Multiphase Flow Physics from Direct Simulation for Model Development

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Part 1: Gas-phase fluctuations from Direct Numerical Simulation using PUReIBM

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Part 2: New Constitutive Model for Granular Stress using Discrete Element Simulations

Graduate Assistant: Vidyapati
Collaborators: S. Sundaresan and G. Tardos
Funding: DE-FG26-07NT43070 (UCR)
Particles (100 to 500 micron) can be larger than the Kolmogorov scale of turbulence.

Large solid particles in a gas: high Stokes number $O(100)$

Fixed particle assemblies are a reasonable approximation (verified by simulation).

High solid volume fraction: not dilute

Non-zero mean slip

Significantly different from the well-documented dilute regime of small “sub-Kolmogorov size” particles of $O(1)$ Stokes number in homogeneous, isotropic turbulence.
Tenneti, S. Garg, R., Subramaniam, S., “Quantification of gas-phase velocity fluctuations in statistically homogeneous gas-solid flow using particle-resolved direct numerical simulation”, *(in review)*
Steady State TKE

\[
\frac{k_f}{|\langle \mathbf{W} \rangle|^2} (\phi, Re_m) = 2\phi + 2.5\phi (1 - \phi)^3 e^{-\phi Re_m^{1/2}}
\]

Gas-phase velocity fluctuations show significant increase with volume fraction: implies transport of RS will be important.
Freely evolving suspensions

Freely moving particles undergoing collisions (elastic and inelastic)

Gas-phase fluctuations in freely evolving suspensions are similar in magnitude to that in fixed particle assemblies because of low collisional dissipation.
Anisotropy in gas-phase fluctuations

Decomposing Reynolds stress into isotropic and deviatoric part

\[ R_{ij}^{(f)} = \left\langle u_i''(f) u_j''(f) \right\rangle = f(\phi, Re_m) \]

\[ b_{ij}^{(f)} = \frac{R_{ij}^{(f)}}{2k(f)} - \frac{1}{3} \delta_{ij} \]

Velocity fluctuation components: parallel and perpendicular to mean flow

\[ u_\parallel'' = u'' \cdot e_\parallel \]

\[ u_\perp'' = u'' \cdot (u''/|u''| - e_\parallel) \]
Anisotropy trends: length scale analysis

Integral length scale of gas-phase fluctuations

\[ L_\parallel = \frac{1}{R_\parallel(0)} \int_0^\infty R_\parallel(r)dr. \]

\[ R_\parallel(r) = \int_{\mathcal{V}(f)} u^{(f)}_\parallel(x) u^{(f)}_\parallel(x, r)dx \]

Measure of inter-particle spacing: weighted average of neighbor particle distances

\[ L_{int} = \frac{\int_{r_{eff}}^r \rho^{(2)}(r)dr}{\int_{r_{eff}}^r \frac{\rho^{(2)}(r)}{r}dr} \]
Multiphase Turbulence Model: Scaling Analysis

Fluid phase TKE equation (homogeneous case)

$$\frac{\partial}{\partial t}\{(1 - \phi) \rho_f k_f\} = -\left\langle u_i''(f) \tau_{ji} n_j^{(s)} \delta (x - x^{(I)})\right\rangle - 2\mu_f \left\langle I_f S_{ij} S_{ij} \right\rangle$$

Interphase TKE transfer

Dissipation

Source

$$\Pi_{k_f} = \langle W \rangle \cdot \left\langle S_{fM}^{(f)} \right\rangle = \frac{18\phi (1 - \phi)^2 \mu_f}{D^2} F(\phi, Re_m) \langle W \rangle^2$$

Steady state

$$\Pi_{k_f} = \rho_f (1 - \phi) \varepsilon_f$$

Scaling of TKE implies a scaling for dissipation: can verify existing models that use Kolmogorov scaling
Multiphase Turbulence Dissipation Models

