CFD-DEM simulations of bubbling fluidization: Identification of critical model parameters

A. Bakshi[a,b*], M. Shahnam[b], T. Li[b], A. Gel[c], C. Altantzis[a,b], W. Rogers[b], A.F. Ghoniem[a]
[a] Massachusetts Institute of Technology, Cambridge, MA-02139
[b] National Energy Technology Lab, Morgantown, WV-26507, USA
[c] ALPEMI Consulting, LLC, Phoenix, Arizona-85044, USA

August 8, 2017

U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

Overall

NATIONAL ENERGY TECHNOLOGY LABORATORY

Objectives

- Identify critical CFD-DEM modeling parameters and their impact on fluidization hydrodynamics in pulsating flows
- Improve TFM constitutive equations after validating critical model and numerical parameters

Summary

Multivariate parametric sensitivity analysis indicates:

1. Choice of metrics is critical: e.g. kn shows little influence on bubble diameter but can significantly affect particle KE. Must choose at least 2 independent dynamic metrics
2. Sensitivity of simulations to friction and restitution depends on choice of tangential damping; high tangential damping => changes in frictional coefficient have little impact on dynamics
3. Spring stiffness is rel. less critical when collision time << flow time; kn = 10 N/m => unphysically high contact deformations => artificially sensitivity to other model parameters

Outline

- Introduction
- Limitations and challenges
- Current application
- Parametric space and sampling
- Quantities of Interest
- MOAT analysis
- *low* spring stiffness
- Friction and restitution
- Friction vs. tangential damping
- Summary

CFD-DEM

Advantages:

- Fundamental understanding of fluidization
- Coupling several particle-scale phenomena
- Constitutive equations for coarse models

Computationally expensive and only small lab-scale systems can be simulated

Frameworks:

Hard sphere
- Instantaneous collisions
- Event-driven time step
- Dilute suspensions

Soft sphere
- Deformations permitted
- Δt = f(collision-time)
- Generally applicable

Non-Linear
- e.g. Hertzian contact is physically relevent
- Collision time can be aritificially increased

Linear
- Simple implementation
- Adapted to multiple applications

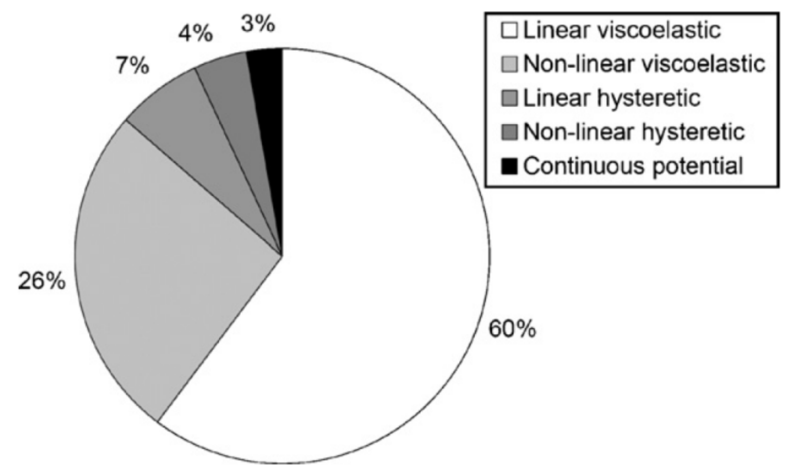


Fig. 1. Relative frequency of different classes of normal force models as found in a randomly selected sample of 100 research papers dealing with DEM simulations of hoppers, drums, mixers, fluidized beds, grates and plug flow.

Kruger-Emden et al 2016

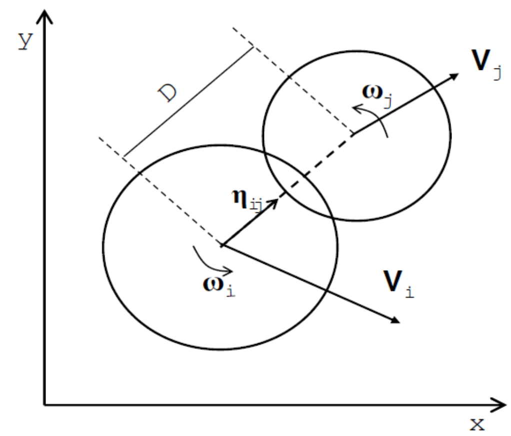
Linear Spring Dashpot (LSD) Model

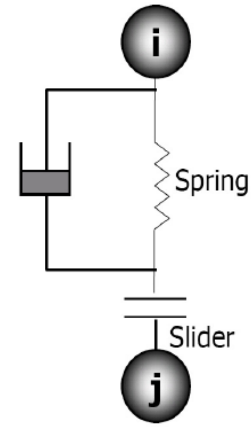
Equations

$$\frac{d\mathbf{X}^{(i)}(t)}{dt} = \mathbf{V}^{(i)}(t)$$

$$m^{(i)}\frac{d\mathbf{V}^{(i)}(t)}{dt} = m^{(i)}\mathbf{g} + \boldsymbol{F_d} + \boldsymbol{F_c}$$

$$I^{(i)}\frac{d\boldsymbol{\omega}^{(i)}(t)}{dt} = \mathbf{T}^{(i)}$$





Contact forces

Spring-dashpot normal force

$$\boldsymbol{F_n}^{(i,j)} = \boldsymbol{F_{n,S}}^{(i,j)} + \boldsymbol{F_{n,D}}^{(i,j)} = -k_n\delta_n\boldsymbol{\xi_n} - \eta_n\boldsymbol{V_n}^{(i,j)}$$

tangential forces are similar, except include friction ..

