Discrete Element Simulation and Modeling of Dense Granular Flows

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NETL Workshop on Multiphase Flow Science 2010

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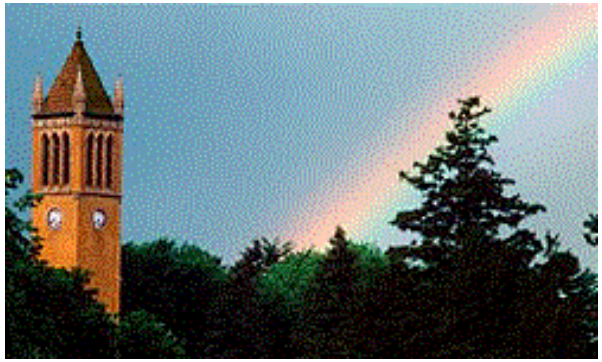


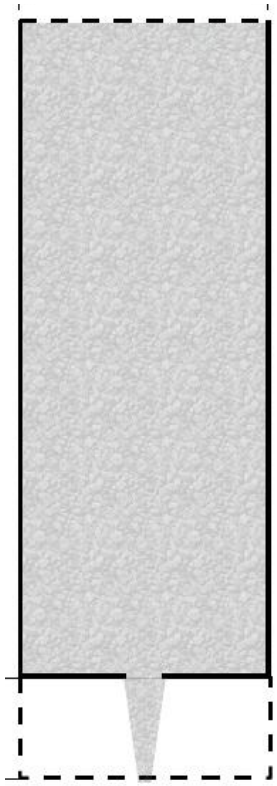
Funding: *DE-FG26-07NT43070* UCR

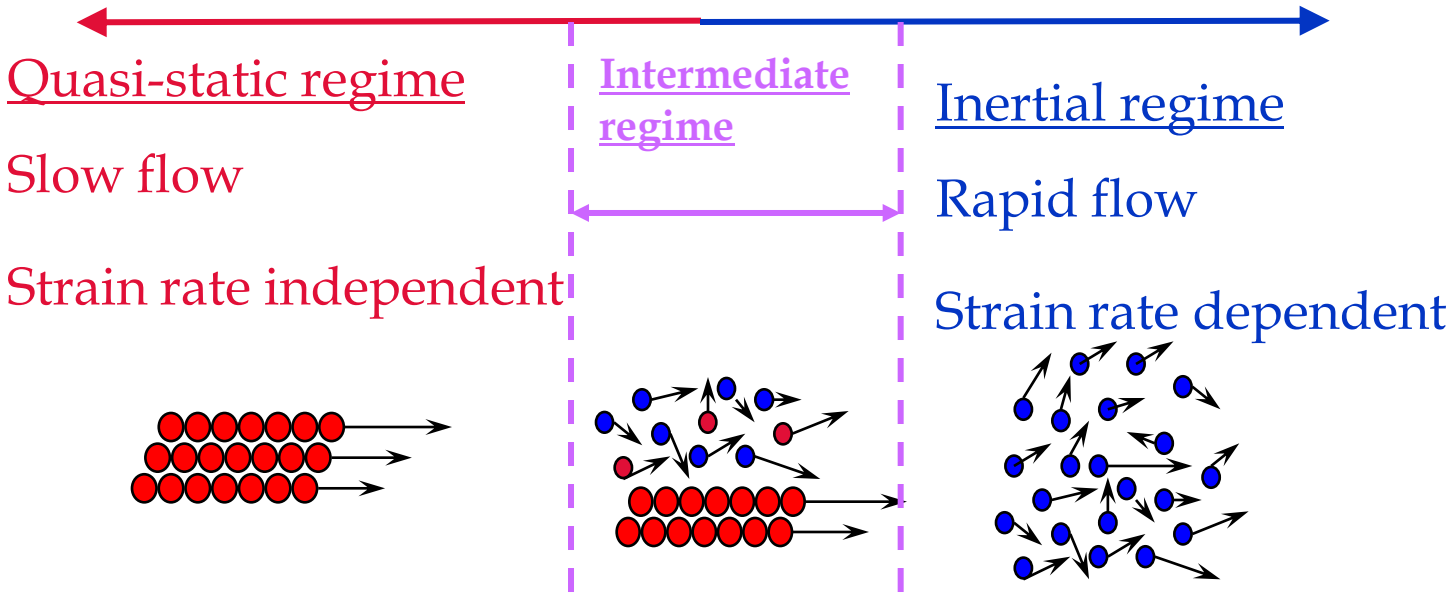
Outline

- Couette cell simulations
  - Established regime transition observed in experiments
  - Database for continuum model assessment
- Homogeneous shear simulations
  - Established intermediate regime map for granular flows
- Silo simulations
  - Assessment of existing continuum models
  - Comparison with experiments
- Inhomogeneous wall shear simulations
  - OP model development and validation

Regime transition in granular flows

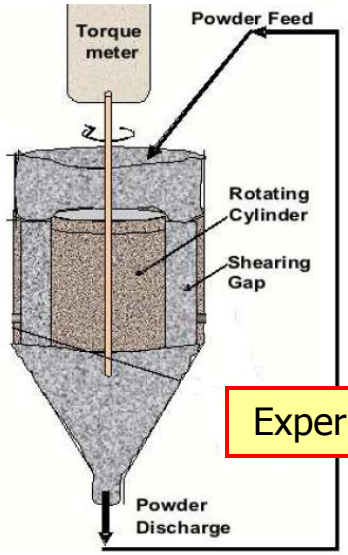
- Dense flow in hoppers, discharge from bins
  - Regime transitions are not sharp
  - Need physics-based models for transitional regime



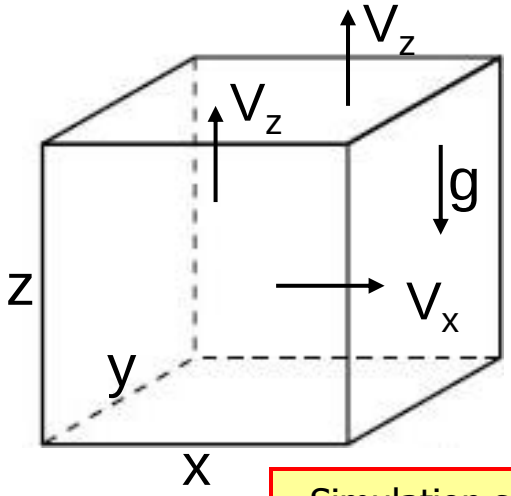


Experiments and DEM simulations reveal that this regime spreads over a range of volume fraction, friction coefficient and shear rate

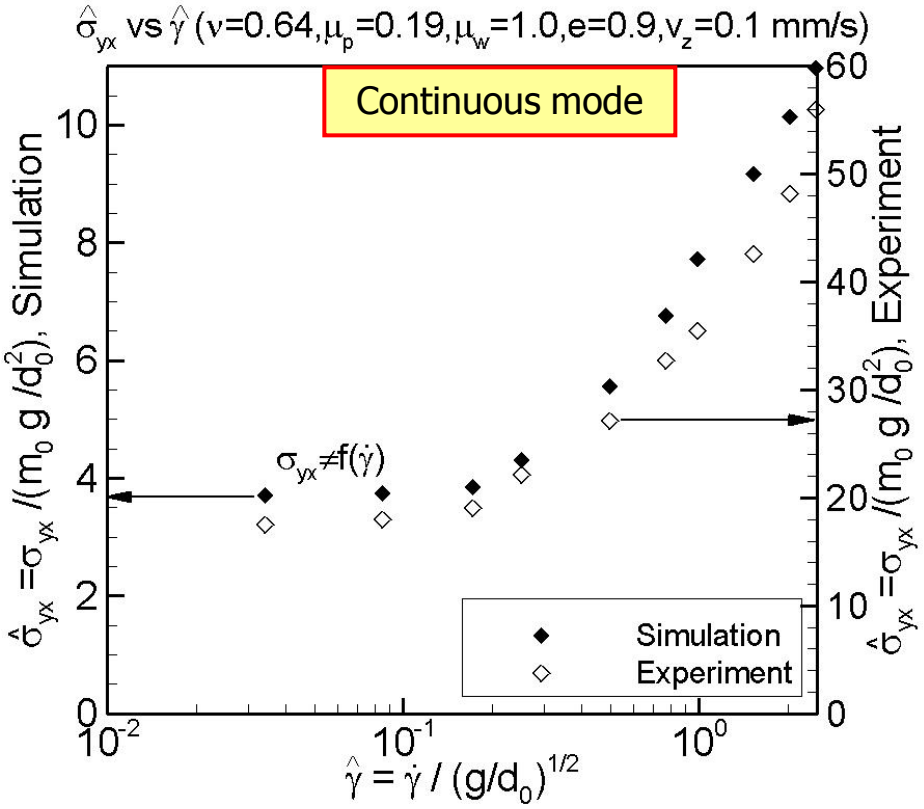
Regime transition in Couette cell



Experimental setup



Simulation setup

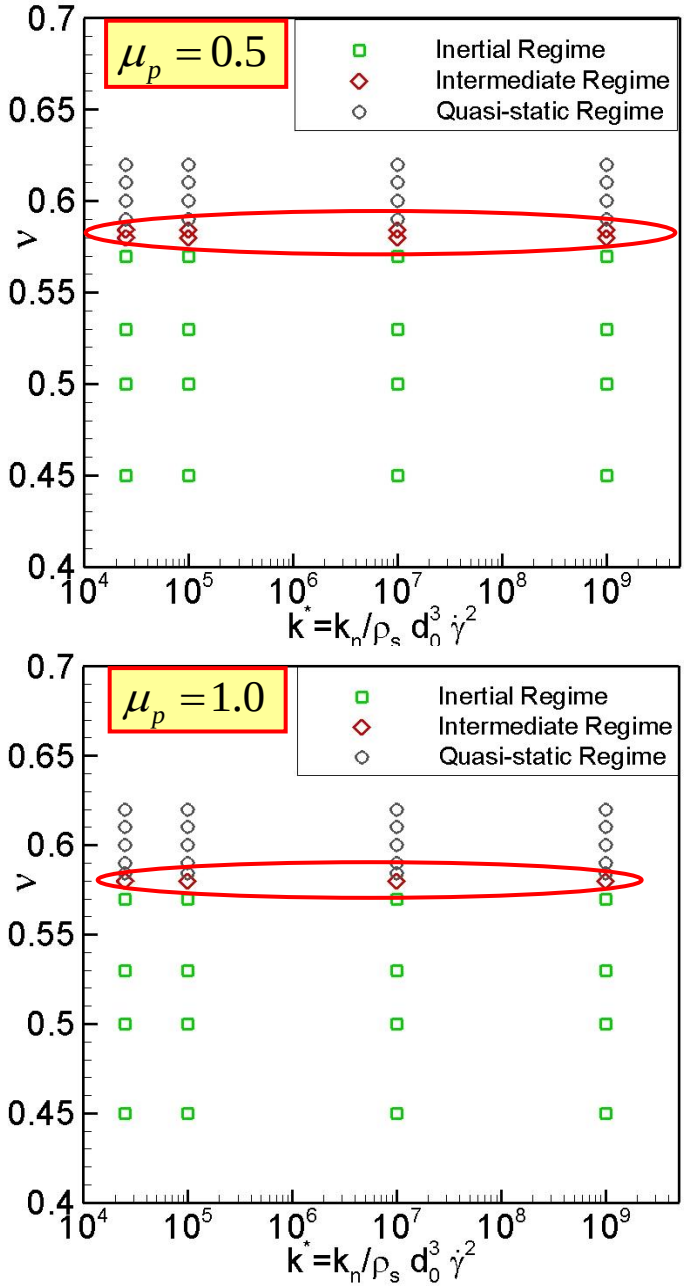


Two distinct regimes present in the flow: quasi-static and intermediate

Vidyapati, M. Kheiripour, J. Sun, S. Sundaresan, G.I. Tardos and S. Subramaniam, *Discrete element simulation of an assembly of spherical particles in Couette device: Comparison with experiments*, In preparation, to be submitted to Powder Technology Journal

Regime map for granular flows

- Identified different regimes of granular flow through DEM simulations of homogeneous flows
  - Identified intermediate regime between quasi-static and inertial (rapid flow) regime
  - Identification based on power law dependence of shear stress on shear rate ($\sigma \propto \dot{\gamma}^n$, with 0<n<2)
  - Experimental results* also verify the existence of the intermediate regime which spans over a range of solid volume fractions and shear rates



