

Investigating Cohesion in Wet Particles Systems

Raffaella Ocone

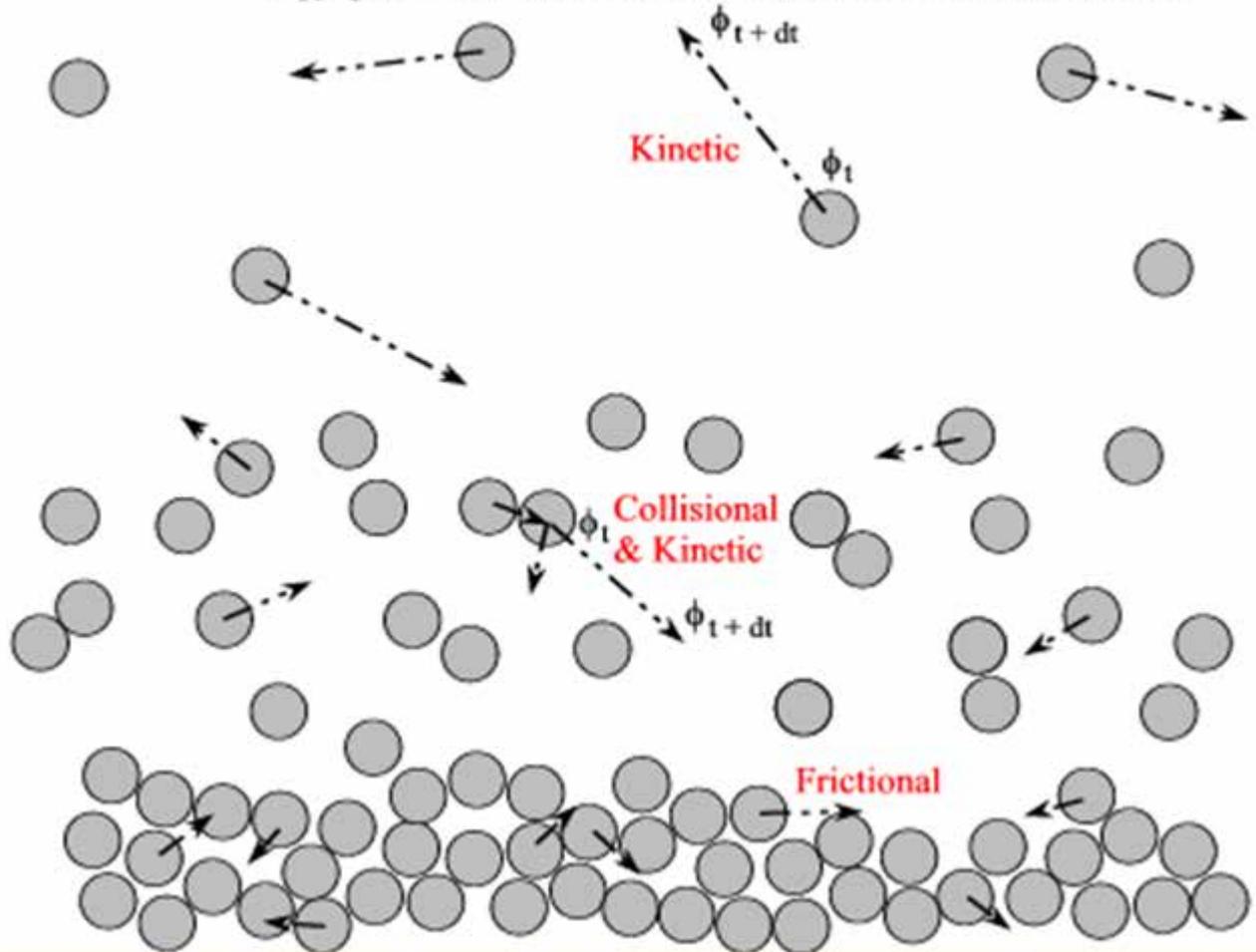
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Regime Map for Particle-Particle Interactions

Copyright of Sebastien Dartevelle, from Sebastien Dartevelle's Ph.D. Thesis



q Rapid flow regime

Binary-collisions
Fluid-like behaviour
KTGF (kinetic theory
of granular flow)

q Intermediate regime

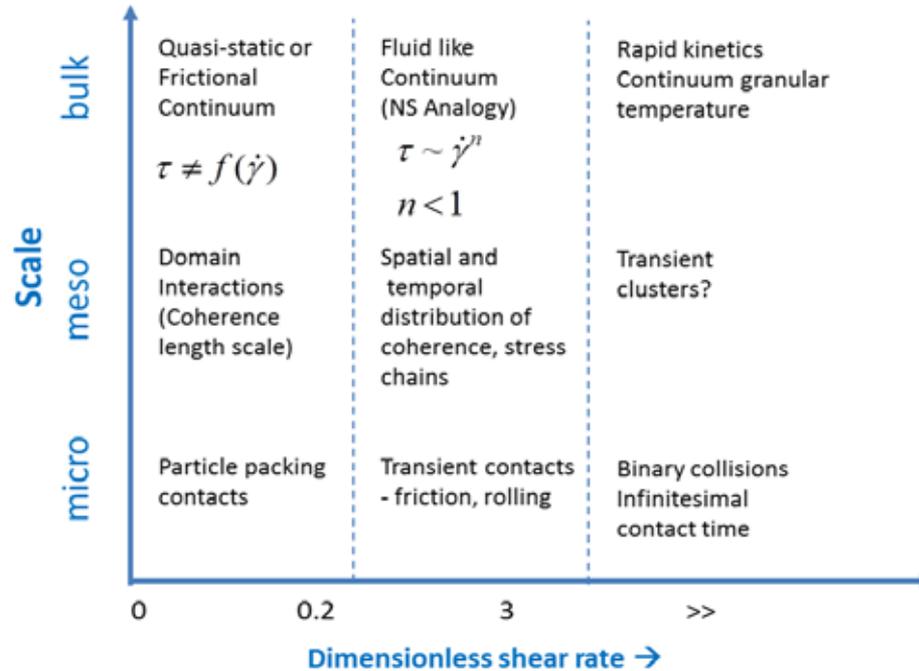
Coexistence of frictional and collisional
stress

q Slow, friction regime

Solid-like behaviour
Particle packing
Enduring contact
Coulomb frictional law

The Classification of Flow Regimes depends on the Applications

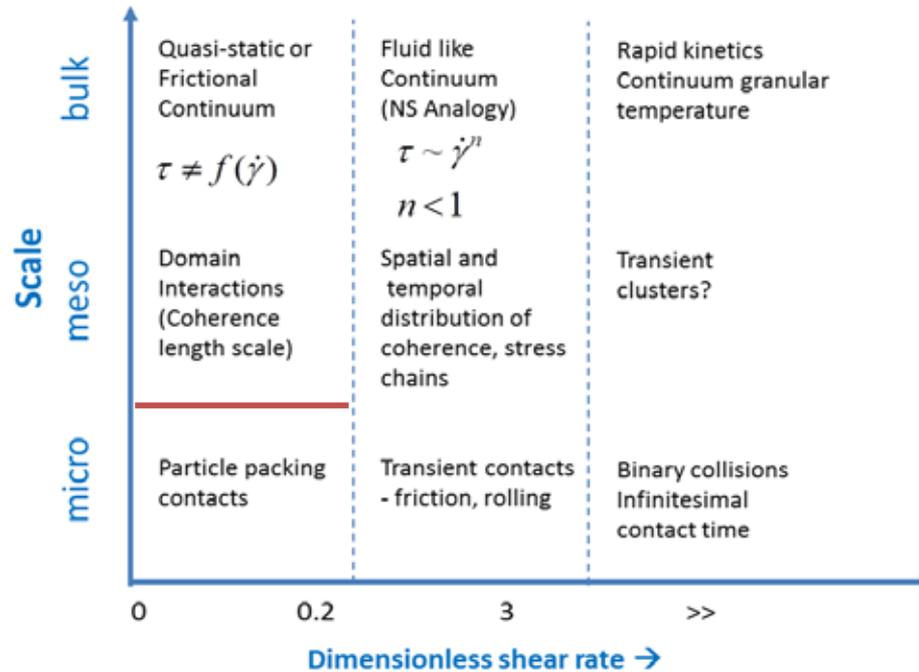
Multi-scale Approach to Particulate Flow – A Regime Map



[courtesy of P Mort]

