Rheological Behavior of Dense Granular Materials: DEM Simulations and Order Parameter Model

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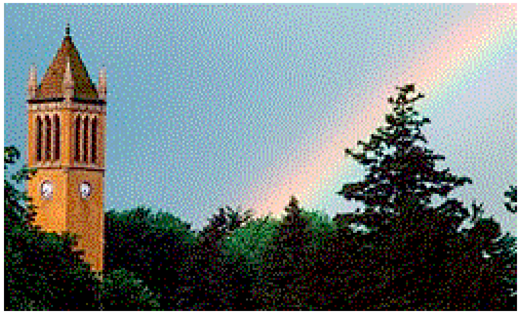
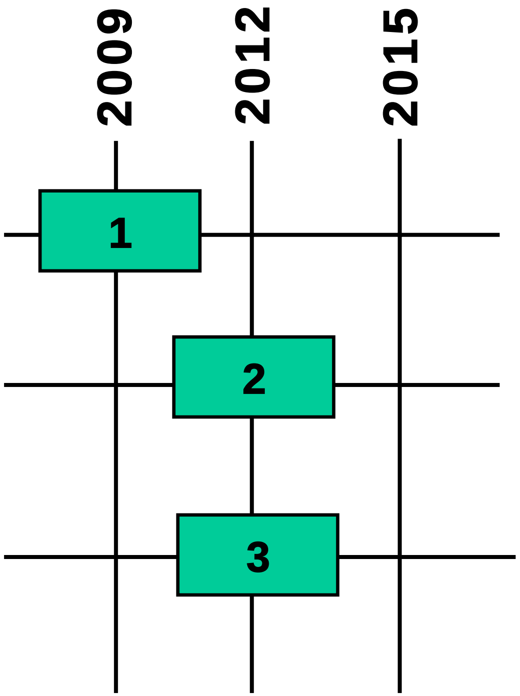


Roadmap for dense granular flow

1. Fundamental aspects of stress and flow fields in dense particulate systems

2. Develop continuum descriptions of dense particulate systems

3. Handle the transition from regimes in which the particles are in enduring contact to regimes in which the particles are in collisional contacts



Rheological Behavior of Dense Assemblies of Granular Materials

Sundaresan, Tardos & Subramaniam

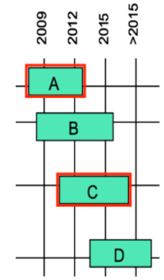
Project Manager: Ron Breault

Annual Review 2009: Iowa State Report

Connection to roadmap

Key questions addressed:

1. Fundamental aspects of stress and flow fields in dense particulate systems
2. Development of constitutive relations for continuum models from discrete models such as DEM or LBM, which are based on fewer assumptions than the continuum approach
3. Handle the transition from regimes in which the particles are in enduring contact to regimes in which the particles are in collisional contacts



Action taken in our project:

- Range of different regimes: quasi-static, intermediate, inertial
  - sensitivity to flow and particle properties?
- DEM simulation validation with experiment?
- Continuum rheological model performance over all regimes?

- Established preliminary regime map
- Compared DEM simulations with Couette cell experiments
- Developed and refined objective order parameter (OP) model: tested in all regimes

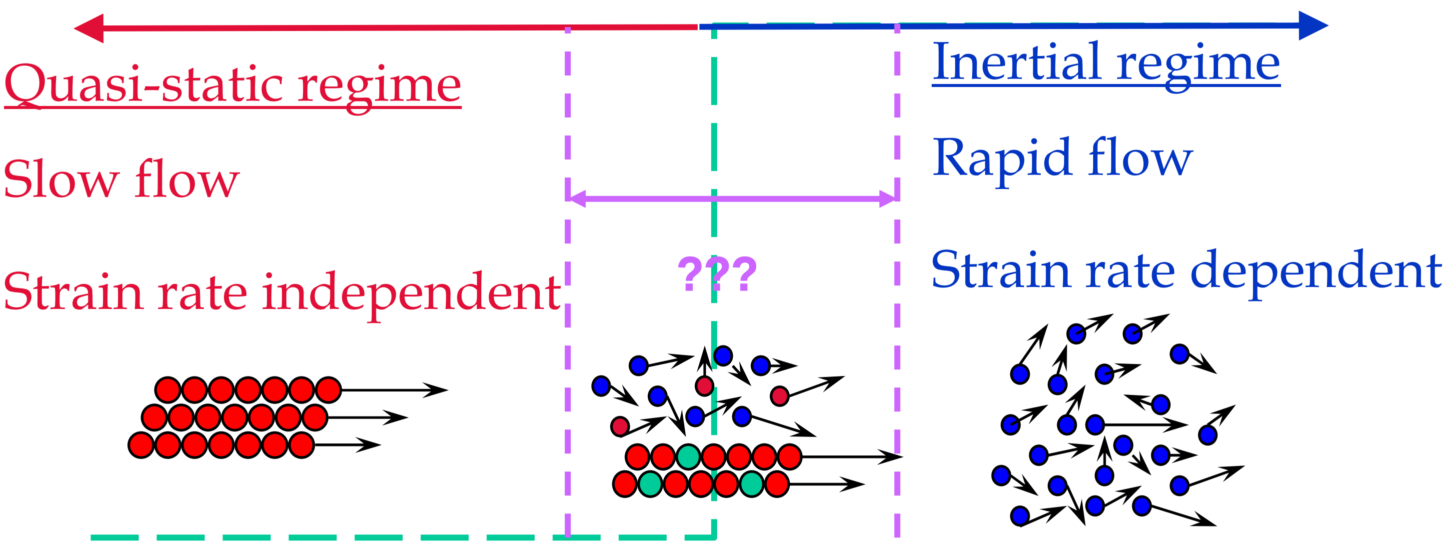
Project tasks and goals

- Develop and validate constitutive models for quasi-static and intermediate regimes
  - Incorporate particle scale properties
  - Capture physics of regime transitions
- Gather simulation data for different flow geometries and compare with experiments

- Developed refined order parameter (ROP) model
  - Order parameter reflects effect of particle and flow properties
- Gathered DEM simulation data for different flow geometries and compared with experiments

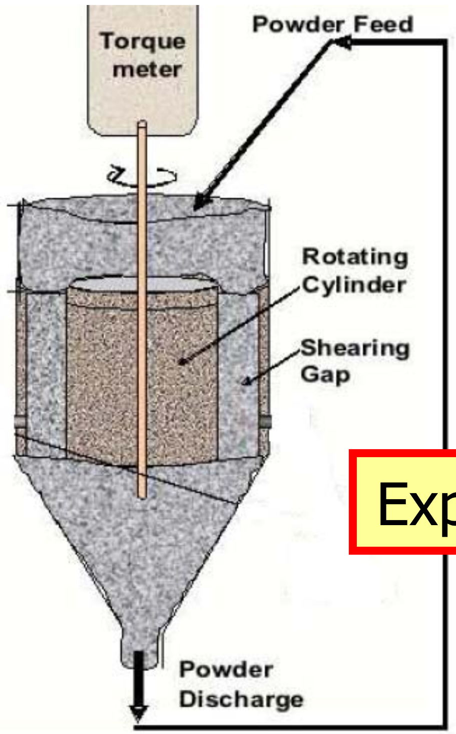
Motivation for current work

- Dense flow in hoppers, discharge from bins
  - Regime transitions are not sharp
  - Need physics-based models for transitional regime

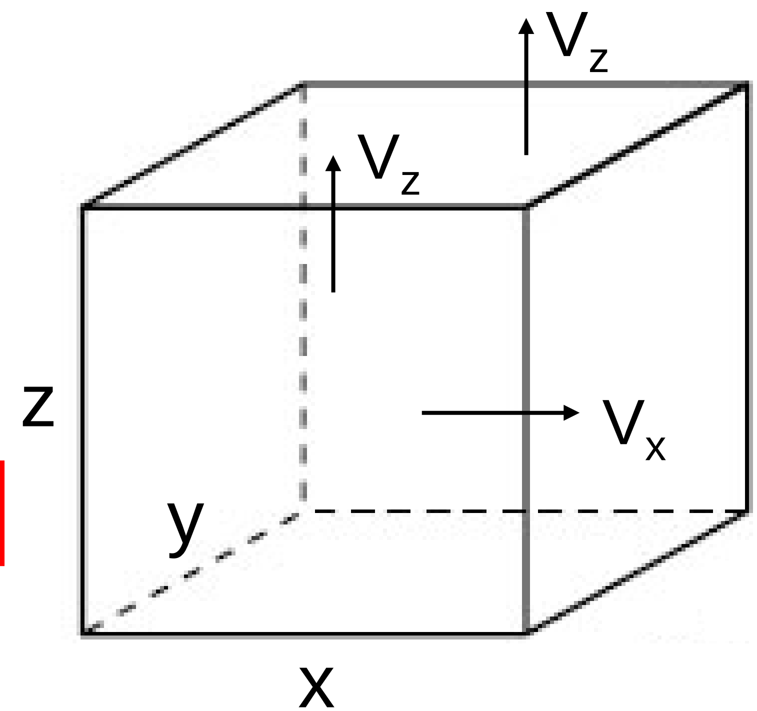


Experiments and DEM simulations reveal that this regime spreads over a range of volume fraction, friction coefficient and shear rate

Simulation of Couette device



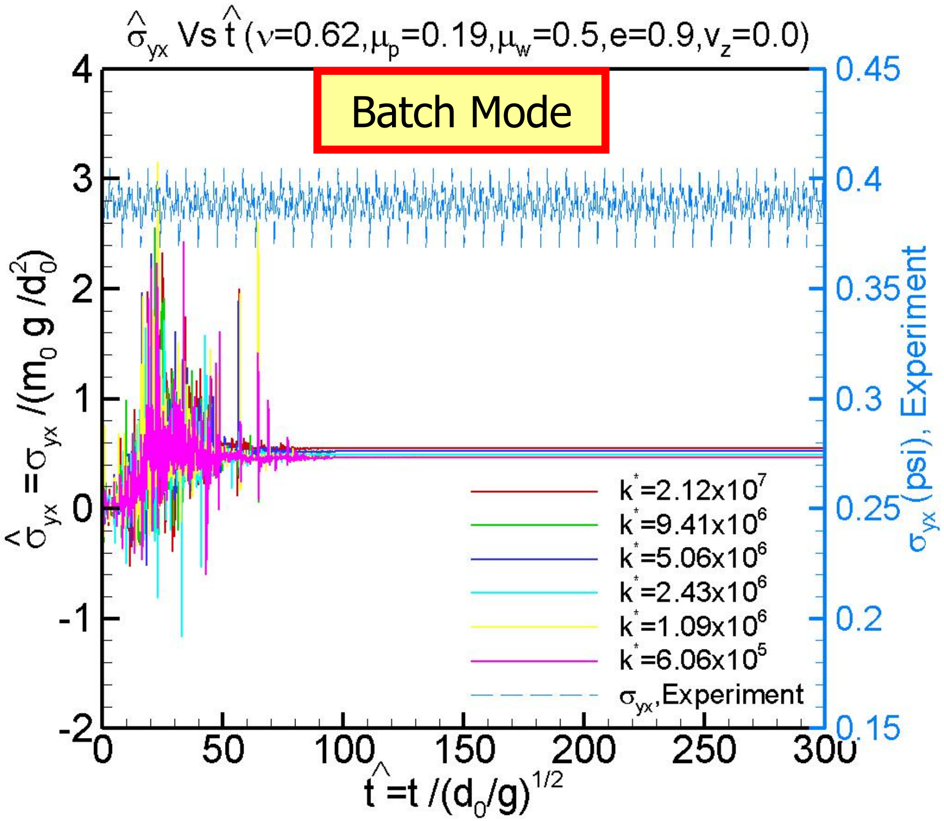
Experimental Setup



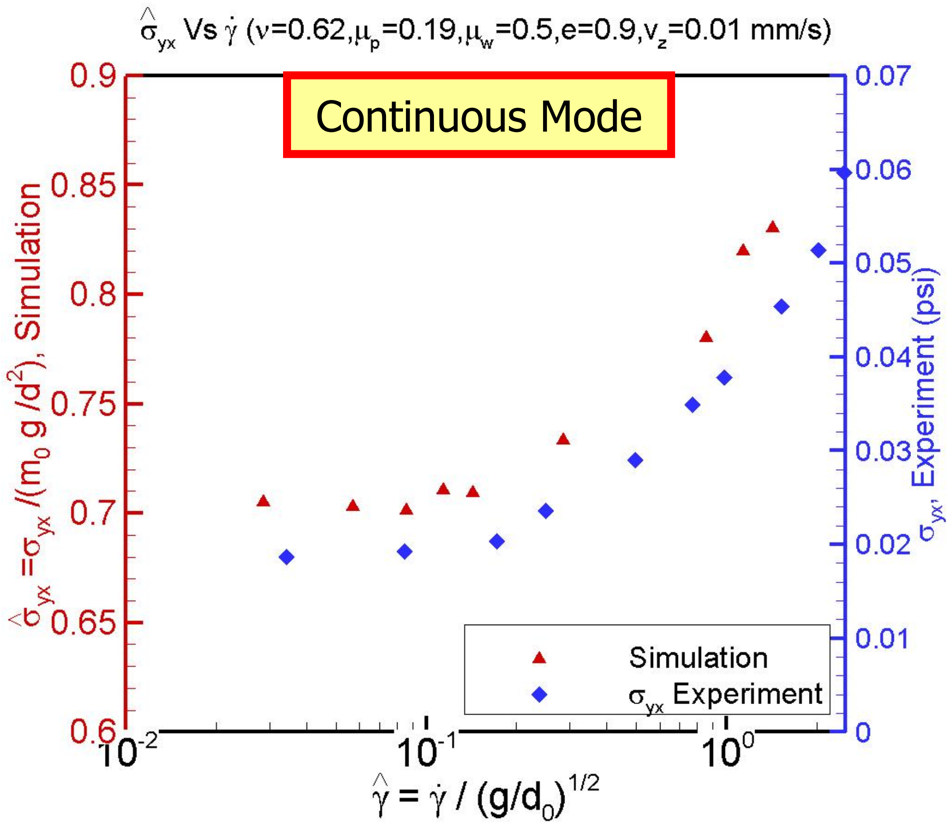
Simulation Setup

- Boundary Conditions
  - y direction (corresponds to radial coordinate): walls (moving in z and x direction)
  - x direction (corresponds to polar coordinate): periodic
  - $z=z_L$, bottom wall and open at top $z=z_H$; gravity in –ve z direction

