Use of an Accurate DNS Method to Derive, Validate and Supply Constitutive Equations for the MFIX Code

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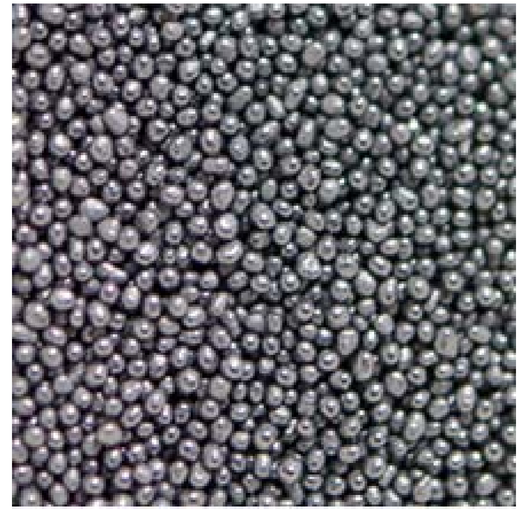
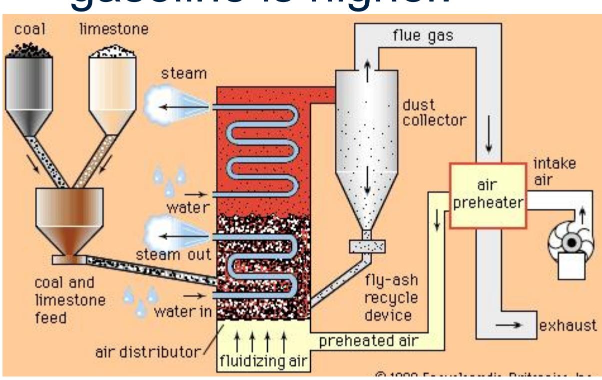
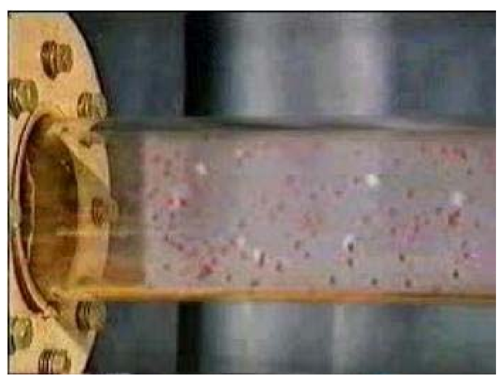
Granular flow

Granular materials are large collections of discrete solid particles whose size is large enough that Brownian motion is irrelevant.



- fluidized beds, pneumatic transport, risers, etc
- Fluid catalytic cracking (FCC) that crack heavy oil with the help of hot catalyst particles, producing light hydrocarbons such as gasoline.
- In the US, fluid catalytic cracking is more common because the demand for gasoline is higher.