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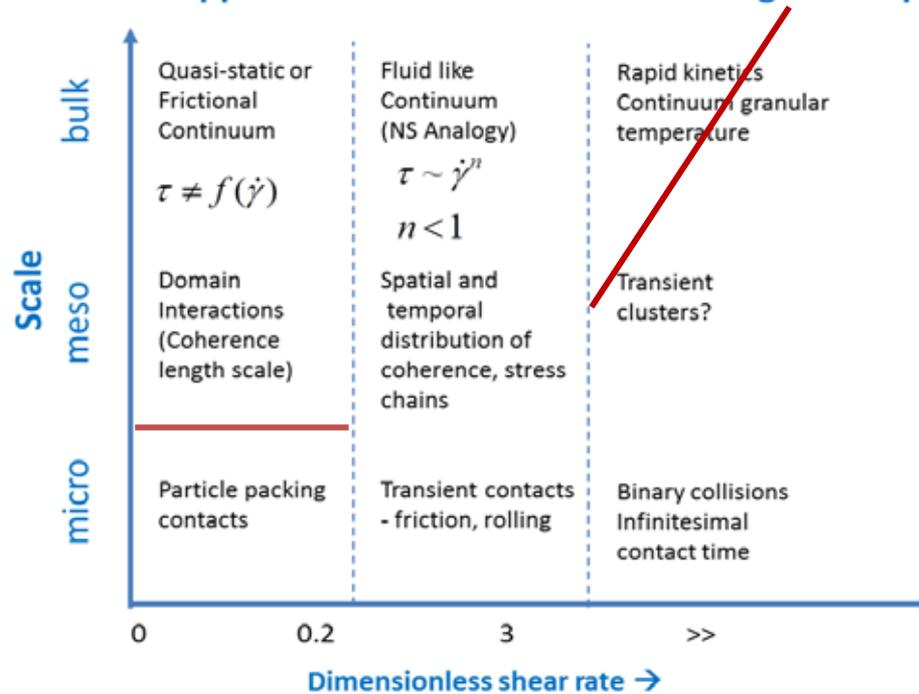
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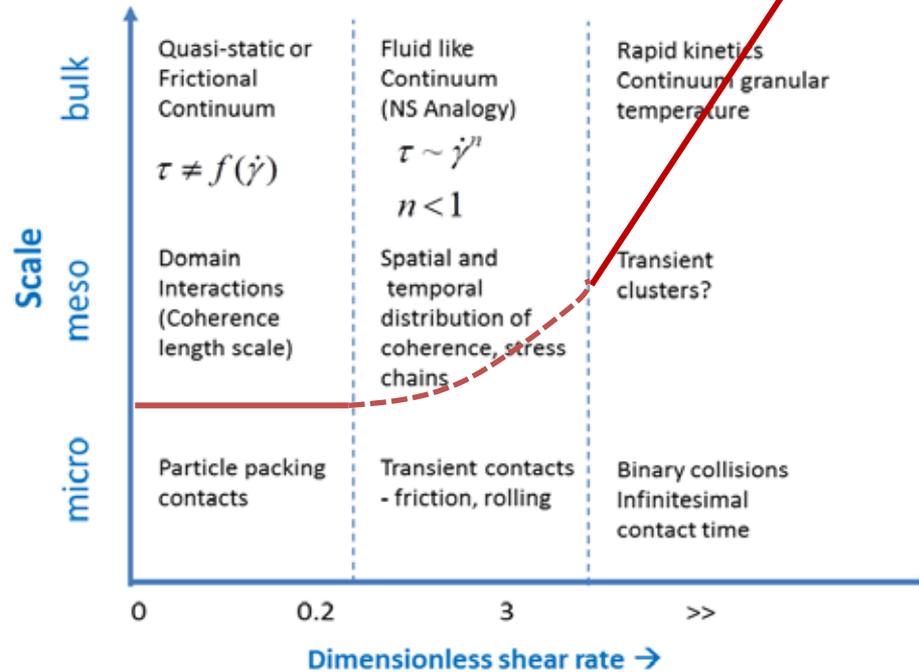
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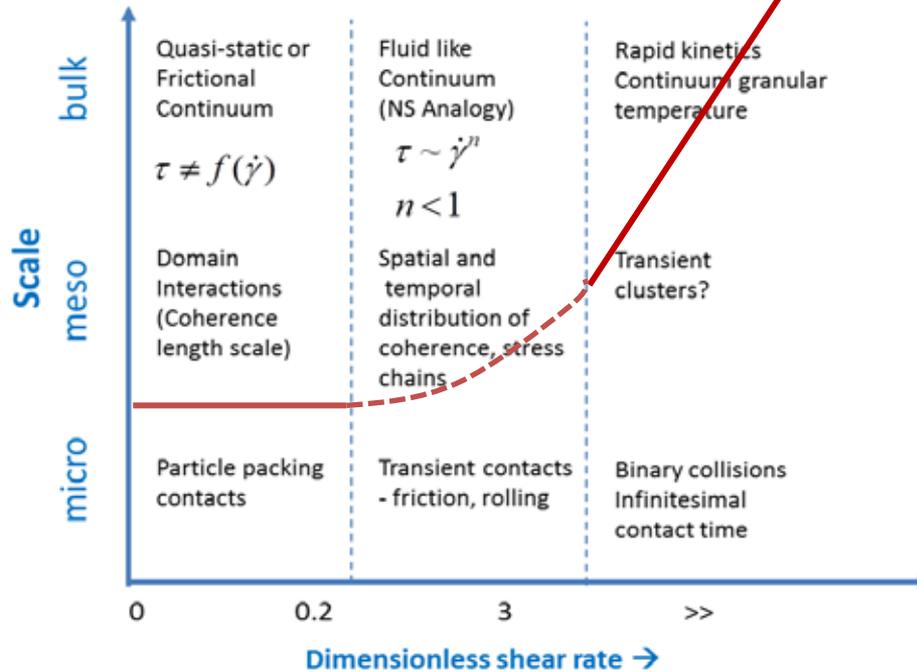
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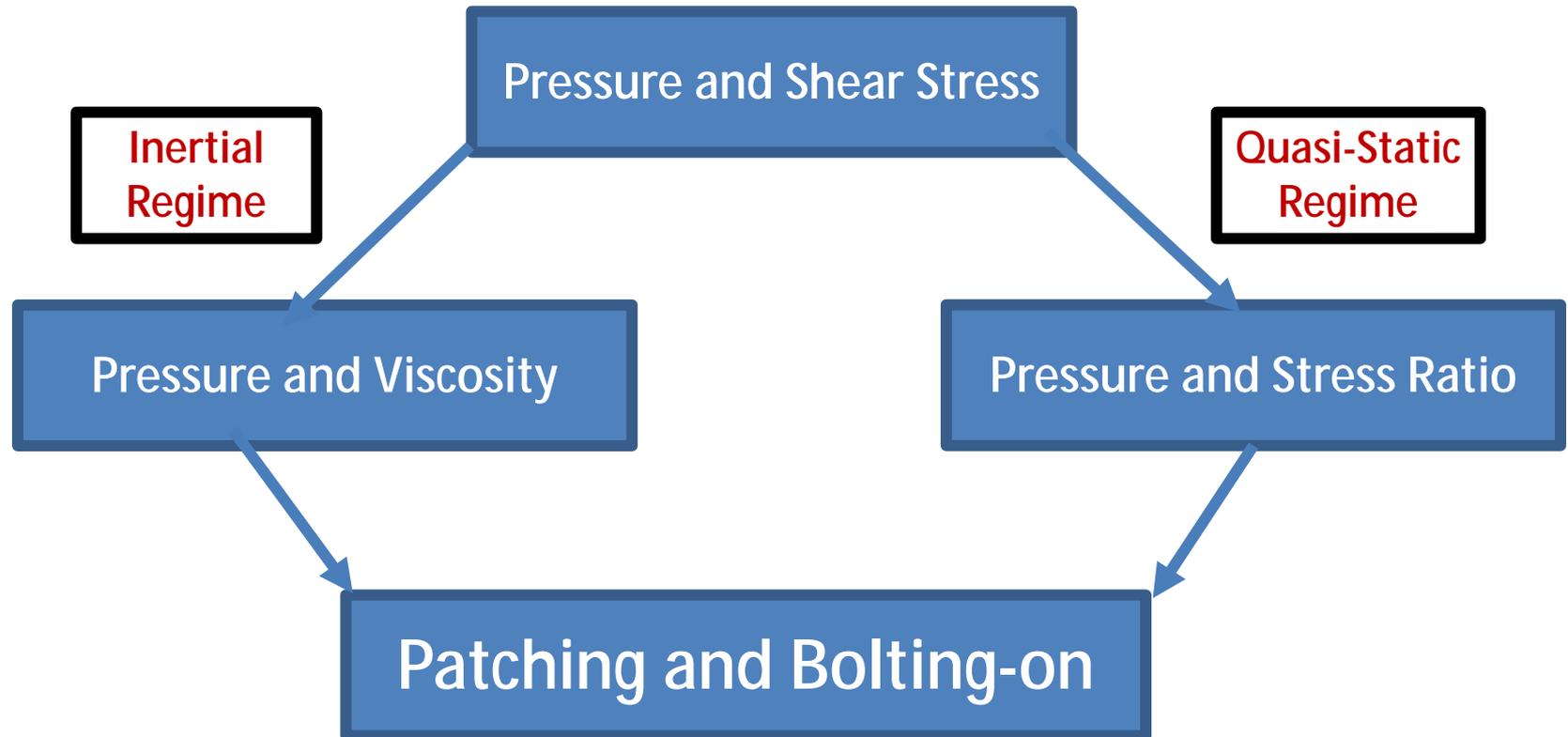
Multi-scale Approach to Particulate Flow – A Regime Map



[courtesy of P Mort]

To understand the bulk properties (meso-scale) we need
RHEOLOGICAL measurements

Constitutive Requirements



Multiscale

+

Averaging

Cohesion

Ø Chemical bonding

Ø Electric charging

Ø van der Waals

Ø Liquid bridges

Cohesion

- Ø Chemical bonding
- Ø Electric charging
- Ø van der Waals
- Ø Liquid bridges

We deal with particles with size ranging from 10^{-3} to 10^4 mm

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7 orders of magnitude!

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Wet Particles

- Ø When particles are wet or are in a moisture-rich environment, capillary forces may be important: these forces are generated by condensed moisture on the particle surface
- Ø The behaviour of wet particles differs significantly from that of dry particles
- Ø Capillary forces, brought about by what are often referred to as “liquid bridges”, are typically stronger than other type of cohesive forces

Inertial Regime

In collaboration with:

Xi Yu and Yassir Makkawi



Proposed Inter-Particle “Cohesive” Model

[Ocone et al, 2000]

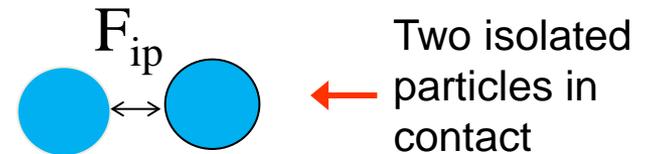
The radial component of the cohesion force is derived:

$$P_c = C_o \frac{6\sqrt{2}F_{ip}\sqrt{T}}{u_t d} |\tilde{N}e_s|$$

Based on experimental data on Group A/B particles, we are taking an average value of $F_{ip}=0.2 \times 10^{-8}$ N

The tangential cohesion force is given by a modified formula of Molerus (1982):

$$t_c = P_c \frac{\rho}{6(1 - e_s)}$$



where C_o is a factor introduced due to uncertainty about the exact value of F_{ip} and F_{ip} is the cohesive force

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[Ocone et al, 2000]

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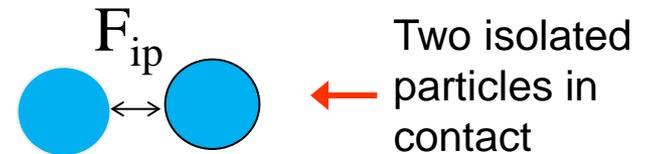
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$$t_c = P_c \frac{1}{\alpha} (\alpha - e_s)$$

BOLTED ON

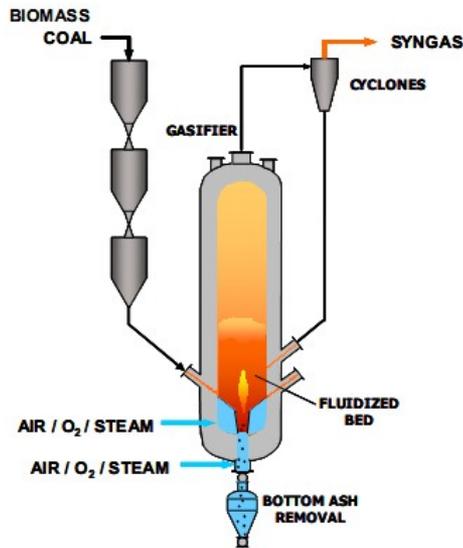


where C_o is a factor introduced due to uncertainty about the exact value of F_{ip} and F_{ip} is the cohesive force

Examples of Wet Fluidised Beds

Coal/biomass gasification

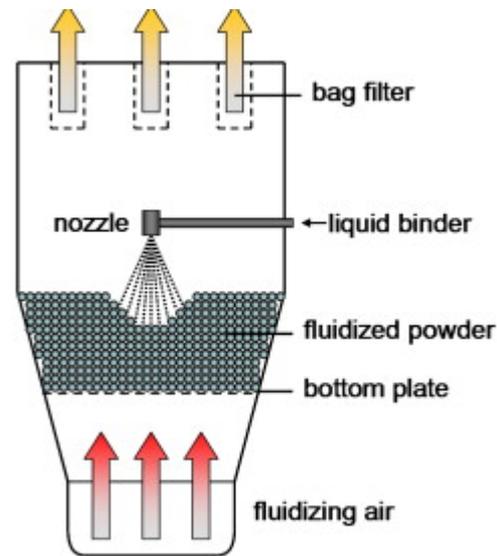
Surface oil/tar leading to agglomeration and severe Degradation and fluidisation



Simple Gasification Process Graphic
(Gas Technology Institute, Illinois, US)

Fluidized bed coating

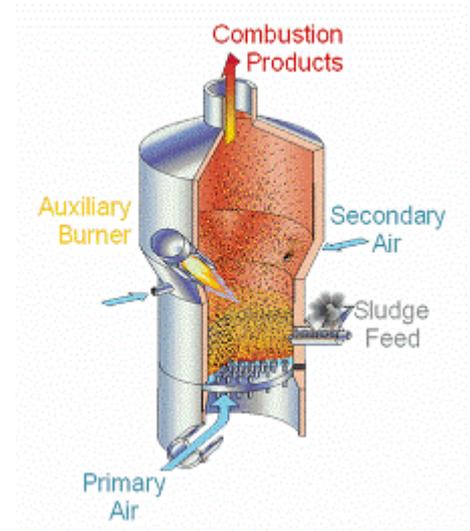
Liquid presence leading to undesired Agglomeration and particles segregation



Schemes of fluidized bed spray granulator
(Fries et al, 2011)

Exothermic fluidized reactor

Temperature control by liquid injection leading to dead zones And overheating at various Parts Of the reactor