Simulation of Couette device



Average shear stress is independent of shear rate: quasi-static regime



Two distinct regimes present in the flow: quasi-static and intermediate

Granular phase transition: Order parameter

- Characterizes the phase or "state" of the granular material

$\rho = 0$ → Pure fluid

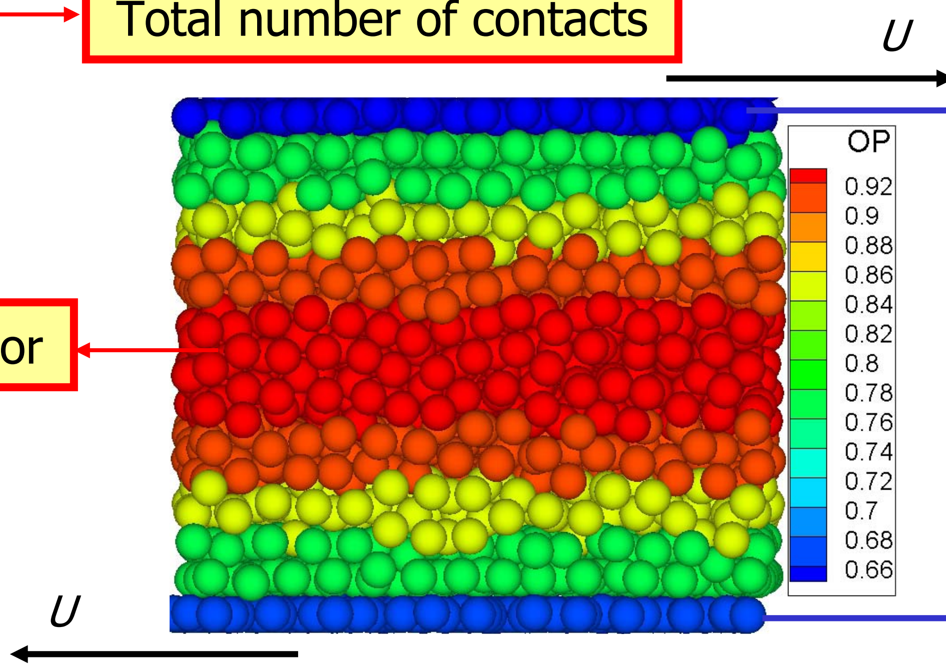
$\rho = 1$ → Pure solid

- Order parameter is defined by

$$\rho = \frac{\langle \overline{Z_s} \rangle}{\langle \overline{Z} \rangle}$$

$\langle \overline{Z_s} \rangle$ → Number of solid contacts

$\langle \overline{Z} \rangle$ → Total number of contacts

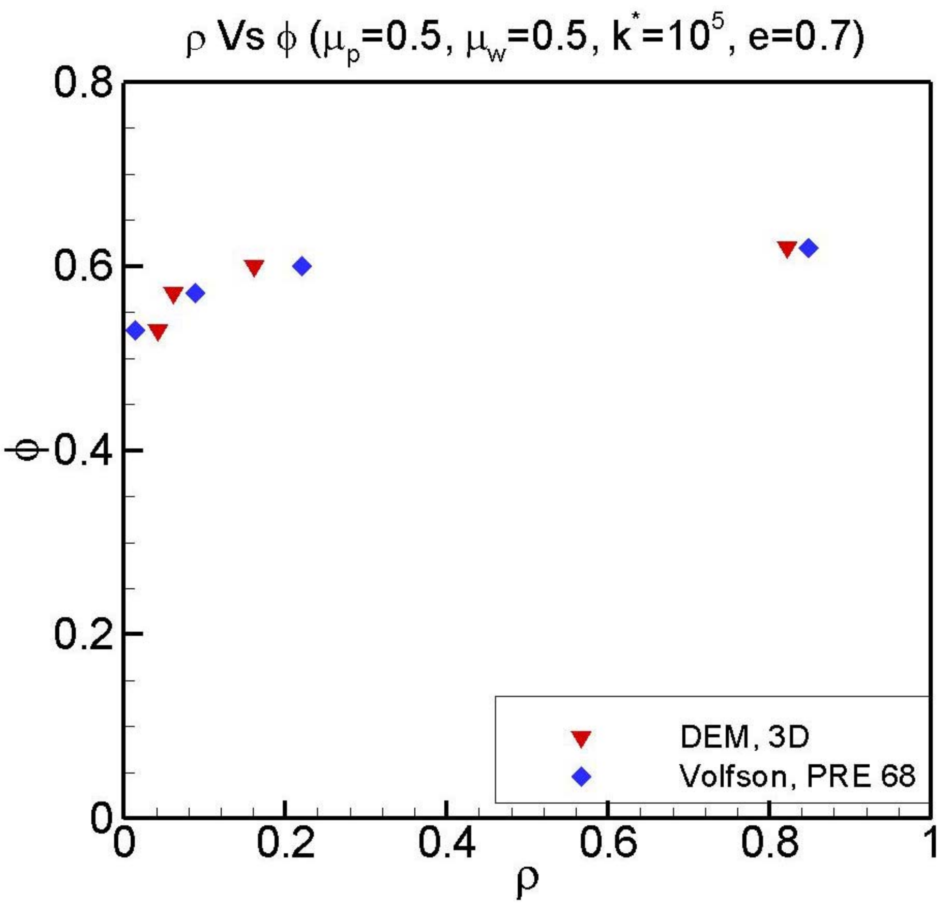


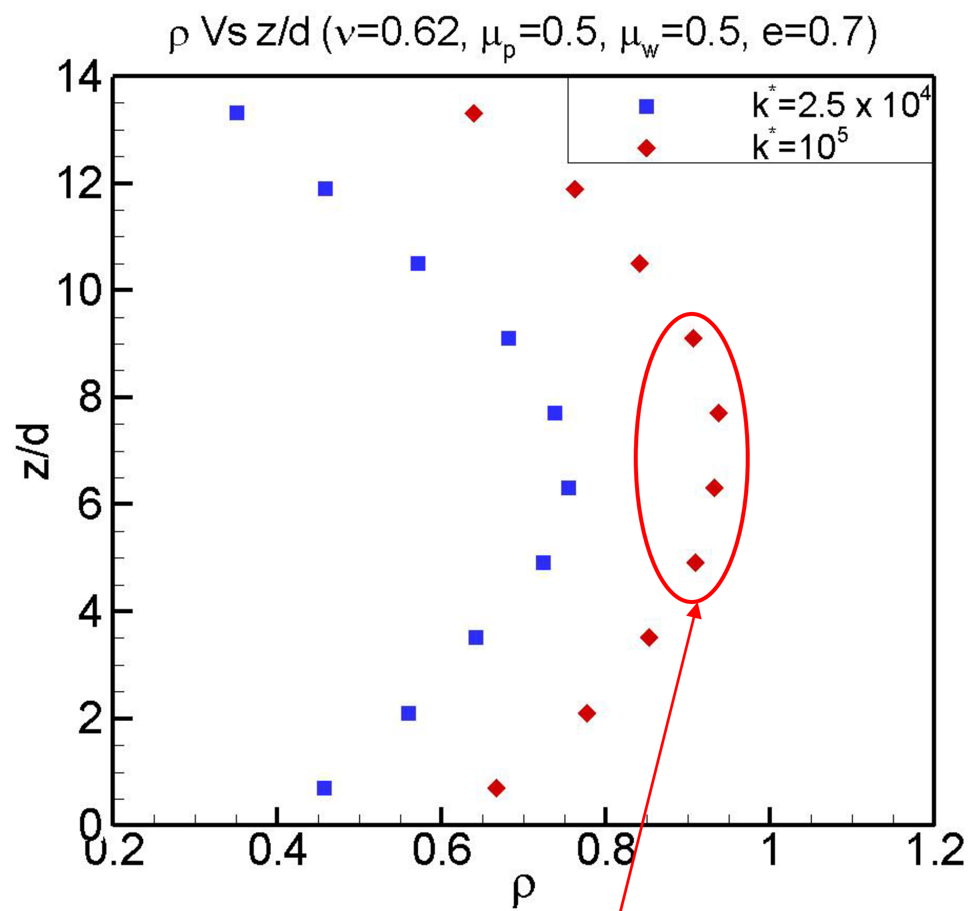
More fluidlike behavior

Solidlike behavior

More fluidlike behavior

Order parameter extraction and validation





Validation of order parameter extraction with existing results

Order parameter captures physics, more solidlike behavior in the center of the channel

Volfson et al., Phys. Rev. E 71, 021302 (2005)

Description of OP model

- Decomposition of total granular stress

$$\sigma_{ij} = \sigma_{ij}^{s} + \sigma_{ij}^{f}$$

Total Stress = Solidlike stress + Fluidlike Stress

- OP model expresses each of the solidlike and fluidlike parts in terms of order parameter and total granular stress tensor

$$\sigma_{ij}^{f} = \sigma_0 \left\{ \alpha \delta_{ij} + \beta b_{ij} + \gamma \left[(\mathbf{b}^2)_{ij} - \frac{1}{3} (\mathbf{b}^2)_{ll} \delta_{ij} \right] \right\}$$

$$\sigma_{ij}^{f} = f\left(\sigma_o, \alpha, \beta, \gamma\right)$$

$$\sigma_{ij}^{s} = \sigma_0 \left\{ (1-\alpha) \delta_{ij} + (1-\beta) b_{ij} - \gamma \left[(\mathbf{b}^2)_{ij} - \frac{1}{3} (\mathbf{b}^2)_{ll} \delta_{ij} \right] \right\}$$

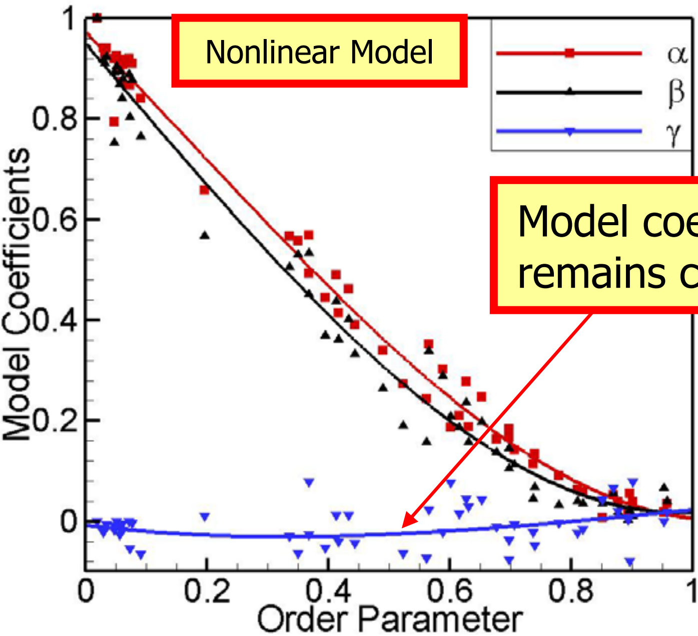
$$\sigma_{ij}^{s} = f\left(\sigma_o, \alpha, \beta, \gamma\right)$$

$\alpha, \beta, \gamma = f$(Order Parameter)

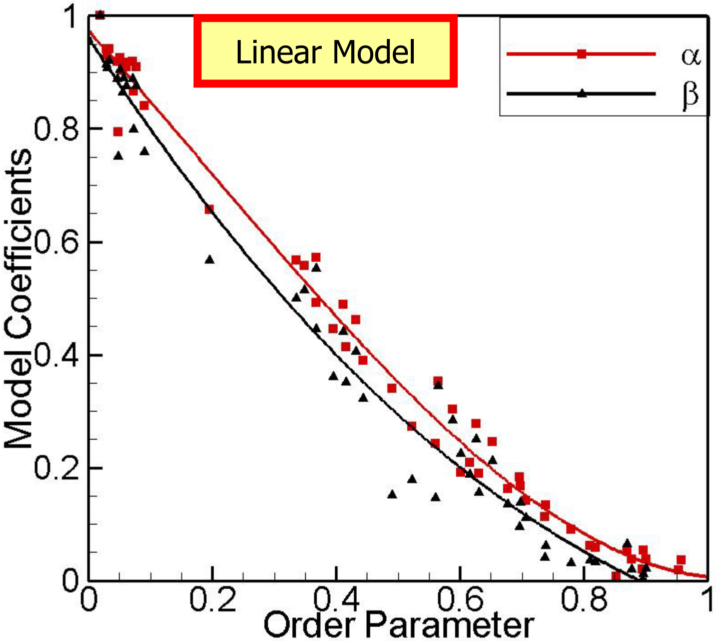
σ_0 Scale of total granular stress

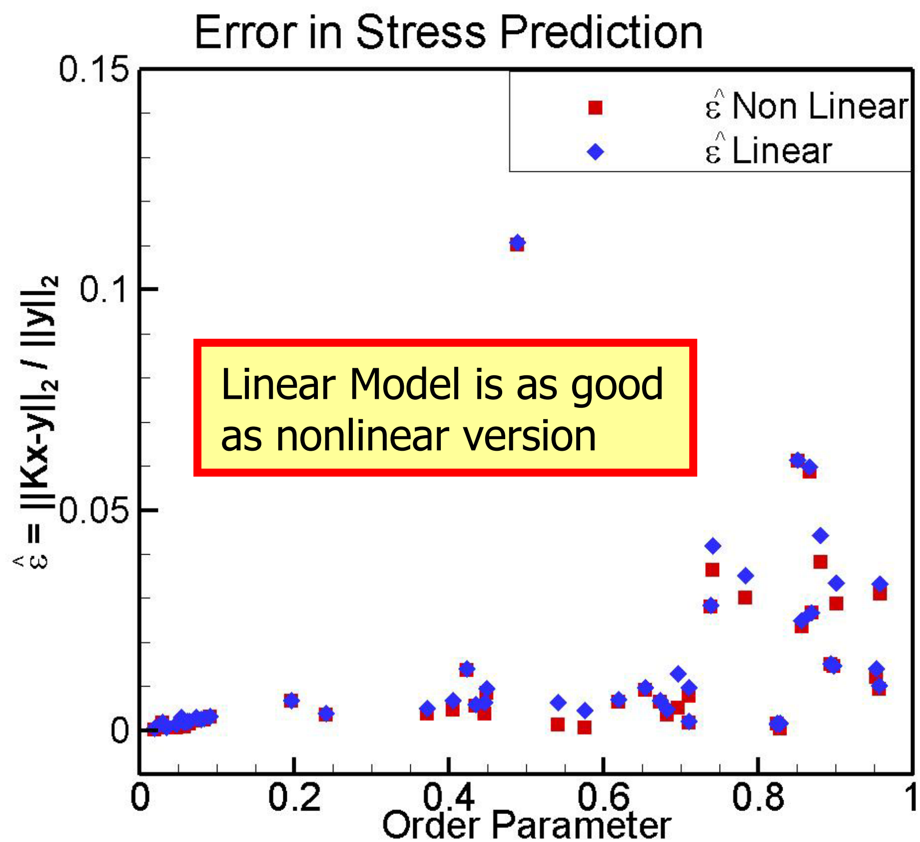
Objective OP Model, Subramaniam Group, *Phys. Rev. E* (2005)