Tardos et al., Powder Technology, vol. 131, 2003

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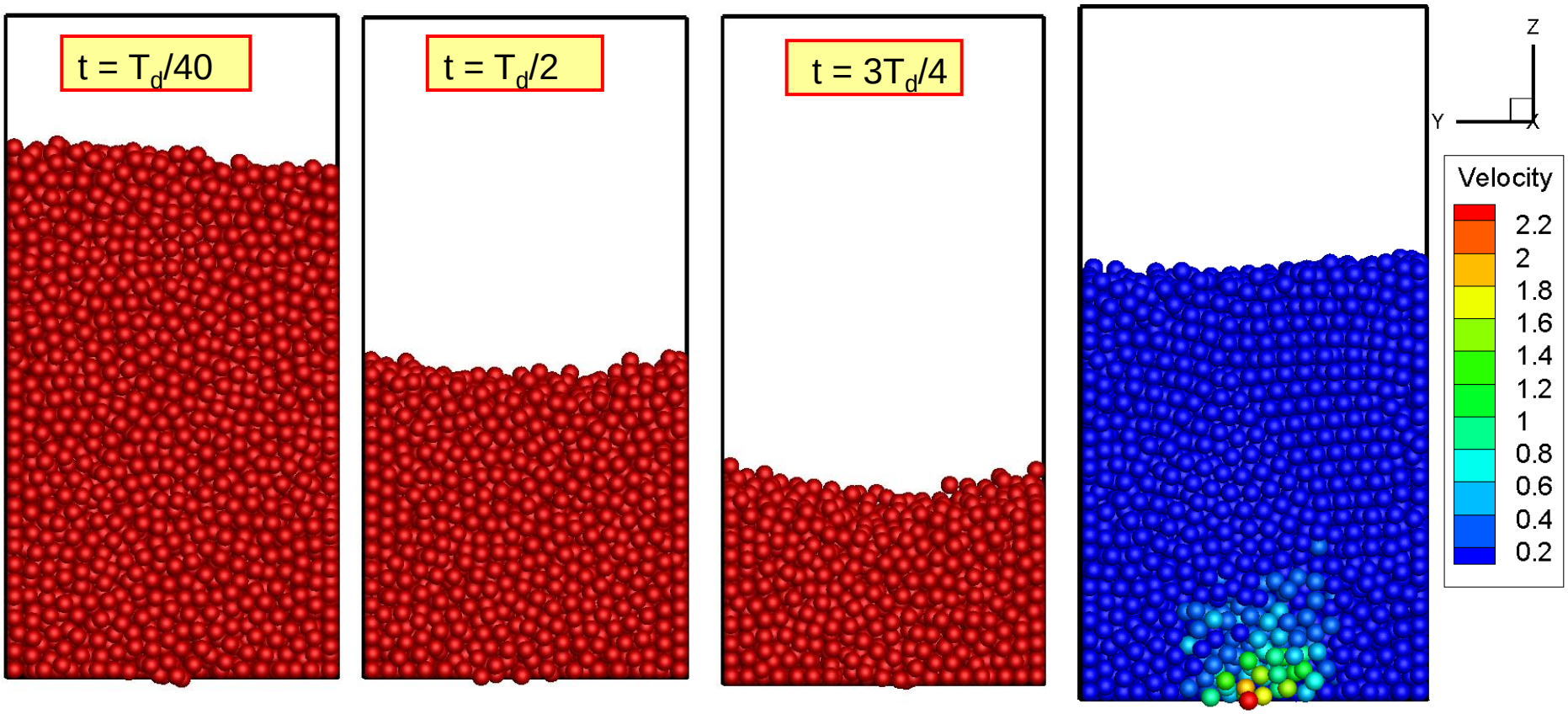
DEM simulation of flat-bottomed silo

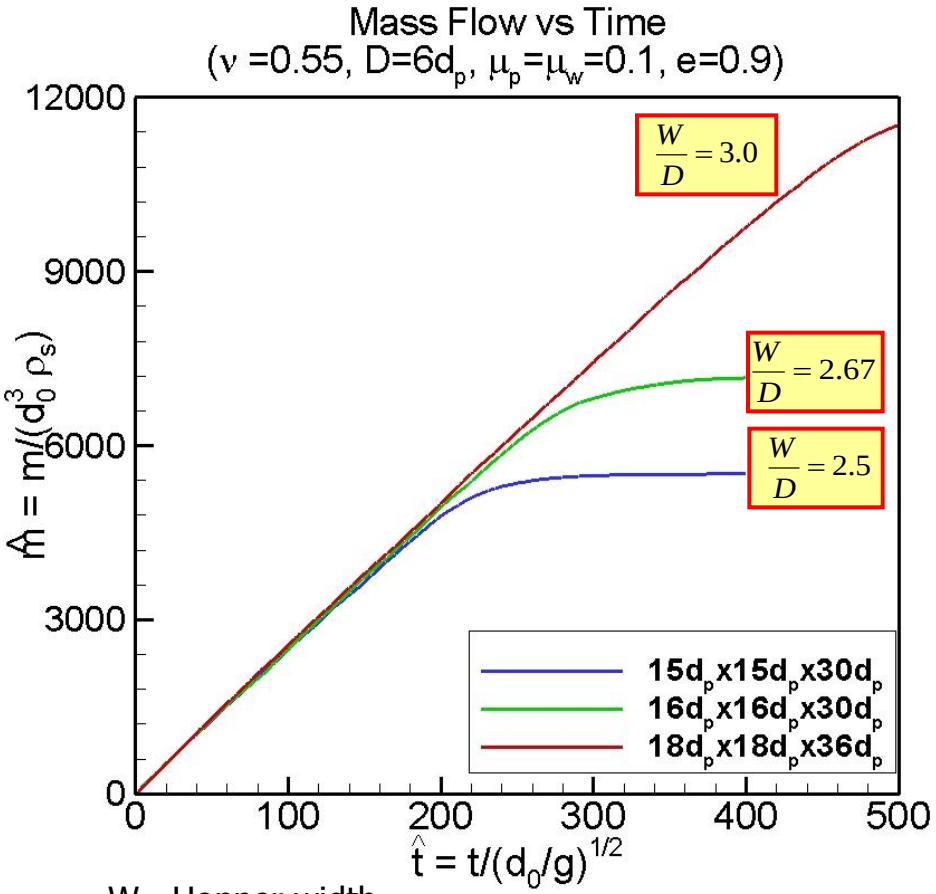
Domain size :$18d_p x 18d_p x 36d_p$

Discharge size (D): $6d_p$



T_d is discharge time scale

Effect of domain size on discharge rate



W Hopper width
D Discharge outlet size
d_p Particle diameter

- Discharge rate obtained from DEM study was compared with Beverloo's correlation

d_p= 0.05 cm, ρ= 2300 kg/m^3, D=6d_p

- Beverloo's correlation

$$\dot{m} = 0.58\rho_b g^{0.5}(D - kd_p)^{2.5}$$

= 4.8x10^{-4} kg/s

- Current DEM study

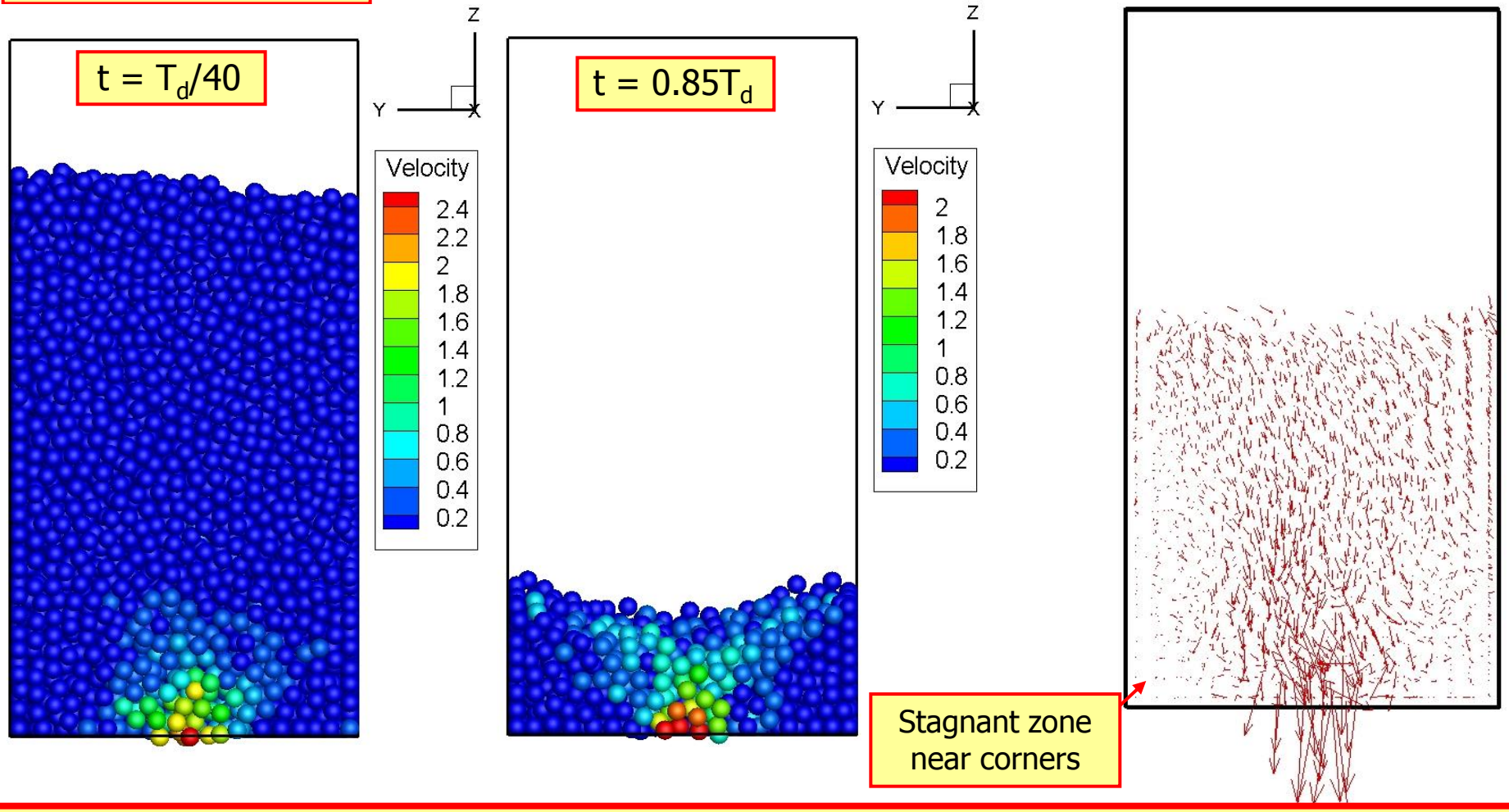
= 7.2x10^{-4} kg/s

Discharge rate is independent of silo dimensions as long as,

W/D>2.5

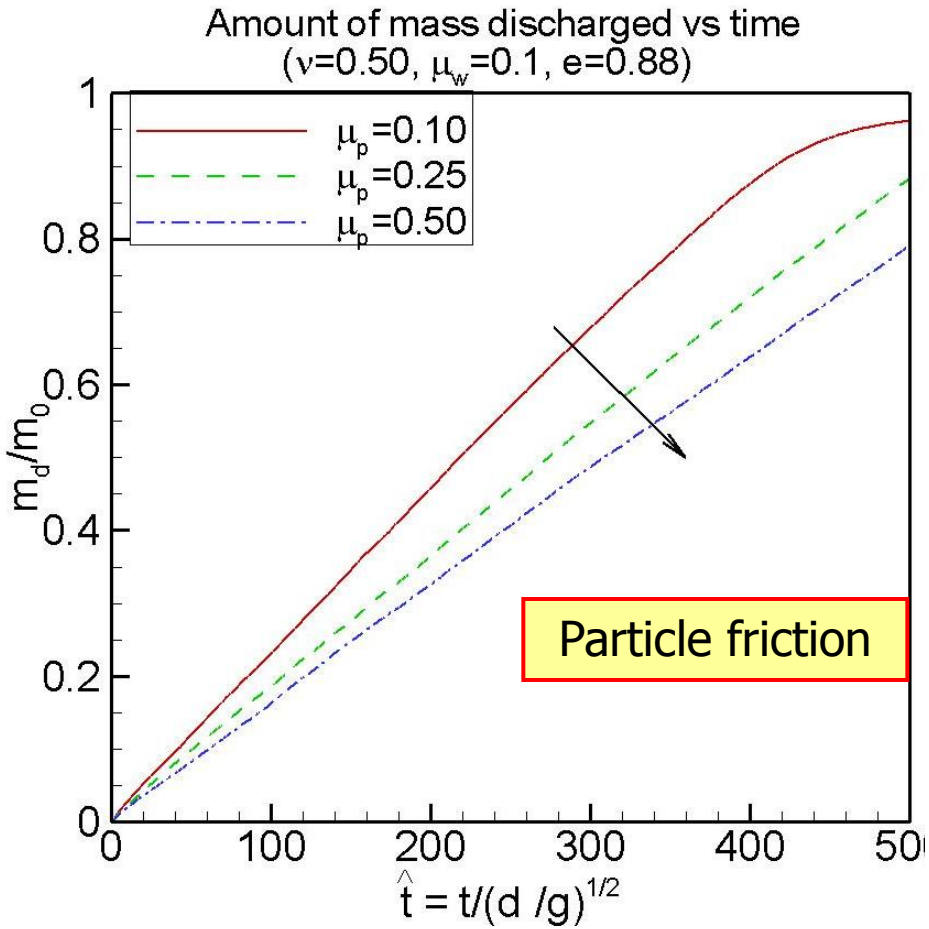
Snapshot of particle velocity magnitude

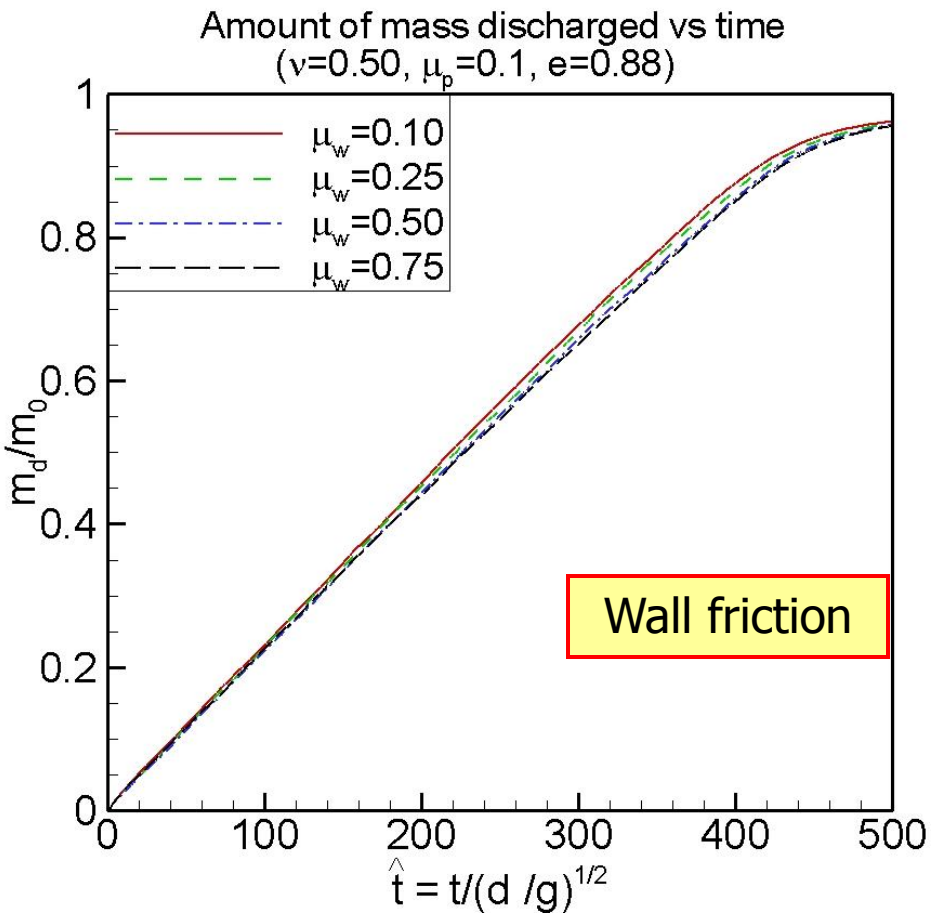
$$v = \sqrt{v_x^2 + v_y^2 + v_z^2}$$



DEM is able to capture the experimental observation of formation of stagnant zone near the silo corner