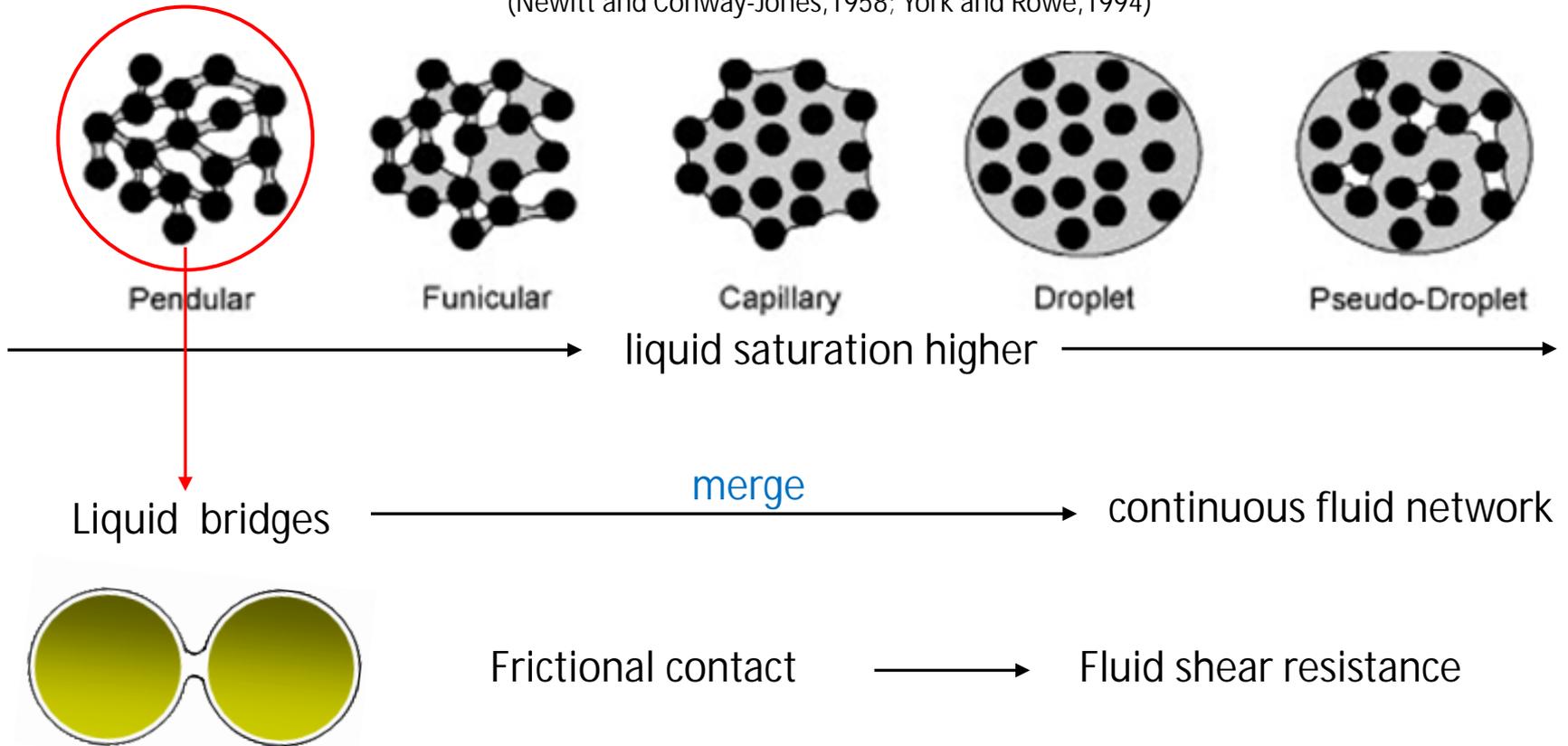


Fluidized Bed Systems, hitachi Zosen Inova, Switzerland)

Slightly Wet Systems

Figure: the different states of saturation of liquid-bound granules

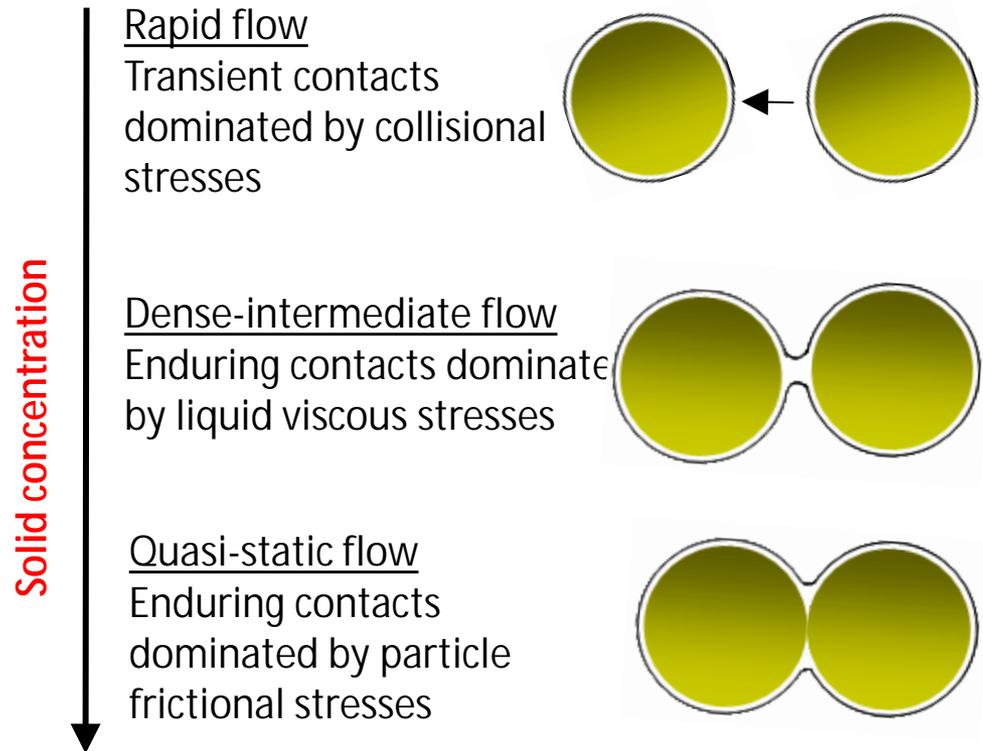
(Newitt and Conway-Jones, 1958; York and Rowe, 1994)



Collisional contacts dissipate energy in both the liquid bridges and particles

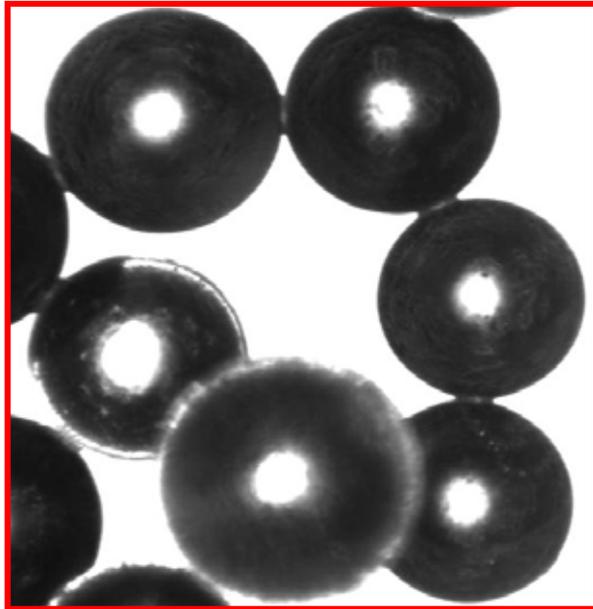
Particle-Particle Interactions in Slightly Wet Suspensions

Hypothesis

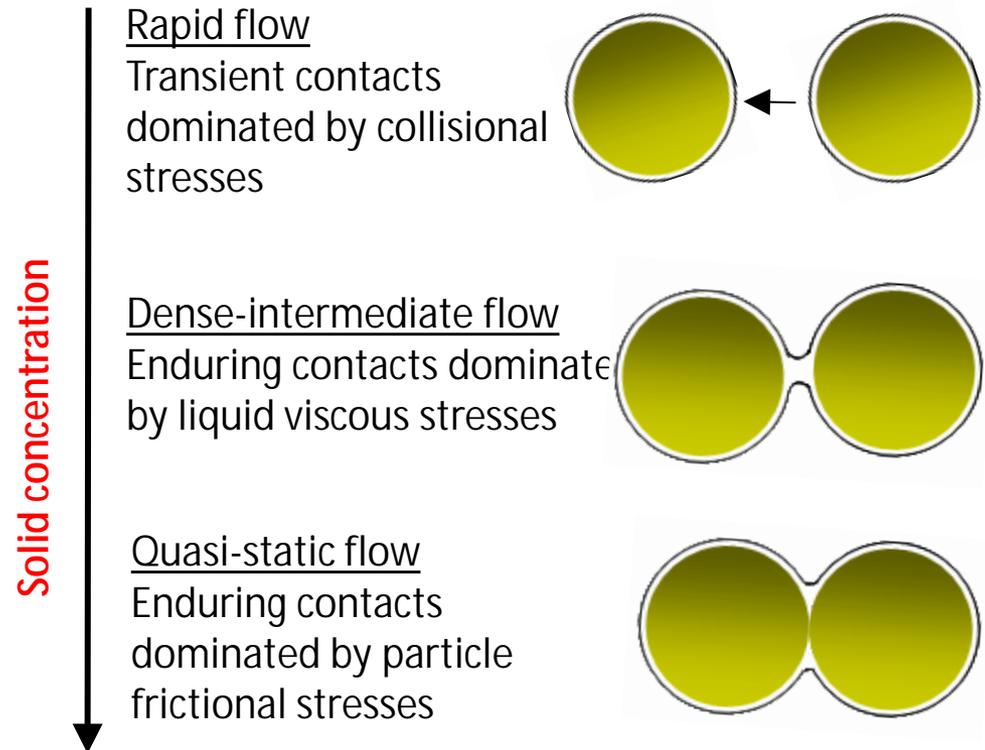


Particle-Particle Interactions in Slightly Wet Suspensions

- q In wet particles flow, direct solid-solid contacts are limited



Hypothesis



Eulerian Modelling of Dry Granular Flow

Solid phase

continuity equation:
$$\frac{\partial(\alpha_s \rho_s)}{\partial t} + \nabla(\alpha_s \rho_s \vec{u}_s) = 0$$

momentum:
$$\frac{\partial(\alpha_s \rho_s \vec{u}_s)}{\partial t} + \nabla(\alpha_s \rho_s \vec{u}_s \vec{u}_s) = -\alpha_s \nabla P - \nabla P_s + \nabla(\bar{\bar{\tau}}_s) + \beta(u_g - u_s) + F$$

Gas phase

continuity equation:
$$\frac{\partial(\alpha_g \rho_g)}{\partial t} + \nabla(\alpha_g \rho_g \vec{u}_g) = 0$$

momentum:
$$\frac{\partial(\alpha_g \rho_g \vec{u}_g)}{\partial t} + \nabla(\alpha_g \rho_g \vec{u}_g \vec{u}_g) = -\alpha_g \nabla P + \nabla(\bar{\bar{\tau}}_g) - \beta(u_g - u_s) + F$$

Energy equation (granular temperature):

$$\frac{3}{2} \left[\frac{\partial(\alpha_s \rho_s T)}{\partial t} + \nabla(\alpha_s \rho_s T) \vec{u}_s \right] = \left(-P_s \bar{\bar{I}} + \bar{\bar{\tau}}_s \right) : \nabla \vec{u}_s - \nabla(\kappa_T \nabla T) - \gamma_T - J_T$$

Well developed KTGF (kinetic theory of granular flow)