New model coefficients from 3D DEM data



Model coefficient γ remains close to zero





Linear Model is as good as nonlinear version

Error incurred in both models < 11%

Refined OP Model: Linear coefficients from 3D DEM data

Advantage: total granular stress can be inverted from solidlike and fluidlike stress relations

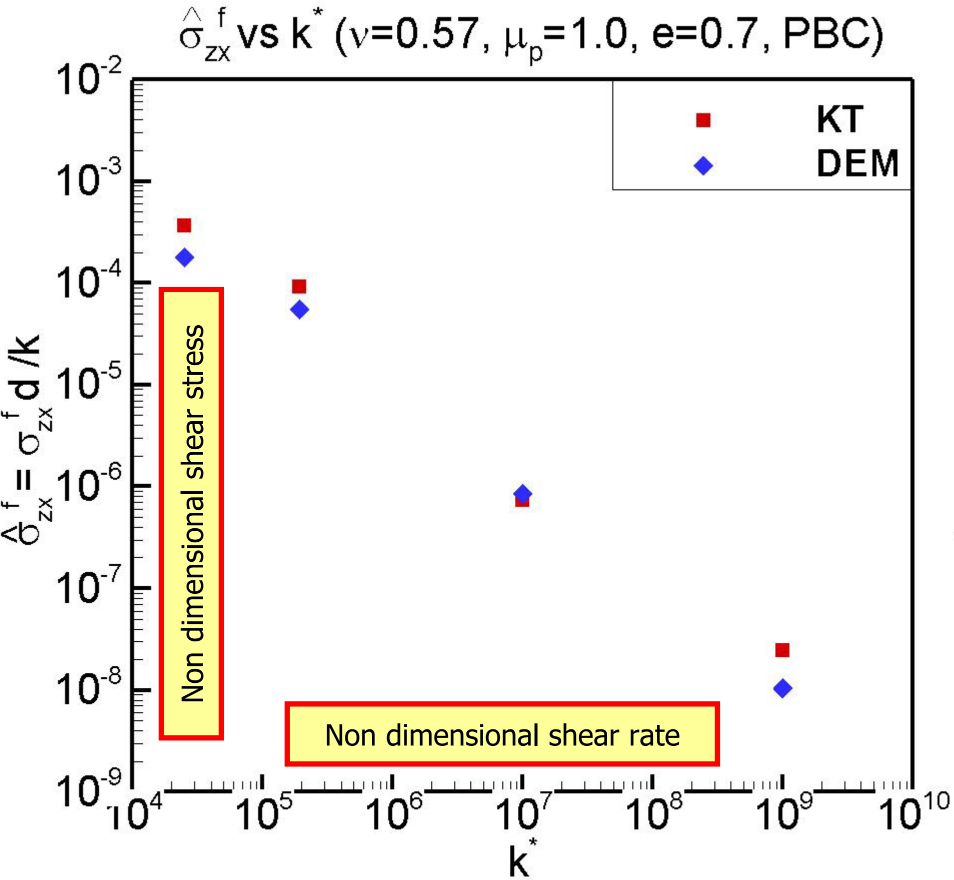
OP constitutive model specification

- To complete the OP constitutive model specification
  - Fluidlike stress is taken from kinetic theory of granular flows

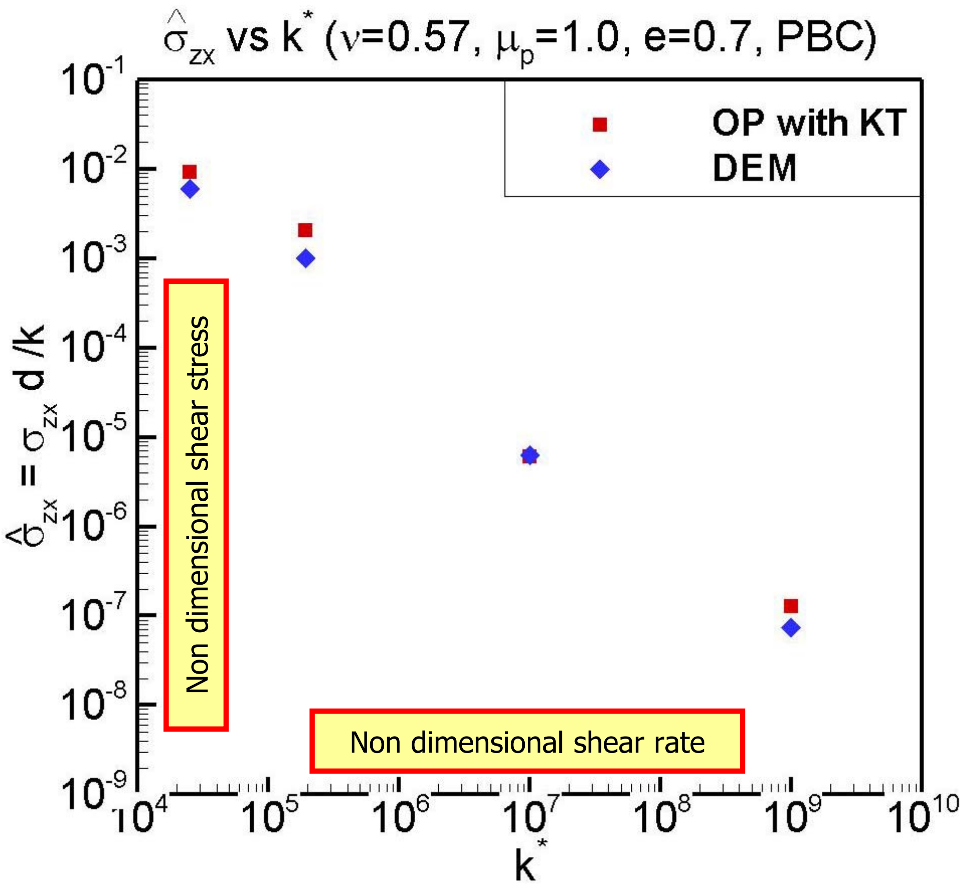
$$\boxed{\sigma_{ij}^{f} \leftarrow KTGF}$$

- Need order parameter and granular temperature
  - Solved transport equation for order parameter (modified Ginzburg Landau equation)
  - Solved granular temperature (pseudo thermal energy) equation
- With new model coefficients and fluid component of the total stress (from KTGF), the ROP-KT model can predict total granular stress

Performance of ROP-KT model



Fluidlike Shear Stress

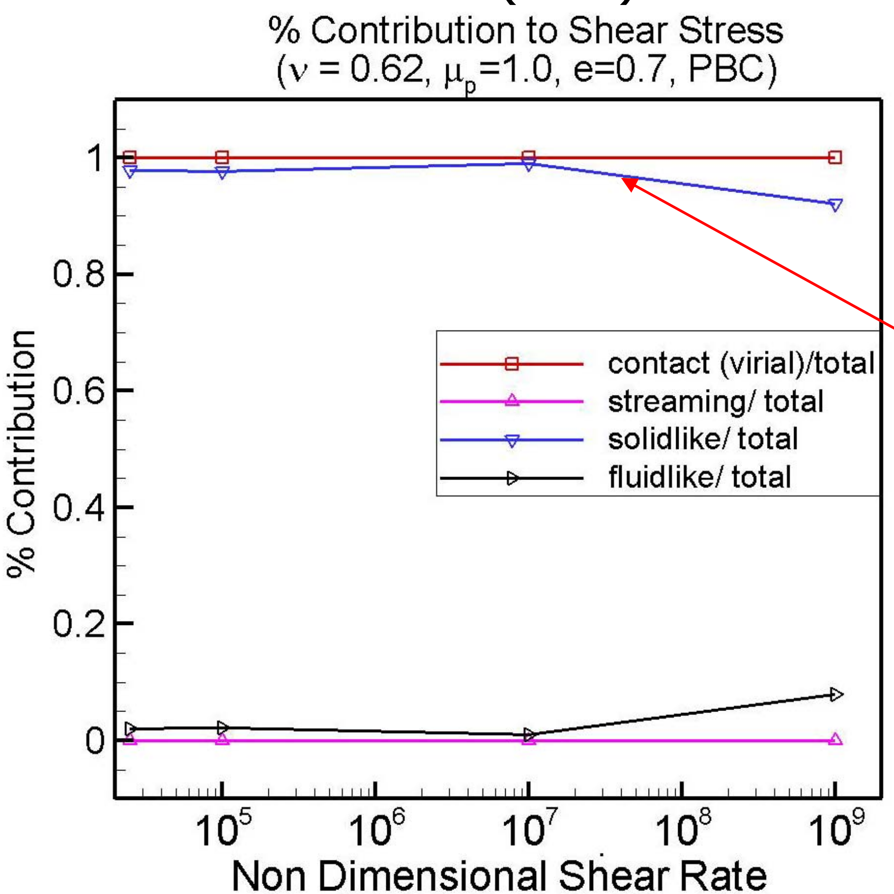


Total Shear Stress

Refined OP model with KT (ROP-KT) performs well for all volume fraction and friction coefficient in the inertial regime

OP coupled with solid stress model (SSM)

- In the quasi-static regime solidlike stress dominates the total granular stress
  - a modification to OP model was proposed by coupling it with solid stress model (SSM)