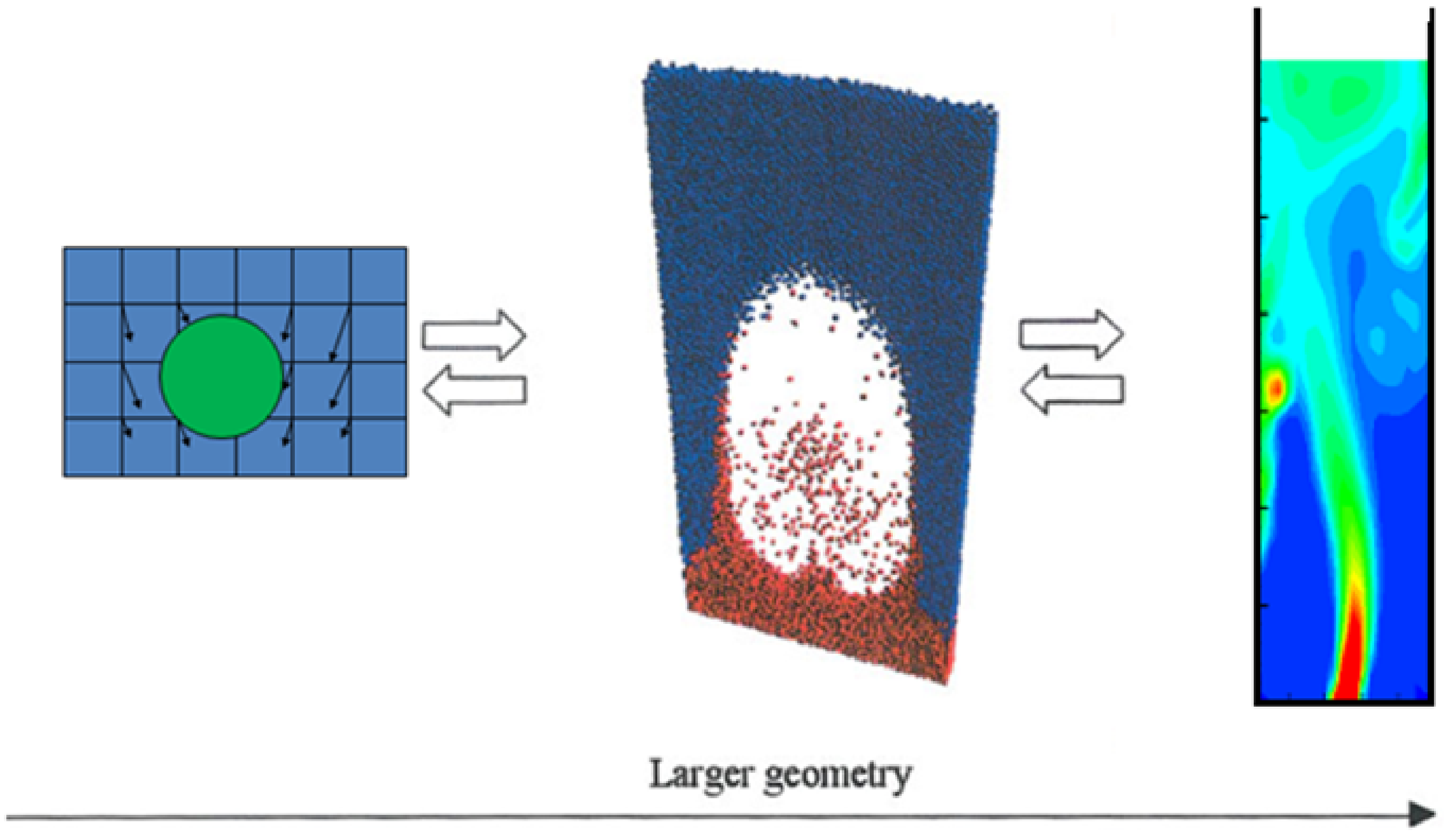


Multiscale Modeling for Particlulate Flows

Resolved Discrete Particle (Direct Numerical Simulation) Model

Unresolved Discrete Particle (Discrete Element) Model

Two-Fluid (Continuum) Model



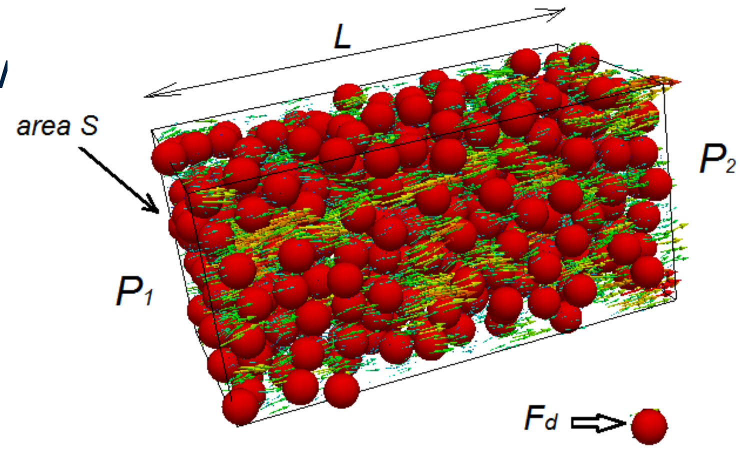
Use DNS to derive the new drag correlation

- Carman-Kozeny equation
  - Based on experiments, for slow flow

$$\nabla p = -\frac{180\phi^2}{(1-\phi)^3 d^2}\mu U$$

  - Dimensionless drag

$$F(\phi,0) = 10\frac{\phi}{(1-\phi)^2}$$

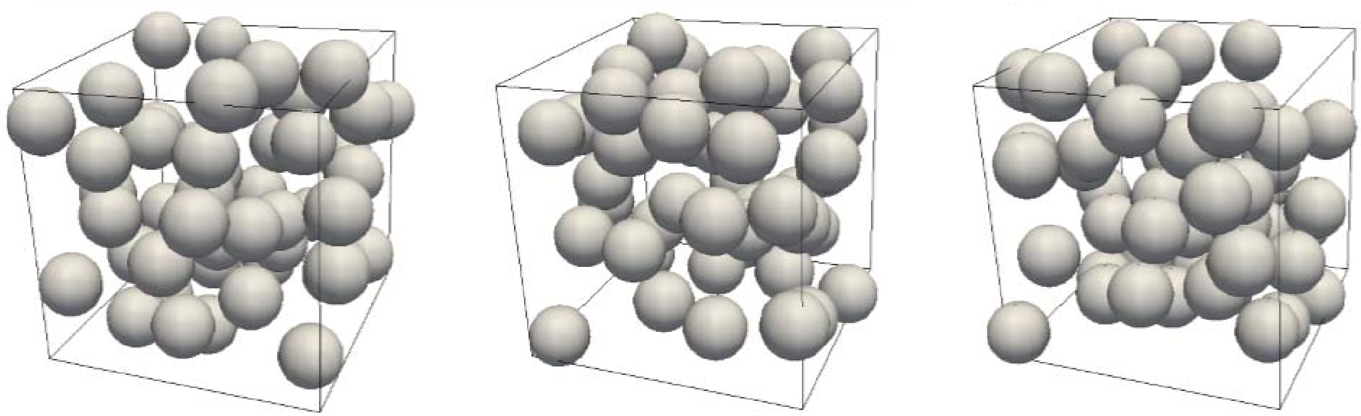


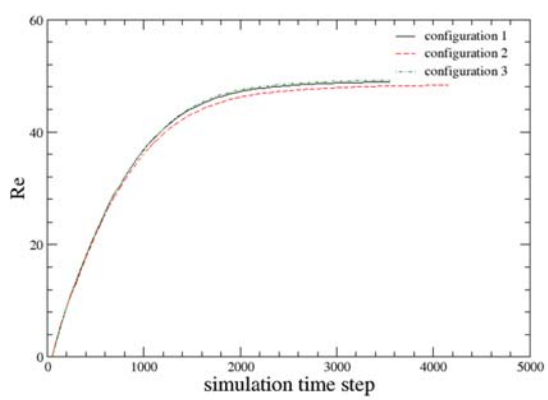
- Ergun equation, based on experiments

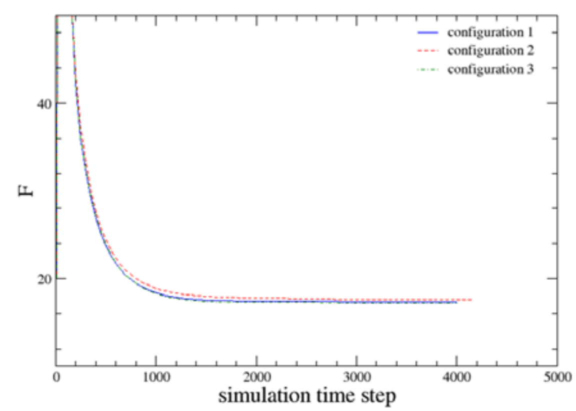
$$F(\phi,\mathrm{Re}) = 8.33\frac{\phi}{(1-\phi)^2} + \frac{0.097}{(1-\phi)^2}\mathrm{Re}$$

Influence of sphere configurations

- Three different random configurations of 50 spheres placed in a cube (solid fraction 0.2873)
- Applied the same pressure gradient