Shear Stress in Particle-Particle Interaction

$$\bar{\tau}_s = \left(\lambda_s - \frac{2}{3} \mu_s \right) (\nabla \cdot \bar{u}_s) \bar{I} + 2\mu_s \bar{S}_s$$

solids shear viscosity $\mu_s = \mu_{s,col} + \mu_{s,kin} + \mu_{s,fr}$

$\mu_{s,fr} = 0$ $0 < \alpha_s < 0.5$ No friction

$\mu_{s,fr} = \frac{P_s \sin \phi}{2\sqrt{I_{2D}}}$ $0.5 < \alpha_s < 0.63$ Particle packing-enduring contact

How to present friction shear stress in slightly wet granular flow?

$$\mu_s = \mu_{s,col} + \mu_{s,kin} + \mu_{s,fr} + \mu_{wet}$$

Wet shear viscosity
(fluid shear resistance)

How to Modify Solid Stress Model

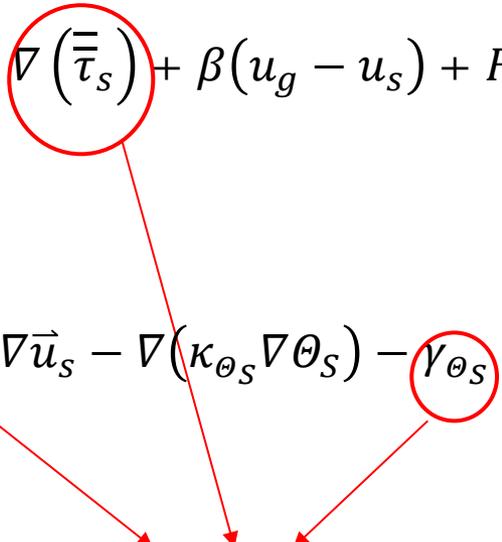
Solid phase momentum

$$\frac{\partial(\alpha_s \rho_s \bar{u}_s)}{\partial t} + \nabla(\alpha_s \rho_s \bar{u}_s \bar{u}_s) = -\alpha_s \nabla P - \nabla P_s + \nabla(\bar{\tau}_s) + \beta(u_g - u_s) + F$$

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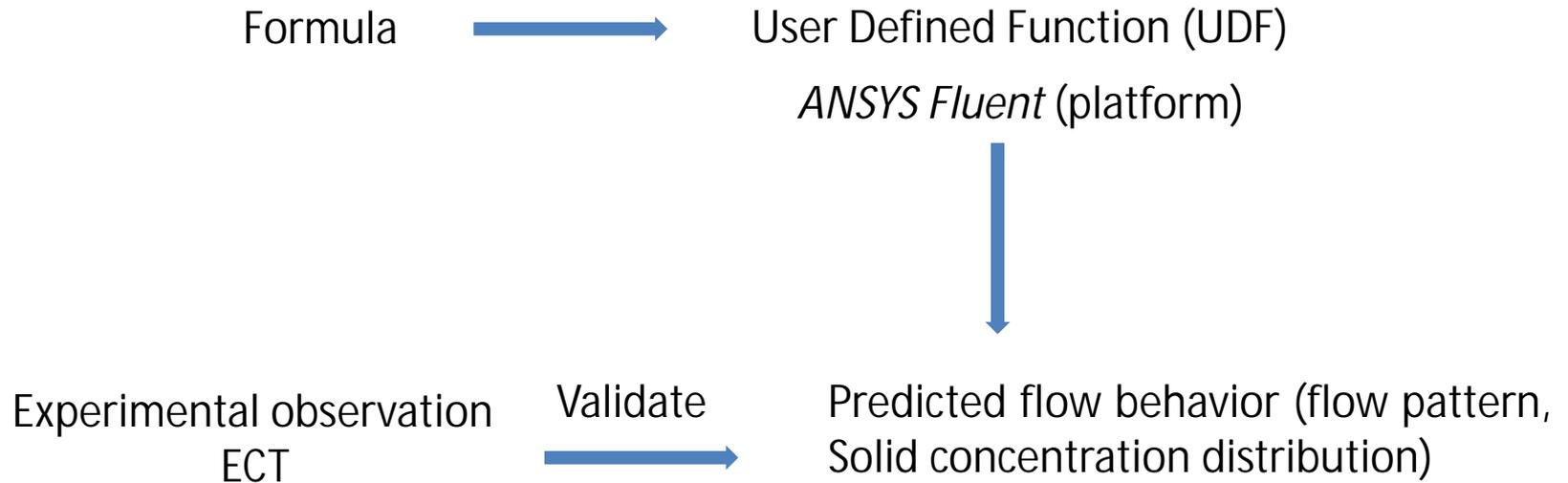
$$\frac{3}{2} \left[\frac{\partial(\alpha_s \rho_s \theta_s)}{\partial t} + \nabla(\alpha_s \rho_s \theta_s) \bar{u}_s \right] = \left(-P_s \bar{I} + \bar{\tau}_s \right) : \nabla \bar{u}_s - \nabla(\kappa_{\theta_s} \nabla \theta_s) - \gamma_{\theta_s} - J_{\theta_s}$$

User Defined Function written in C language



Big Picture

How to incorporate shear stress (based on liquid bridge) in slightly wet particle flow?



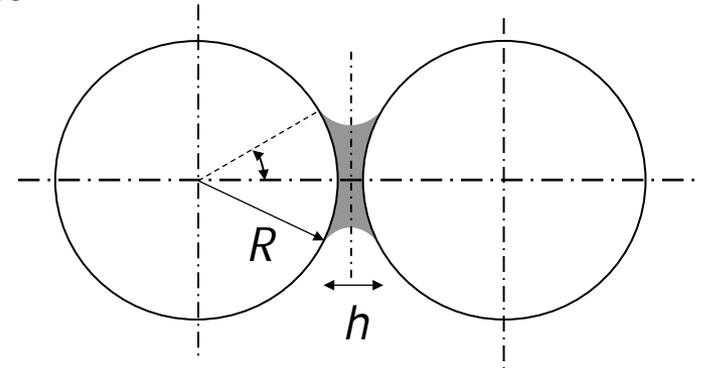
Liquid Bridge Stresses

q For this, we may start from the interparticle force at single particle level:

$$\dot{F}_{liquid} = \frac{3}{8} \pi \mu_{liquid} d_p^2 \frac{\dot{u}}{h}$$

q Interparticle approach velocity can be estimated from granular temperature:

$$\dot{u}_s = \frac{3}{2} \sqrt{\pi \theta_s}$$



Normal stress

q For this, it is required to determine the force per unit area:

$$P_{liquid} = \frac{9}{16h} \pi \mu_{liquid} \sqrt{\pi \theta_s} \left(\frac{6\alpha_s}{\pi} \right)^{2/3}$$

Equivalent shear viscosity

q Analogue to Coulomb friction law

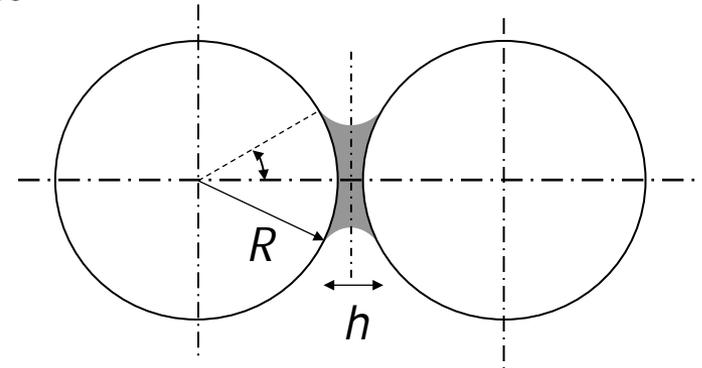
$$\mu_{wet} = \frac{\sqrt{2} P_{liquid} \eta}{|\bar{S}|}$$

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← Interparticle gap



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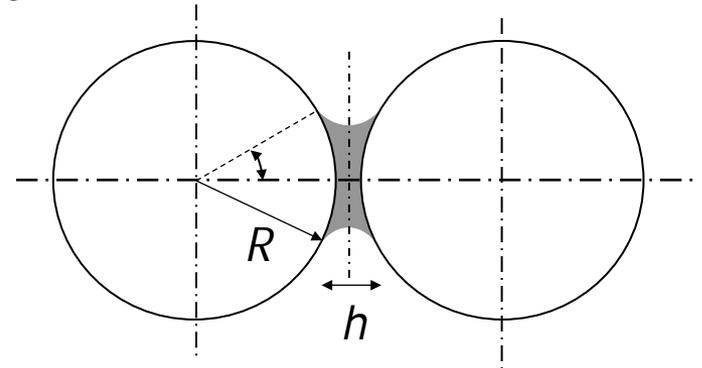
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"lubrication" coefficient

Criteria to Turn on/off the Effect of Liquid Bridges

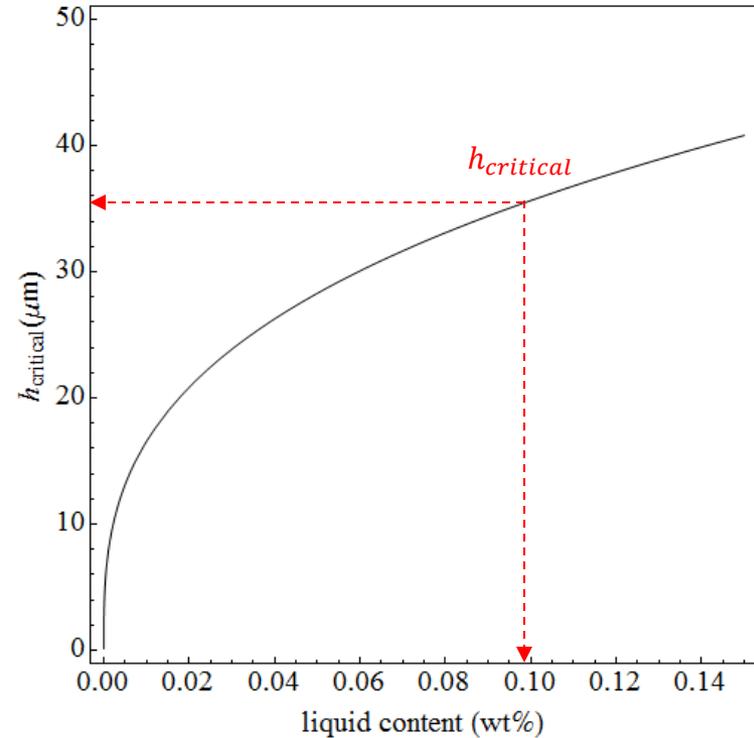
q We need to specify a critical interparticle gap distance at which liquid bridges become dominant:

$$P_{liquid} = \frac{9}{16h} \pi \mu_{liquid} \sqrt{\pi \theta_s} \left(\frac{6\alpha_s}{\pi} \right)^{2/3} \quad \text{if } h_a < h \leq h_{critical}$$

$$P_{liquid} = 0 \quad \text{if } h > h_{critical}$$

$$h_{critical} = 0.8d_p \sqrt[3]{\left(\frac{M_L}{M_S}\right) \left(\frac{\rho_S}{\rho_L}\right)} \quad \text{Lian et al. (1992)}$$

$h_a = 2 \sim 10 \mu\text{m}$ particle surface asphericity



$$d_p = 350 \mu\text{m}, \rho_L = 969 \text{kg/m}^3, \rho_S = 2500 \text{kg/m}^3, \\ m_s = 4.5 \text{kg}$$