$$\boldsymbol{F_{t,S}}^{(i,j)} = \begin{cases} -k_t\delta_t\boldsymbol{\xi_t} & \text{if } k_t\delta_t \le \mu\left|\boldsymbol{F_{n,S}^{(i,j)}}\right| \\ -\mu\left|\boldsymbol{F_{n,S}^{(i,j)}}\right|\boldsymbol{\xi_t} & \text{otherwise} \end{cases}$$

Analytical solution:

Normal damping related to spring stiffness, restitution

$$\eta_{\mathrm{n}m\ell} = \frac{2\sqrt{m_{\mathrm{eff}}k_{\mathrm{n}m\ell}}\,|\ln e_{\mathrm{n}m\ell}|}{\sqrt{\pi^2 + \ln^2 e_{\mathrm{n}m\ell}}}$$

(normal) contact duration depends on spring stiffness, restitution

$$t_{col} = \sqrt{\frac{m_{eff}}{k_{nml}}}\sqrt{\pi^2 + ln^2 e_{nml}}$$

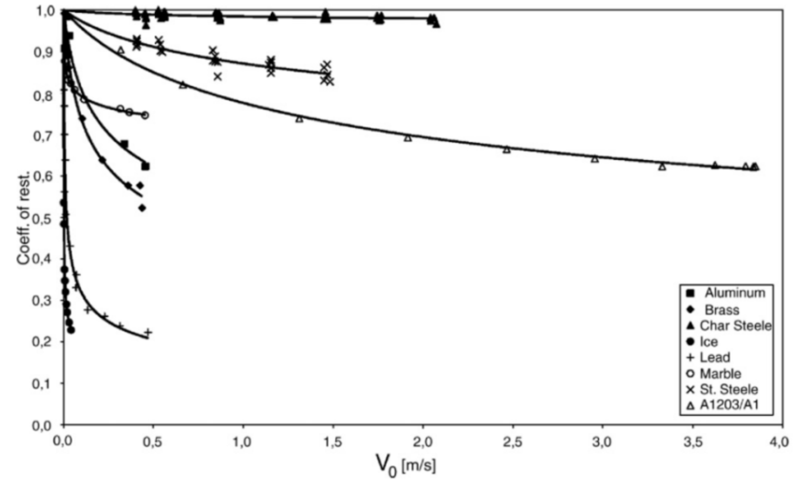
Limitations and challenges

1. Oblique, multi-particle collisions and interactions are difficult / impossible to measure
2. Normal restitution, contact duration depend on material properties, V_0 and humidity
3. Based on material properties, kn ~ 10^6 makes simulations computationally infeasible

⇒ **Model parameters are often tuned, but ..**

1. 2D simulations have significantly lower coordination numbers and require over-tuning
2. Sensitivity studies limited to at most two parameters = f(nominal settings of others)
3. Choice of metrics: statics vs. dynamics, bubbles vs. solids mixing; focus on specific/limited metrics could undermine system dynamics

Lack of guidelines for model development and validation, and inconsistent findings in literature



Kruggel-Emden et al 2007

Application

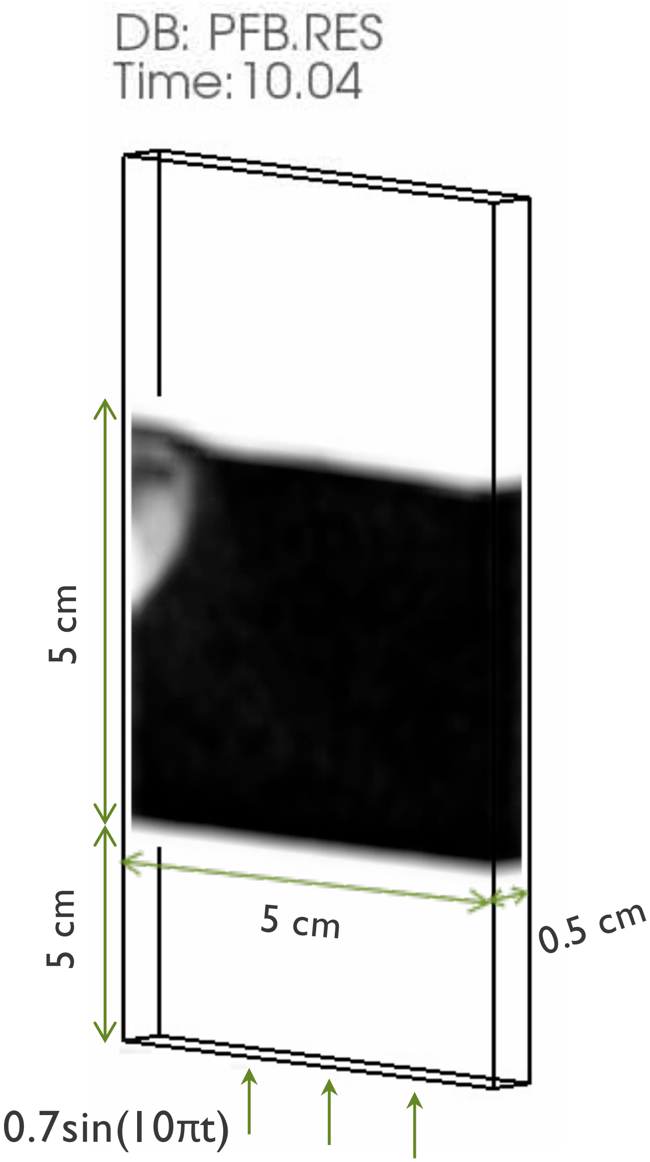
Simulation Setup

- Pulsating beds alternate between granular and kinetic dominated regimes
- Domain size chosen for alternate 1-1 bubbling
- 166380 Geldart B particles (0.4 mm, 2500 kg/m^3)