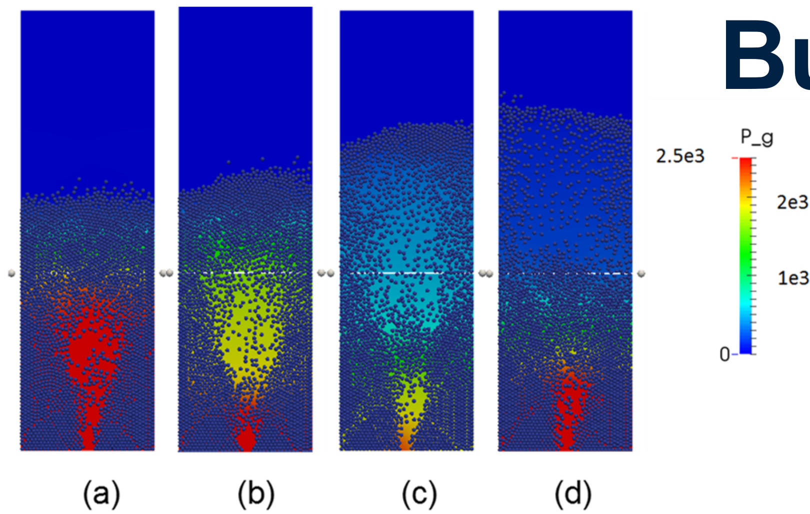
New drag correlation

- Final correlation for the drag model:

$$F = 1 + 9.5\varphi/(1-\varphi)^3 + 9.5\varphi(1-\varphi)^3 + (0.002 + 0.8\varphi^{1.5} + 52\varphi^8)\,\mathrm{Re}$$

  - Based on over 150 simulation data.
  - Applicable to solid fraction 0.05~0.63 and
  - Easy to be implemented in MFIX

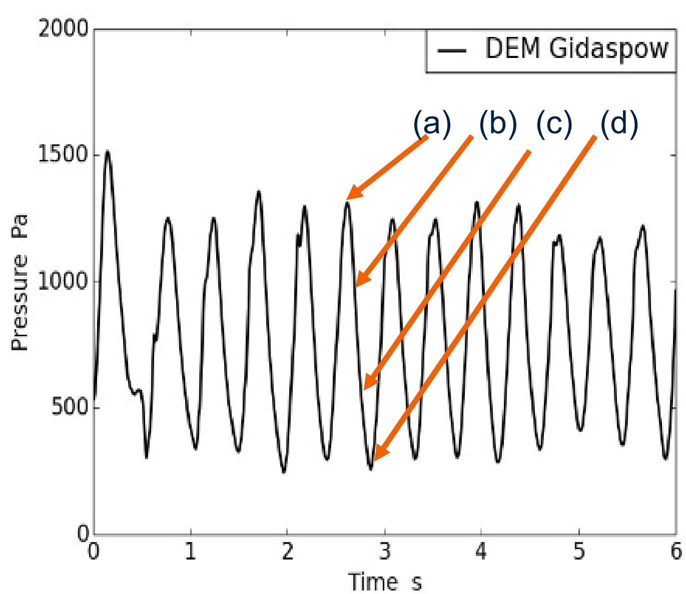
Bubble dynamics

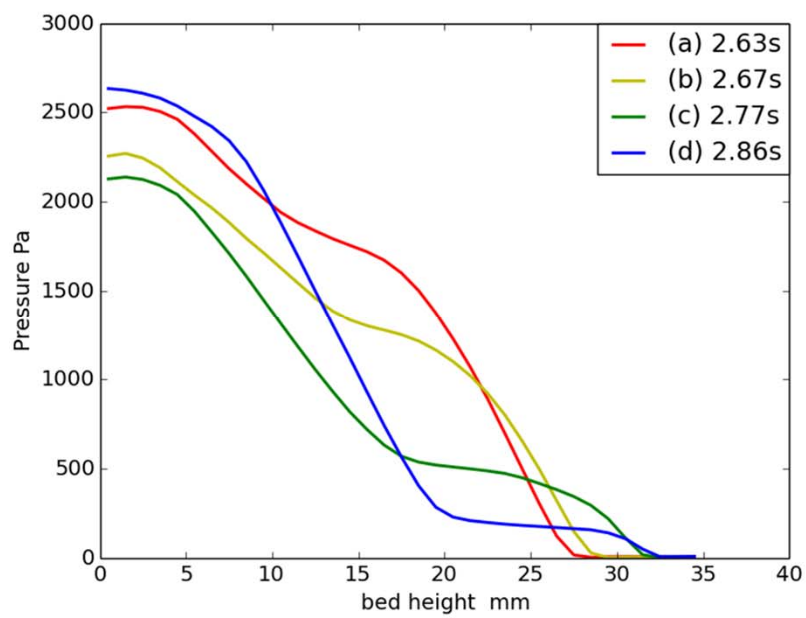


Pressure fluctuation measured at 20 mm bed height

Pressure changes from top to bottom in a cycle

Formation of a bubble in a fluidized bed from DEM simulation. Gas pressure is shown in color, measured pressure changed from maximum value (a) to minimum value (d) in a cycle. (b), (c) and (d) are snapshots 0.04s, 0.14s, and 0.23s after snapshot (a).

