Stokes flow only)
  - presence of other particles on drag
  - instantaneous fluid velocity
- *Does account* for
  - instantaneous particle velocity

Idealized First Case: KTGF derivation

Balance Equations (Solid-Phase Momentum & Granular Energy)

$$D_t \mathbf{U} + \frac{1}{mn}\nabla \mathbf{P} = \boxed{-\frac{\beta_{St}}{m}\left(\mathbf{U}-\mathbf{U}_g\right)} + \mathbf{g}$$

mean drag

$$D_t T + \frac{2}{3n}\left(\nabla \cdot \mathbf{q} + P_{ij}\nabla_j U_i\right) = -\zeta T \boxed{-\beta_{St} T}$$

sink due to viscous drag

source due to fluid-dynamic interactions: missing!

Zeroth Order Solution to Kinetic Equation

- Same form for HCS (i.e., same scaling solution is used)

Constitutive Relations Modified by β

- Shear viscosity $\eta^k = nT\left(\nu_\eta - \frac{1}{2}\zeta^{(0)} \boxed{+\frac{\beta_{St}}{m}}\right)^{-1}\left[1-\frac{2}{5}\left(1+\alpha\right)\left(1-3\alpha\right)\phi\chi\right]$
- Conductivity κ^k
- Dufour coefficient μ^k

Case II: 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)

Comments

- IBM-based coefficients will depend on n, Re_m & Re_T
- In limit of low Re_m:
  - $\beta_{IBM} = f(n)$ only
  - $\gamma_{ij} = f(n)$
  - $B_{ij} = f(n, \mathrm{Re}_T)$

Case II: KTGF derivation in low Re_m limit

Balance Equations (Solid-Phase Momentum & Granular Energy)

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

mean drag

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

sink due to viscous drag

source due to fluid-particle fluctuations

Zeroth Order Solution to Kinetic Equation

- HCS solution is *non-isotropic*, which is contrary to physical expectations for no spatial gradients (**P** can be nondiagonal, **q** can be nonzero)
- If γ_{ij} and B_{ij} are scalars instead of tensors ($\gamma_{ij}=\gamma\delta_{ij}$ and $B_{ij}=B\delta_{ij}$):
  - solution is *isotropic*
  - scaling solution is possible (key for derivation of constitutive relations)

Comments

- Constitutive relations: *all* are modified by coefficients

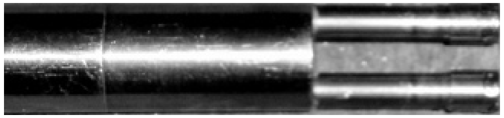
Next step: Incorporate explicit relation for coefficients & evaluate impact

Task 4.3: Experiments in a Low-velocity Fluidized Bed

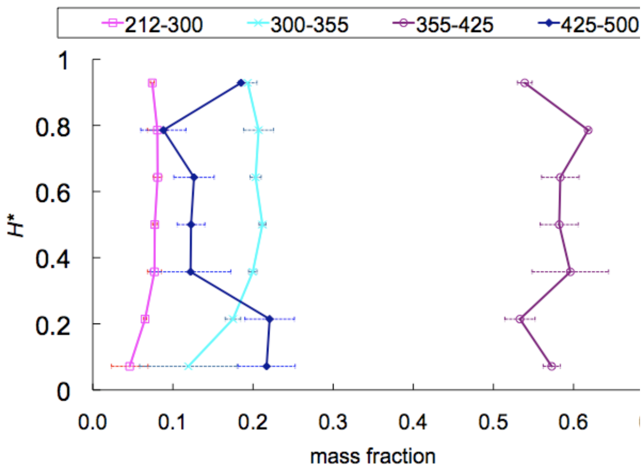
- Basic idea: use a suite of validation sets with increasing levels of "physics" to test new theories: *low-velocity fluidized bed does not involve gas-phase turbulence or significant particle-particle interactions (kinetic theory)*

- Existing experimental data at University of Colorado
  - Segregation data for binary mixtures (glass / PS) (Joseph et al., *AIChE J.*, 2007)
  - Bubbling data for binary mixtures (glass / PS) (Summer 2007)

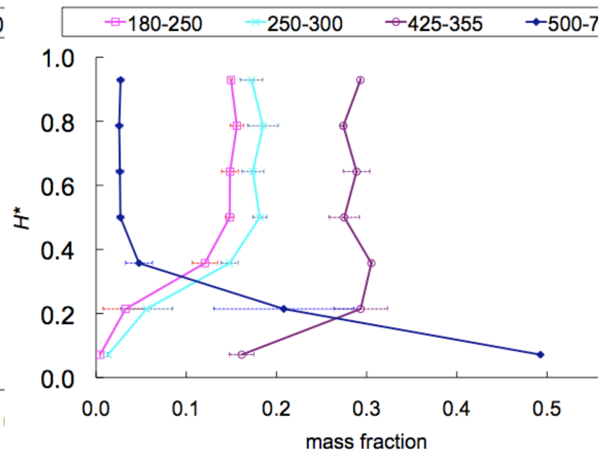
- New data
  - Segregation data for continuous PSD's (sand) (Current)



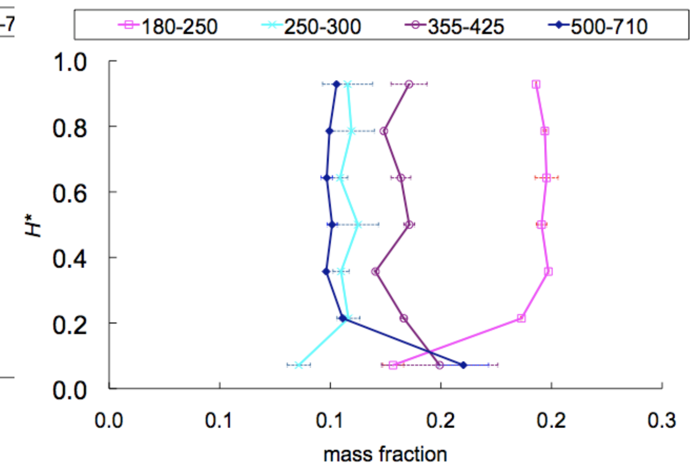
Lognormal PSD: Non-monotonic segregation behavior



$\sigma / d_{ave} = 10\%$



$\sigma / d_{ave} = 30\%$



$\sigma / d_{ave} = 70\%$