Assumptions:

1. Gidaspow drag model is applicable
2. Simulations using resolution 2.5 particle diameters are *grid independent* (Liu et al 2016, Radl and Sundaresan 2014)
3. Time and space integration are less critical than model parameters (Kruggel-Emden et al 2011, Hanley et al 2016)

Uncertainties from these assumptions will be quantified in the next phase



$U/U_{mf} = 1.3 + 0.7\sin(10\pi t)$
$U_{mf} = 2.6$ m/s

Parametric Range

System dynamics change significantly depending on choice of parameters

e_n = 0.98
μ = 0.33
η_t/η_n = 0.90
k_n = 10 N/m

High dissipation

e_n = 0.50
μ = 0.33
η_t/η_n = 0.63
k_n = 1000 N/m

Low dissipation

e_n = 0.98
μ = 0.05
η_t/η_n = 0.90
k_n = 215 N/m

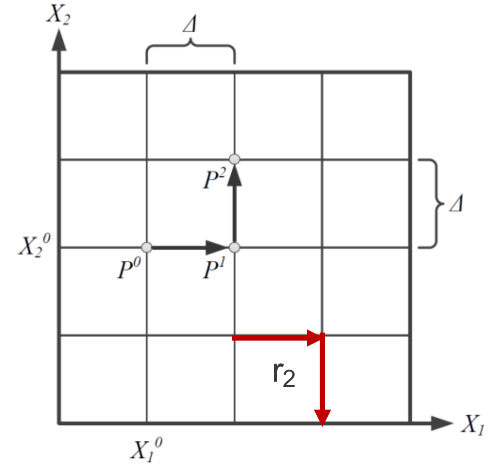
Parametric Range

Nominal setting and range based on commonly reported values in literature

Label	Model parameter			Range		
	Physical representation	Symbol	Units	Nominal	Min.	Max.
p_1	normal spring stiffness p-p (10^{p_1})	k_n	[N/m]	2.00	1.00	3.00
p_2	normal spring stiffness p-w (10^{p_2})	$k_{n,w}$	[N/m]	2.00	1.00	3.00
p_3	friction coefficient p-p	μ	-	0.30	0.05	0.90
p_4	friction coefficient p-w	μ_w	-	0.30	0.05	0.90
p_5	normal restitution p-p	e_n	-	0.90	0.50	0.98
p_6	normal restitution p-w	$e_{n,w}$	-	0.90	0.50	0.98
p_7	tangential-normal stiffness ratio p-p	k_t/k_n	-	0.29	0.10	0.90
p_8	tangential-normal stiffness ratio p-w	$k_{t,w}/k_{n,w}$	-	0.29	0.10	0.90
p_9	tangential-normal damping ratio p-p	η_t	-	0.50	0.10	0.90
p_{10}	tangential-normal damping ratio p-w	$\eta_{t,w}$	-	0.50	0.10	0.90
p_{11}	collision-DEM time-step ratio	τ_{col}/τ_{DEM}	-	50	20	50
p_{12}	fluid equations tolerance ($10^{p_{12}}$)		-	-4.00	-6.00	-3.00
p_{13}	DEM-fluid grid interpolation width		[Δx]	0.80	0.40	1.00

MOAT Sampling

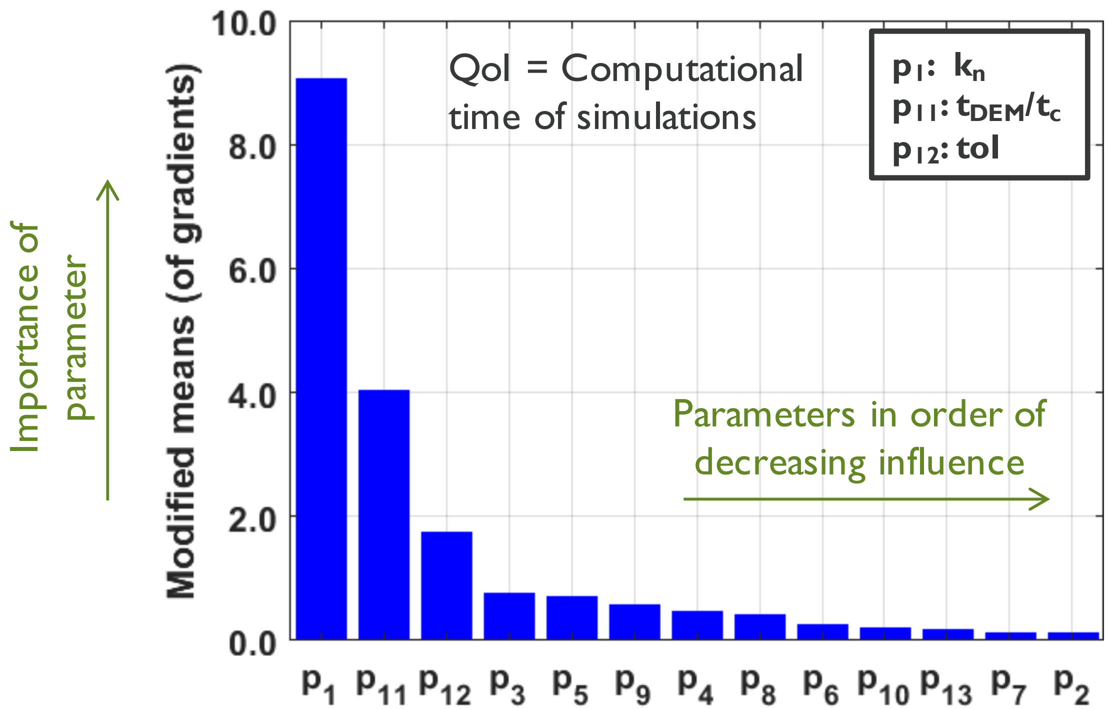
- Used in complex models: ecological, building and traffic simulations …
  - Qualitative screening, best for quantifying most sensitive factors
- Parameters discretized at 4 levels, assuming uniform distribution
- First point and orientation (*walk*) are randomly chosen
- One replication constitutes (p+1) simulations
- Multiple replications required for uniform sampling and convergence
- Sensitivity to x_i = average of *elementary effects* $F(x_i)$ across all replications