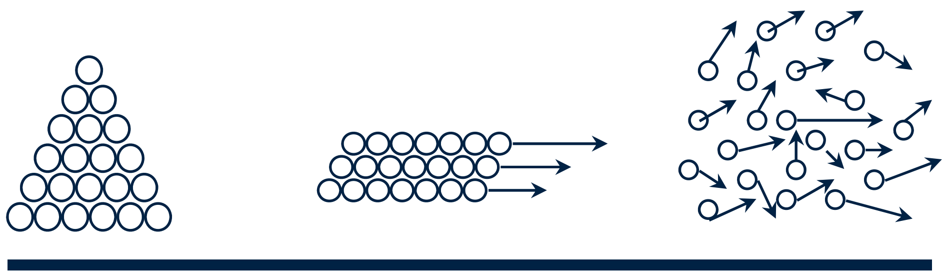




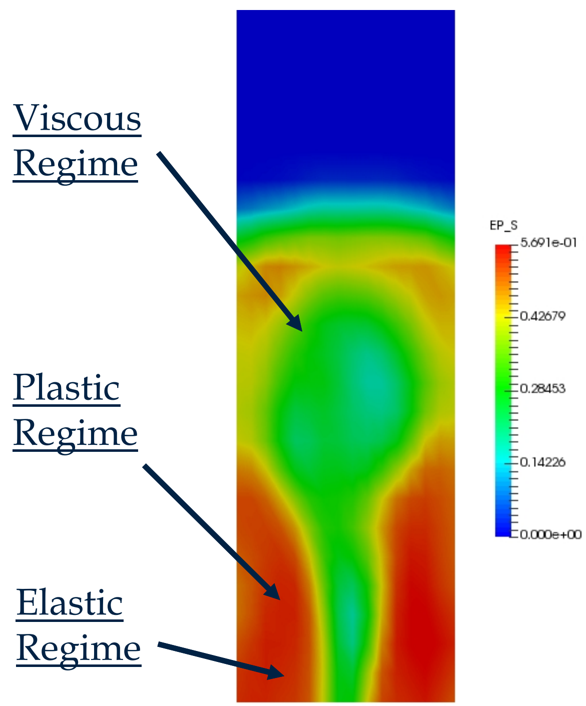
Gas pressure along with bed height, corresponding to the four snapshots at different time in Figure 2.

Granular flow regimes

Elastic Regime	Plastic Regime	Viscous Regime.
Stagnant	Slow flow	Rapid flow
Stress is strain dependent	Strain rate independent	Strain rate dependent
Elasticity	Soil mechanics	Kinetic theory



Kinetic theory is used to model the solid particles as a continuum phase in TFM method.



Granular flow can show different behaviors (from fluid like behaviors to solid like behaviors) in a fluidized bed, kinetic theory deteriorates in the dense regime

Kinetic Theory of Granular Flow

Boltzmann equation: $$\frac{\partial f}{\partial t} + v \cdot \nabla f = J[f, f]$$

Binary collision integral: $$J[f, f] = d^2 \int dv_2 \int \Theta(g \cdot n)(g \cdot n)\left[\frac{1}{e_n^2} f_2(v_1', x_1, v_2', x_1 - dn, t) - f_2(v_1, x_1, v_2, x_1 + dn, t)\right] dn$$

Multiplying a generic function of the velocity, $\phi(v)$ and integrate over v

$$\frac{\partial}{\partial t}\langle n\phi\rangle + \frac{\partial}{\partial x}\langle n\phi v\rangle = \int \phi \, J[f, f] dv$$

If we let $\phi = 1, v \; and \; v^2$, balance equations for mass, momentum, and energy could be derived:

$$D_t \rho + \rho \nabla \cdot u = 0$$

$$\rho D_t u + \nabla \cdot \sigma = 0$$

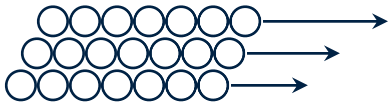
$$\frac{3}{2} \rho D_t T + \nabla \cdot q + \sigma : \varepsilon + \Gamma = 0$$

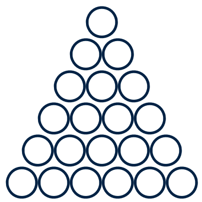
$$\sigma_{ij} = m \int V_i V_j f(v, x, t) dv$$