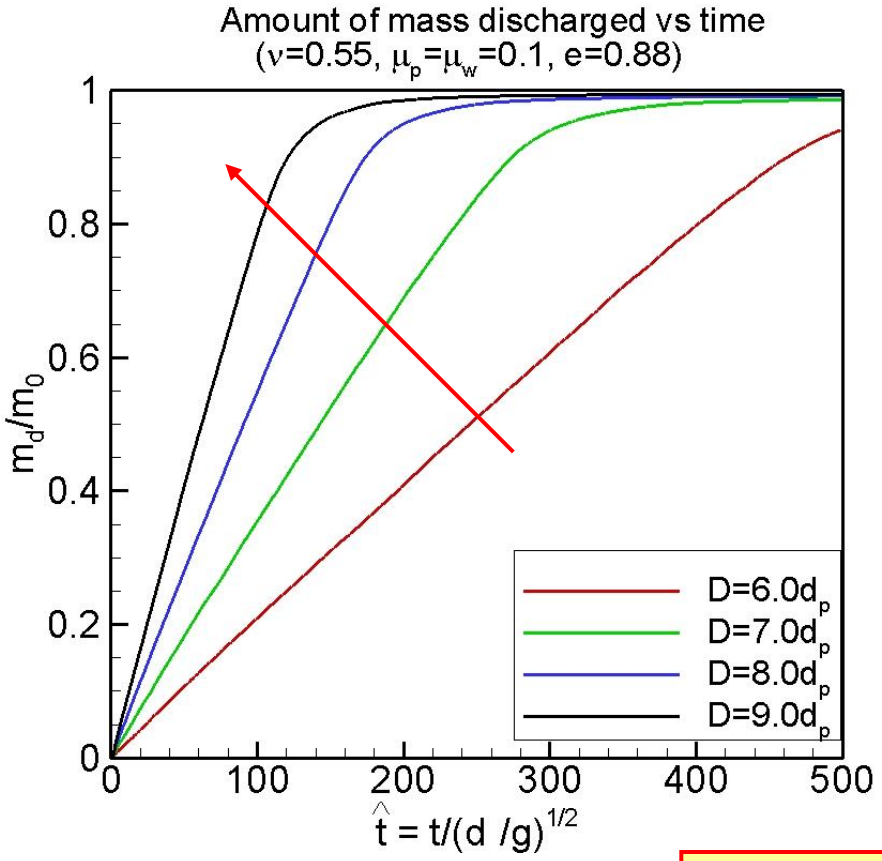
Effect of friction on discharge rate

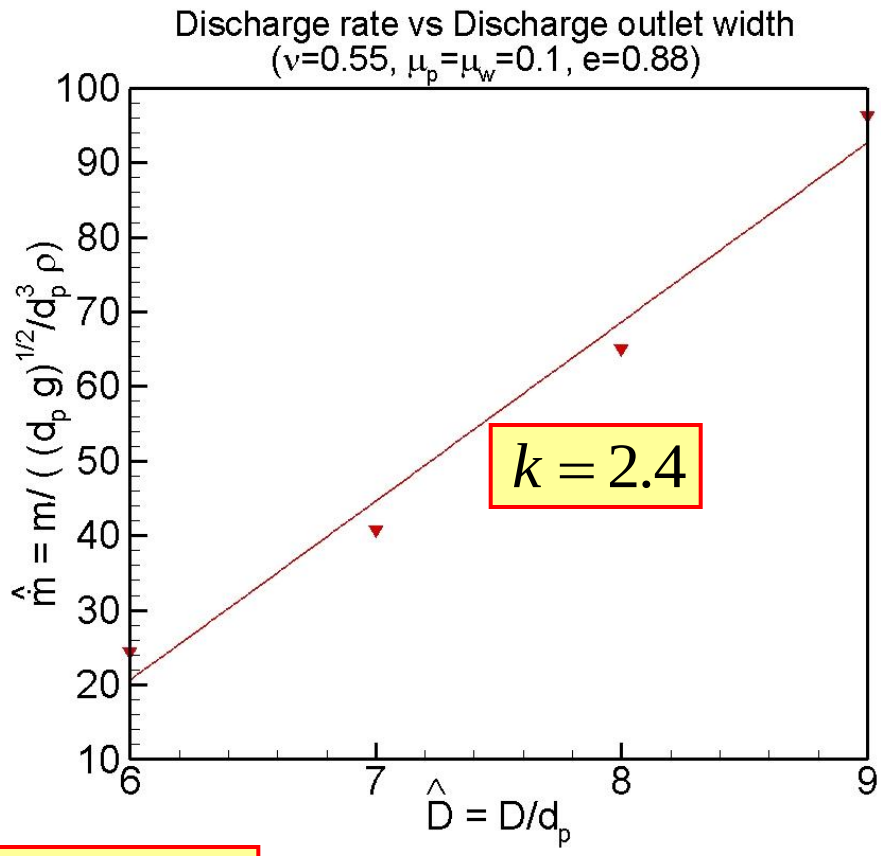




Discharge rate is almost independent of the wall friction coefficient

Effect of discharge outlet size

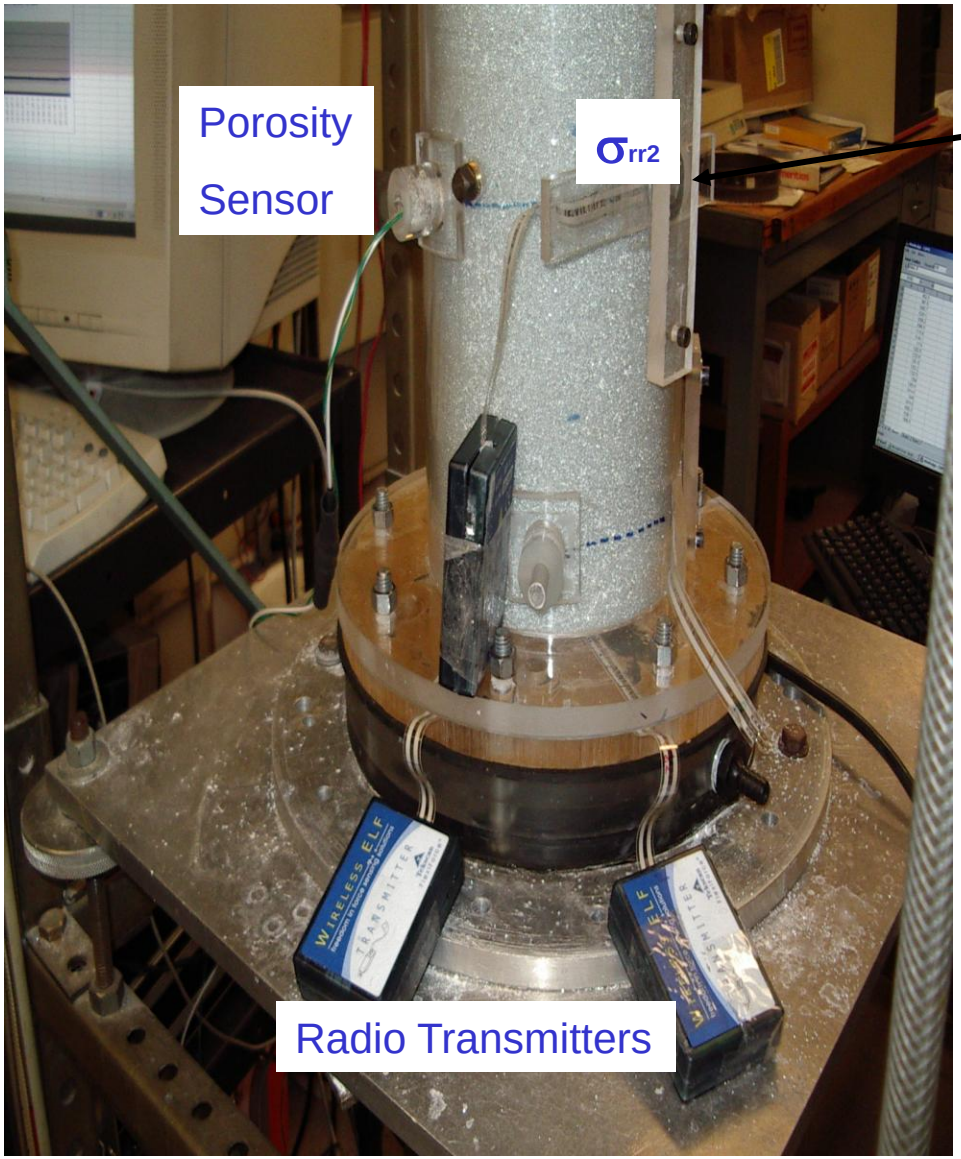




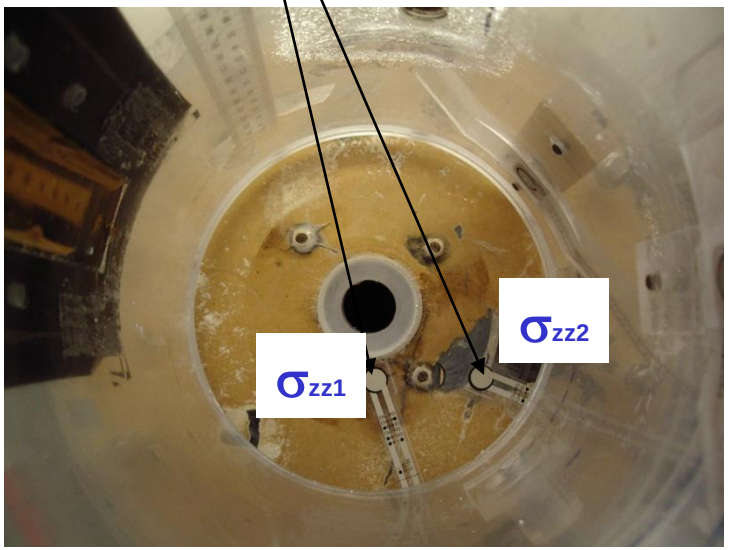
$$\dot{m} \propto (D - kd_p)^{5/2}$$

Size of the discharge outlet is the most important parameter which controls the discharge rate from silo