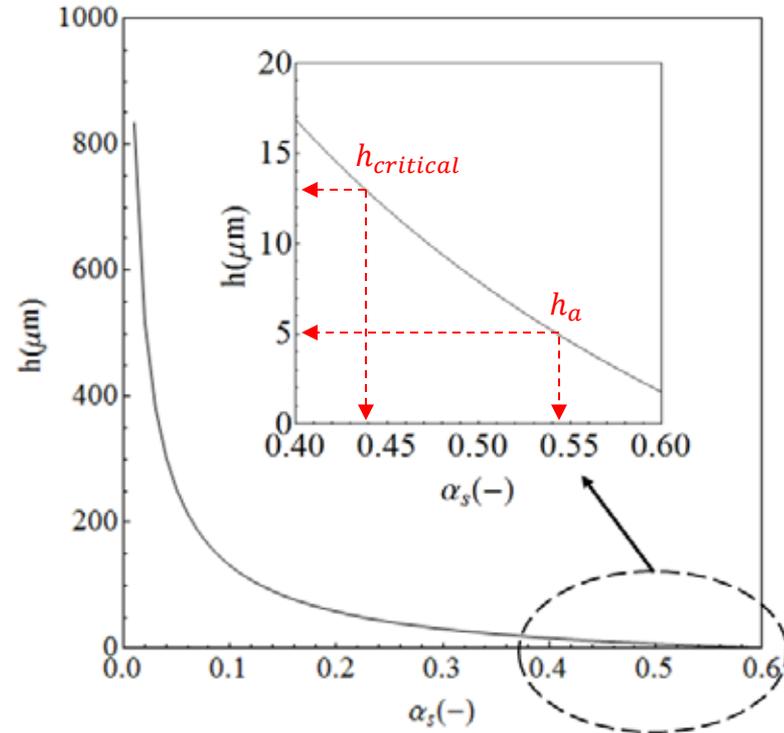
(1) Lian et al., A theoretical study of the liquid bridge forces between two rigid spherical bodies, *Int J. of interface Science*, 1992

Void and Inter-Particle Gap Distance Relation

q In randomly packed spheres, the gap distance can be expressed in terms of solid volume fraction⁽¹⁾:

$$h = d_p \left(\sqrt{\frac{1}{3\pi\varepsilon_s} + \frac{5}{6}} - 1 \right)$$

The critical solid fraction at liquid bridge rupture can be estimated once the rupture distance is known



(1) L.V. Woodcock, in "Proc. of a workshop on glass forming liquids", edited by Z. I. P. Bielefeld (Springer Lecture Series in Physics, 277, 1985) p. 113.

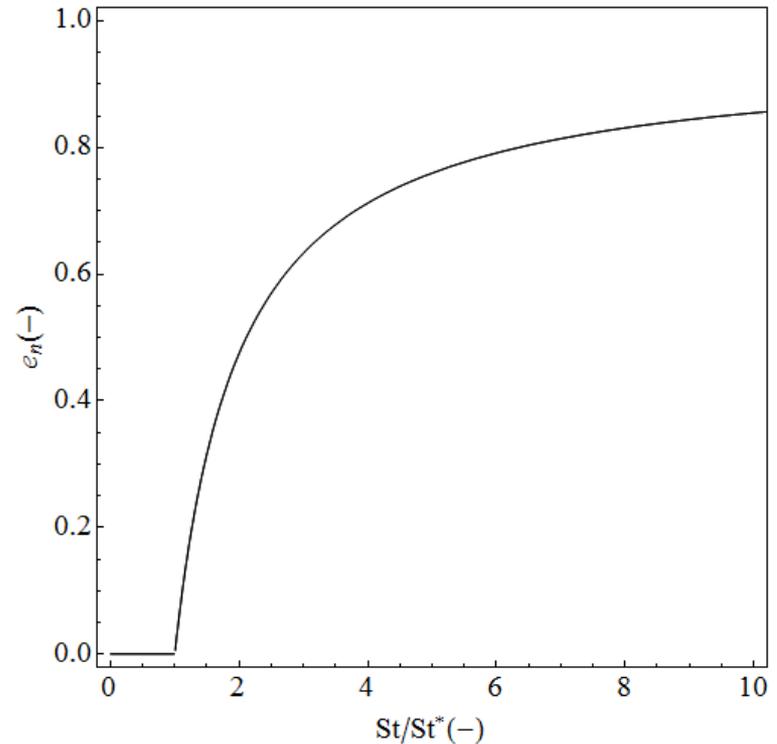
Restitution Coefficient of Wet Particles

$$St = \frac{8m\dot{u}}{3\pi\mu d_p^2}$$

$$St^* = \left(1 + \frac{1}{e_{dry}}\right) \ln\left(\frac{h}{h_a}\right) \quad \text{critical Stokes number}$$

$$e_{wet} = \begin{cases} e_{dry} \left(1 - \frac{St^*}{St}\right) & \text{if } h_a < h \leq h_{critical} \text{ and } St > St^* \\ 0 & \text{if } St \leq St^* \\ e_{dry} & \text{if } h > h_{critical} \text{ and } St > St^* \end{cases}$$

$$\gamma_{\theta_s} = \frac{12(1 - e_{wet}^2)g_{0,SS}}{d_s \pi^{1/2}} \alpha_s^2 \rho_s \theta_s^{3/2}$$

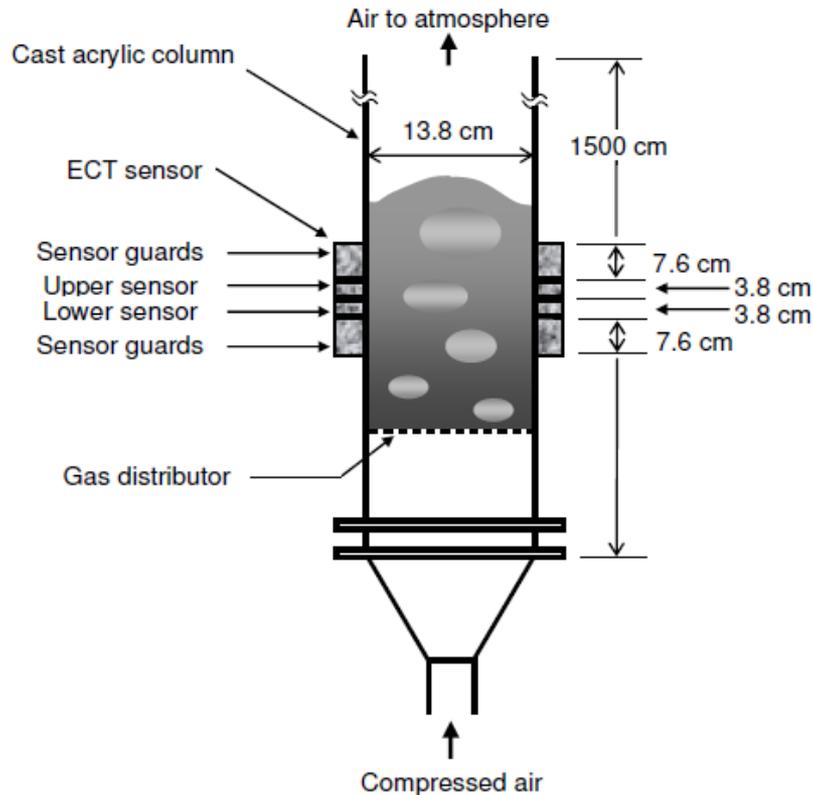


$$d_p = 350\mu\text{m}, \rho_L = 969\text{kg/m}^3, \rho_s = 2500\text{kg/m}^3 \\ \mu = 0.4945 \text{ kg/(m.s)}$$

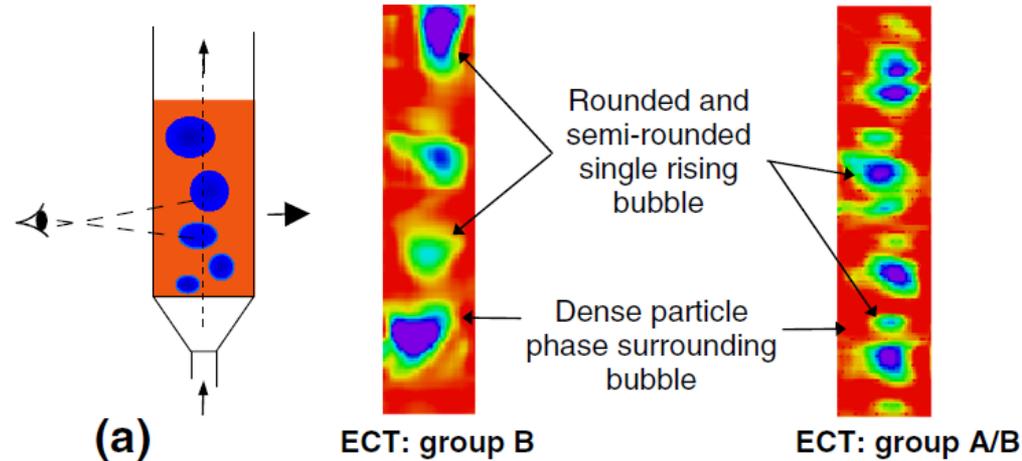
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Experimental Results (ECT) in Dry Particle-Flow



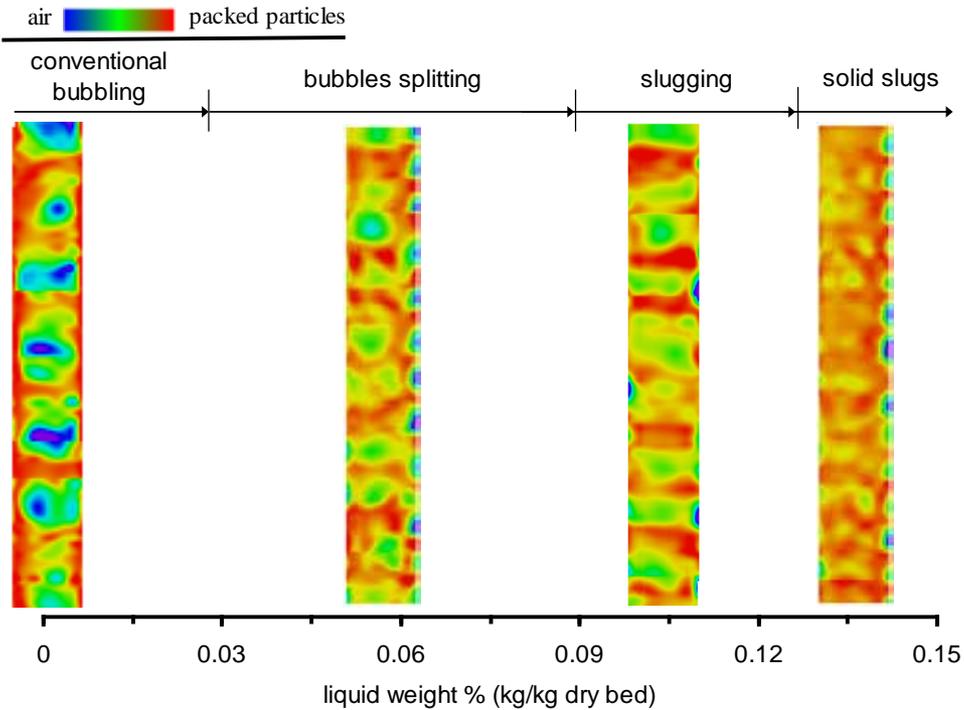
Experimental setup



(Makkawi et al, 2006)
Solid volume fraction

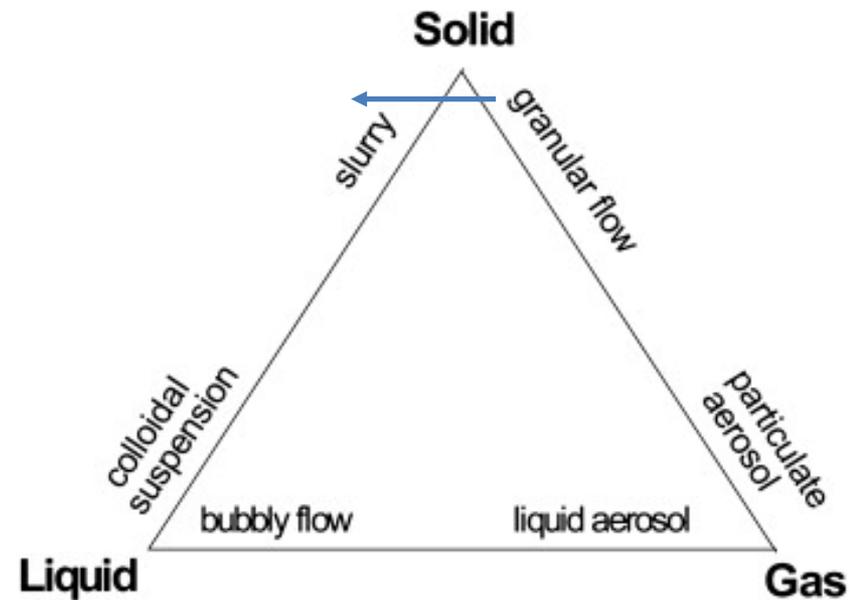
ECT (electrical capacitance tomography) is a diagnostic imaging tool in the medical field