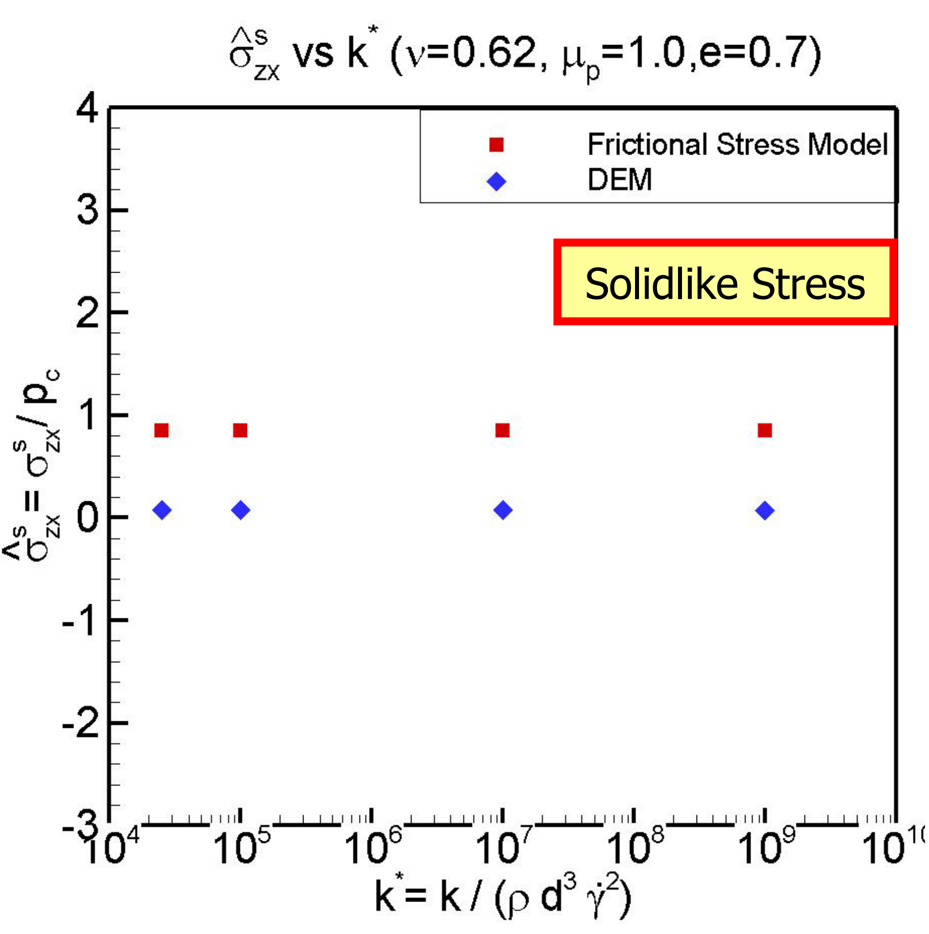


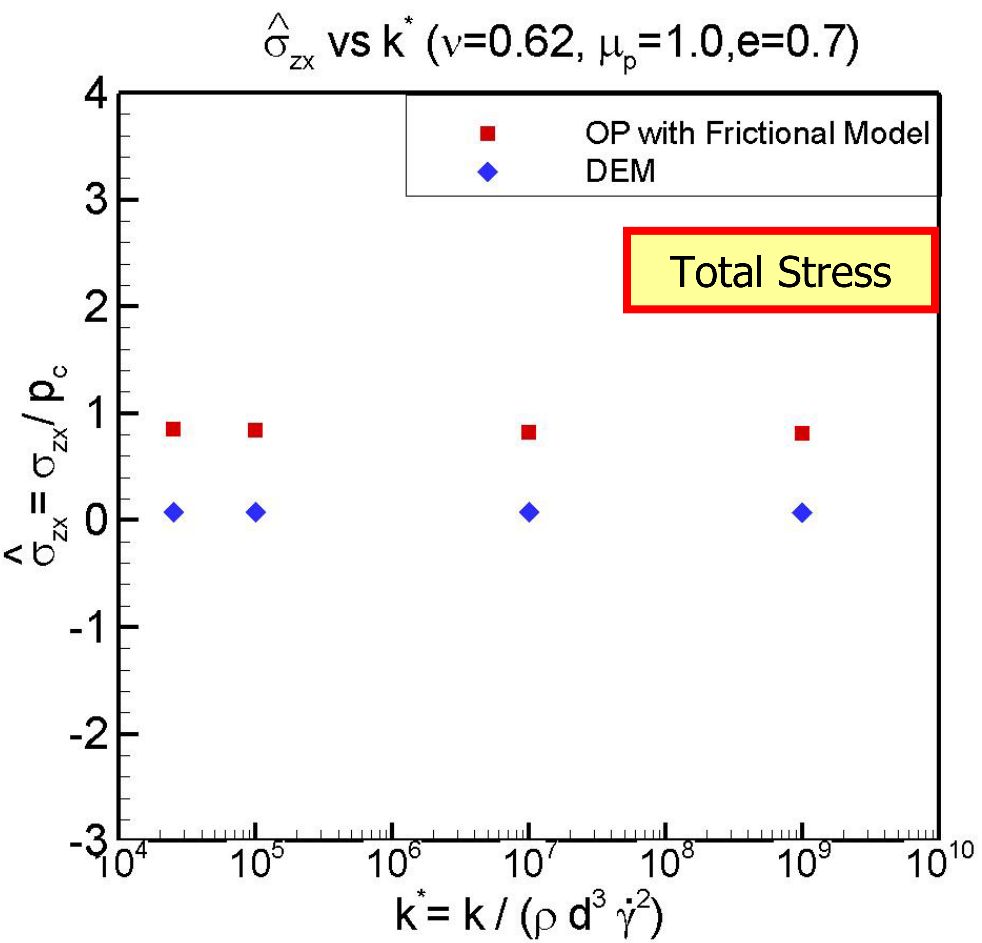
$$\boxed{\sigma_{ij} = f(\rho, \sigma_{ij}^{s})}$$

$$\boxed{\sigma_{ij}^{s} \leftarrow SSM}$$

Contribution from solidlike stress is more than 95% in the dense regime

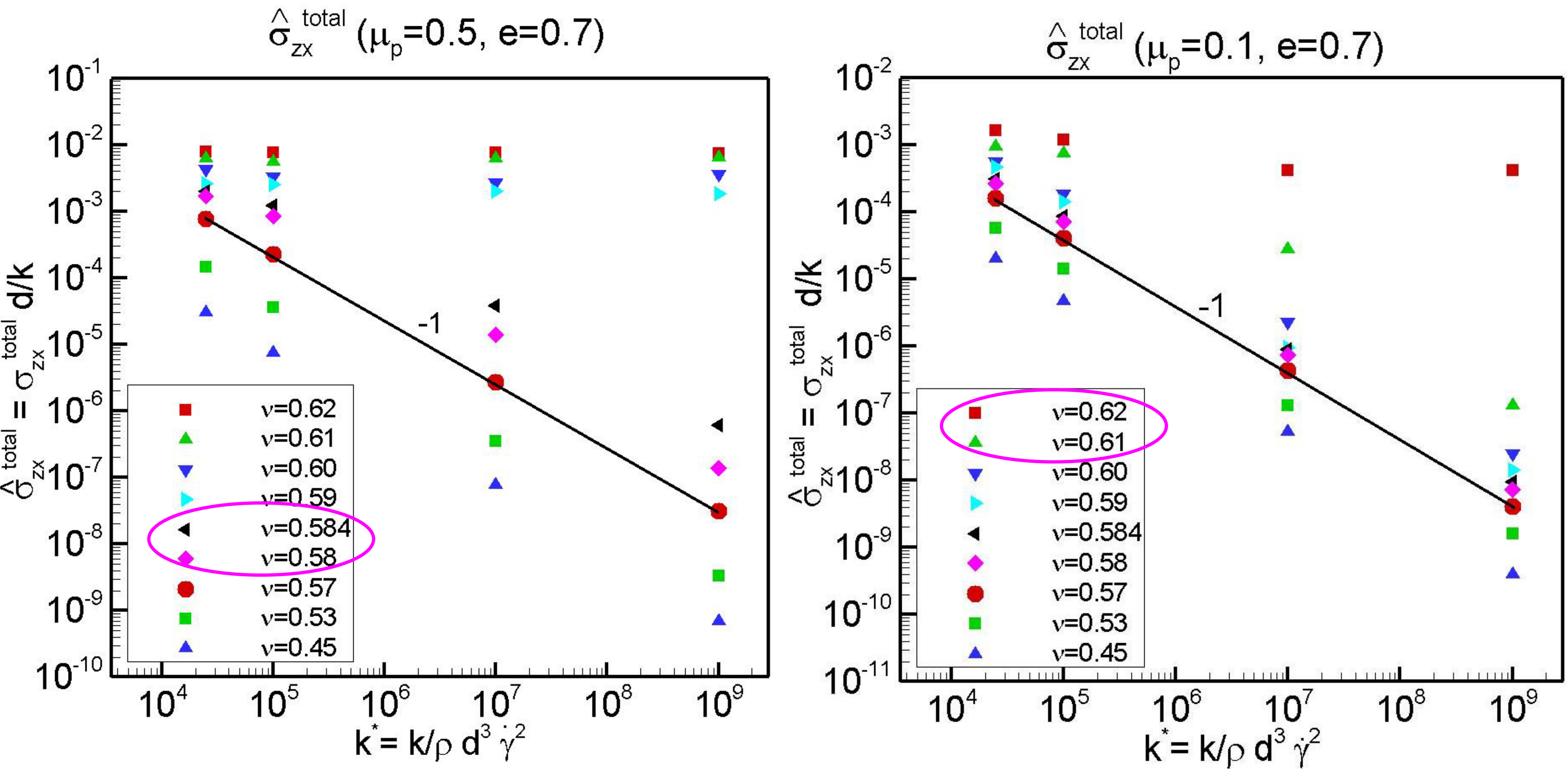
Performance of OP model coupled with SSM





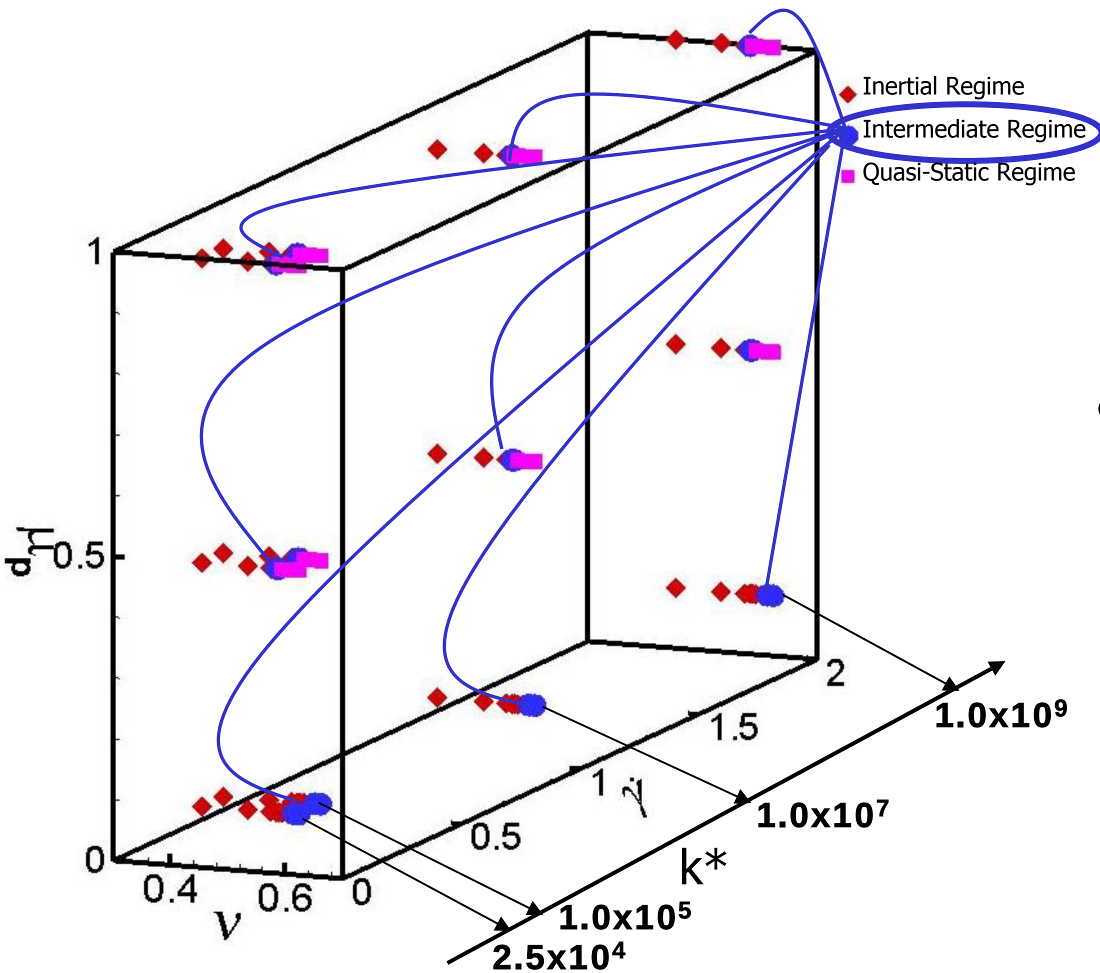
- Able to capture trend, but not magnitude
- Propose to use Princeton's "Dissipative Plasticity Model" in quasi-static regime

Identification of intermediate regime



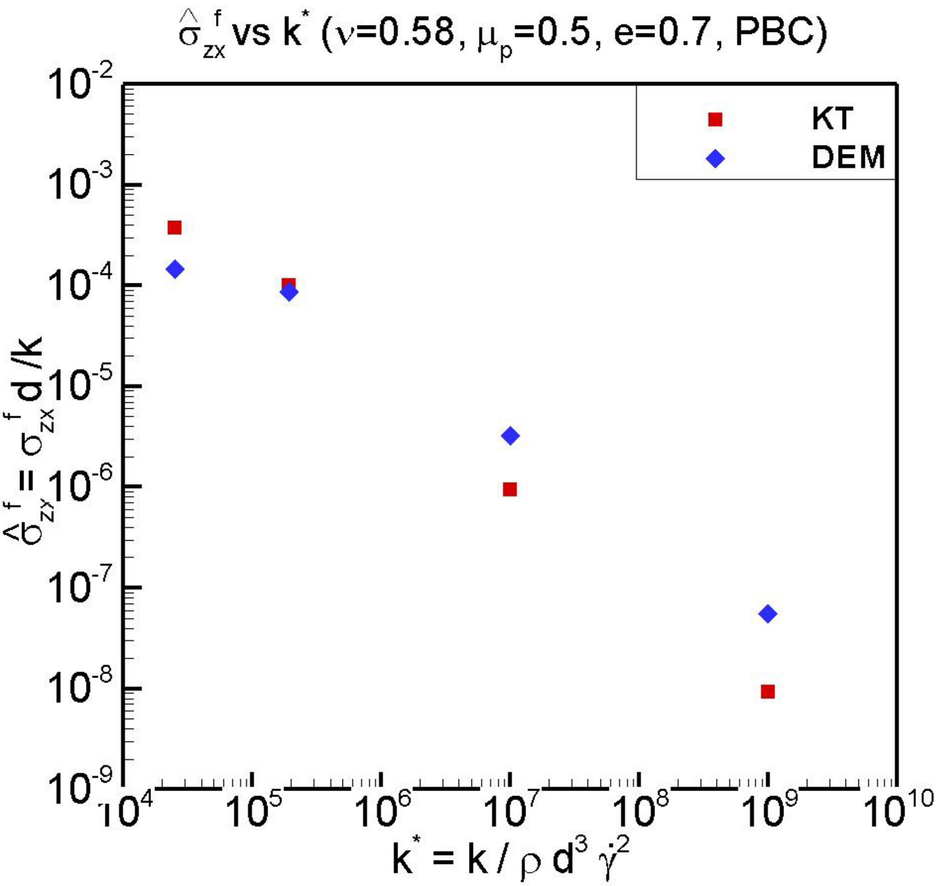
Identified range of intermediate regime using DEM data