Experiments on flat bottom silo

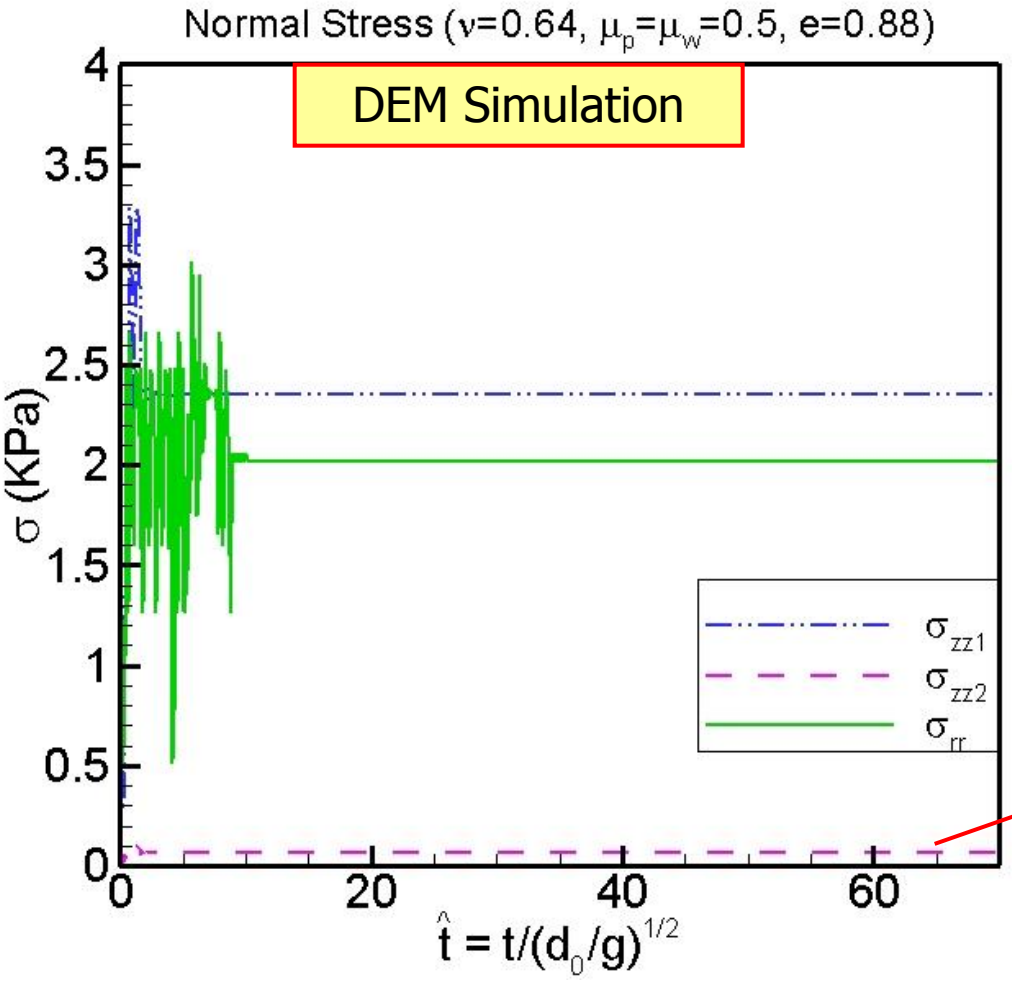


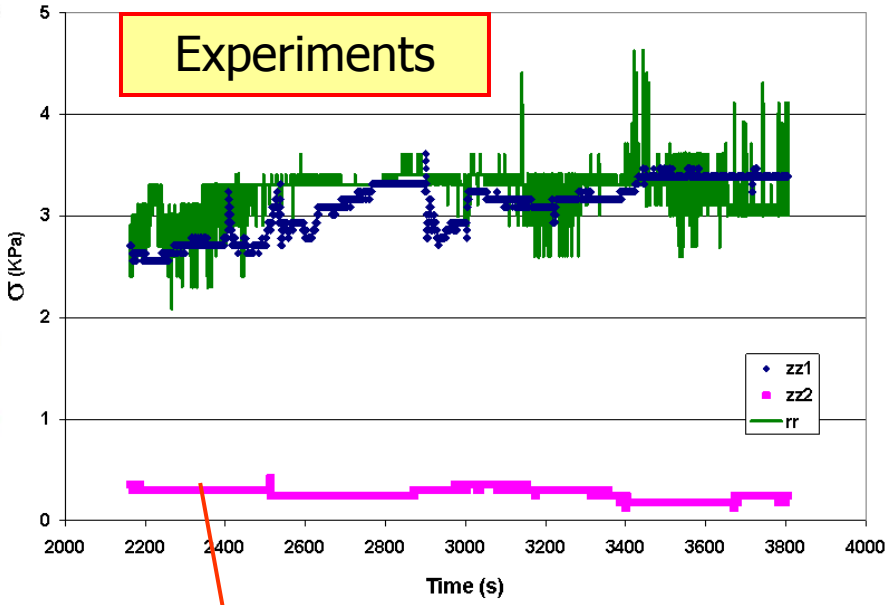
Stress Sensors



•Bottom Plate: view from above

Comparison of normal stresses



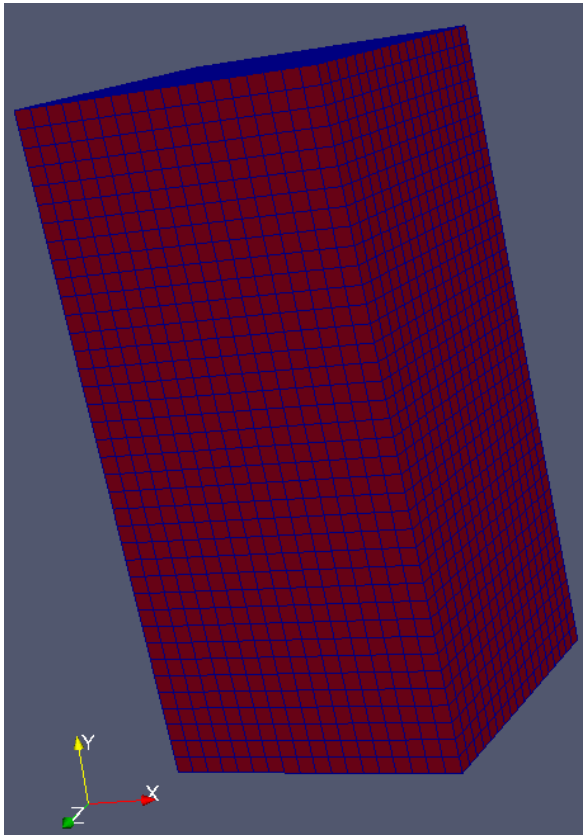


Both studies verify that normal stress on the bottom plate (away from the discharge outlet) is very small

DEM simulations were able to reproduce the observations found in experiments

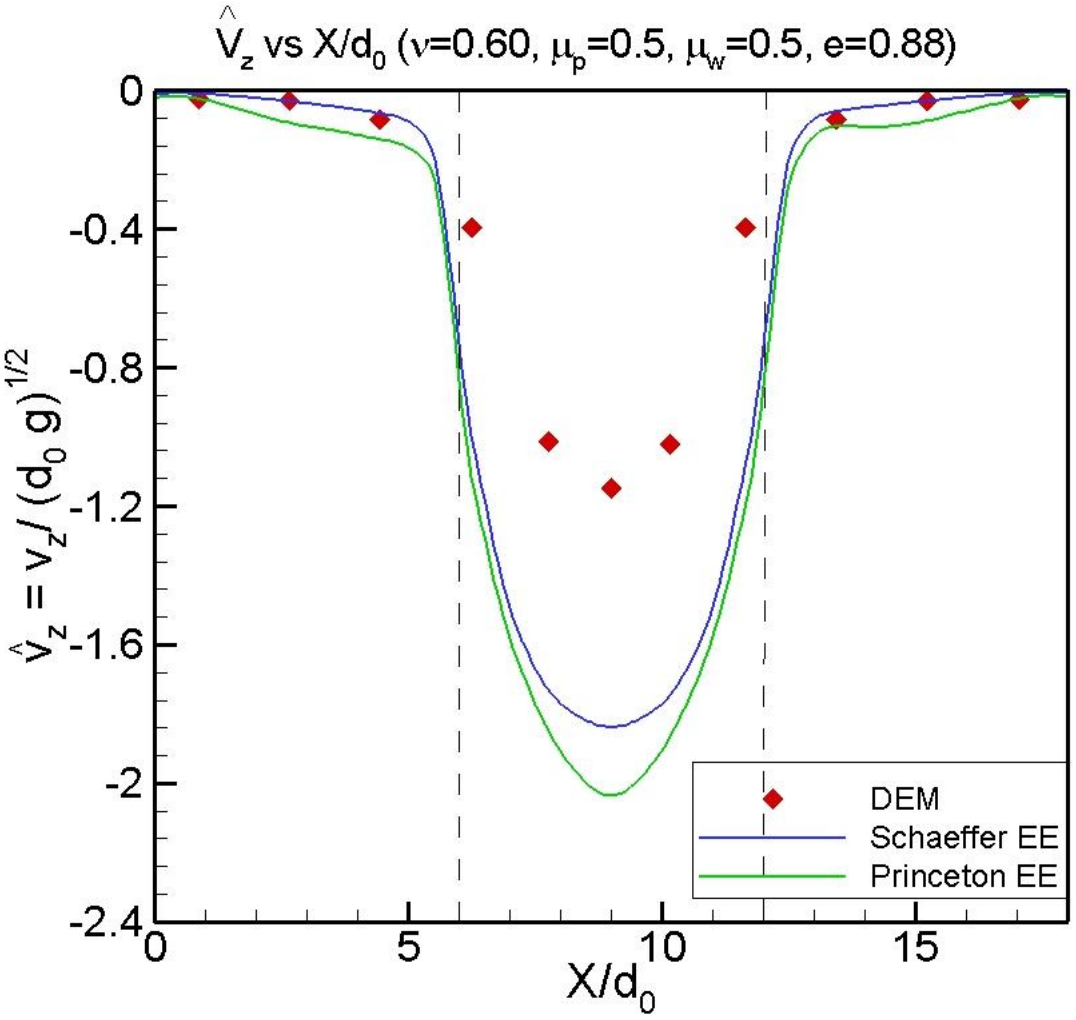
Comparison of continuum models with DEM

- Quantitative assessment of continuum models by comparing with DEM
- 3D MFIX continuum simulations (square outlet) compared to DEM (circular outlet)
- Boundary conditions for continuum simulations
  - Partial slip wall boundary conditions (Johnson and Jackson) for solid phase all vertical walls
  - Free slip BC for gas at the wall
  - At top and bottom boundary gas pressure was set to atmospheric, whereas normal continuation condition (zero gradient) applied for other variables



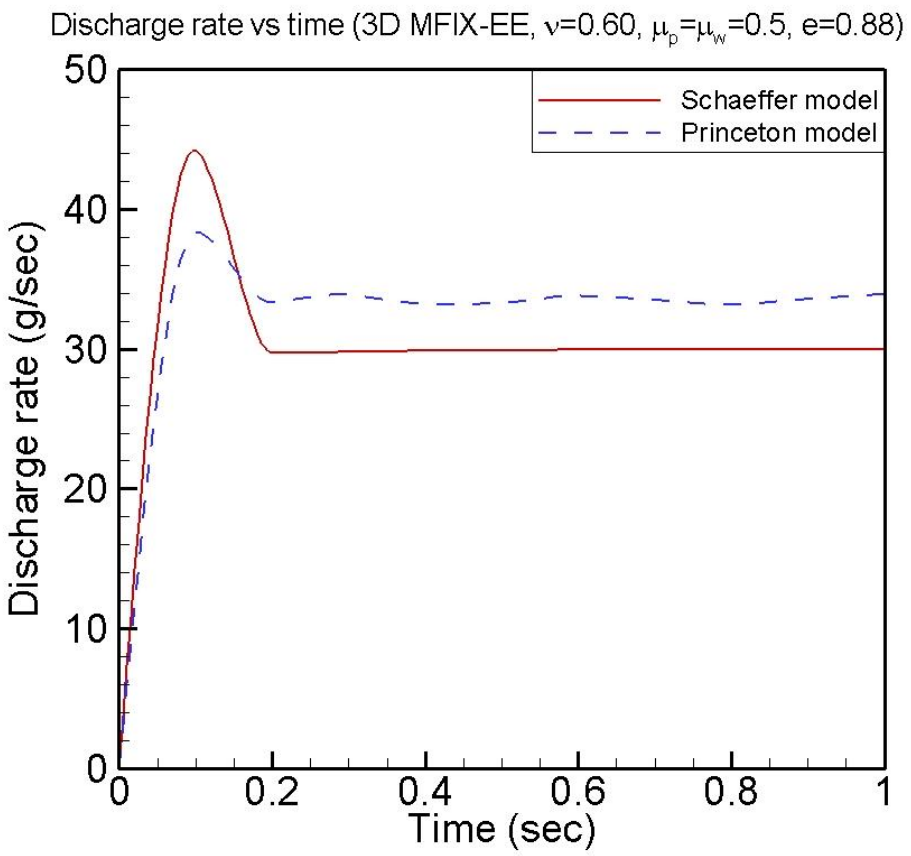
3D flat-bottomed silo

Solid velocity prediction



Solid velocity predicted by both the continuum models are higher than the DEM data

Discharge rate prediction



- Schaeffer frictional model
  - discharge rate (W) = 29.94 g/sec
- Princeton frictional model
  - discharge rate (W) = 33.28 g/sec
- Current DEM study
  - discharge rate (W) = 23.94 g/sec
- Beverloo correlation

$$\dot{m} = 0.58 \rho_b g^{0.5} (D - k d_p)^{2.5}$$

  - discharge rate (W) = 17.25 g/sec

Both the continuum models over predict discharge rate when compared with DEM study

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Granular phase transition: Order parameter