Experimental Results (ECT) in Slightly Wet Flow



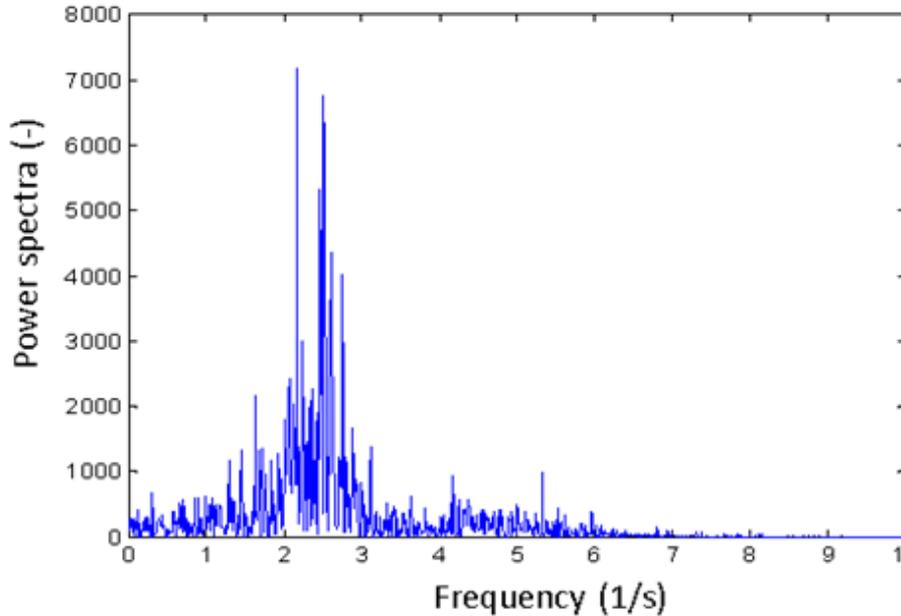
Operating conditions: fluidisation velocity=0.8 m/s, bed of 350 mm diameter glass bead, bed weight=3.5 kg, column diameter=15 cm, liquid used is silicon oil (density=969 kg/m³, surface tension=0.0165 N/m and dynamic viscosity=0.4945 kg/(m.s))

Lines: Types of two-phase system

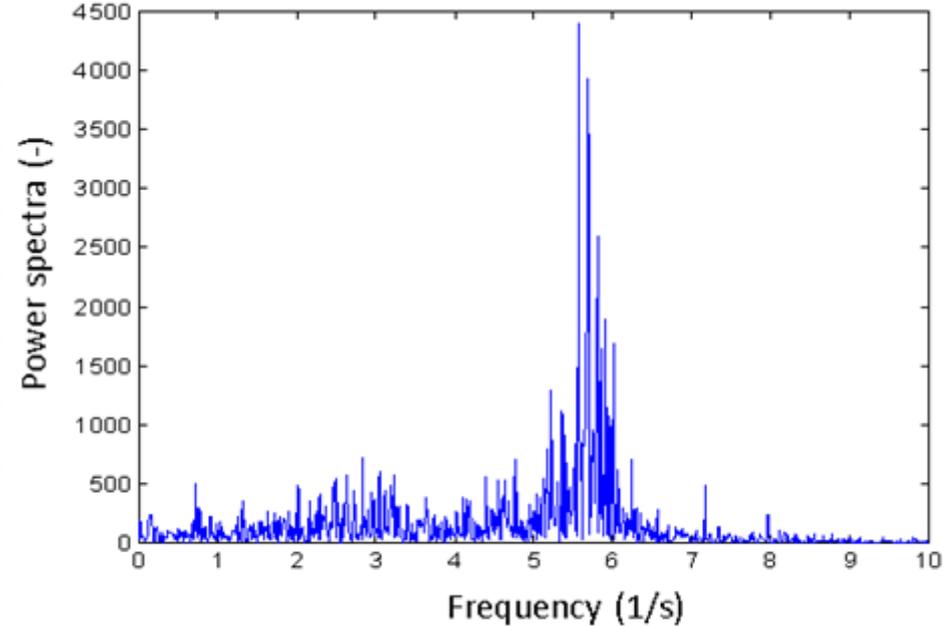


Evolution of slightly wet system
In three-phase diagram

Fast Fourier Transform Analysis



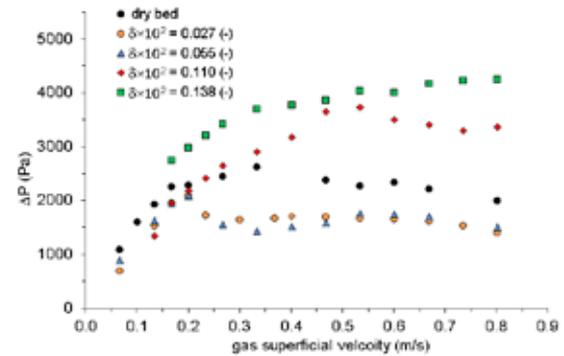
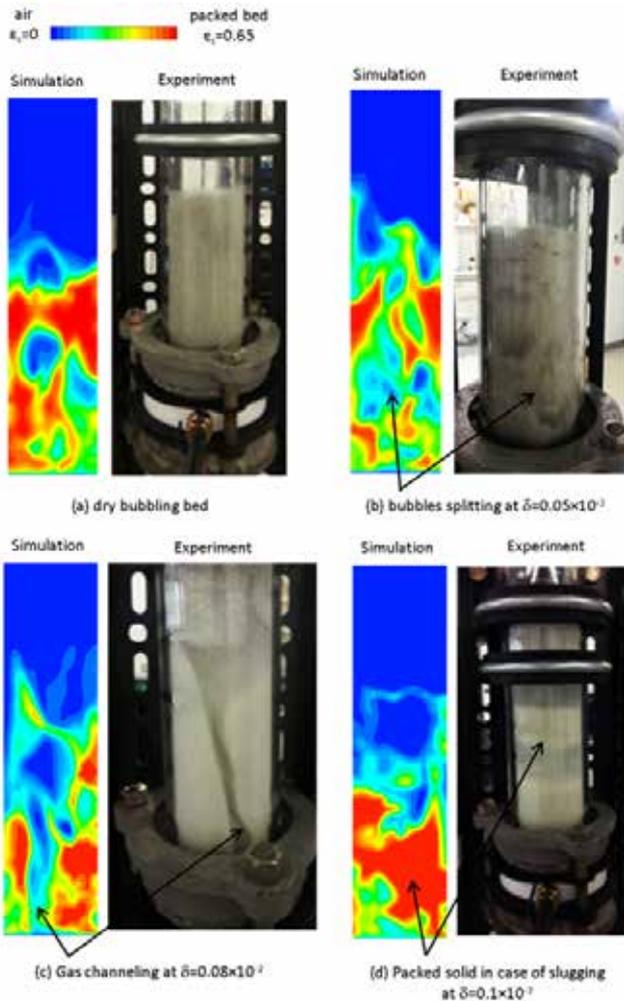
(a) FFT of dry bed



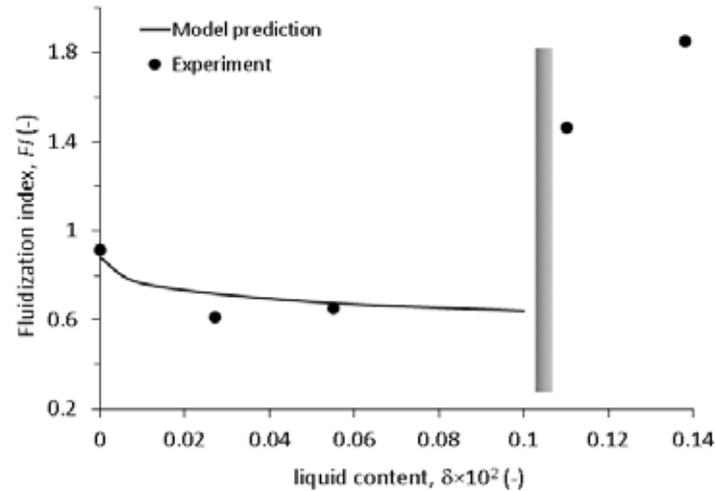
(b) FFT of wet bed

Fast Fourier Transform (FFT) analysis of solid fraction fluctuation obtained by ECT measurement in a bubbling fluidized bed (a) dry (b) wet at $\delta = 0.055 \times 10^{-2}$. The solid fraction data represents the spatial average fluctuations at 7.6 cm above the distributor and was produced in a 15 cm diameter column with the bed material consisting of 3.5 kg glass beads fluidized at the gas velocity of 0.8 m/s.

Fluidisation Analysis



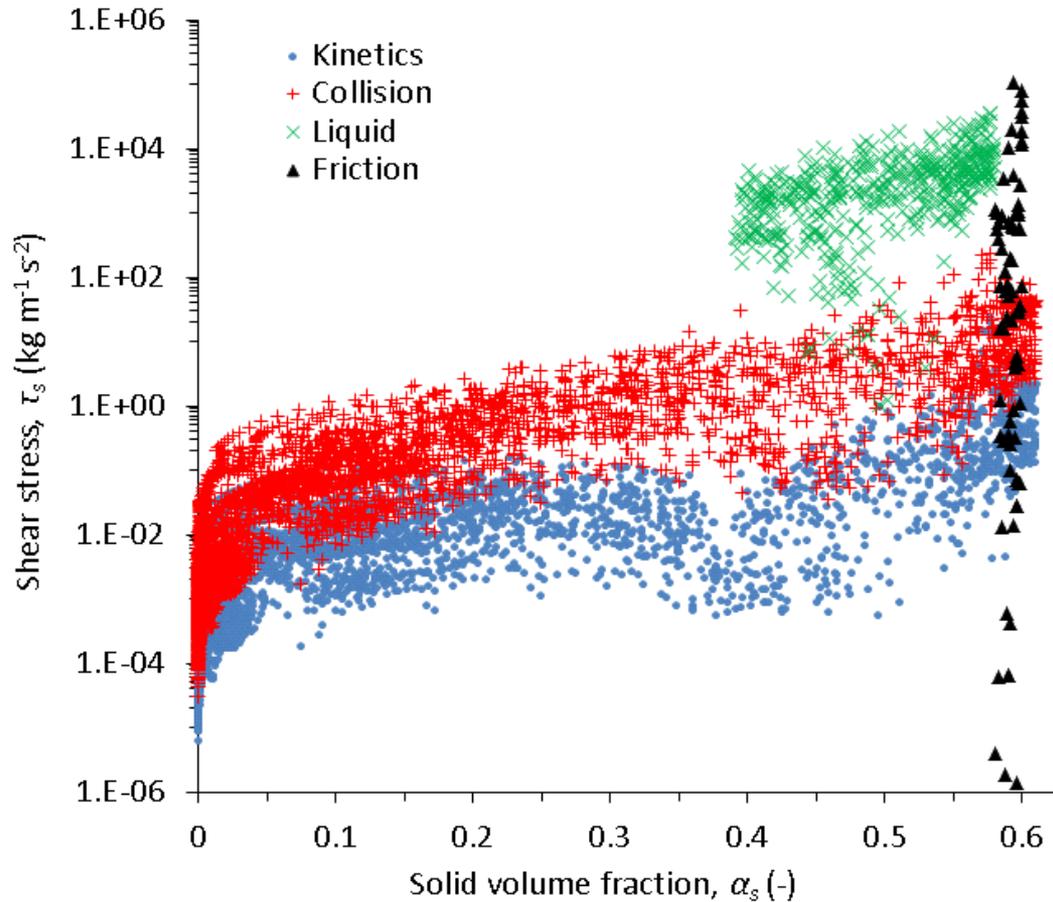
Experimental fluidised bed pressure drop at various gas velocities