$$q = \frac{m}{2} \int |V| V^2 f(v, x, t) dv$$

$$\Gamma = -\frac{m}{2} \int V^2 J(f, f) dv$$

Discrete Element Method results as benchmark

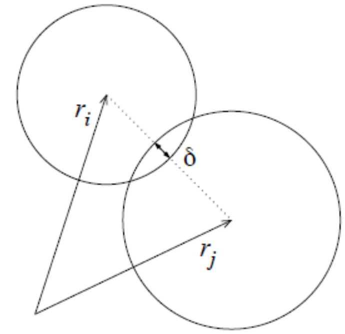




Particle-particle interactions

Soft-sphere collision scheme

To resolve the particle collisions,
DEM time step = $T_{coll}/50$



$$F_{ij}^{n} = k_n \delta_{ij} n_{ij} - \gamma_n m_{eff} v_{ij}^{n}$$

$$F_{ij}^{t} = -k_t u_{ij}^{t} - \gamma_t m_{eff} v_{ij}^{t}$$

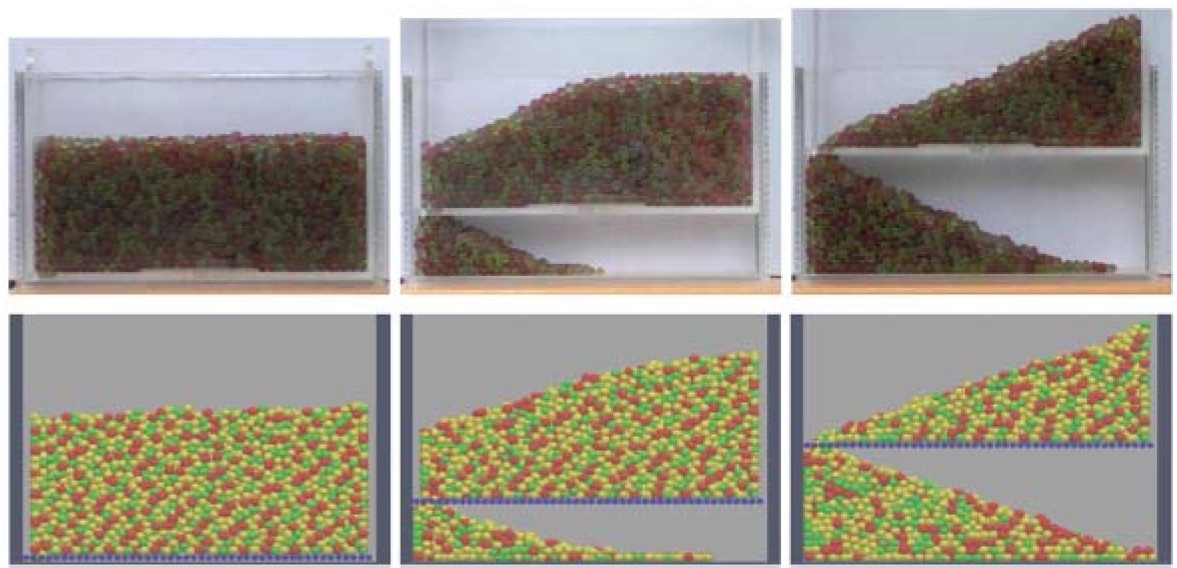
$$m_{eff} = m_i m_j / (m_i + m_j)$$

$$e = \exp\left(-\gamma_n \pi / \sqrt{4k_n / m_{eff} - \gamma_n^2}\right)$$

$$m_i \frac{d^2}{dt^2} r_i = f_i$$

$$I_i \frac{d}{dt} \omega_i = t_i$$

$$t_{coll} = \pi\left(2k_n / m - \gamma_n^2 / 4\right)^{-1/2}$$



Snapshots of side discharge of glass beads from experiment (top row) and simulation with a rolling friction coefficient of 5×10−5 m (bottom row) *

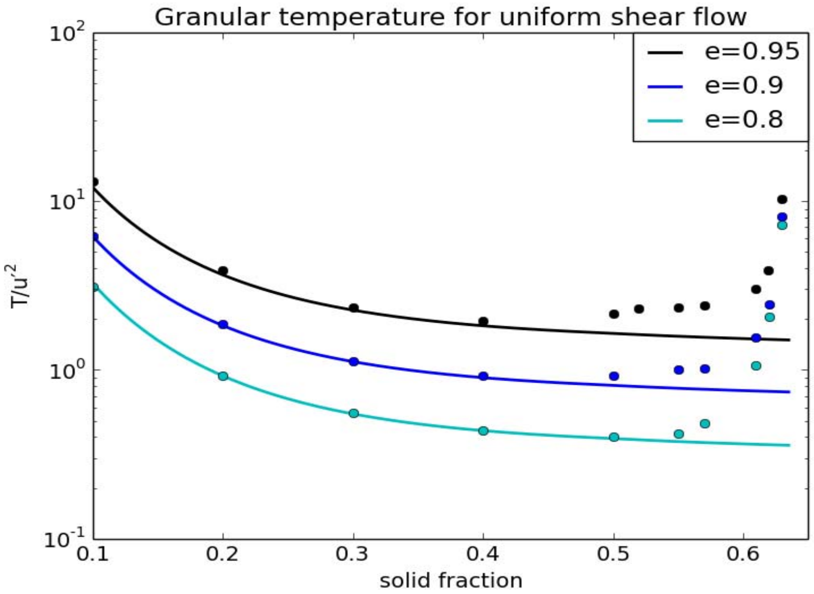
Li, T., et al. (2012). "Open-source MFIX-DEM software for gas-solids flows: Part II—Validation studies." Powder technology **220**: 138-150.

Kinetic theory cannot match DEM results in dense region

Assumptions:

- Velocity distribution only determined by collisions
- Inelastic collision (kinetic energy dissipated during collision)
- Instant binary collision

However in dense regime, where sustained multi-particle contacts prevail, the kinetic theory will overestimate the energy dissipation rate and the model may suffer inaccuracy.



*S. Chialvo, andS. Sundaresan, "A modified kinetic theory for frictional granular flows in dense and diluteregimes," Physics of Fluids (1994-present) **25**, 070603 (2013).

Challenges/Objectives

- Kinetic theory can handle large scale simulation but it may suffer inaccuracy when system is dense
- DEM is computational expensive, cannot be applied to industrial level simulation

Improve the continuum modelling of granular flow

In detail:

- To extend current kinetic theory to cover dense system where sustained multi-particle contacts prevail
- To use DEM result to verify and improve Kinetic Theory modeling in dense system

to facilitate the modeling of a wide range of flow system.

Modified Kinetic Theory for multi-body collision in dense region

Inelastic hard sphere model: event driven model with a varied time step, unlike soft sphere Discrete Element Method (DEM)

Three drawbacks:

1. The number of collisions per unit time can diverge, i.e. "inelastic collapse"
2. All interactions are binary, multiparticle contacts cannot occur
3. No static limit (No way to represent enduring contacts between particles)

Proposed modifications to the IHS model: "contact duration" concept, so that it can store some contact energy

$$e = \begin{cases} 1 \;\; if \; t < t_c \\ e \; if \; t \geq t_c \end{cases} \quad t: time\ since\ last\ contact$$

Luding, S. and A. Goldshtein (2003). "Collisional cooling with multi-particle interactions." Granular matter **5**(3): 159-163.

Modified Kinetic Theory for multi-body collision in dense region

Based on the modification to IHS, the energy dissipation rate was modified* :

$$p(t_c + dt) = p(t_c)(1 - t_E^{-1} dt) \qquad p(t_c) = \exp(-\tau_c)$$

$$\tau_c = t_c / t_E$$

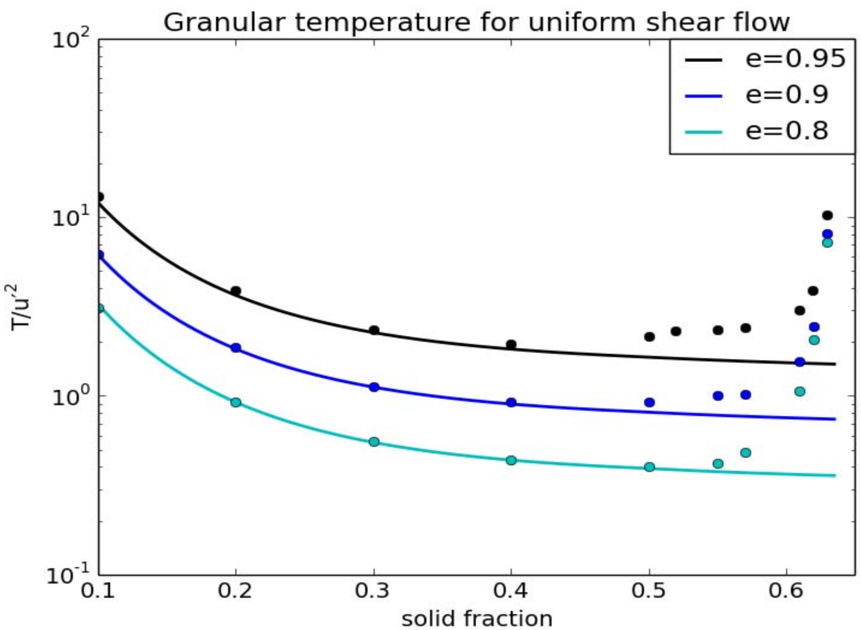
$$K = p(t_c)^2 = \exp\left(-24 \frac{\mathrm{t_c}}{\mathrm{d}} \phi g_0 \sqrt{\frac{T}{\pi}}\right)$$