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

$\rho = 0$ → Pure fluid

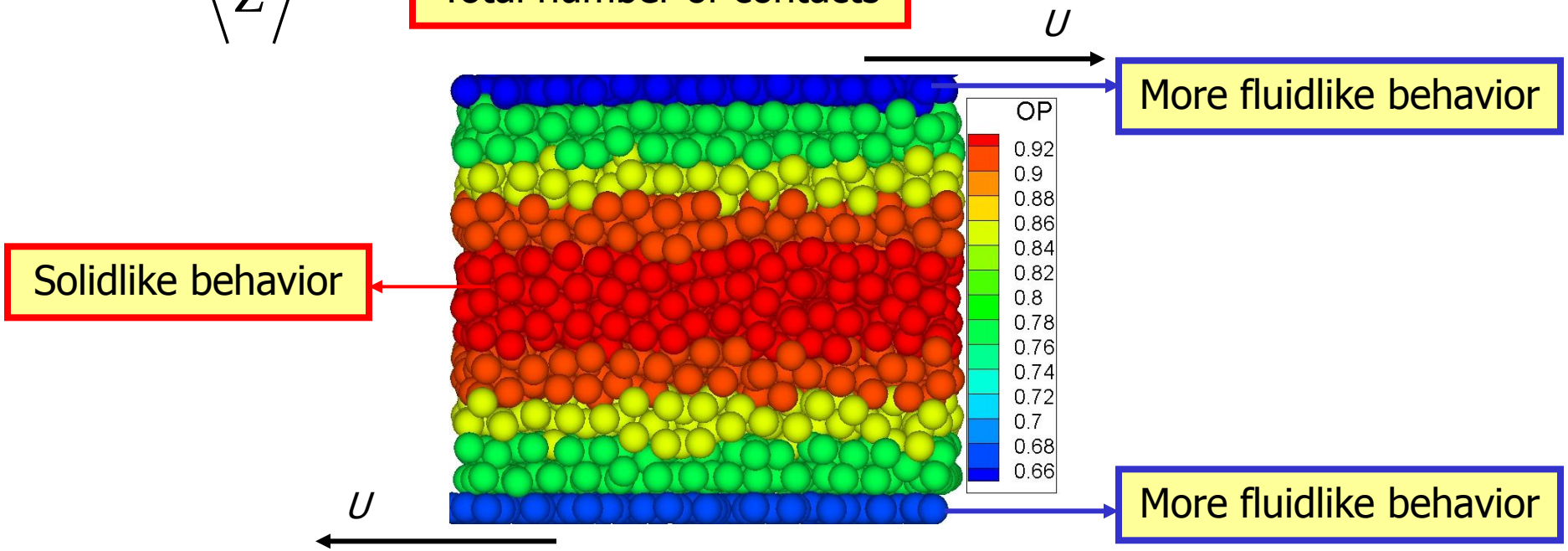
$\rho = 1$ → Pure solid

- 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



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

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

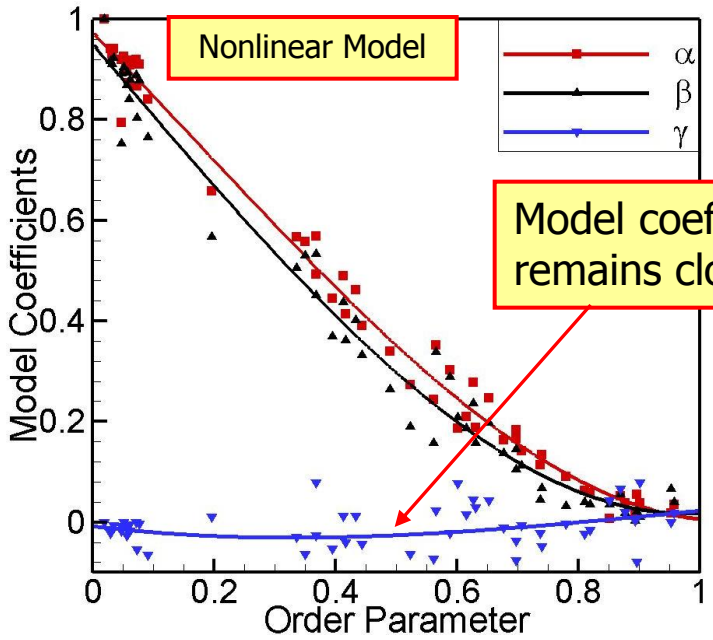
$$\sigma_{ij}^{s} = \sigma_0 \left\{ (1-\alpha) \delta_{ij} + (1-\beta) b_{ij} - \gamma \left[(\mathbf{b}^2)_{ij} - \frac{1}{3}(\mathbf{b}^2)_{ll}\delta_{ij} \right] \right\} \rightarrow \sigma_{ij}^{s} = f(\sigma_o, \alpha, \beta, \gamma)$$

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

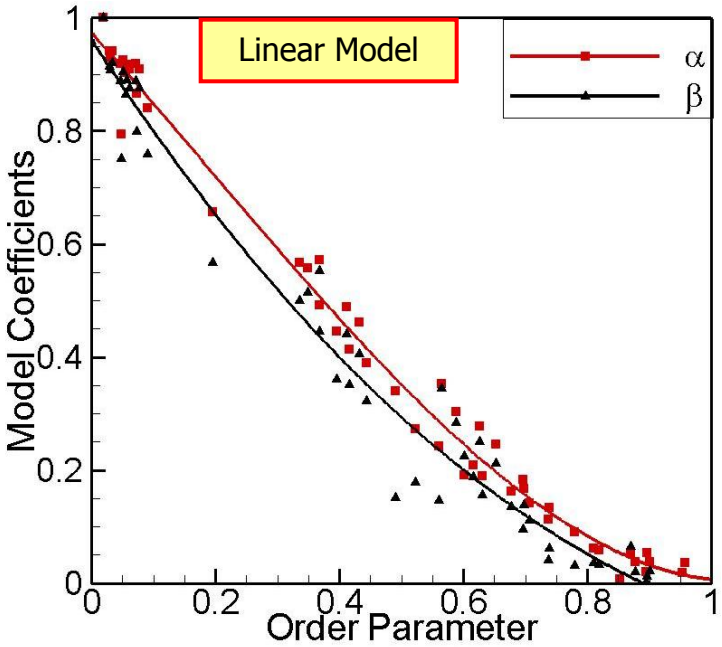
σ_0 Scale of total granular stress

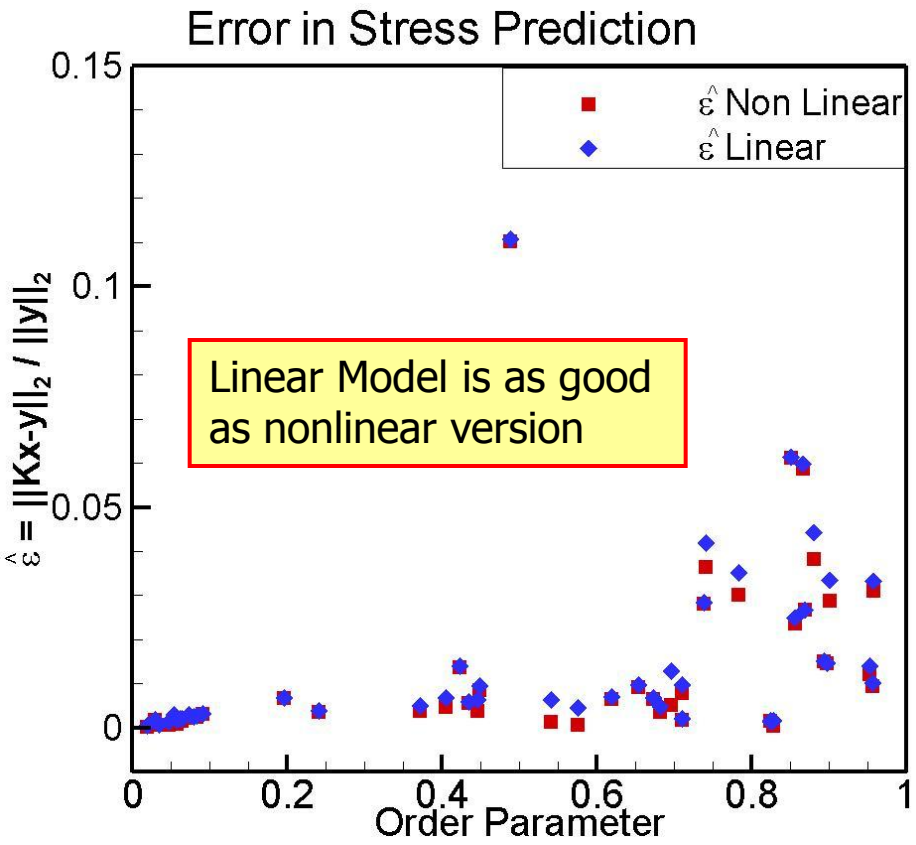
Objective OP Model, Subramaniam Group, *Phys. Rev. E* (2005)

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

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

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

*Volfson et al., Phys. Rev. Lett., vol. 90, 254301 (2003)

Solution for order parameter

- Order parameter was obtained by solving generic Ginzburg-Landau (GL) equation

$$\frac{D\rho}{Dt} = D\nabla^2\rho - F(\rho,\delta)$$

$$F(\rho,\delta) = (1-\rho)\left\{\rho^2 - 2\rho_*\rho + \rho_*^2 \exp\left[-A(\delta^2 - \delta_*^2)\right]\right\}$$

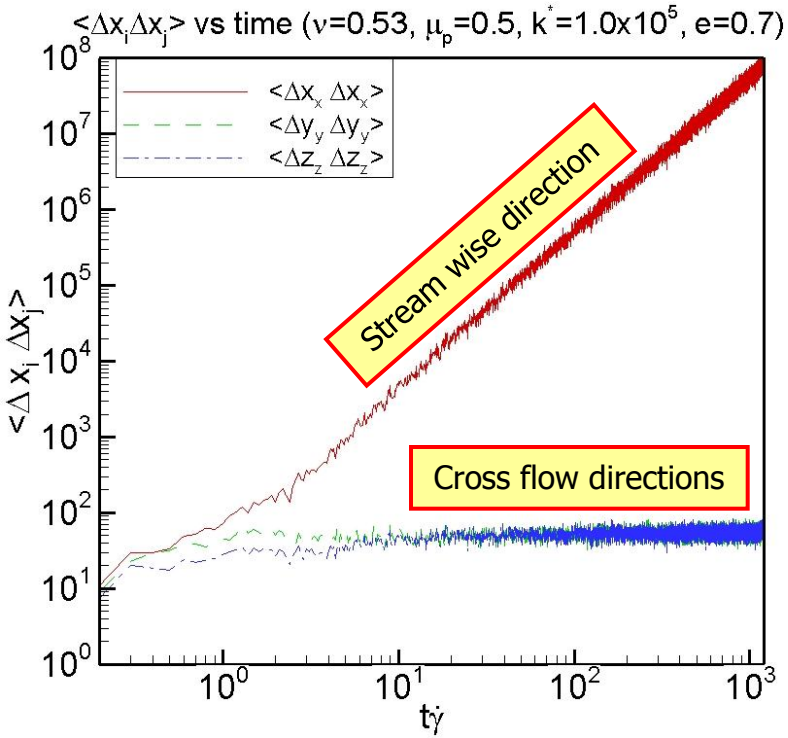
$$\rho_* = 0.6, A = 25, \text{ and } \delta_* = 0.26$$

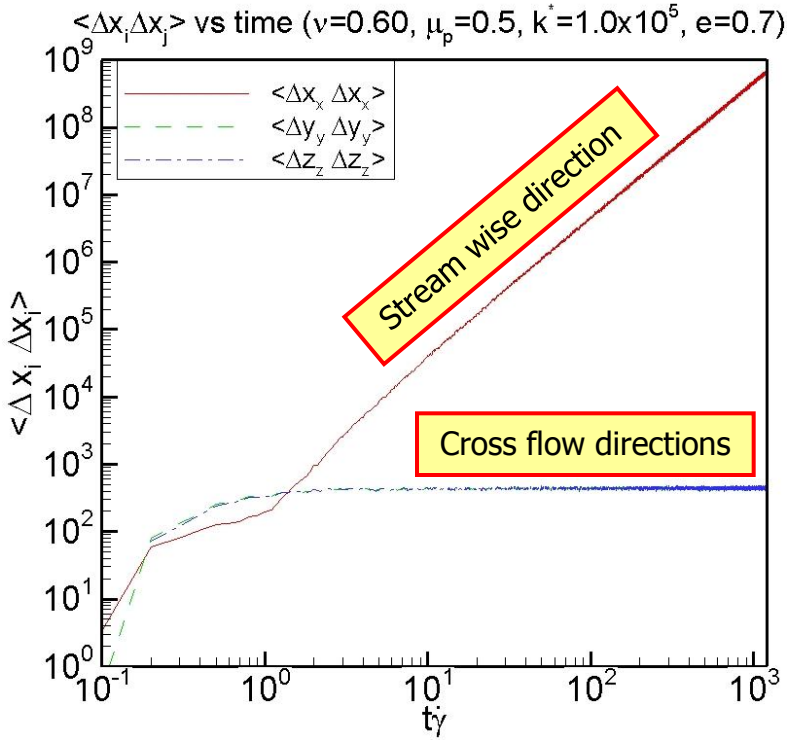
- Solution of GL equation requires the knowledge of diffusion coefficient and proper boundary conditions for the order parameter
- Diffusion coefficient was calculated by using two different methods
  - From mean square displacement (MSD) of enduring contacts
  - From velocity autocorrelation function

Extraction of diffusion coefficient: MSD

- Diffusion coefficient was approximated by calculating the MSD of "enduring contacts" and use of Einstein relation

$$\left\langle r^2(t)\right\rangle = \frac{1}{N_c}\sum_{i=1}^{N_c}\left[X_c^i(t) - X_c^i(0)\right]^2$$





Diffusion coefficient is anisotropic with largest component along direction of mean motion

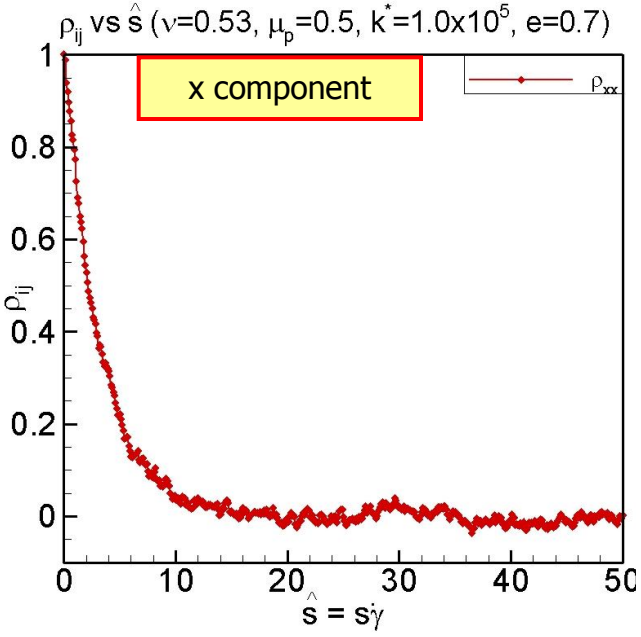
Diffusion coefficient: Velocity autocorrelation

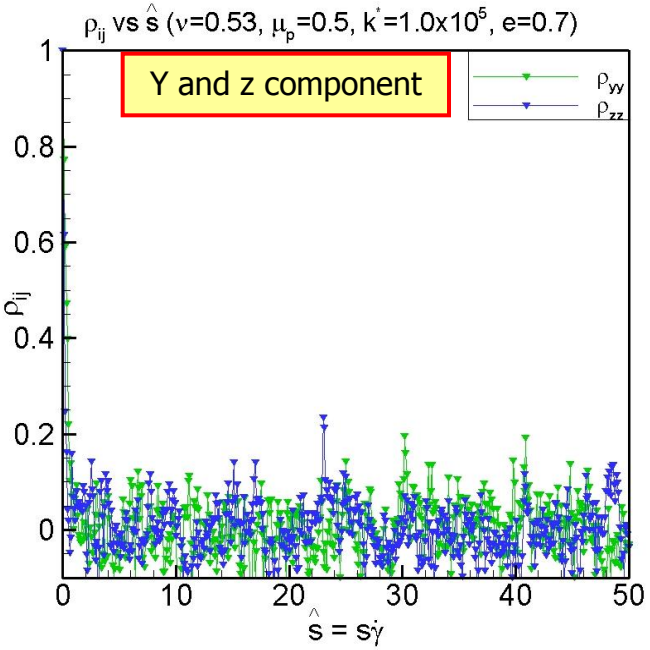
- Diffusion tensor can also be determined using velocity autocorrelation function (VACF)

$$D_{ij} = \left(\left\langle u_i^2 \right\rangle \left\langle u_j^2 \right\rangle\right)^{1/2} \tau_{ij}$$

$$\tau_{ij} = \int_0^\infty \rho_{ij}(s)\,ds$$

$$\rho_{ij}(s) = \frac{\left\langle u_i(t)\,u_j(t+s)\right\rangle}{\left\langle u_i^2\right\rangle^{1/2}\left\langle u_j^2\right\rangle^{1/2}}$$