Comparison of the predicted and experimentally determined fluidisation index $Ff = \frac{\Delta PA}{W_{bed}g}$

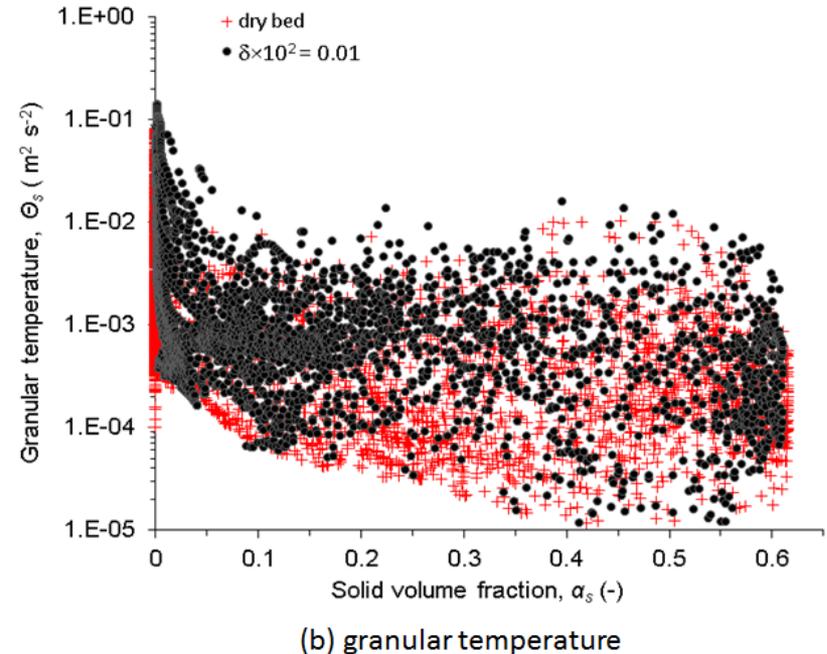
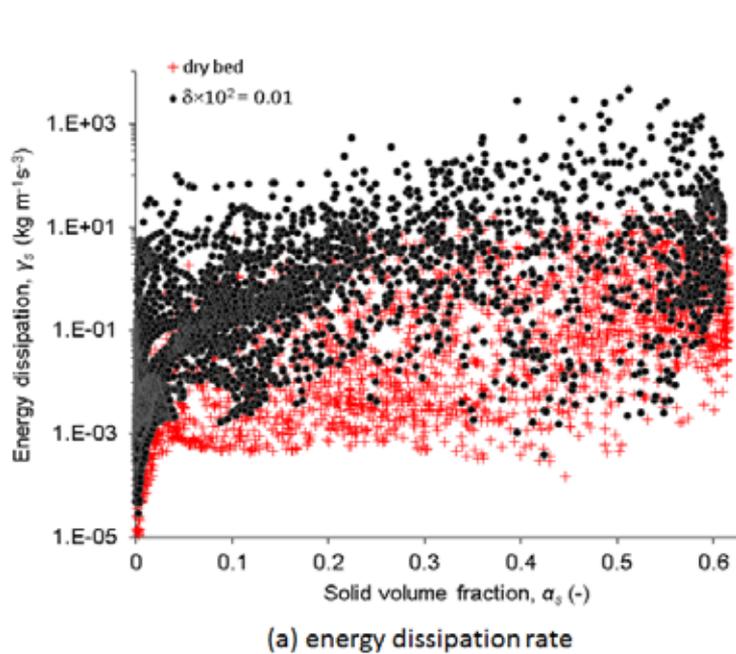
In highly cohesive powders, the experimentally determined FI was found to be greater than 1.4 (De Jong et al, 1999). The model failed to provide a stable solution at $d > 0.1 \times 10^{-2}$

Results



Predicted solid shear stress in a slightly wet fluidised bed of 15 cm diameter at the gas velocity of 0.8 m/s and liquid amount of $\delta = 0.1 \times 10^{-2}$

Results



Predicted (a) energy dissipation rate and (b) granular temperature as function of the solid concentration in dry and a slightly wet fluidized bed of 15 cm diameter at the gas velocity of 0.8 m/s

Conclusions

- ∅ The proposed model combines theories of liquid bridge forces with the kinetic theory of granular flow (KTGF)
- ∅ The model is capable of predicting characteristic hydrodynamic features of slightly wet, non-porous particles in a bubbling fluidised bed
- ∅ The experimental measurement produced by electrical capacitance tomography (ECT) have shown distinct hydrodynamic features characterised by bubbles splitting, gas channelling, slugging and de-fluidisation as the liquid presence in the bed increases
- ∅ The proposed model allows, for the first time, continuum modelling of slightly wet solid fluidisation, thus extending the existing classic two-fluid modelling beyond its traditional boundaries.

Quasi-Static Regime

Lyes Ait Ali Yahia, Riccardo Maione and Ali Ozel



Shear Test

Evaluation of the stresses needed to generate shear leading to either compaction or dilation states under a given applied normal stress

Shear Test

Evaluation of the stresses needed to generate shear leading to either compaction or dilation states under a given applied normal stress

FT4 Powder Rheometer -



- Automated device
- 48mm diameter – shear head
 - 18 blads – 2mm height

Shear Test

Evaluation of the stresses needed to generate shear leading to either compaction or dilation states under a given applied normal stress

FT4 Powder Rheometer -



- Automated device
- 48mm diameter – shear head
 - 18 blads – 2mm height



Constitutive models combining DEM simulations and experimental results

Shear test procedure

Shear head applies a normal stress (s) by moving downward

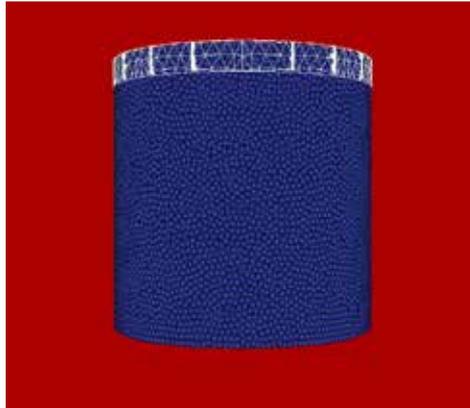
Shear test procedure

Shear head applies a normal stress (s) by moving downward



Once the desired normal stress is reached, the shear head induces a shear stress (t)

Shear test procedure



Shear head applies a normal stress (s) by moving downward



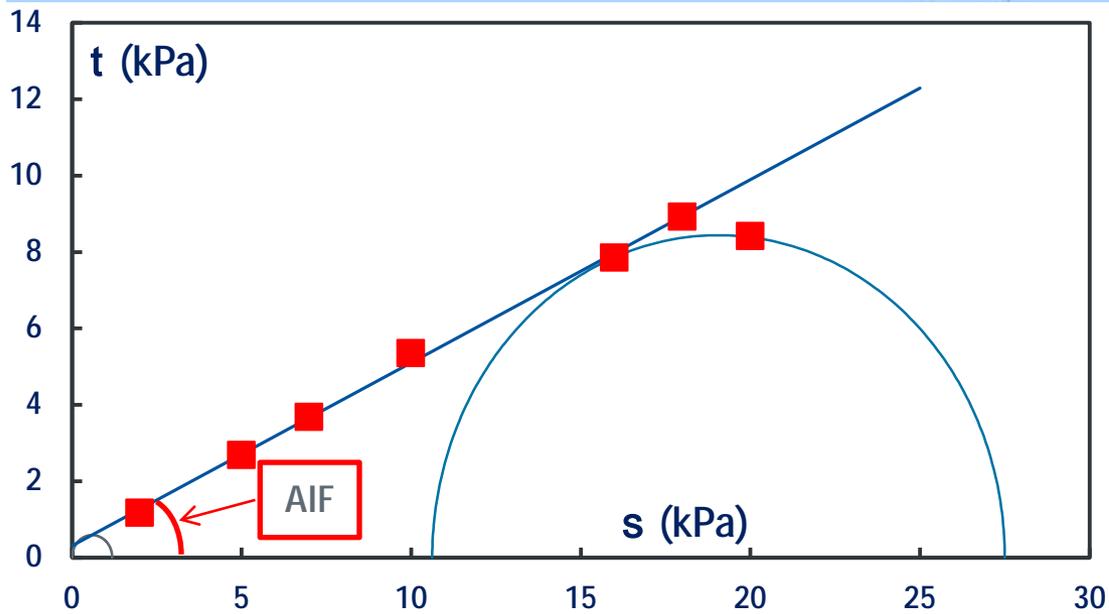
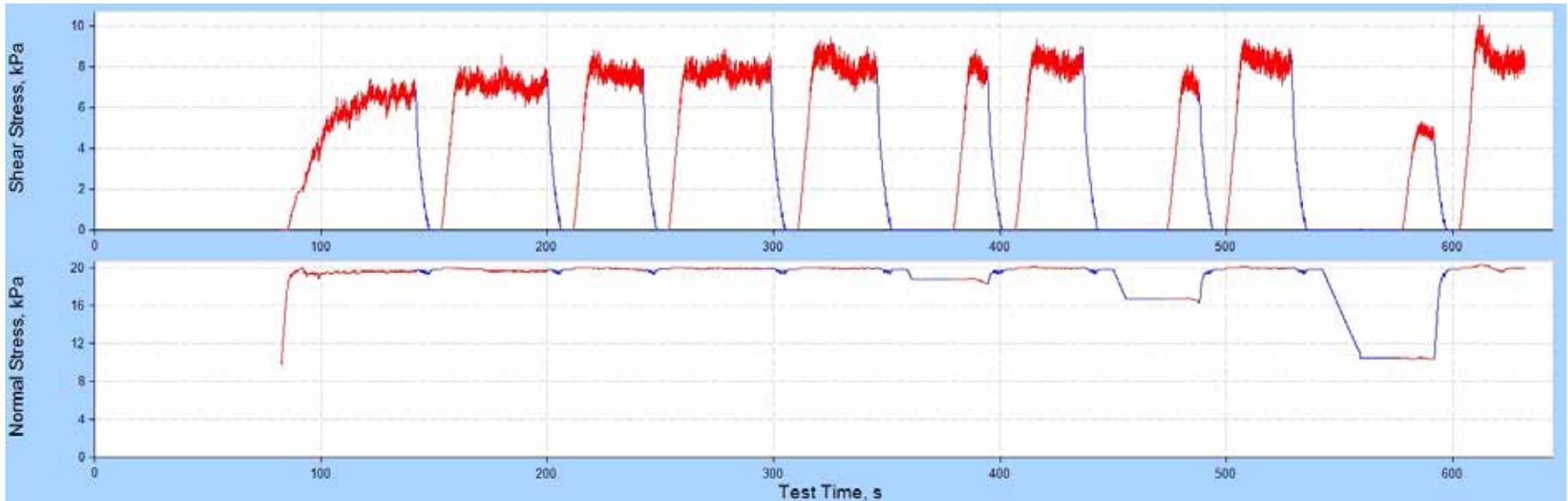
Once the desired normal stress is reached, the shear head induces a shear stress (t)