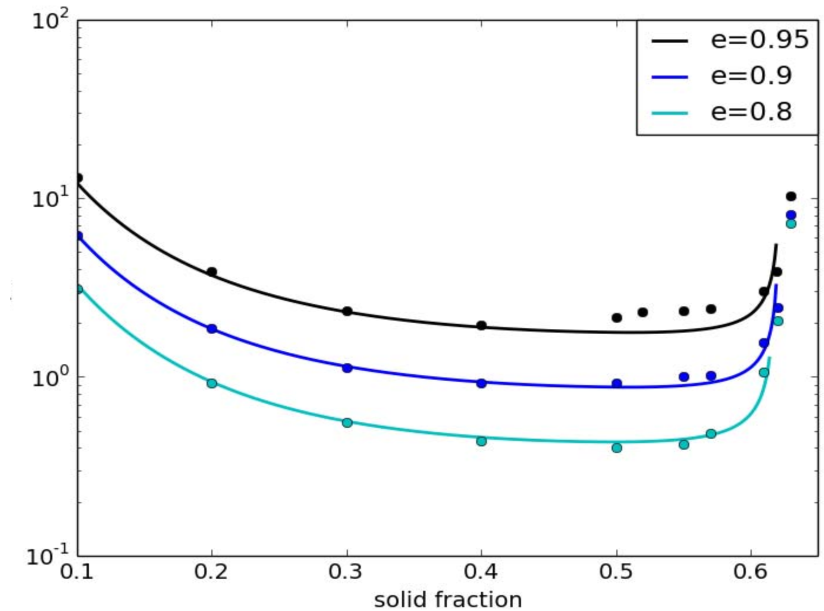
$$\Gamma = \frac{12}{\sqrt{\pi} d} \rho \phi^2 g_0 (1 - e^2) K$$

$$t_E^{-1} = \frac{12}{\mathrm{d}} \phi g_0 \sqrt{\frac{T}{\pi}}$$

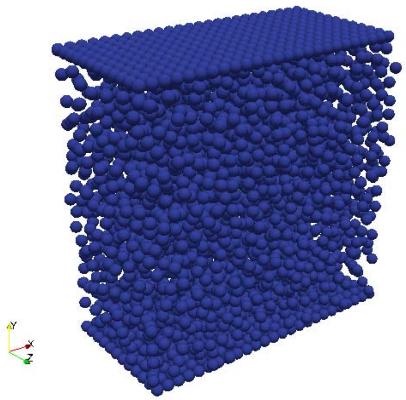
*S. Luding, andS. McNamara, "How to handle the inelastic collapse of a dissipative hard-sphere gas with the TC model," Granular Matter **1**, 113 (1998)

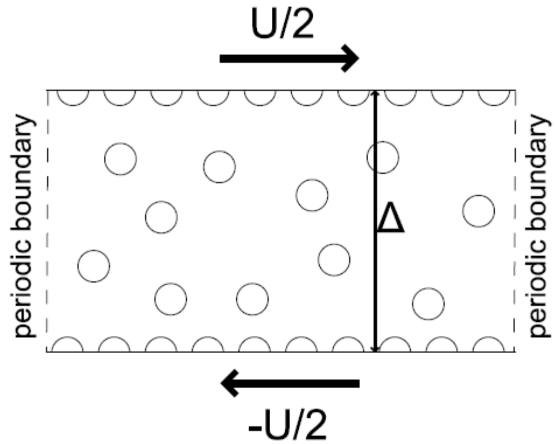
Modified Kinetic Theory applied on uniform shear flow



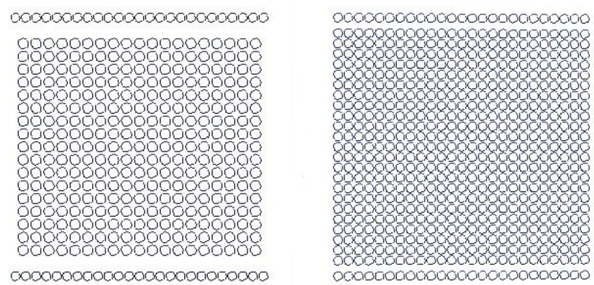


Modified Kinetic Theory applied on plane shear flow

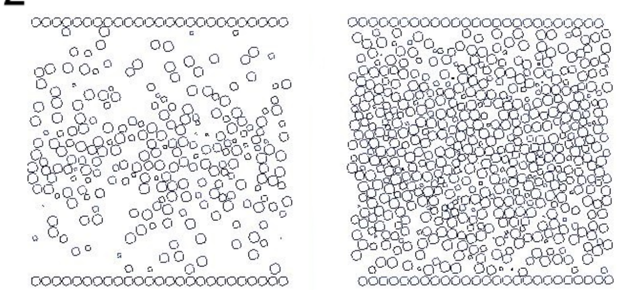




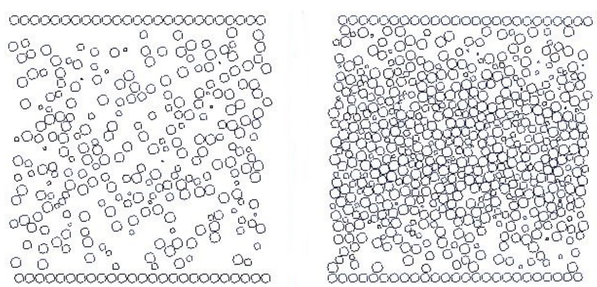
D=0.8 cm
Rho=2.7 g/cm^3
e=0.9
L x H x W=20 cm x 20 cm x 10 cm
U=20 cm/s