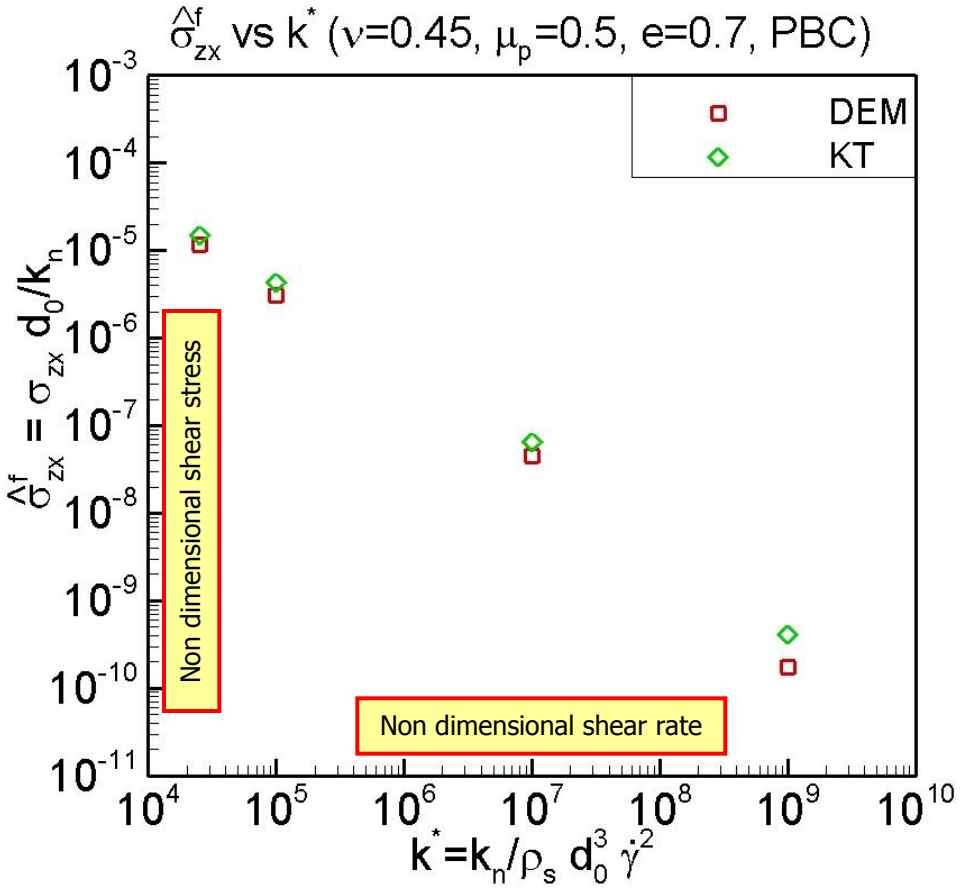


% difference in diffusion coefficient prediction

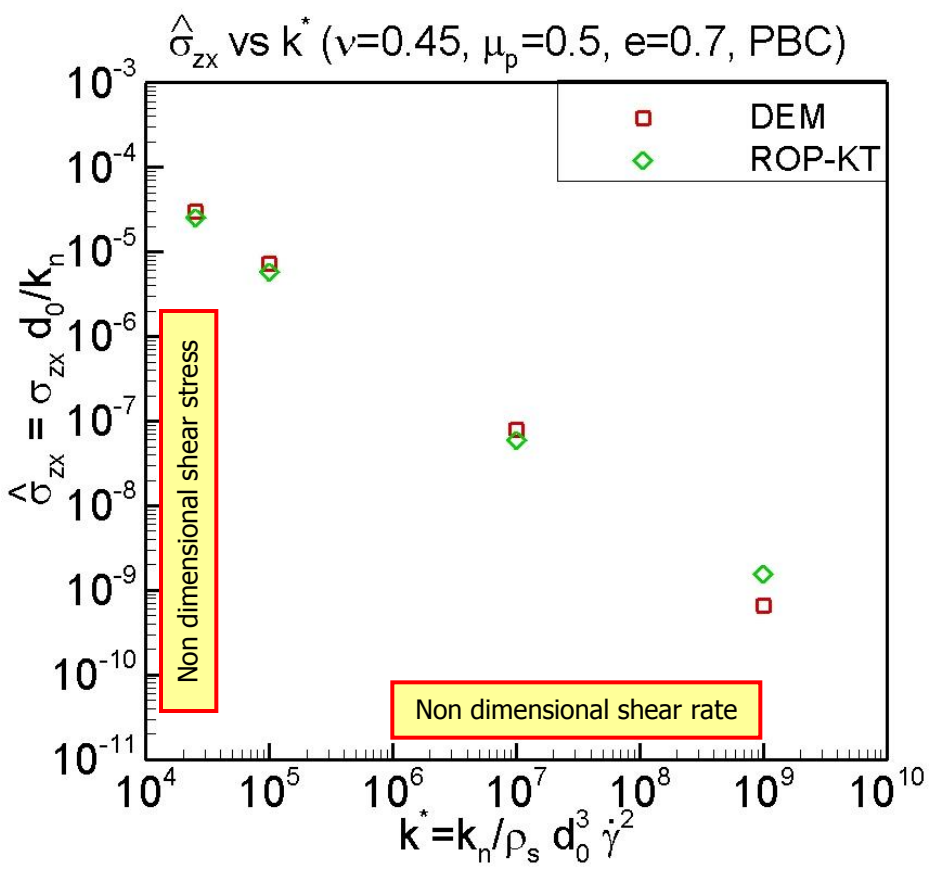
υ	D_{MSD}	D_{VACF}	% diff.
0.45	1.046	1.242	18.65
0.53	1.017	1.176	15.60
0.57	1.012	1.133	11.85
0.60	1.007	1.093	8.53
0.62	1.005	1.052	4.63

Both MSD and VACF predict the largest diffusion in along direction of mean motion within maximum difference of 18%