Kolmogorov scaling

Dissipation is assumed to take place on a length scale corresponding to \( l_{\text{diss}} \)

\[
\prod k_f = \rho_f (1 - \phi) \varepsilon_f
\]

\[
\varepsilon_f \sim k_f^{3/2} / l_{\text{diss}}
\]

\[
\left( \frac{k_f}{E_f} \right)^{3/2} = \left( \frac{l_{\text{diss}}}{D} \right) 36 \sqrt{2} \phi (1 - \phi)^2 \frac{F(\phi, \text{Re}_m)}{\text{Re}_m}.
\]

\[
\frac{k_f}{E_f} = \left( \frac{l_{\text{diss}}}{D} \right)^2 18 \phi (1 - \phi) F(\phi, \text{Re}_m).
\]

Taylor microscale
Taylor microscale scaling is appropriate for gas-solid flows with finite sized particles.
1. Presence of finite sized particles with mean slip velocity generate high level of *non-turbulent* gas-phase velocity fluctuations

2. Developed a correlation for kinetic energy for monodisperse suspensions

3. Strong anisotropy: depends on Re & volume fraction

4. From scaling analysis it is found that Taylor microscale type scaling for the dissipation of TKE is appropriate for gas-solid flows with finite sized particles

5. Correlation and the turbulence model extend to bidisperse suspensions in terms of SMD (not shown)
Part 1: Gas-phase fluctuations from Direct Numerical Simulation using PUReIBM

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Part 2: Constitutive Model for Granular Stress using Discrete Element Simulations

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Existence of different regimes using DEM

Even in a simple problem such as the discharge from a silo, different regimes coexist.

Regime map is established from DEM data of homogeneously sheared granular flow.

3D DEM simulation of flat bottomed silo
Regime classification: Red = Inertial regime; Blue = Quasi-static regime.
Challenges for continuum models

Vidyapati and Subramaniam, S., “Granular flow in Silo discharge: DEM simulations and model assessment”, (in prep)
None of these models captures the correct scaling of shear stress with shear rate in the intermediate regime.
Granular phase transition: Order Parameter

\[ \text{OP} = \frac{\langle Z_s \rangle}{\langle Z \rangle} \]

- Number of solid contacts
- Total number of contacts

Different regimes in granular shear cell (GSC) experiment

Order Parameter is indeed capable of capturing granular ‘phase’ transition from solidlike to fluidlike behavior

It was postulated\(^1\) that free energy density function has two local minima at \( \rho = (\text{completely solidlike}) \) and \( \rho = (\text{completely fluidlike}) \).

\[
F(\rho, \delta) = \int_{\rho} \rho (\rho - 1)(\rho - \delta) \, d\rho
\]

\[
\frac{D\rho}{Dt} = D_c \nabla^2 \rho - \frac{\partial F(\rho, \delta)}{\partial \rho}
\]

\(^1\)Aranson et al., *Phys. Rev. E*, vol. 65, 061303 (2001)
OP dynamics from DEM simulations

OP extracted from DEM simulations using two different contact models

- Hooke
- Hertzian

\[ F_{n_{ij}} = f(\delta_{ij}/d)(k_n\delta_{ij}n_{ij} - \gamma_n m_{\text{eff}} v_{n_{ij}}) \]

\[ F_{t_{ij}} = f(\delta_{ij}/d)(-k_t u_{t_{ij}} - \gamma_t m_{\text{eff}} v_{t_{ij}}) \]

**Hookean contact model:**

\[ f(\delta_{ij}/d) = 1 \]

**Hertzian contact model:**

\[ f(\delta_{ij}/d) = \sqrt{\delta_{ij}/d} \]

Discovered existence of a third stable granular phase which is neither completely solidlike nor completely fluidlike
New formulation of free energy density function

\[ F^*(\rho, \delta) = \int_\rho \rho (\rho - 1)(\rho - \rho_3)(\rho - \delta)(\rho - \delta^*) \, d\rho \]

\( \rho_3 \) third stable phase of granular material

\[ \frac{D\rho}{Dt} = D_c \nabla^2 \rho - \frac{\partial F^*(\rho, \delta)}{\partial \rho} \]

* Graph showing the free energy density function \( F^*(\rho, \delta) \) with different values for \( \delta \) and \( \rho \).