(a): t=0sec (left: 3507 particles; right: 7500 particles)

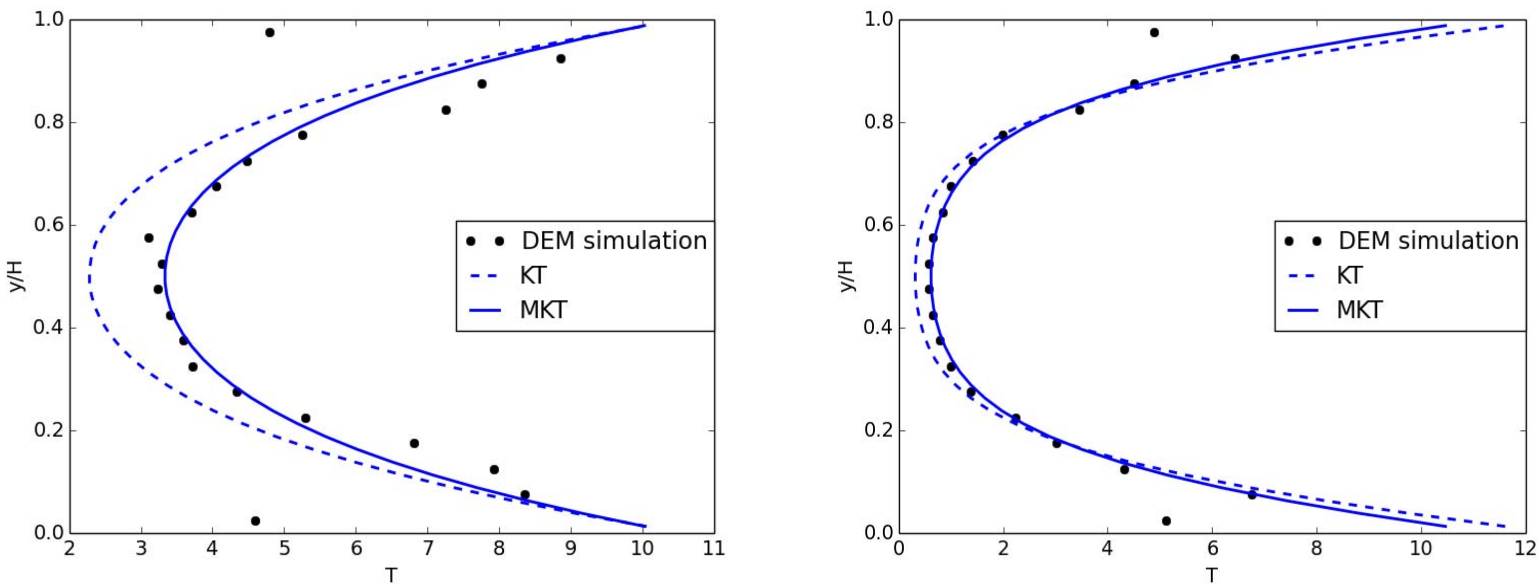


(c): t=60sec (left: 3507 particles; right: 7500 particles)



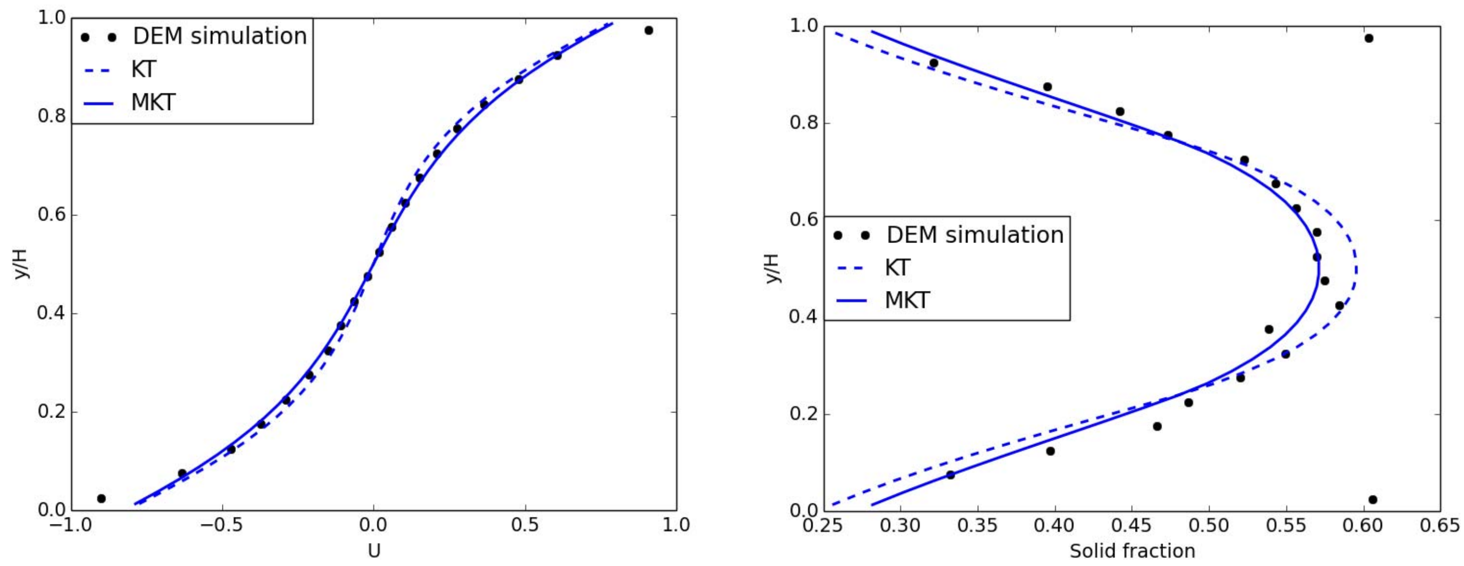
(b): t=10sec (left: 3507 particles; right: 7500 particles)