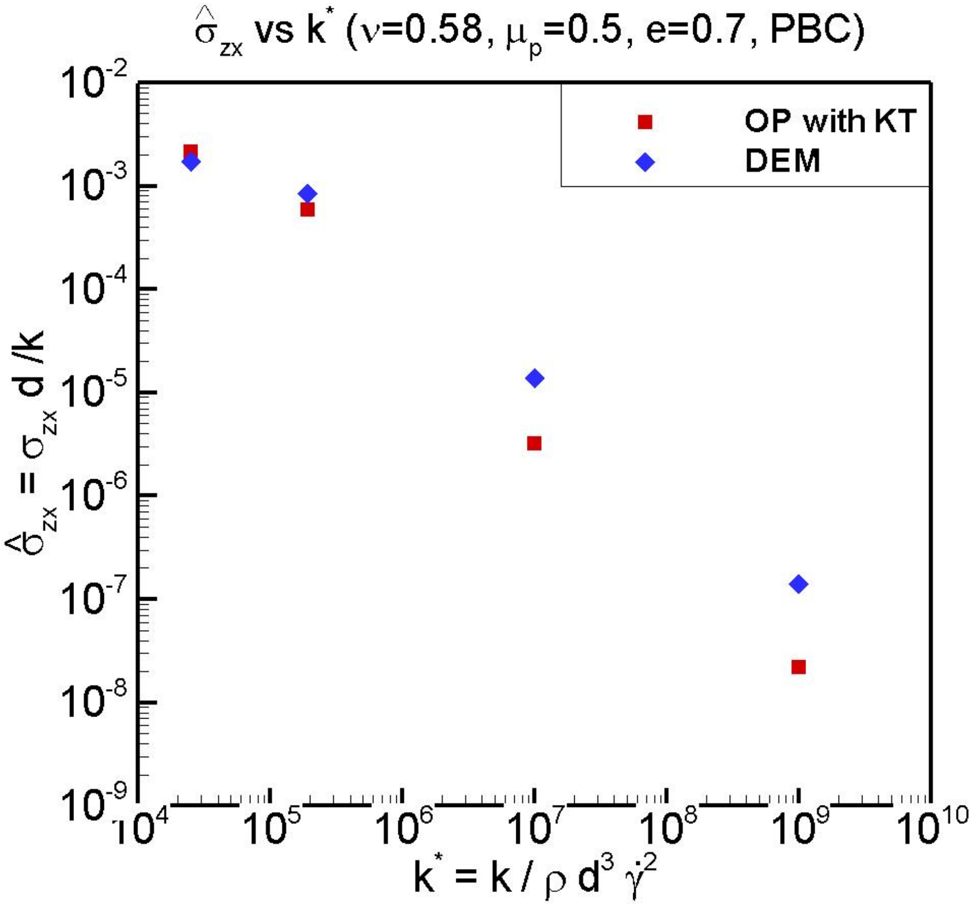
Regime map for granular flows



- Total number of DEM simulation performed
  - PBC ~ 140
  - Wallshear ~ 120
- To explore parameter space more intelligently, future plan is to use computational search tools like
  - cyber guided exploration
  - data mining ideas

ROP-KT performance in intermediate regime



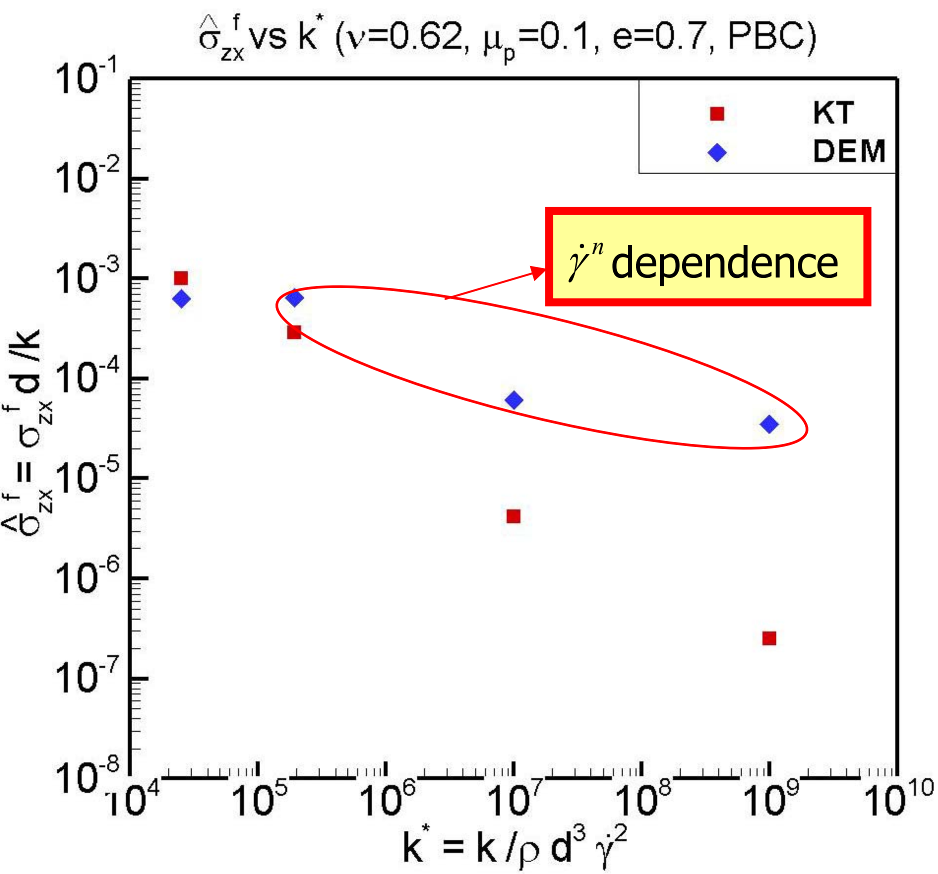


Fluidlike Shear Stress

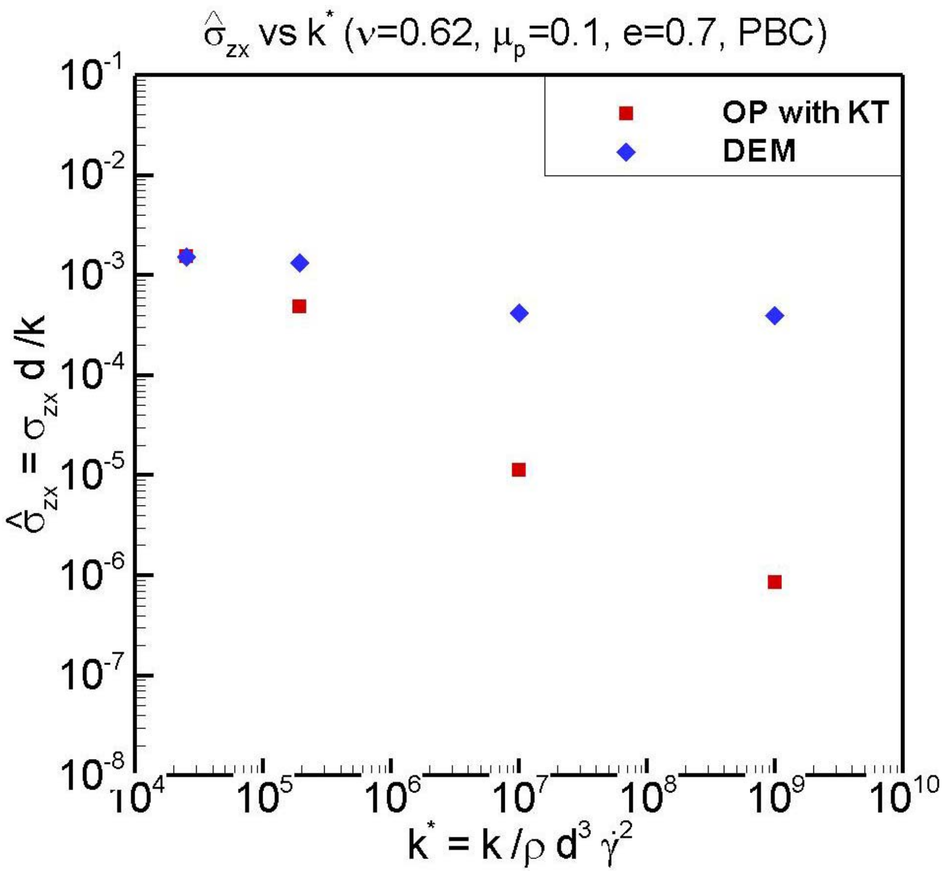
Total Shear Stress

As expected ROP-KT obeys inertial scaling and deviates from DEM in intermediate regime

ROP-KT performance in intermediate regime



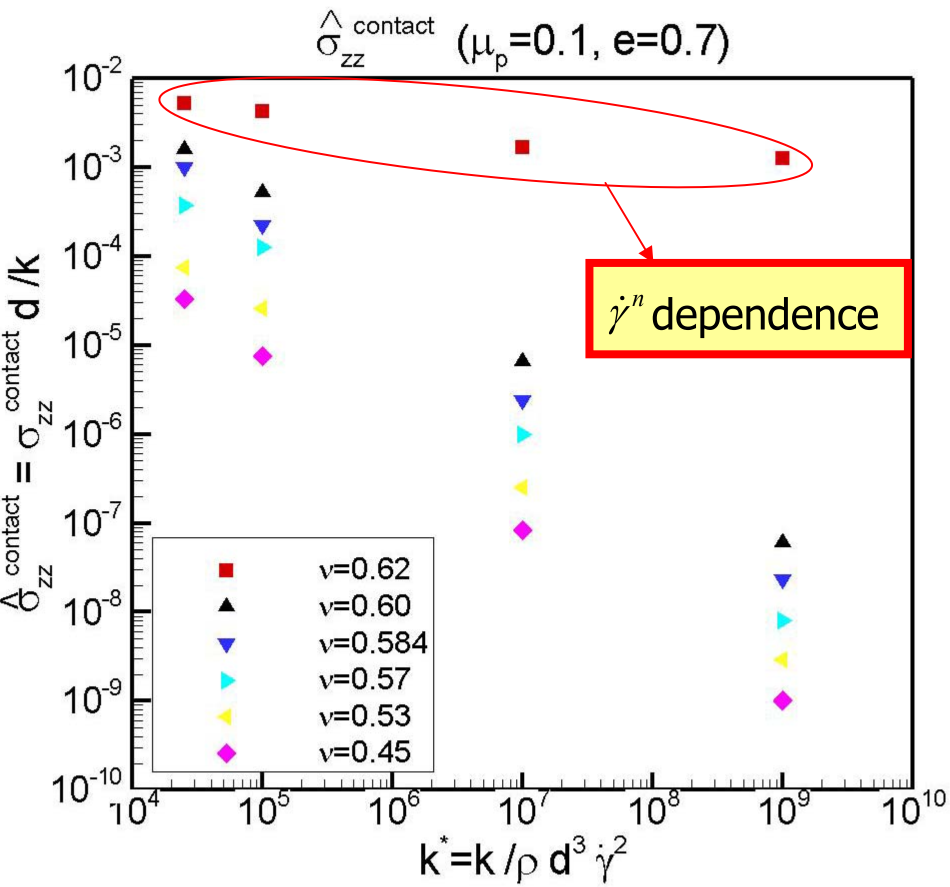
Fluidlike Shear Stress

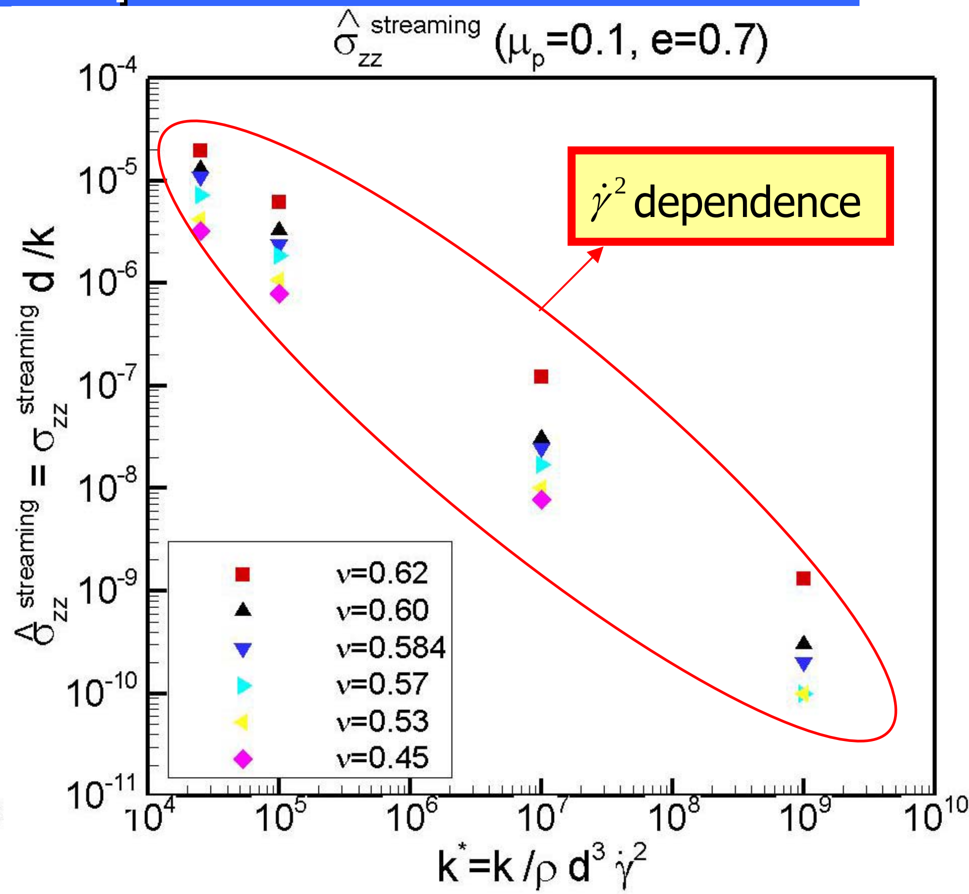


Total Shear Stress

ROP-KT model predictions deviate even more from DEM data at higher volume fraction