Ge and Menendez 2014

$$F(X_1) = \frac{QoI(p^1) - QoI(p^0)}{\Delta}$$

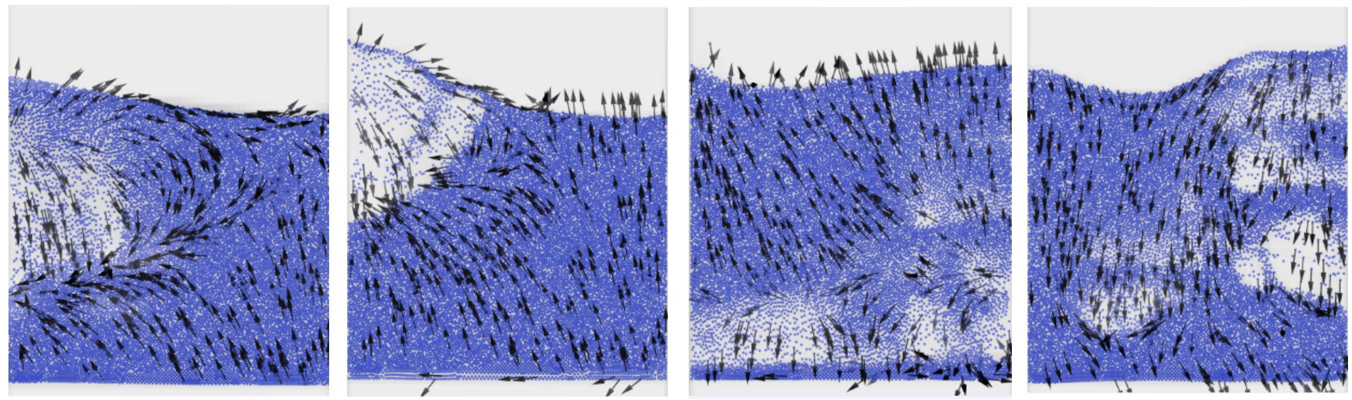
$$F(X_2) = \frac{QoI(p^2) - QoI(p^1)}{\Delta}$$



Quantities of Interest (QoI)

PSUADE + MATLAB

Sampling



CFD-DEM simulation data (50 Hz, 10-40s)

MS3DATA (2D slices)

Analysis

Bubbling and solids dynamics are related in freely bubbling beds

- alternating granular and bubbling regimes
- short bed height => bubble dynamics are not always sensitive