* Graph showing the density \( \rho \) over time \( \gamma_t \) for different values of \( \nu \) and \( \mu \).

* Graph illustrating the DEM simulation results with \( \rho_{DEM} = 0.737 \) and \( \rho_{GL} = 0.703 \), showing a % difference of 4.61%.
The third stable granular phase is quantified using structural quantity such as pair correlation function.
Quantification of third phase

Average coordination number is more sensitive to the phase change as indicated by stable OP values, than the fabric tensor.
Stress tensor in granular media

\[
\sigma_{\alpha\beta}^{\text{tot}} = \frac{1}{V} \left[ \sum_{i} m^{(i)} v_{\alpha}^{(i)} v_{\beta}^{(i)} + \sum_{i} \sum_{j, j \neq i} \frac{1}{2} r_{\alpha}^{(i)(j)} f_{\beta}^{(i)(j)} \right]
\]

DEM reveals that streaming part of the total stress is negligible (<3%) in the intermediate and dense regimes.

Streamlining stress << contact (virial) stress

Accurate modeling of contact (virial) stress is critical in the intermediate regime.

Developed the **Relative Acceleration** model: a statistical model based on evolution of the pair-correlation.
Relative acceleration concept

• The term $\langle r^{(i)(j)}_\alpha \Delta A^{(i)(j)}_\beta \rangle$ can be computed using the idea of relative acceleration

$\langle \Delta A^{(i),(j)} | \mathbf{r}, \mathbf{w} \rangle = \langle A^{(i)} | \mathbf{r}, \mathbf{w} \rangle - \langle A^{(j)} | \mathbf{r}, \mathbf{w} \rangle = \langle A | \mathbf{r}, \mathbf{w} \rangle$

$r = r^{(i)} - r^{(j)} \quad w = v^{(i)} - v^{(j)}$

• The conditional relative acceleration can be decomposed as

$\langle \Delta A | \mathbf{r}, \mathbf{w} \rangle = \langle \Delta A | \mathbf{r} \rangle + \langle \Delta A | \mathbf{w} \rangle$

• In LD (Langevin dynamics), the term $\langle \Delta A | \mathbf{w} \rangle$ can be modeled in terms of inelasticity and damping

$\Delta A^{(i)(j)}_\beta = A^{(i)} - A^{(j)}$

Representative volume $V$

Location of contacting neighbor defined by $g(r)$ at contact

$\langle N_c \rangle$ represents average number of contacts or number of red dots in volume $V$
Relative acceleration model

- RA model for normal component of contact stress

\[ \sigma_{\alpha\beta} = \frac{1}{2V} N_{CN} \left\langle N(V) \right\rangle k_n R_{\alpha\beta} \int_0^{r_c} r^{(i)(j)} \delta^{(i)(j)} g(r) \, dr \]

\[ r^{(i)(j)} = d - \delta^{(i)(j)} \]

for small normal overlaps one can write the contact stress as

\[ \sigma_{\alpha\beta} = \frac{1}{2V} N_{CN} \left\langle N(V) \right\rangle k_n R_{\alpha\beta} d \int_0^{r_c} \delta^{(i)(j)} g(r) \, dr \]

Model Inputs:

1. Average coordination number
2. Fabric tensor
3. Pair Correlation (r<r_c) or Force PDF
Preliminary model prediction using DEM data

- Model inputs \( (N_{CN}, R_{\alpha \beta}, \delta^{(i)(j)}, g(r)) \) directly taken from data of DEM

\[ \hat{\sigma}_{zz} \text{ vs } k^*(v=0.62, \mu_p=0.1, e=0.7, \text{PBC}) \]