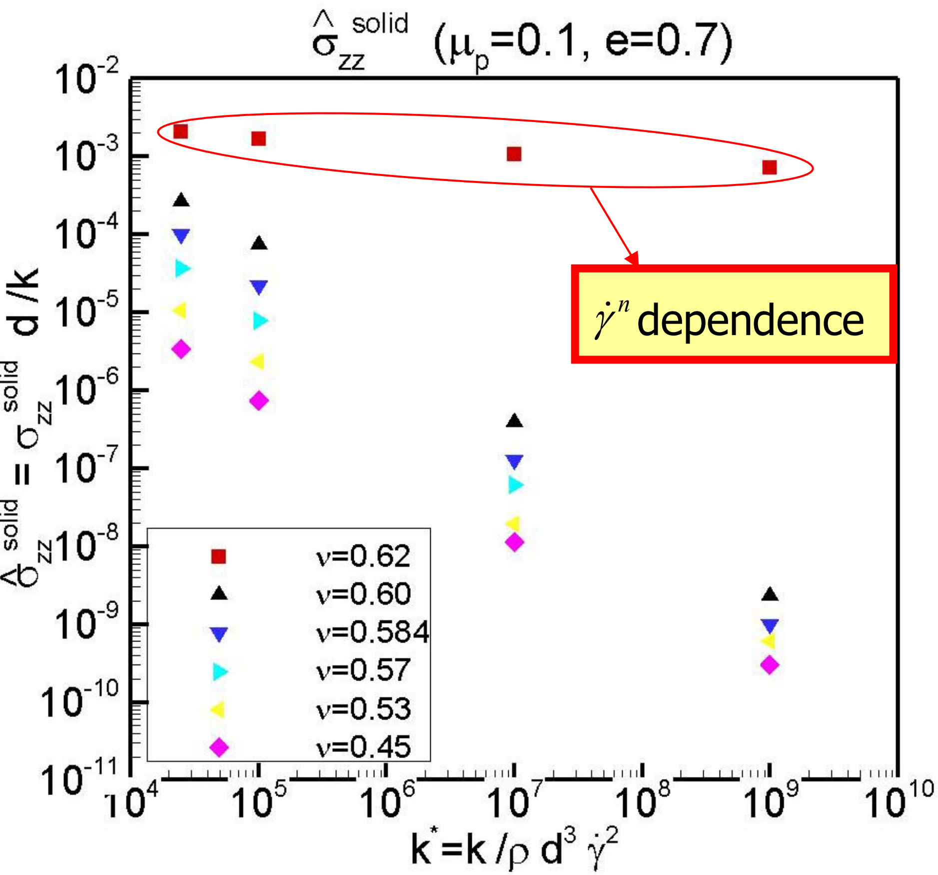
Decomposition of stresses

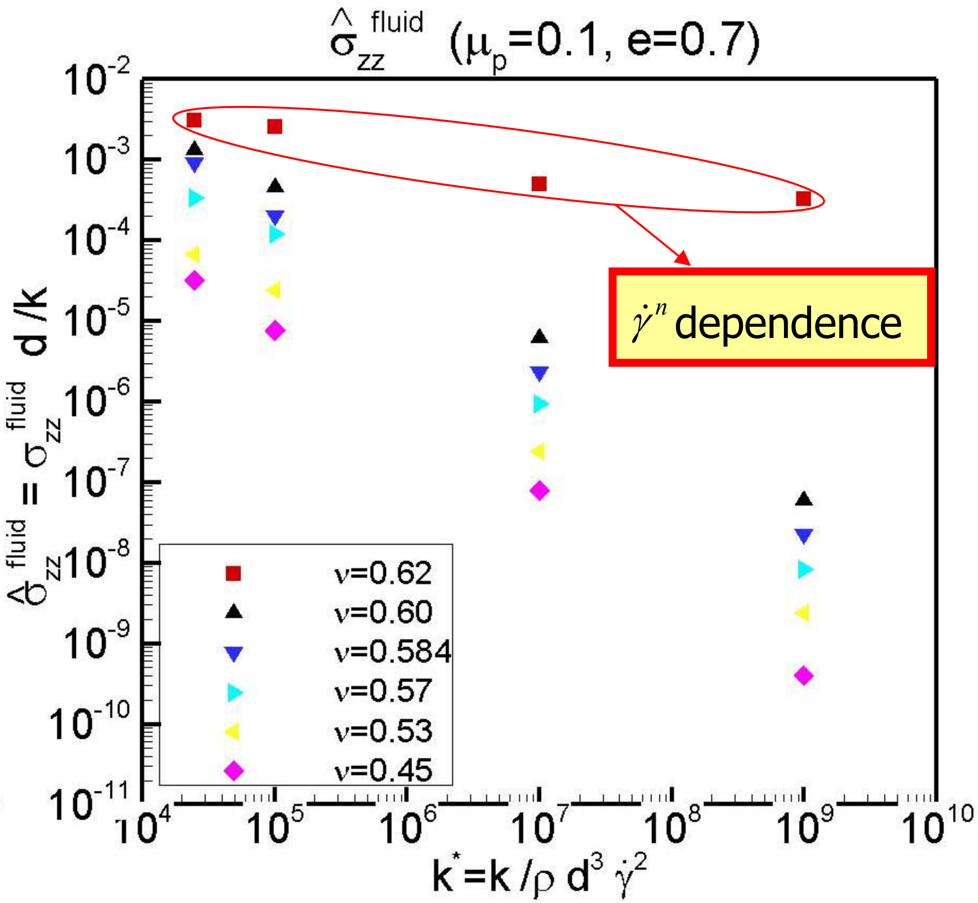




Contact (virial) part of the stress exhibits $\dot{\gamma}^n$ dependence, while streaming part exhibits $\dot{\gamma}^2$ dependence in intermediate regime

Decomposition of stresses



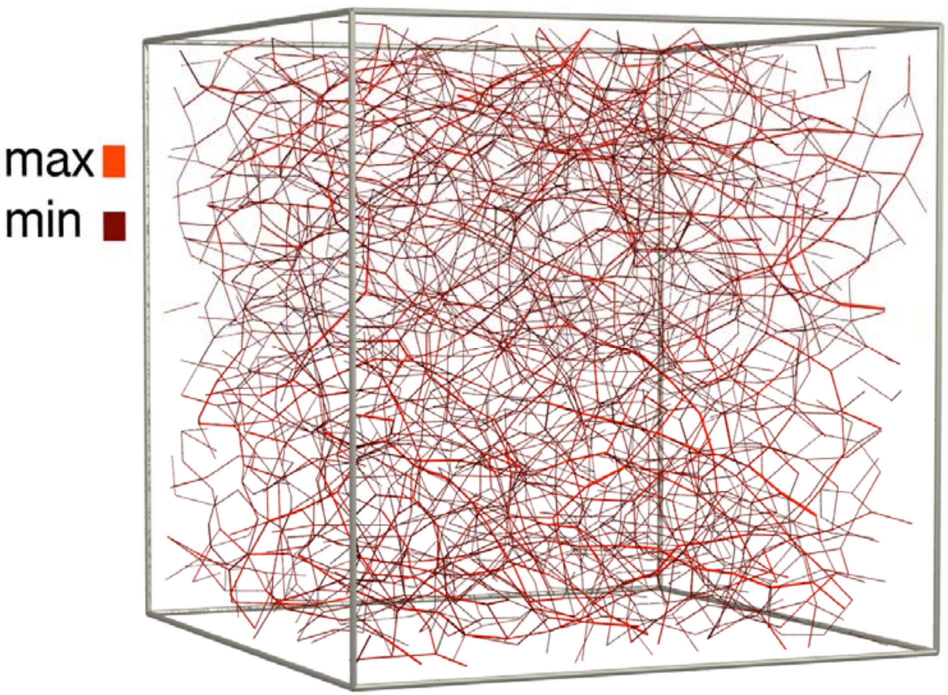


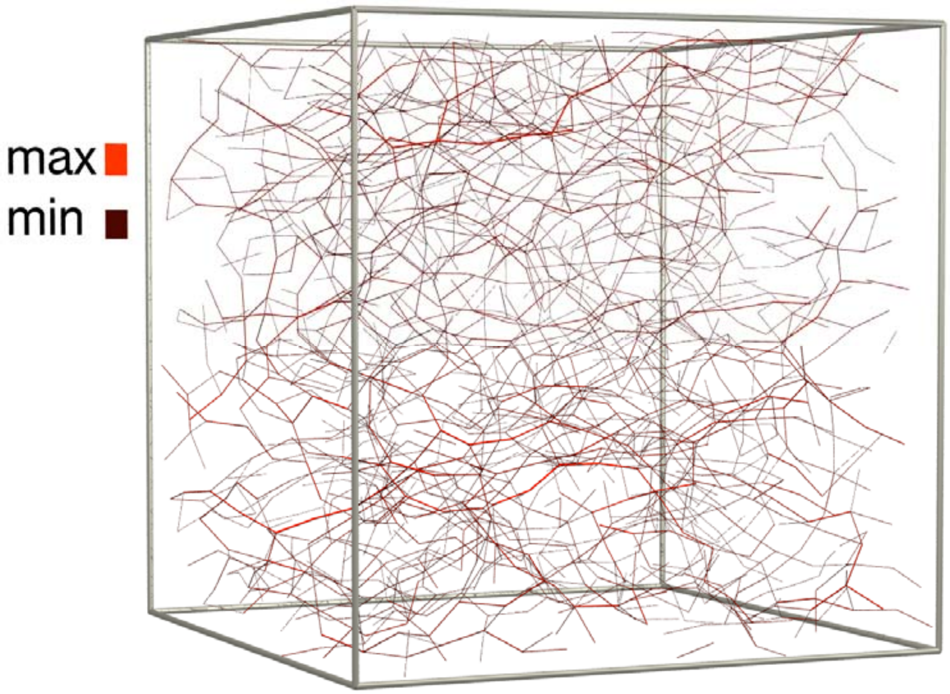
Both solidlike and fluidlike part exhibits $\dot{\gamma}^n$dependence on shear rate in the intermediate regime

Role of force networks

$\phi = 0.62, \mu_p = 0.1$

$\phi = 0.58, \mu_p = 1.0$





$$\frac{\mathbf{F_{n,max}}}{\overline{\mathbf{F_n}}} = \mathbf{5.34}$$

$$\frac{\mathbf{F_{n,max}}}{\overline{\mathbf{F_n}}} = \mathbf{4.94}$$

Strong force networks in the intermediate regime correlate with stress variation as $\dot{\gamma}^n$

Current Efforts

1. Further refinement of OP model to improve its performance in the intermediate regime
2. Study the role of force networks in intermediate regime
   - o Extract the length and time scales associated with them
3. Establish a scaling relation for the intermediate regime
4. Investigate constitutive models for non-Newtonian fluids/polymer rheology as candidates for the intermediate regime

Paper:

Vidyapati, M. Kheripour-Langrudi, J. Sun, S. Subramaniam, G.I. Tardos and S. Sundaresan, “Discrete element simulation of an assembly of spherical particles in Couette device: Quantitative comparison with experiments, In preparation, to be submitted to NETL special issue Journal (2009)