Bubbling dynamics

1. Diameter ~ dissipation

$$\bar{d}_b = \sqrt{\frac{\sum d_b^2}{n_b}}$$

2. x-location ~ pattern

$$\bar{x}_b = \frac{\sum |x_b|}{n_b}$$

Solids dynamics

1. rms velocity ~ mixing time

$$\mathrm{KE_t} = \sum_i^N \frac{1}{2} m v_i^2$$

2. average height ~ distribution

$$\mathrm{PE_t} = \sum_i^N m g h_i$$

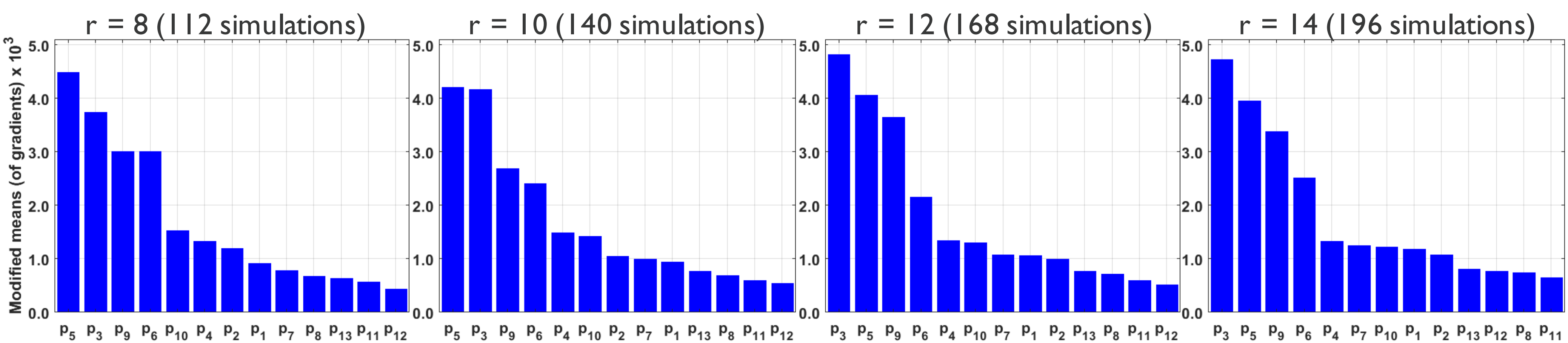
MOAT Analysis

NATIONAL ENERGY TECHNOLOGY LABORATORY

Statistical convergence – bubble diameter

- Replications required for sampling uniformity in parametric space
- # replications for convergence depends on Non-linearity / coupling of parameters
- How many *critical* parameters are of interest?
- Bubble diameter: top 4 parameters identified within 6 replications (although ranking + magnitudes only converge at 12 replications)

p_1: k_n
p_2: k_{nw}
p_3: μ
p_4: μ_w
p_5: e_n
p_6: e_{nw}
p_7: k_t/k_n
p_8: k_{tw}/k_{nw}
p_9: η_t/η_n
p_{10}: η_{tw}/η_{nw}
p_{11}: t_{DEM}/t_c
p_{12}: tol
p_{13}: w_{DES}



MOAT Analysis

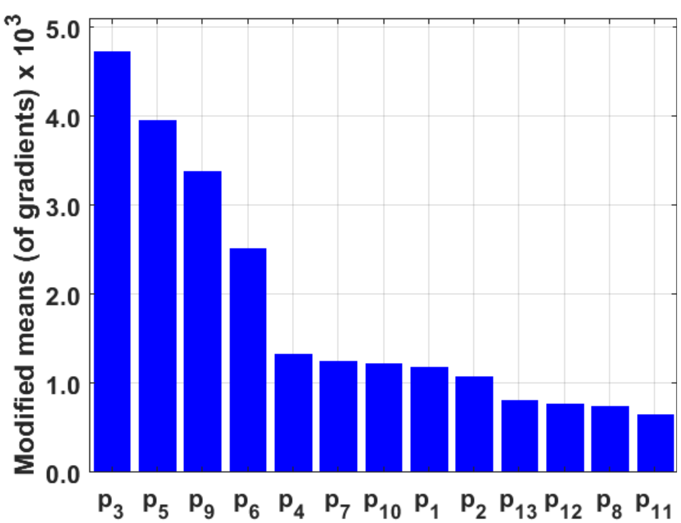
NATIONAL ENERGY TECHNOLOGY LABORATORY

All metrics

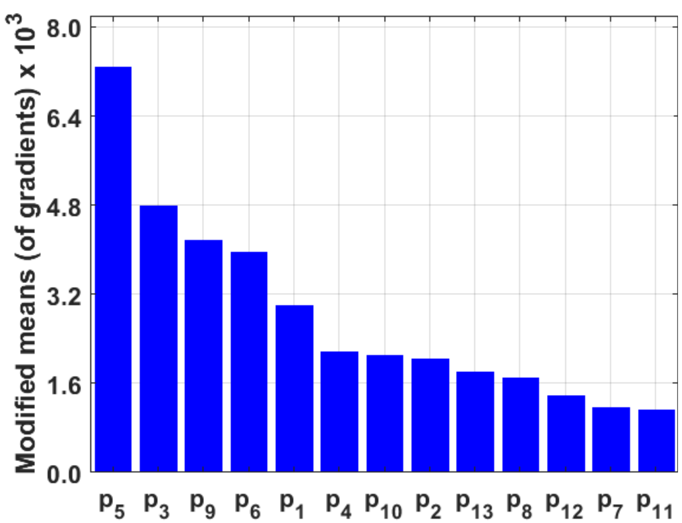
- Different QoI are affected by different parameters
- Besides friction (p3, p4) and restitution (p5, p6), tangential damping (p9) has significant influence
- Spring stiffness (p1) affects particle KE but not bubble diameter
- Tangential / normal spring stiffness ratio (p7, p8), and *numerical* parameters- # DEM time steps (p11), interpolation width (p12) are relatively irrelevant

p_1: k_n
p_2: k_{nw}
p_3: μ
p_4: μ_w
p_5: e_n
p_6: e_{nw}
p_7: k_t/k_n
p_8: k_{tw}/k_{nw}
p_9: η_t/η_n
p_{10}: η_{tw}/η_{nw}
p_{11}: t_{DEM}/t_c
p_{12}: tol
p_{13}: w_{DES}