Non dimensional shear rate
Non dimensional stress
Accurate \( \dot{\gamma}^n \) dependence

\[ \hat{\sigma}_z \text{ vs } k^*(v=0.61, \mu_p=0.1, e=0.7, \text{PBC}) \]

Non dimensional stress
Non dimensional shear rate

Preliminary results confirm the correct scaling of stress-strain scaling in intermediate regime
Particle-resolved Direct Numerical Simulation for gas-solid flows, and Discrete Element Simulations for granular flows, are useful approaches for understanding multiphase flow physics and for model development.
Contour plot of equivalent $R\lambda$ generating the same energy in velocity fluctuations as the non-turbulent fluctuations arising from the presence of particles in gas-solid flow.
Convergence of $k_f$ at $Re_m =$ 20

- Squares: $D_m = 10$
- Triangles: $D_m = 20$
- Diamonds: $D_m = 30$

Volume fraction: 0.3
Volume fraction: 0.4
Convergence of $k_f$ at $\text{Re}_m =$

Volume fraction: 0.3
Freely evolving suspensions

Freely moving particles with inelastic collisions

Similarity of $k(f)$ among fixed and moving particles

\[
\langle I^{(f)} \rho^{(f)} \rangle \frac{d}{dt} k^{(f)} = \left\{ \begin{array}{l}
\langle W_i \rangle \langle \tau_{ji} \dot{n}_j^{(s)} \delta (x - x^{(I)}) \rangle \\
- \langle u_i^{(s)} \tau_{ji} \dot{n}_j^{(s)} \delta (x - x^{(I)}) \rangle \\
- 2\mu^{(f)} \langle I^{(f)} S_{ij} S_{ij} \rangle
\end{array} \right.
\]

unsteady term

\[
\langle I^{(s)} \rho^{(s)} \rangle \frac{d}{dt} k^{(s)} = \left\{ \begin{array}{l}
\langle W_i \rangle \langle \tau_{ji} \dot{n}_j^{(s)} \delta (x - x^{(I)}) \rangle \\
- \langle u_i^{(s)} \tau_{ji} \dot{n}_j^{(s)} \delta (x - x^{(I)}) \rangle \\
+ \Gamma^{(s)}_{coll}
\end{array} \right.
\]

interphase TKE transfer

Small compared to others

Evolution equation the same as fixed beds

\[\text{Re}_m = 20\]
Cross correlations are almost zero
Anisotropy is along mean flow direction
The normal correlations in perpendicular plane are similar
Reynolds stress is axi-symmetric along the mean flow

\[ b_{11}(Re_m, \phi) = \frac{a}{1+be^{-cRe_m}}e^{-d\phi/(1+ee^{-fRe_m})} \]
\[ b_{22}(Re_m, \phi) = b_{33}(Re_m, \phi) = -\frac{b_{11}(Re_m, \phi)}{2} \]
\[ b_{ij}(Re_m, \phi) = 0, \quad i \neq j \]

\[ a = 0.523 \]
\[ b = 0.303 \]
\[ c = 0.114 \]
\[ d = 3.526 \]
\[ e = 1.809 \]
\[ f = 0.005 \]
Strength of gas-phase velocity fluctuations depend strongly on only the total solid volume fraction and the Reynolds number based on Sauter mean diameter.
Multiphase Flow Turbulence Model

Mean momentum equation: fluid phase

\[ \frac{\partial}{\partial t}\{\rho_f (1 - \phi) \langle u_i(f) \rangle\} + \frac{\partial}{\partial x_j}\{\rho_f (1 - \phi) \langle u_i(f) \rangle \langle u_j(f) \rangle\} \]

\[ = - (1 - \phi) \langle g_i(f) \rangle - \frac{\partial}{\partial x_j}\left\{\rho_f \left\langle I_f u_i''(f) u_j''(f) \right\rangle\right\} \]

\[ - \left\langle \tau_{ji} n_j^{(s)} \delta (x - x(I)) \right\rangle. \]