Granular temperature and velocity profile



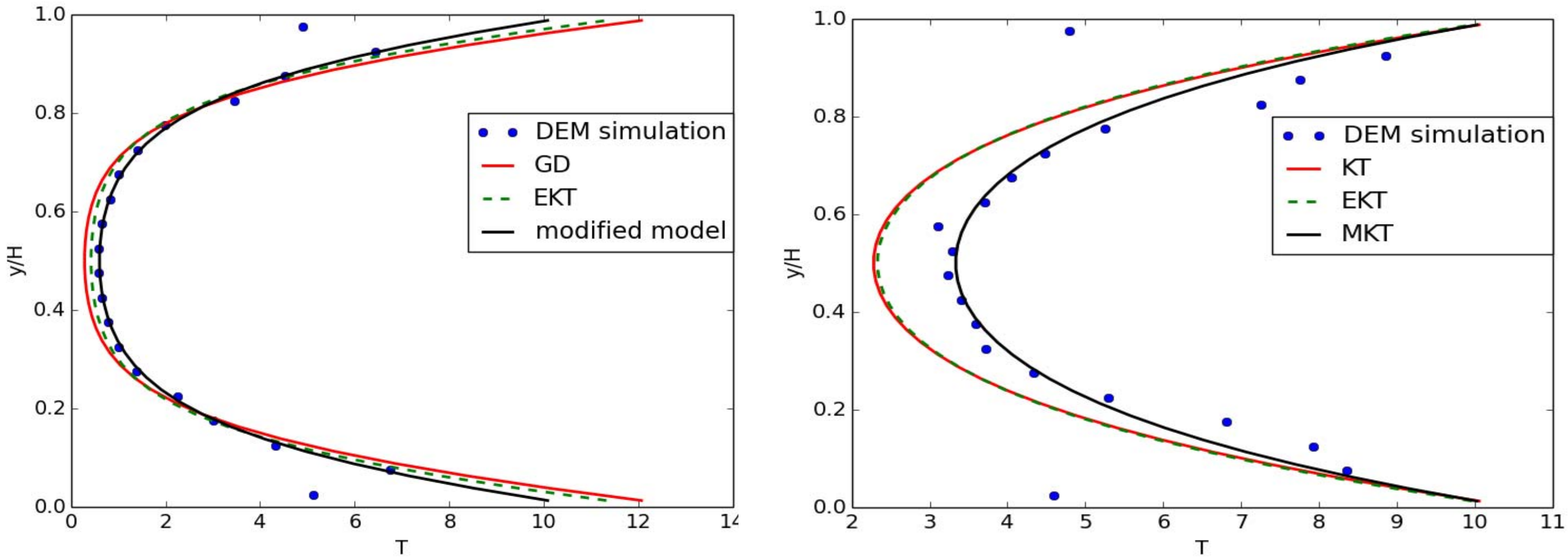
Profile of granular temperature T along the y direction. DEM result (dots) and theoretical solution from the KT model (dashed line), theoretical solution from this model (line) at e=0.95 (left) and e=0.9 (right)

Solid volume fraction profile



Profiles of velocity U and solid volume fraction ϕ along the y direction. DEM result (dots) and theoretical solution from the KT model (dashed line), theoretical solution from this model

Comparison between EKT and our modified KT



Result comparison between t-c modification and extended kinetic theory (EKT) e=0.9 left, e=0.95 right

LIST OF PAPERS PUBLISHED, STUDENTS SUPPORTED UNDER THIS GRANT

Archival journal publications:

- Feng, Z-G., Ponton, M. E. C., Michaelides, E. E., and Mao, S. (2014). “Using the Direct Numerical Simulation to Compute the Slip Boundary Condition of the Solid Phase in Two-Fluid Model Simulations.” Powder Technology. j.powtec.2014.01.020
- Feng, Z-G (2014). “Direct Numerical Simulation of Forced Convective Heat Transfer from a Heated Rotating Sphere in Laminar Flows,” ASME J. of Heat Transfer, ” Journal of Heat Transfer. doi:10.1115/1.4026307.
- Feng, Z-G, and Samuel Gem Musong. "Direct numerical simulation of heat and mass transfer of spheres in a fluidized bed." Powder Technology 262 (2014): 62-70.
- Musong, S. and Feng, Z-G (2015). “Mixed Convective Heat Transfer from a Heated Sphere at an Arbitrary Incident Flow Angle in Laminar Flows,” Int. J. Heat and Mass Transfer, vol. 78, pp. 34-44.
- Feng, Z-G, Alatawi, E. S., Roig, A., and Sarikaya, C.(2016). “A resolved Eulerian-Lagrangian simulation of fluidization of 1204 heated spheres in a bed with heat transfer.” ASME Journal of Fluid Engineering. Vol. 138, No.4: 041305.
- Musong, S. G., Z-G Feng, Efstathios E. Michaelides, and Shaolin Mao (2016). "Application of a Three-Dimensional Immersed Boundary Method for Free Convection From Single Spheres and Aggregates." Journal of Fluids Engineering 138, no. 4 (2016): 041304.
- Duan,Y., Feng. Z-G, Michaelides, E. E ., and Mao, S. (2017). “Modified Kinetic Theory Applied to the Granular Flows.” Physics of Fluids. Accepted.

Book Chapter:

- Feng, Z-G and Michaelides, E. (2016). The Immersed Boundary Method. In Efstathios E Michaelides, Clayton T Crowe, John D Schwarzkopf (Ed.), Multiphase Flow Handbook, Second Edition. CRC Press Taylor & Francis Group. Pages: 126-144.

Student involved in the project:

- Miguel Cortina, Yifei Duan, Samuel Musong (PhD candidates)
- Adams Roig, Kody Smajstrla, Cenk Sarikaya, Steven Cooks (master students)
- Silvia Murguia, Carlos Mendez, Joshua Moran (Undergraduate students)

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