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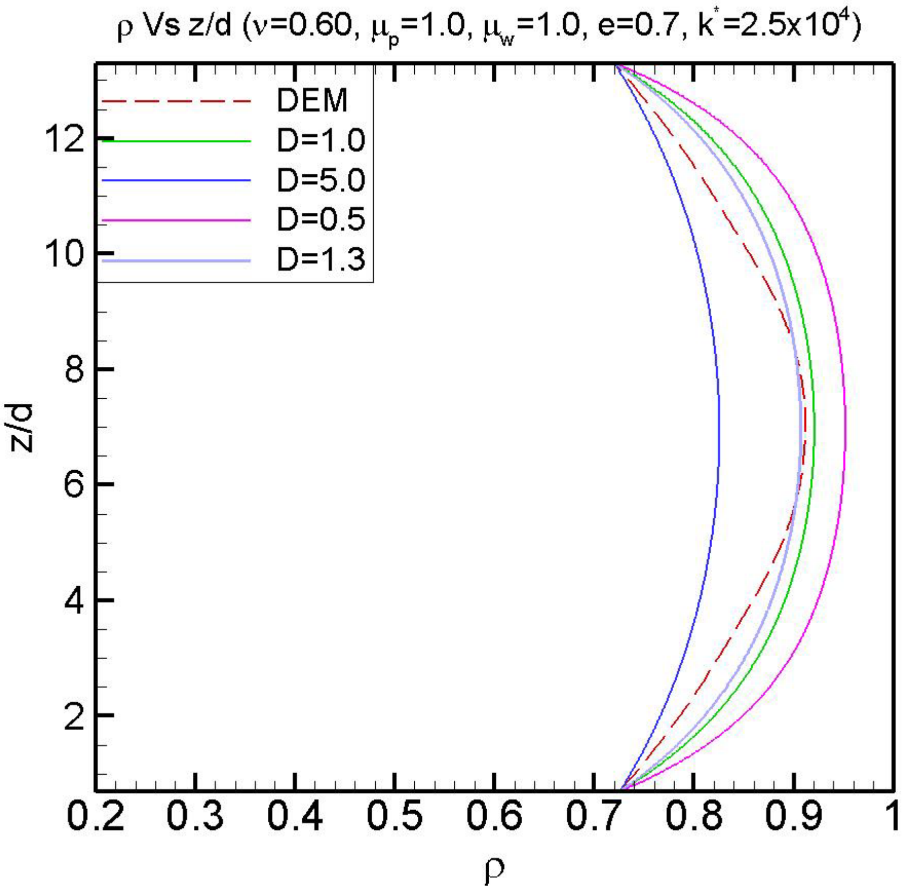
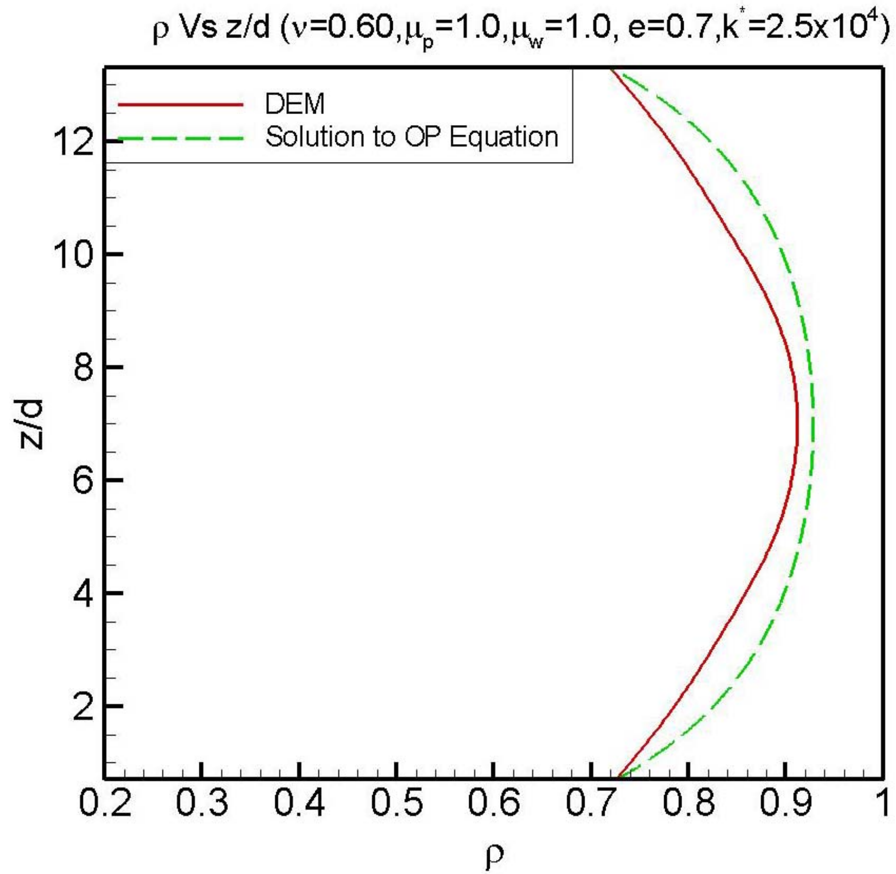
Back Up

Order parameter against channel height

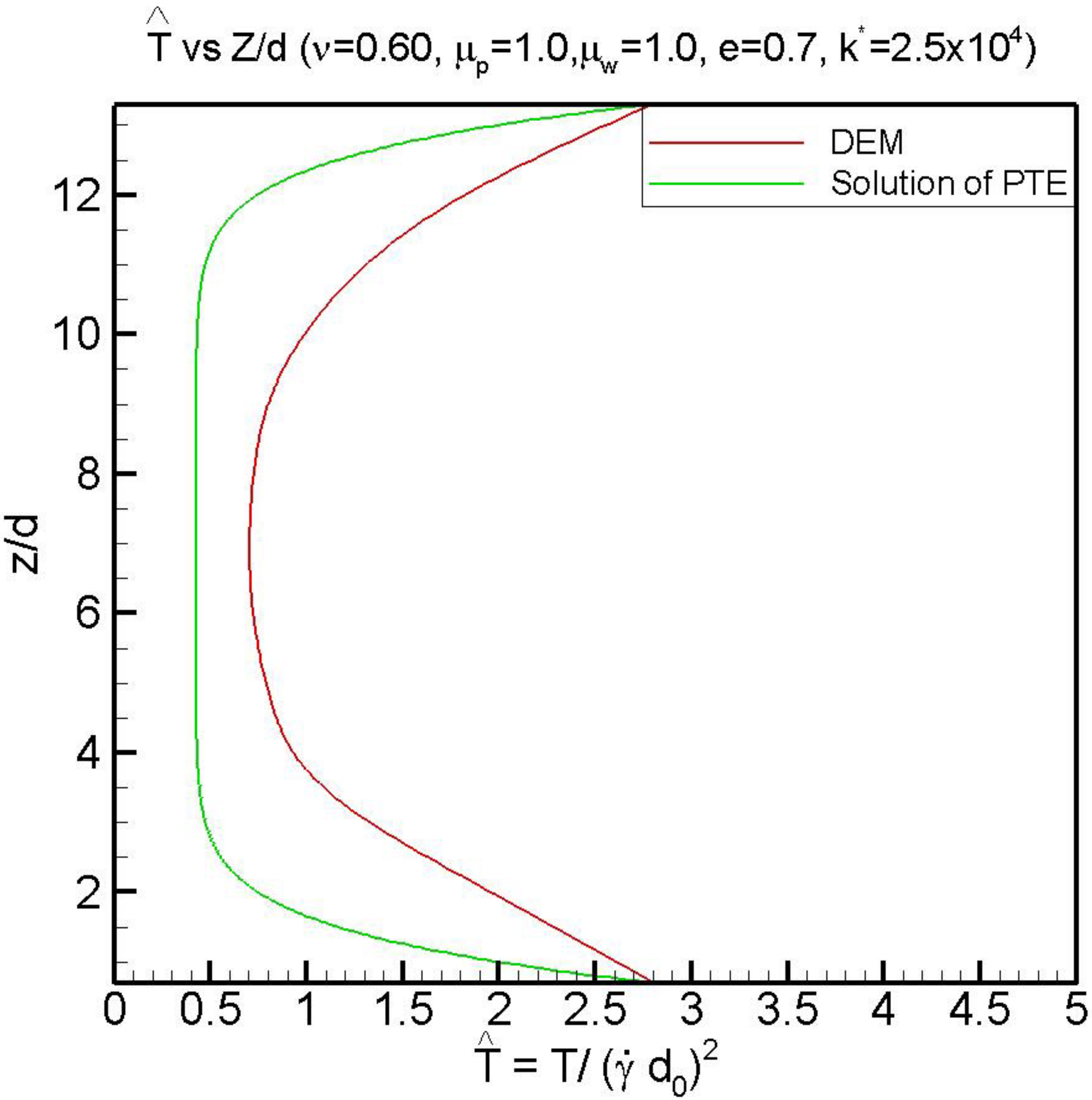




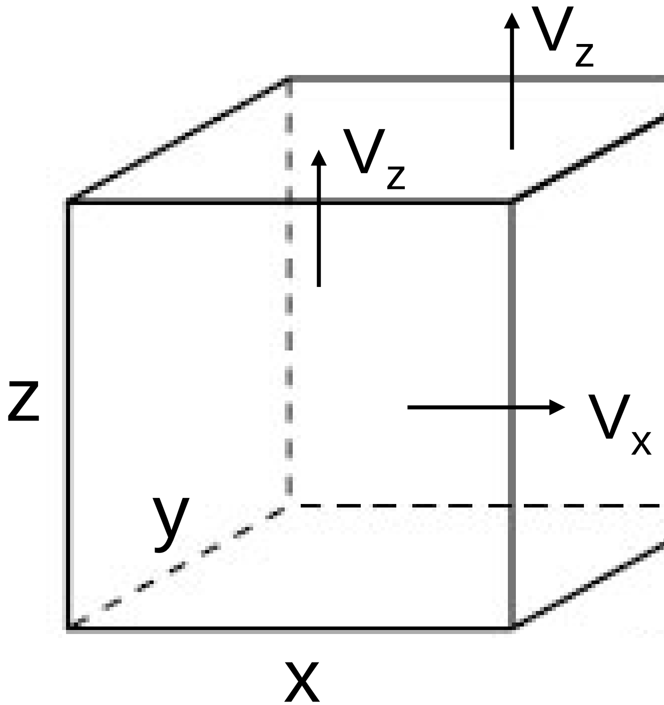
By curve fitting the diffusion coefficient

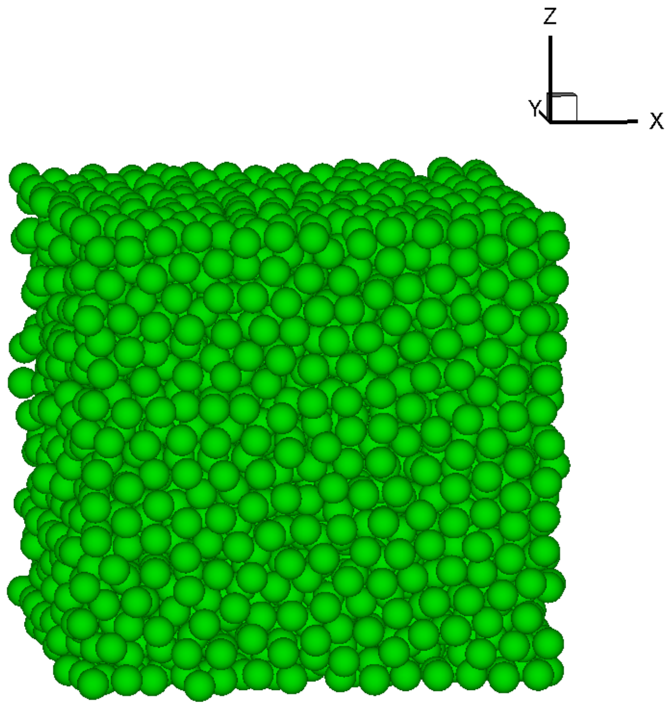
From solution of OP equation

Solution of temperature equation



Simulation of Couette device

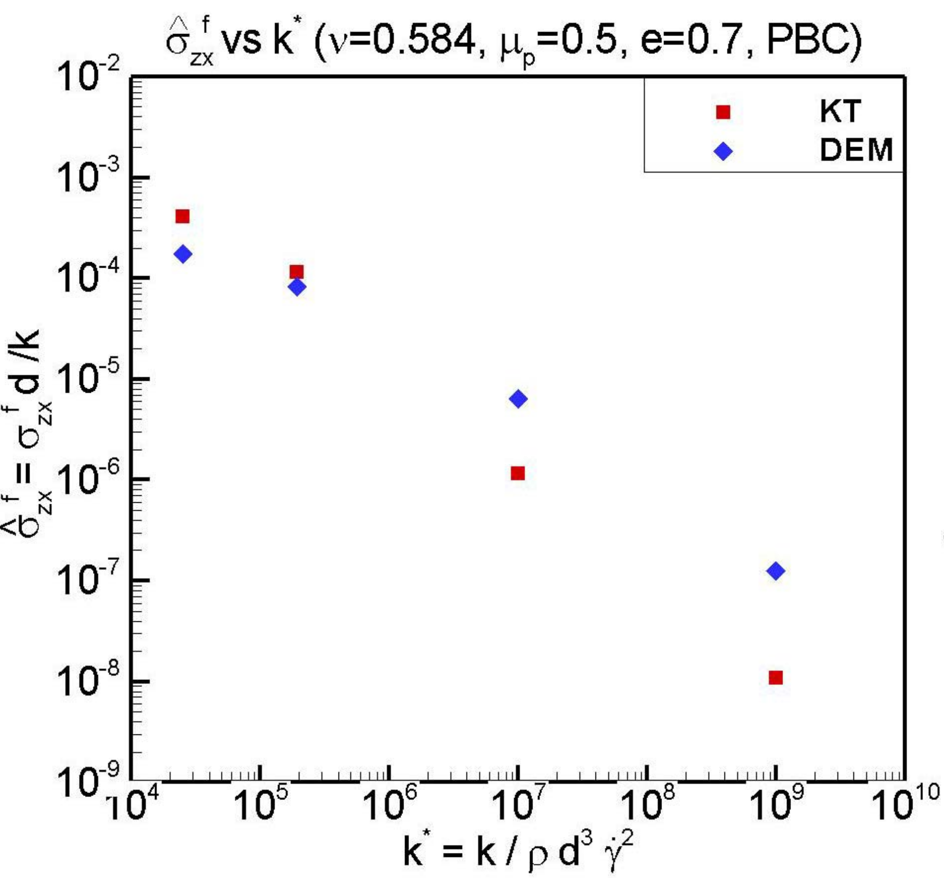




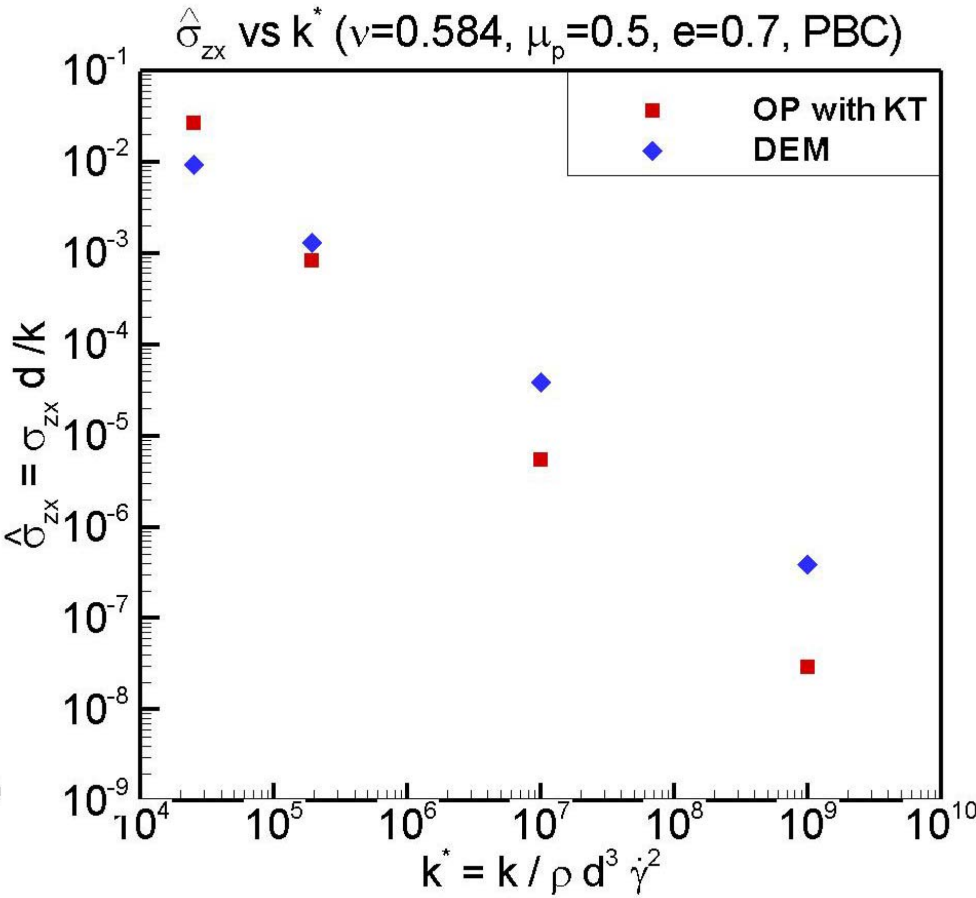
- Average stresses were measured at inner side and bottom wall, by computing forces on each wall of these walls.