ROP model performance, inertial regime



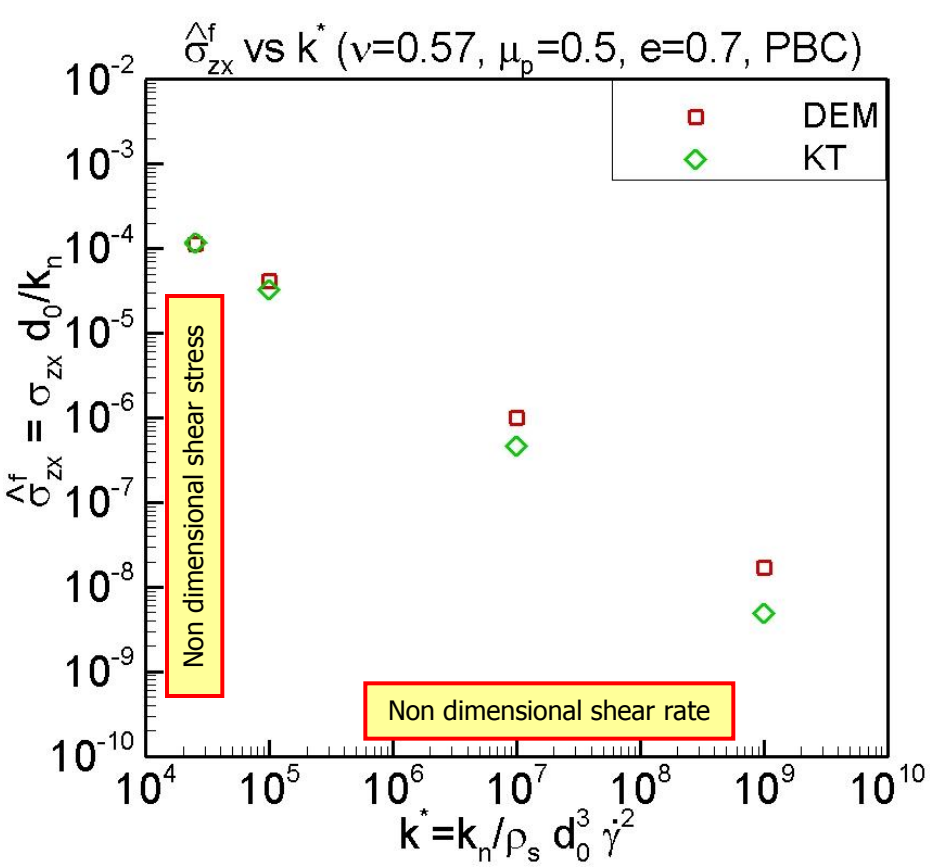
Fluidlike Shear Stress



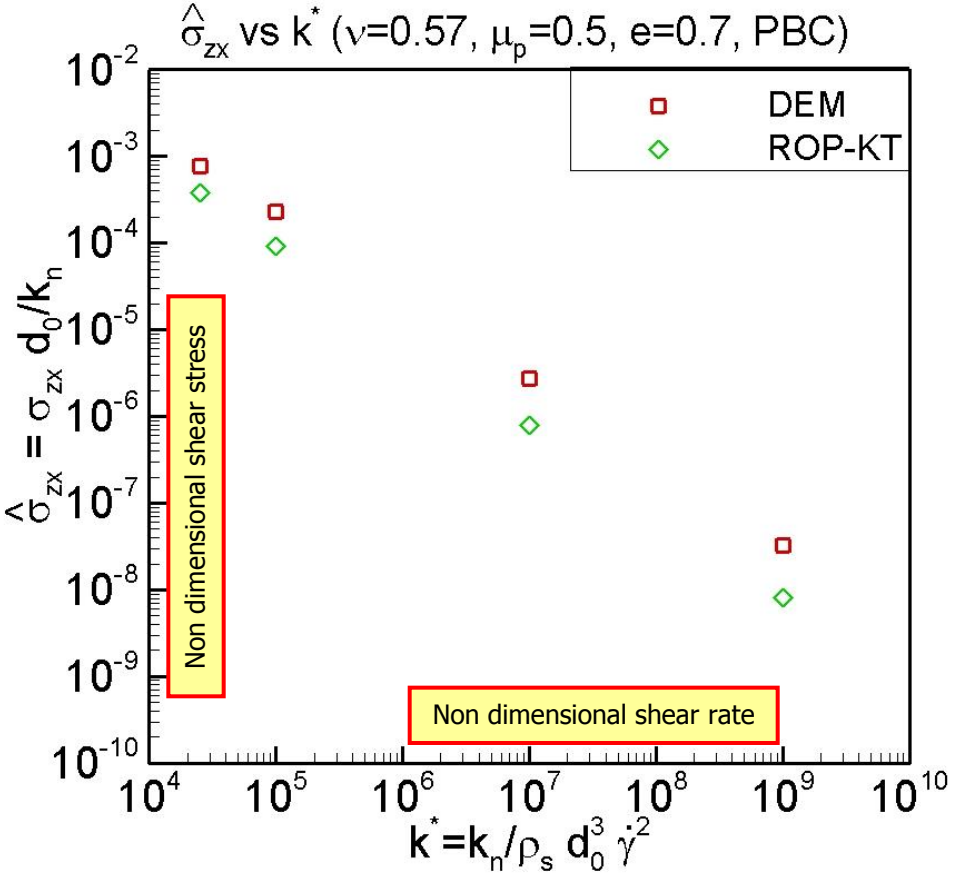
Total Shear Stress

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

ROP model performance, near transition



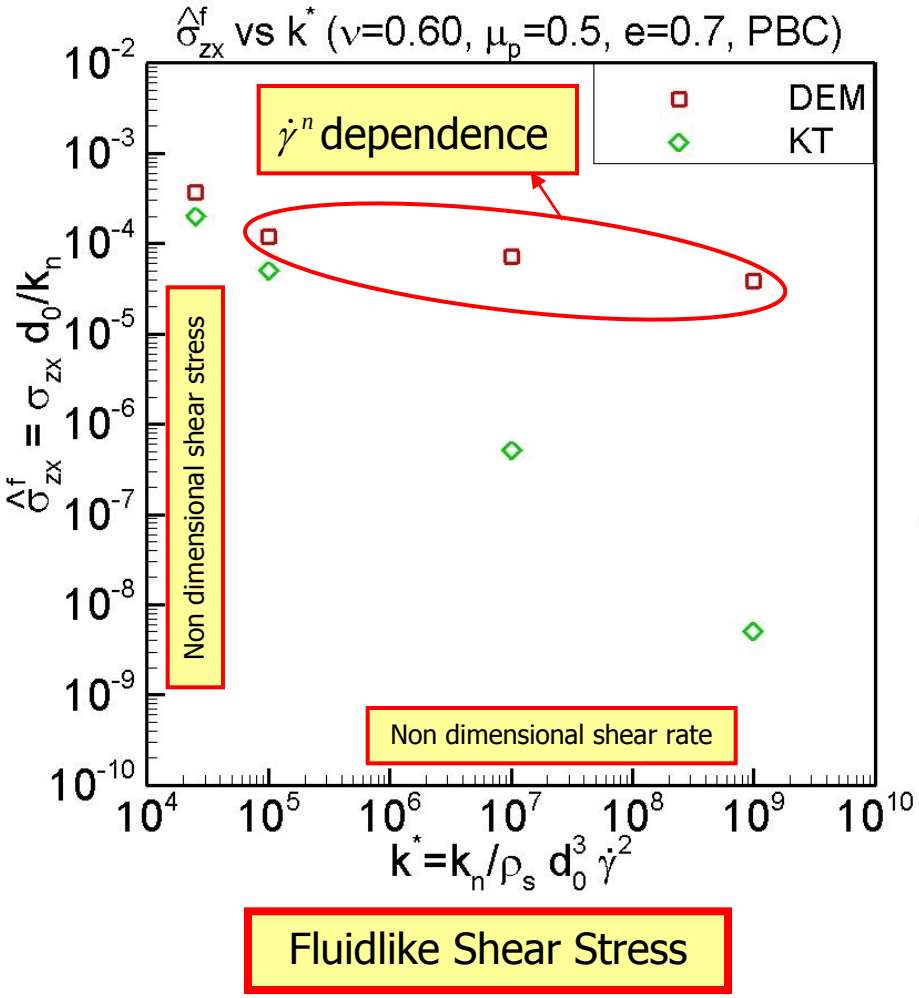
Fluidlike Shear Stress



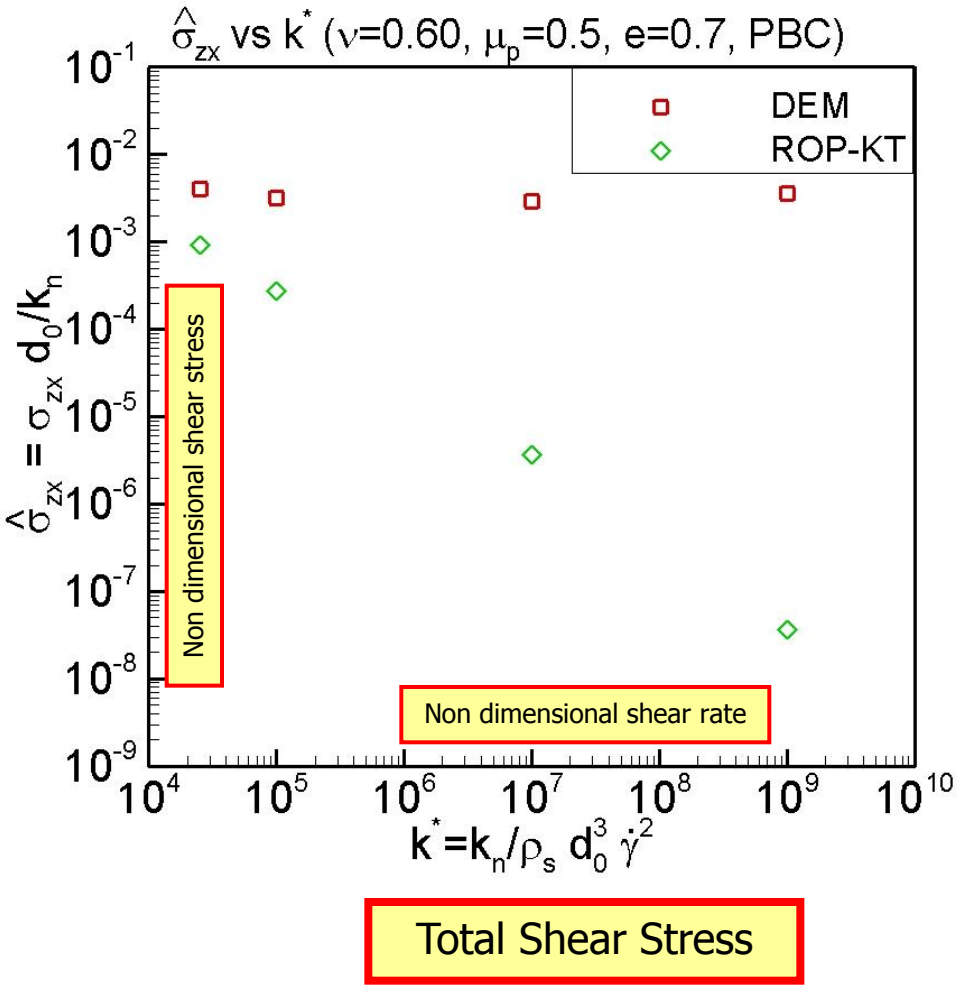
Total Shear Stress

Near the transition regime the ROP-KT model performs reasonably well (within accuracy of 15%)

ROP model performance, intermediate regime



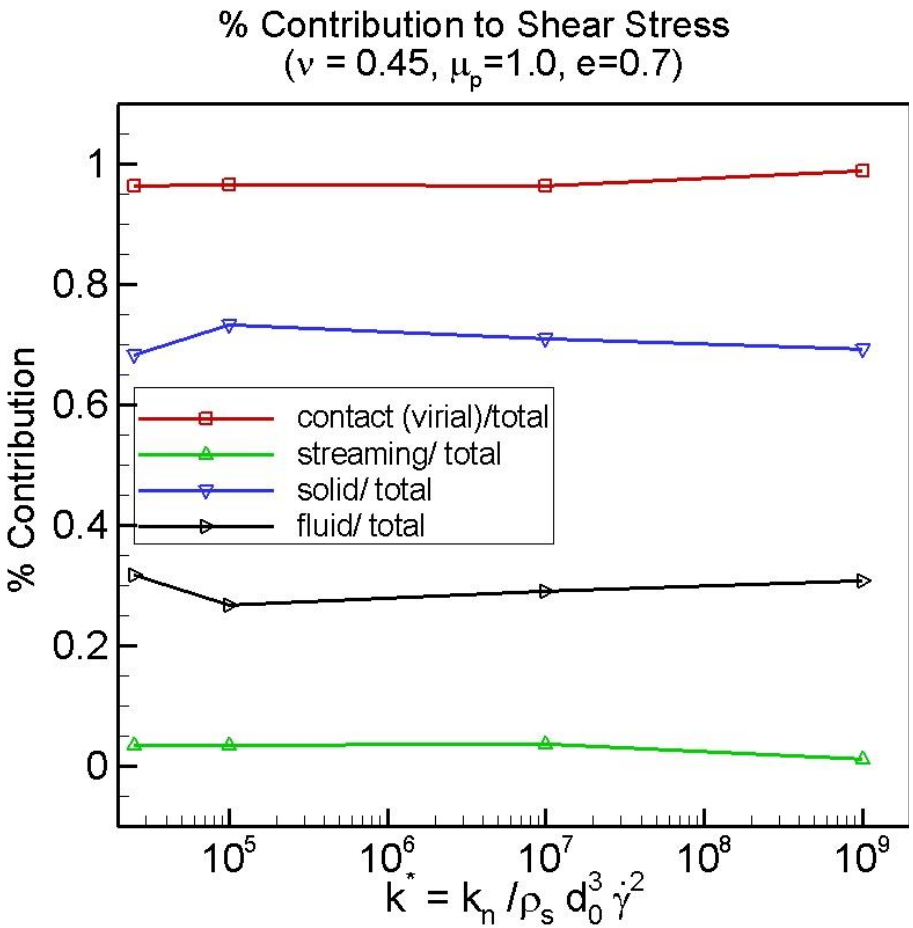
Fluidlike Shear Stress

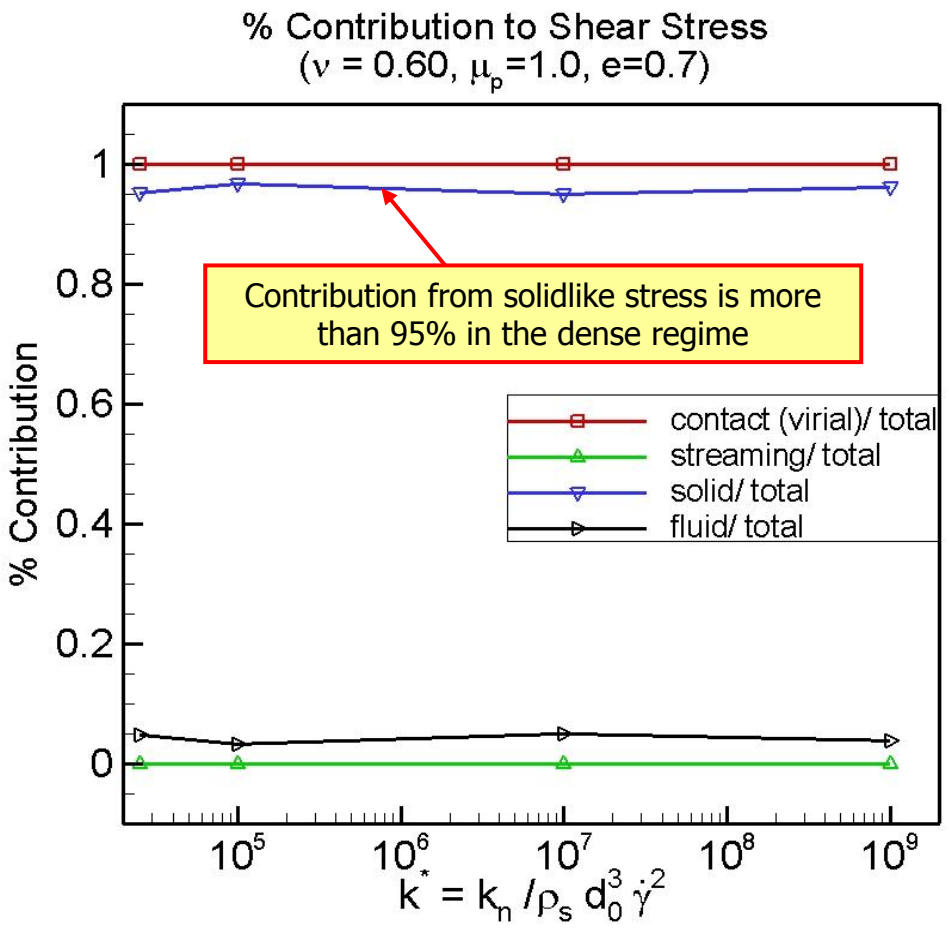


Total Shear Stress

In the intermediate regime the ROP-KT model is not able to predict the correct trends of shear stress with shear rate

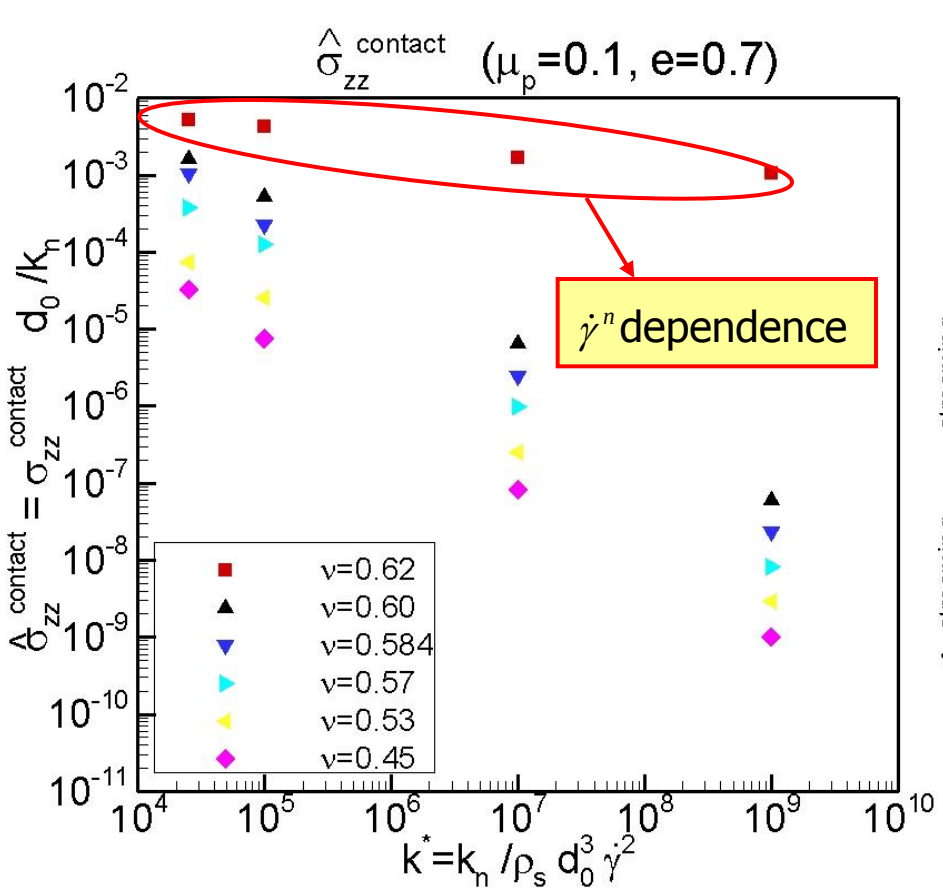
% contribution of the total stress



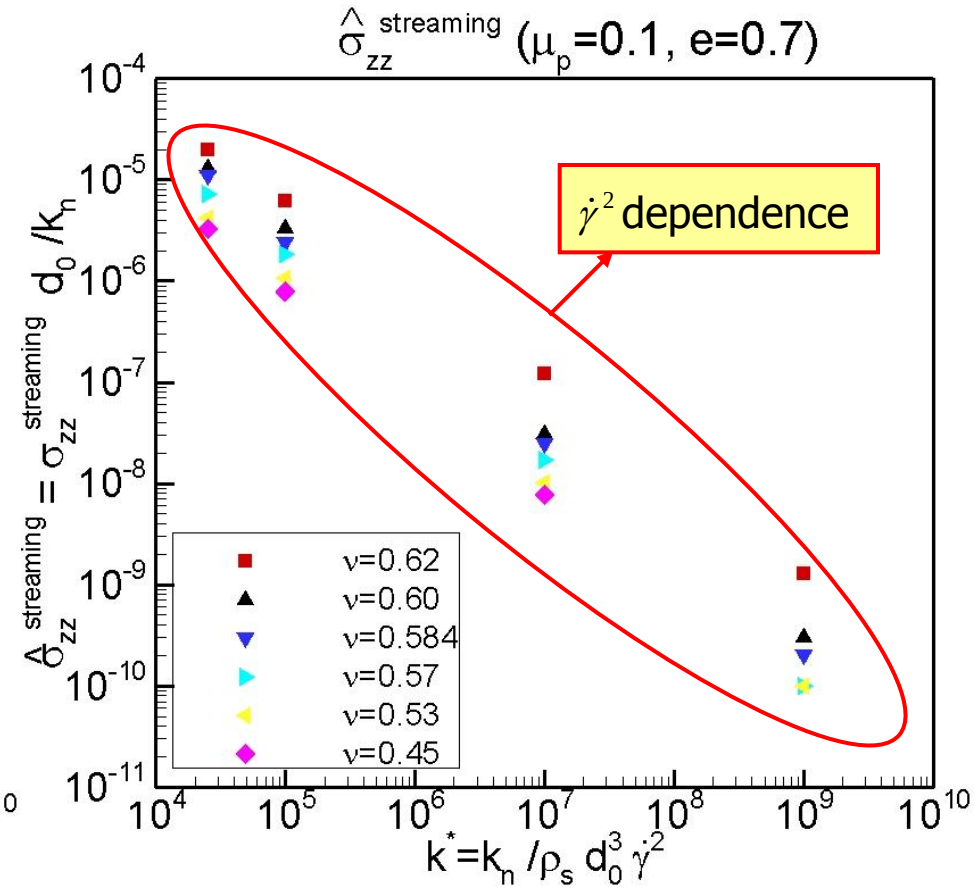


In dense regime the contribution from the solidlike stress dominates over the fluidlike stress contribution