Drag law

\[ (1 - \phi) \rho_f \frac{k_f}{\varepsilon_f} \frac{\partial}{\partial x_j} \langle u_i(f) \rangle \]

Turbulence model

Existing multiphase turbulence models are extensions of single-phase turbulence models.
Back-Up
Granular phase transition: Order parameter

- Characterizes the phase or “state” of the granular material

\[
\text{OP} = \begin{cases} 
0 & \text{Pure fluid} \\
1 & \text{Pure solid} 
\end{cases}
\]

- Order parameter is defined by \(^1\)

\[
\text{OP} = \frac{\langle Z_s \rangle}{\langle Z \rangle}
\]

- Number of solid contacts
- Total number of contacts

Solidlike contacts \(^1\)

- Solidlike stress
  - stress from solidlike contacts

Fluidlike stress

- stress from fluidlike contacts
  + streaming stress

Total granular stress

- Solidlike stress + Fluidlike stress

A fit for steady values of OP with solid volume fraction and friction coefficient is proposed based on the data obtained from DEM simulations.

\[
\rho_3 = \begin{cases} 
  a \sin(b \pi \nu \mu_p) & 0 < \nu \leq \nu^* \\
  A \log(B \nu^2 \mu_p) + C \exp(\nu^2 - \mu_p) & \nu^* < \nu < \nu_{\max}
\end{cases}
\]

\[a = 0.804, \ b = 0.678, \ A = 0.5547, \ B = 6.769, \ C = 0.6847\]
Assessment of proposed hypothesis

\[
\frac{D\rho}{Dt} = D_c \nabla^2 \rho - \frac{\partial F^*(\rho, \delta)}{\partial \rho}
\]

\[
F^*(\rho, \delta) = \int_0^\rho \rho(\rho-1)(\rho-\rho_3)(\rho-\delta)(\rho-\delta^*)d\rho
\]

\(\delta^*=0.85, \delta=0.28, \nu=0.60, \mu_p=0.5\)

\(\rho_{DEM} = 0.737, \rho_{DL} = 0.703\)

\% difference = 4.61\%

\(\nu = 0.60\)

\(\rho \text{ vs } \gamma t \) \((\nu=0.62, \mu_p=0.5, k=1.0 \times 10^5, e=0.7)\)

\(\delta^*=0.85, \delta=0.28, \nu=0.62, \mu_p=0.5\)

\(\rho_{DEM} = 0.780, \rho_{DL} = 0.754\)

\% difference = 3.64\%
Quantification of third phase

Co-ordination number (N_{CN}): average number of contacts per particle

\[ N_{CN} = \frac{\sum_i N_c^{(i)}}{N} \]

- number of contacts for \( i \)th particle
- total number of particles

Fabric tensor \( R_{ij} \): describes the anisotropy of the contact distribution in granular media

\[ R_{ij} = \frac{1}{N_c} \sum_{c \in V} n_i n_j \]

Pair correlation function (g(\( r \))): probability of finding a particle at a distance \( r \) away from given reference particle

\[ g(r) = \frac{N_r}{N \times V_r \times n} \]

[Volume of sphere formula]

\[ V_r = 4\pi r^2 \, dr \]

\( n \) : Number density
Regime classified based on relationship between stress-strain

**Inertial regime**

\[ \sigma \propto \dot{\gamma}^2 \]

**Intermediate regime**

\[ \sigma \propto \dot{\gamma}^n, 0 < n < 2 \]

**Quasi-static regime**

\[ \sigma \neq f(\dot{\gamma}) \]

\[ k^* = k_n / \rho_s d_0 \dot{\gamma}^2 = 2.5 \times 10^4 \]

\[ k^* = k_n / \rho_s d_0 \dot{\gamma}^2 = 10^9 \]