- To measure the variation of stresses along the depth of granular layer, multiple sensors were placed at different heights.

OP model performance in intermediate regime

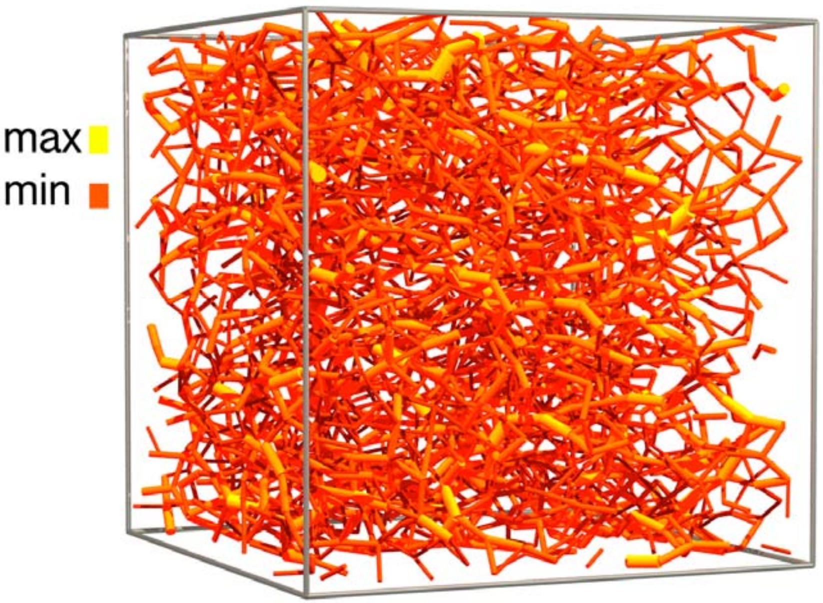


Fluidlike Stress

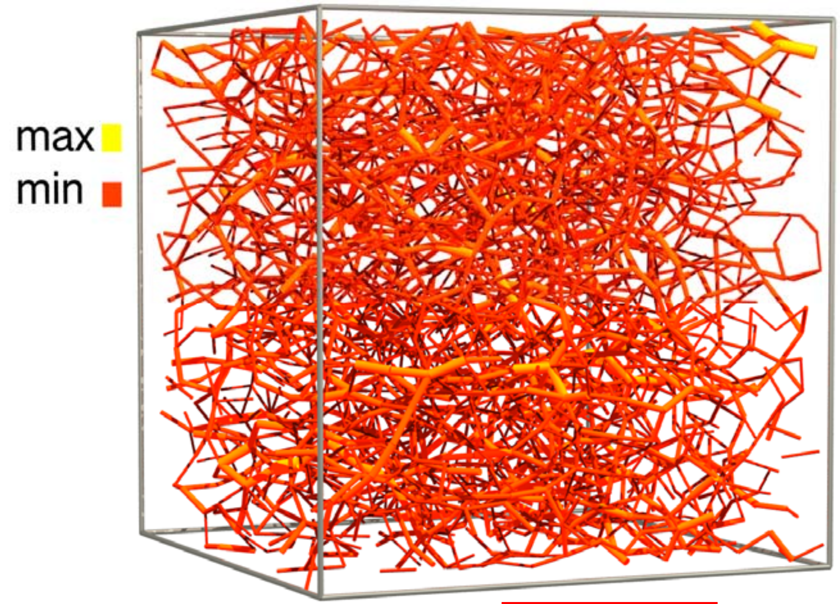


Total Stress

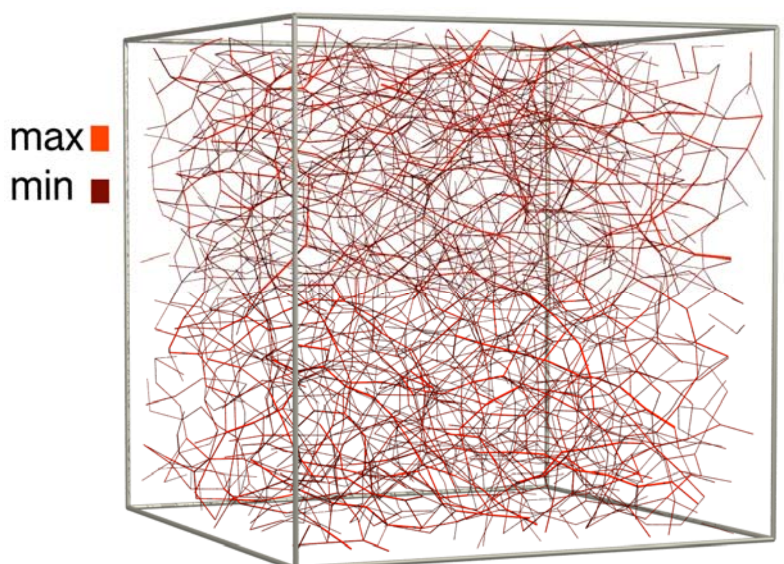
Force Network, volume fraction 0.62



$\mu_p = 1.0$



$\mu_p = 0.5$



$\mu_p = 0.1$

Simulation of Couette device

- LAMMPS code used for simulation,
- Need to resolve correct scaling for input parameters,
  - Scaling based on gravity
  - Scaling based on applied shear rate

Timescale	Gravity Based	Shear Based
t_0	$\sqrt{\dfrac{d_0}{g}}$	γ^{-1}

$$d_0 = 0.05 \text{ cm}, \quad \text{g} = 981 \text{ cm/s}^2, \; \gamma_{\max}^{-1} = 130 \text{ s}^{-1}$$

$$t_0 \text{ (gravity)} = 7.13 \times 10^{-3} s, \quad \text{t}_0 (\mathit{shear}) = 7.7 \times 10^{-3} \text{ s}$$

Timescale based on gravity (free fall time) seems to be limiting

Overview of tasks performed in year 1

- Verified numerically convergent DEM simulation and validated with existing results.
- Developed, setup and post processed “constant volume” DEM simulations of shear flow.
- Developed, setup and post processed “constant normal stress” DEM simulations of shear flow.
- Boundary effect analysis performed by simulating,
  - Flat frictional wall and roughened bumpy wall
- Constant applied normal stress simulations, compared with CCNY overburden experiments: Similar trends were observed.

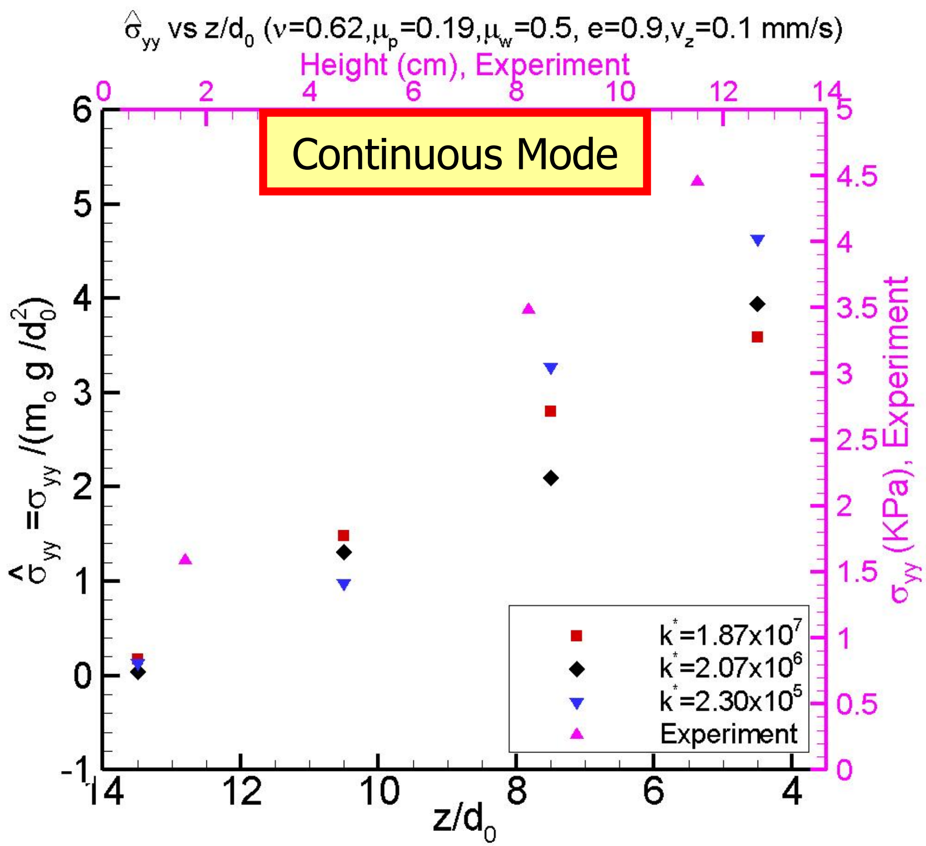
Overview of tasks for year 2

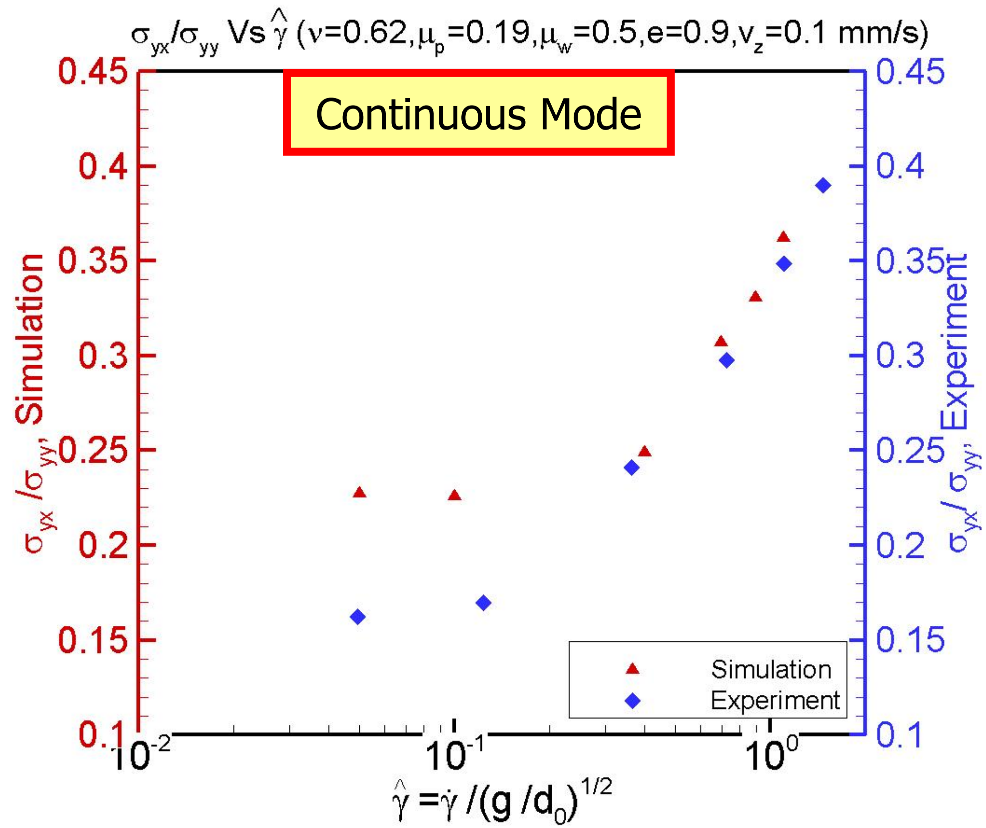
- Assessment of order parameter based continuum model using DEM data
  - Extraction of order parameter and new model coefficients from 3D DEM simulation
- Refinement of order parameter based continuum model
  - Coupling it with KTGF (ROPKT)
  - Coupling it with solid stress model (ROPSSM)
- Assessment of refined OP model for all regimes of granular flow i.e. inertial, intermediate and quasi-static regime.
- Comparison of DEM results with experimental data
  - Simulation of Couette device using DEM code

Highlights of Results

1. Extraction of order parameter, new model coefficients calculation from 3D DEM data and validation with existing results.
2. Refined OP model coupled with KTGF predicts correct stresses in the inertial regime, but fails to capture the entire intermediate regime.
3. Identification of exact intermediate regime by DEM data.
4. Decomposition of stresses and force network analysis gives physical inside of intermediate regime.
5. Simulations performed with Couette device exhibits the similar trends as in experiments.

Simulation of Couette device





Stress varies linearly against depth of the granular layer

Ratio remains constant at lower shear rates and equal to friction coefficient