Decomposition of stresses



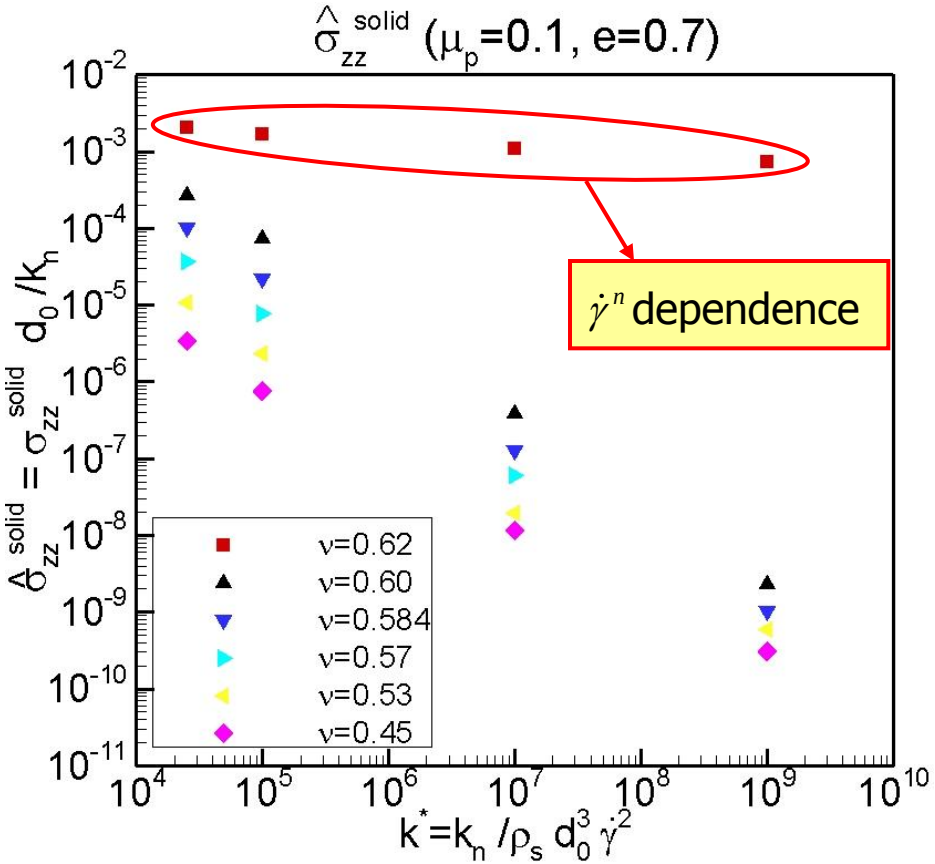
Contact (virial) stress



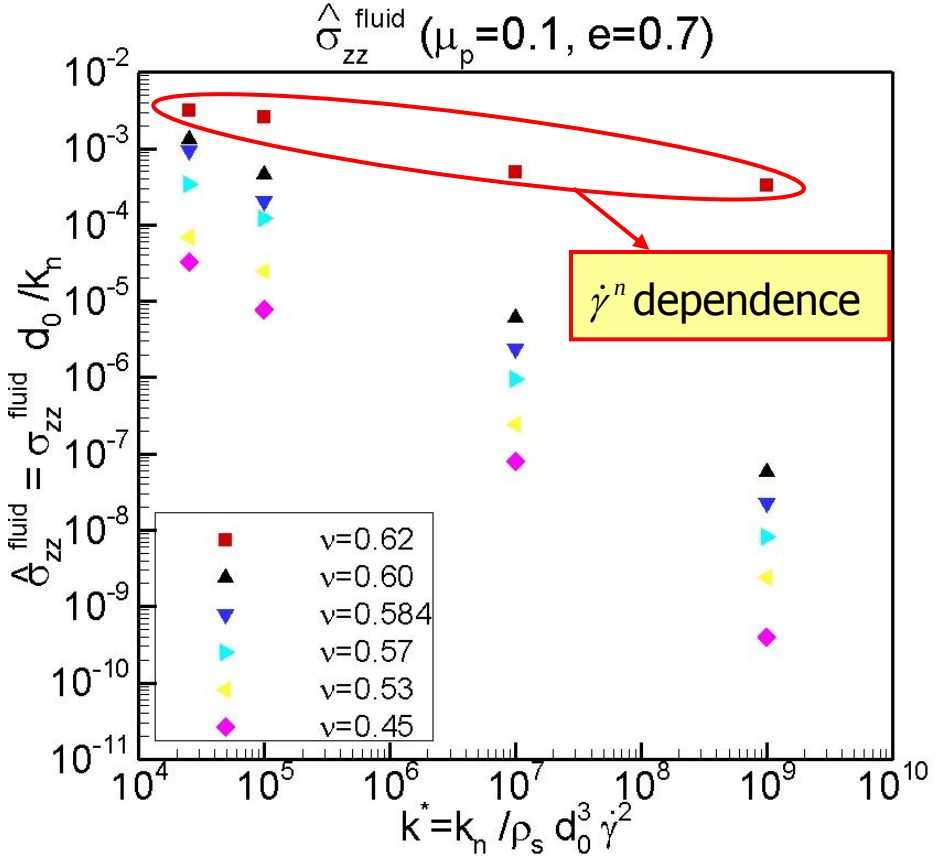
Streaming stress

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



Solidlike stress



Fluidlike stress

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

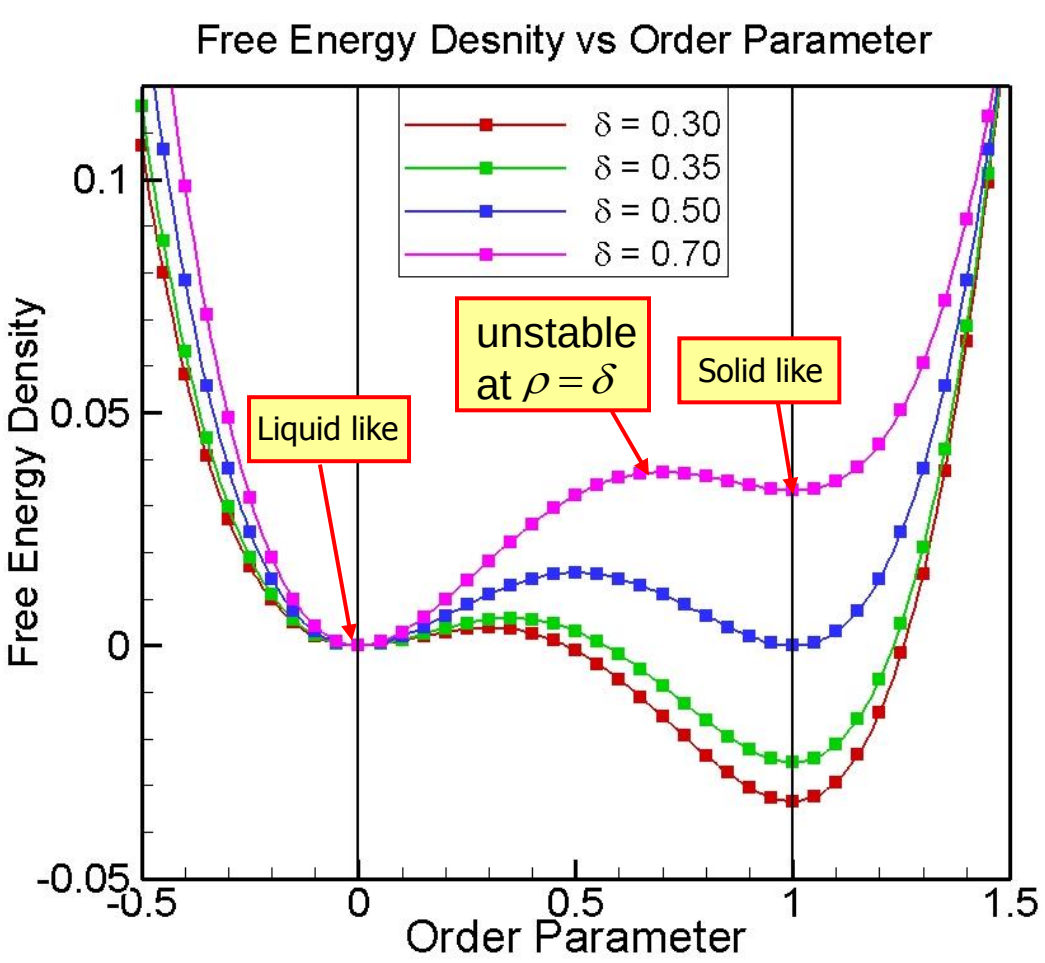
Outline

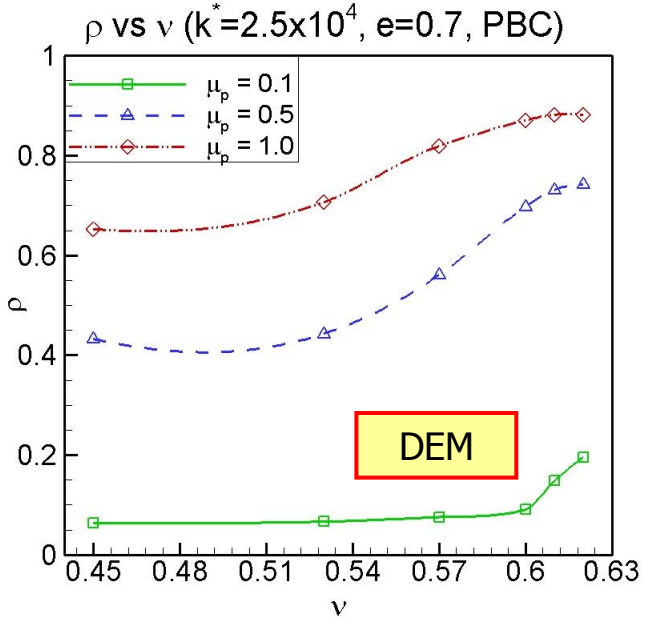
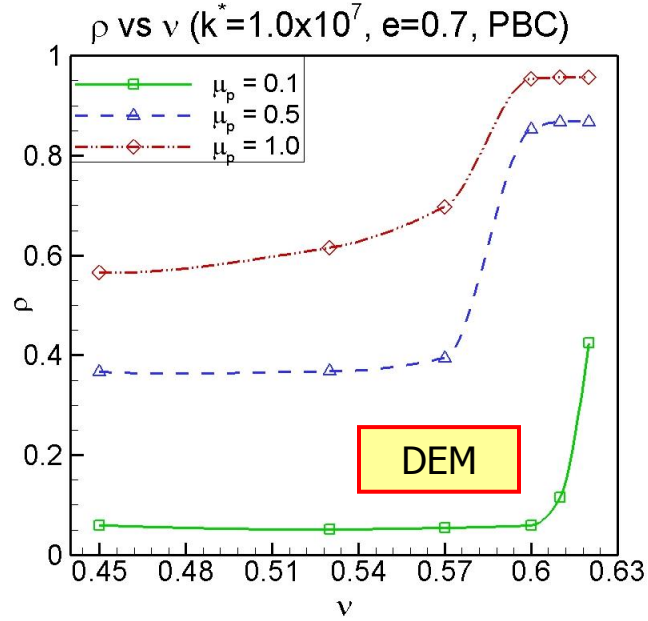
- Couette cell simulations
  - Established regime transition observed in experiments
  - Database for continuum model assessment
- Homogeneous shear simulations
  - Established intermediate regime map for granular flows
- Silo simulations
  - Assessment of existing continuum models
  - Comparison with experiments
- Inhomogeneous wall shear simulations
  - OP model development and validation

Current Efforts

- Coupling the ROP model with the "Dissipative plasticity model" developed by Princeton team for the solidlike contribution of the total granular stress in dense regime
- New formulation of the free energy density function to accommodate the third stable value of the order parameter at the steady state

Free energy density function



$$F(\rho,\delta) = \int_{o}^{\rho} \rho(\rho-1)(\rho-\delta)\,d\rho$$

$$\delta = \frac{\sigma_{zx}}{\sigma_{zz}}$$