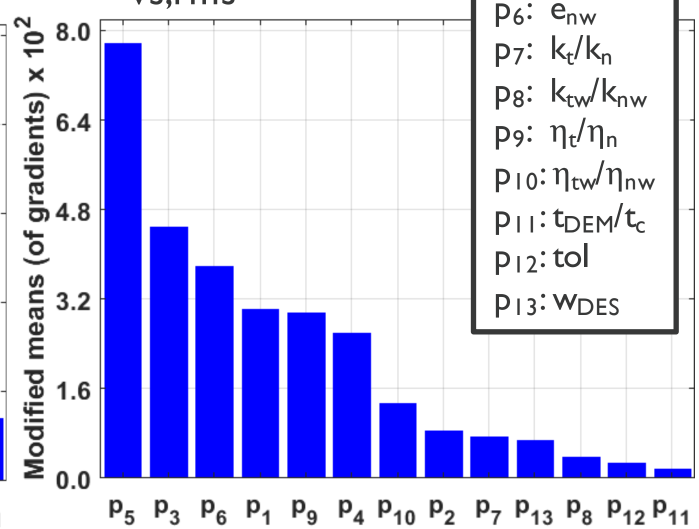
bubble diameter



bubble x-location



vs,rms

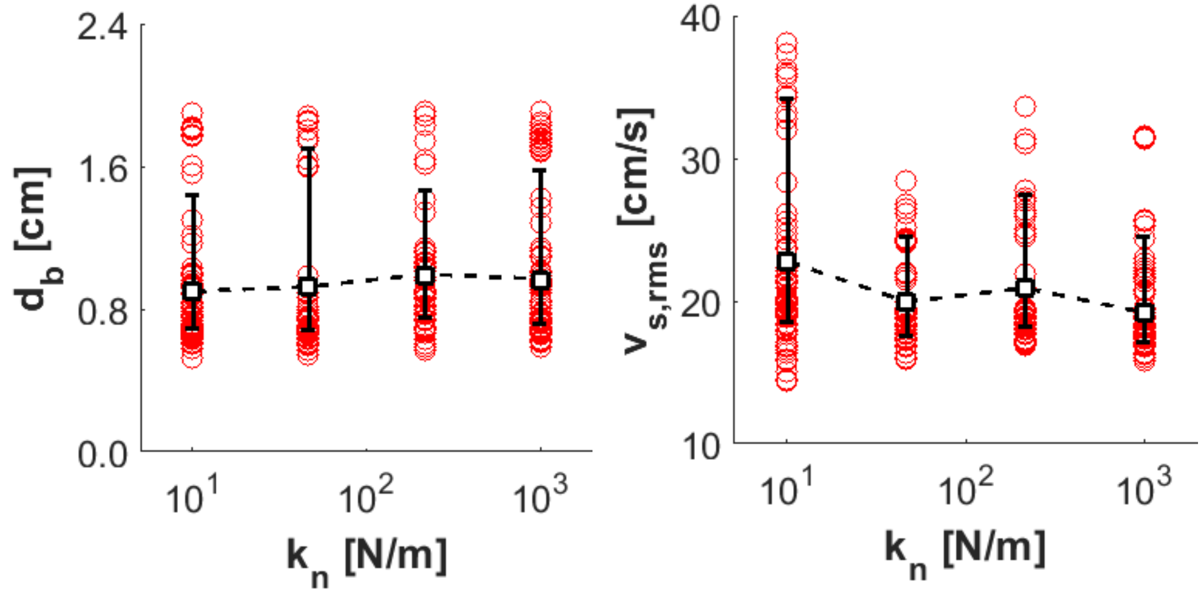


Spring Stiffness

Scatter plots obtained by segregating ~250 simulations based on spring stiffness

Significant spread in KE for kn = 10 N/m, even though bubble diameter predictions fairly consistent

- Artificially high contact deformations amplifies influence of other model parameters



Spring Stiffness

4 simulations with all other parameters at their nominal settings
- Similar bubble diameter and x-location
- KE (rms vs) increases as kn decreases

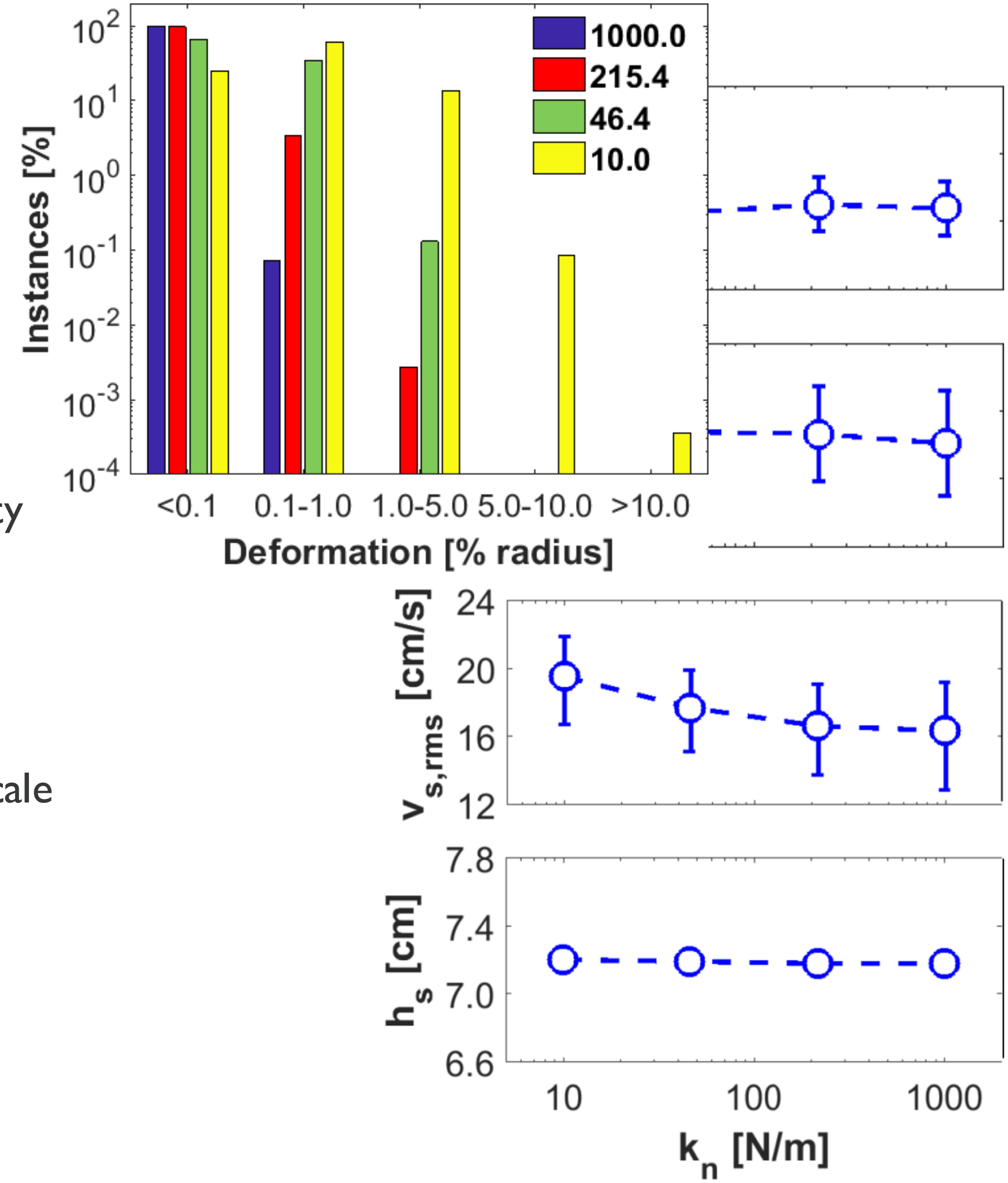
Lower stiffness
⇒ higher contact deformations (>5%)
⇒ more compact dense phase & lower permeability
⇒ faster bubble flow
⇒ faster solids flow around bubbles

Acceptable choice must dependent on flow-time scale

$$\frac{\text{Collision time}}{\text{Flow time}} = \sqrt{\frac{m_{eff}}{k_n}}\sqrt{\pi^2 + \ln^2 e}\,\frac{v_{s,rms}}{H_0}$$

= 0.30% for kn = 10 N/m

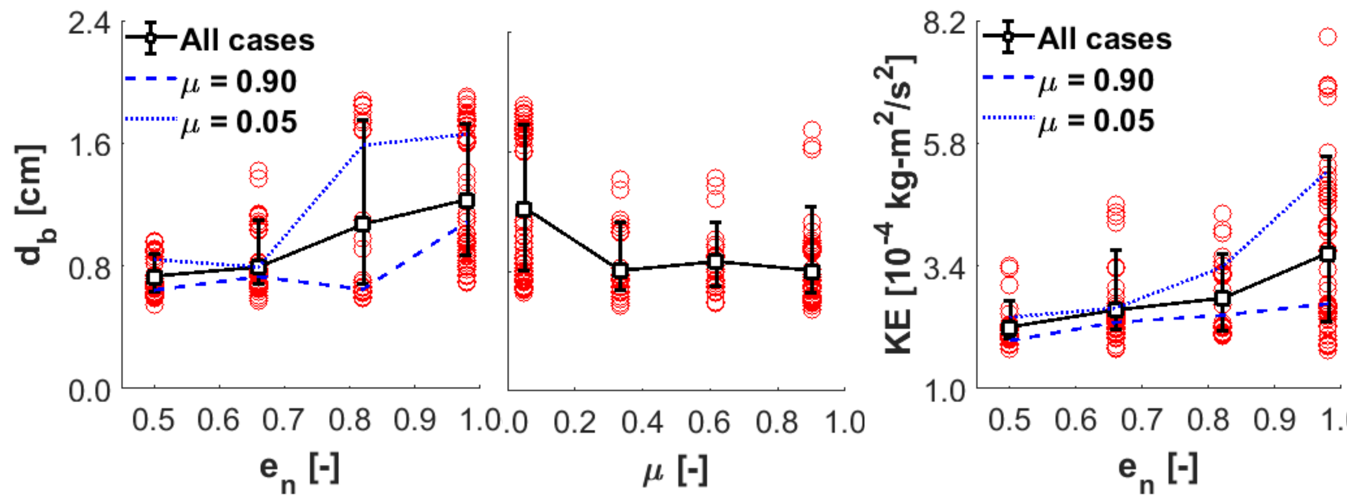
= 0.02% for kn = 1000 N/m



Friction & restitution

Dissipation in system has significant influence on bubble growth and particle KE

- diameter increases at higher restitution / lower friction
- beyond friction = 0.3, exact value doesn't matter



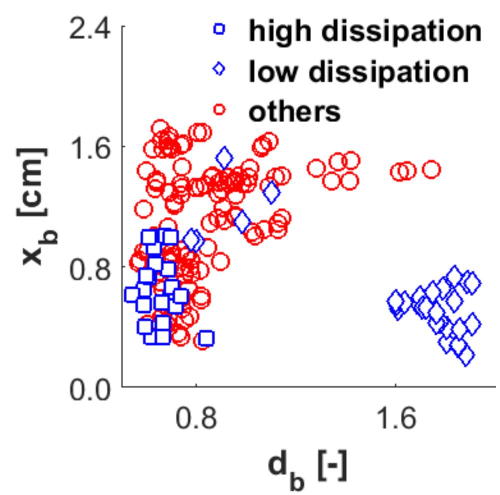
Patterns depend on bubble size

<u>*Low* dissipation</u>

- en = 0.82, 0.98 and mew= 0.05
- large bubbles rising through center

<u>*High* dissipation</u>

- en = 0.50, 0.66 and mew> 0.05
- small bubbles which collapse soon



High x_b indicates bubbles observed close to walls and higher likelihood of patterns

Friction vs. tangential damping

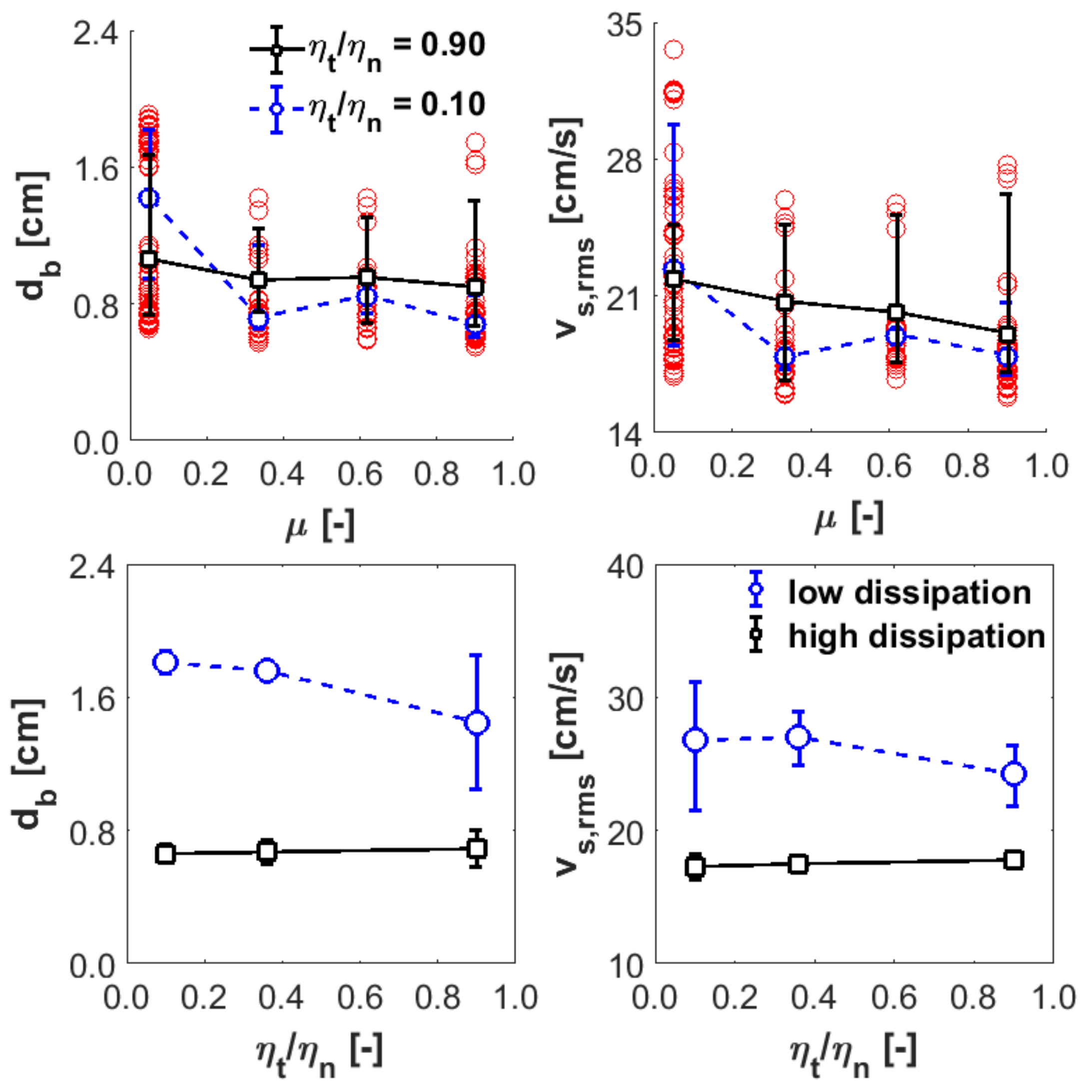
NATIONAL ENERGY TECHNOLOGY LABORATORY

Mixed reports in literature regarding the influence of friction

Tangential damping coefficient has received little attention

MFiX: $$\frac{\eta_t}{\eta_n} = 0.5$$

Deen et al: $$\frac{\eta_t}{\eta_n} = \frac{2}{7}\frac{\ln e_t}{\ln e_n}$$



Conclusions:

- Sensitivity of QoI to friction is high iff damping coefficient is low
- In low dissipation regime (high en, low friction), choice of tangential damping is critical

Summary

Key takeaways:

1. Important to investigate at at least 2 independent dynamic metrics
2. Artificially low kn has adverse consequences on particle KE; lower bound must be based on comparison of flow and collision time-scales.
3. Sensitivity of simulations to friction and restitution depends on tangential damping, and is the primary source of inconsistencies in literature
4. Pattern formation is unlikely in very high dissipation (no bubbles) or very low dissipation (high coalescence) regimes

Next steps:

- Generalized criterion for spring stiffness
- Friction vs. tangential damping – are these two sides of the same coin?
- Quantitative sensitivity analysis accounting for uncertainty in numerical parameters, drag
- Validate simulations and calibrate uncertain parameters using experimental data
- Why the Two Fluid Model is unable to capture patterns successfully
  - bubble formation and displaces solids motion
  - relaxation of particles during granular regime