The shear stress (t) increases until the powder bed fails

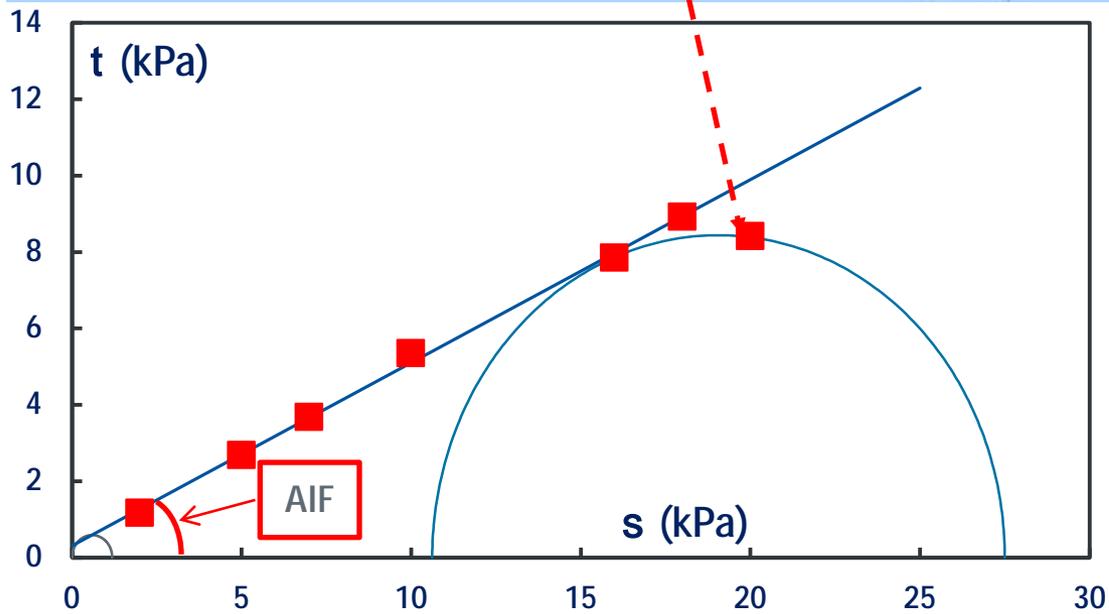
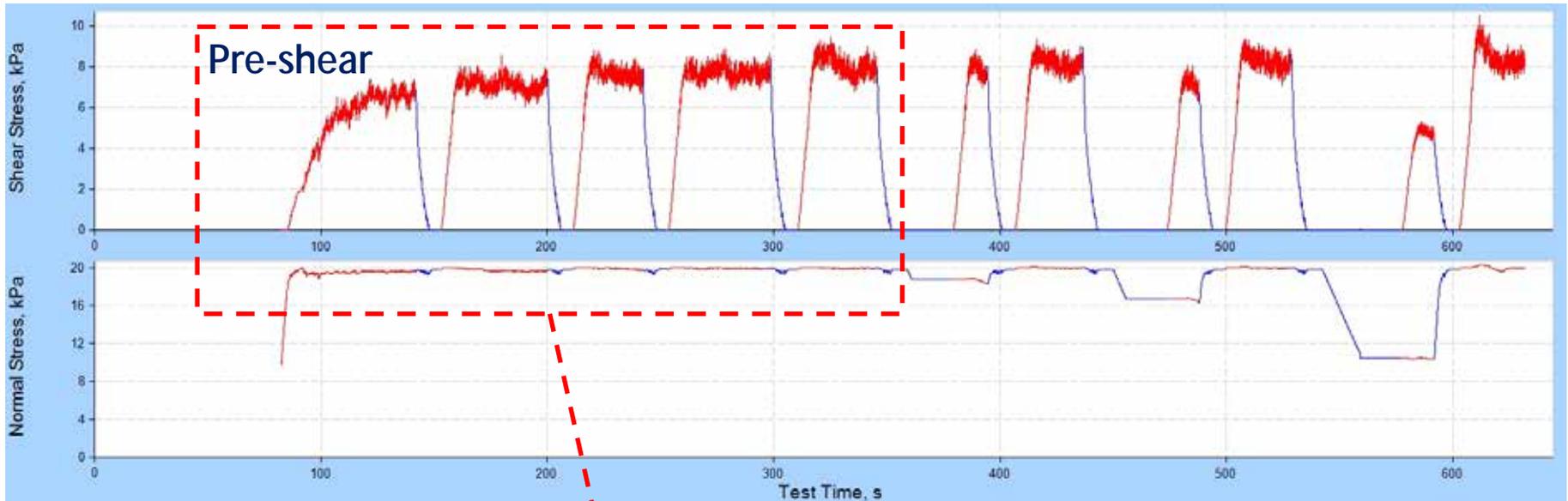
Shear Test - Experiments

0.5mm diameter dry glass beads



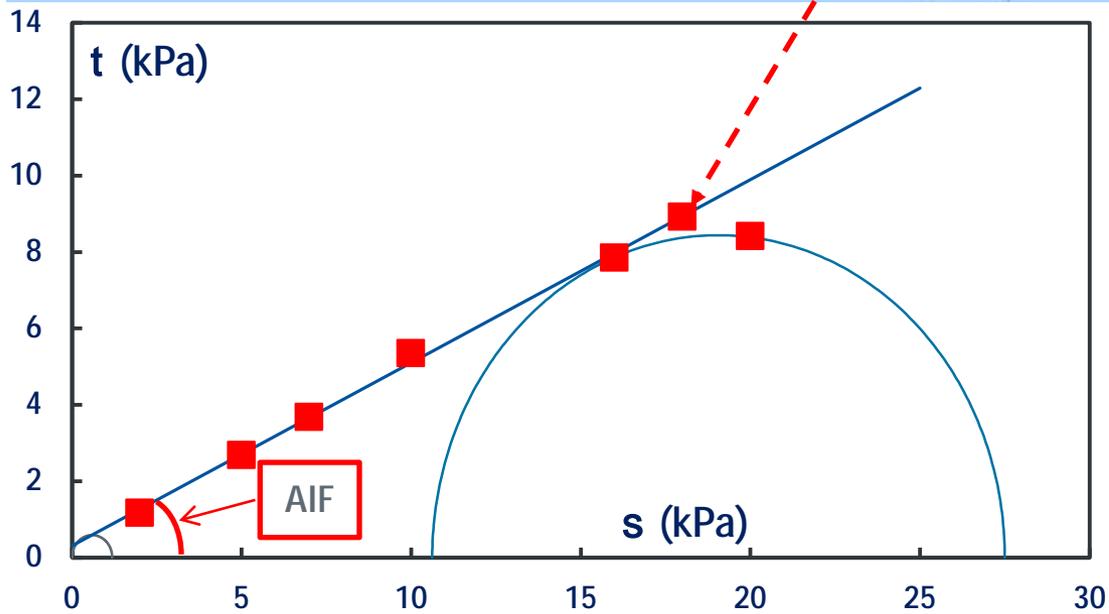
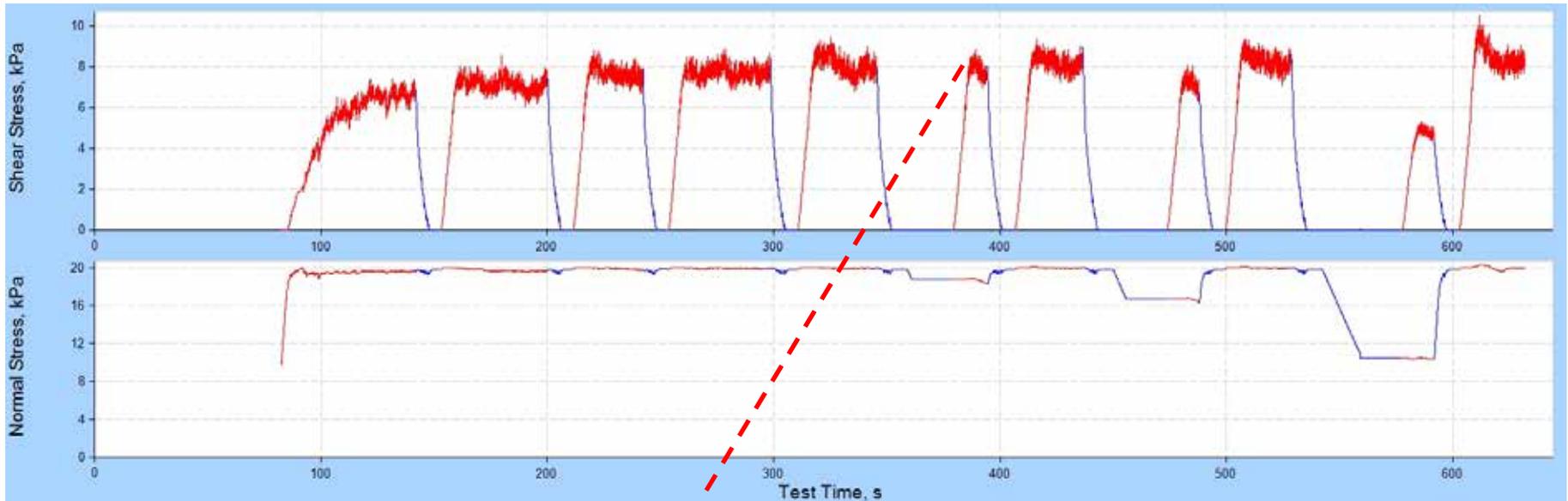
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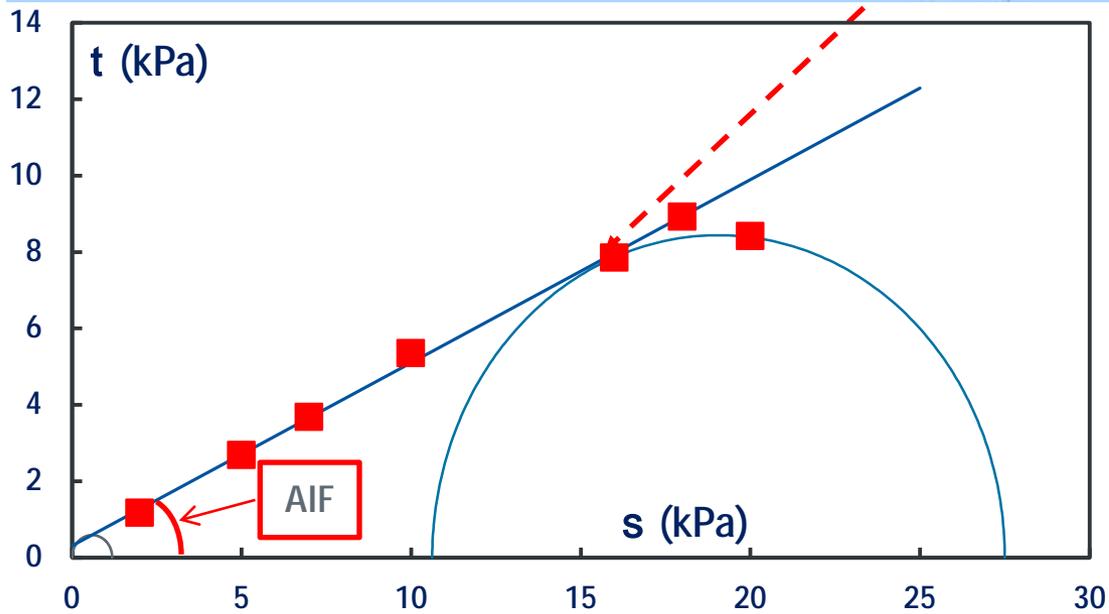
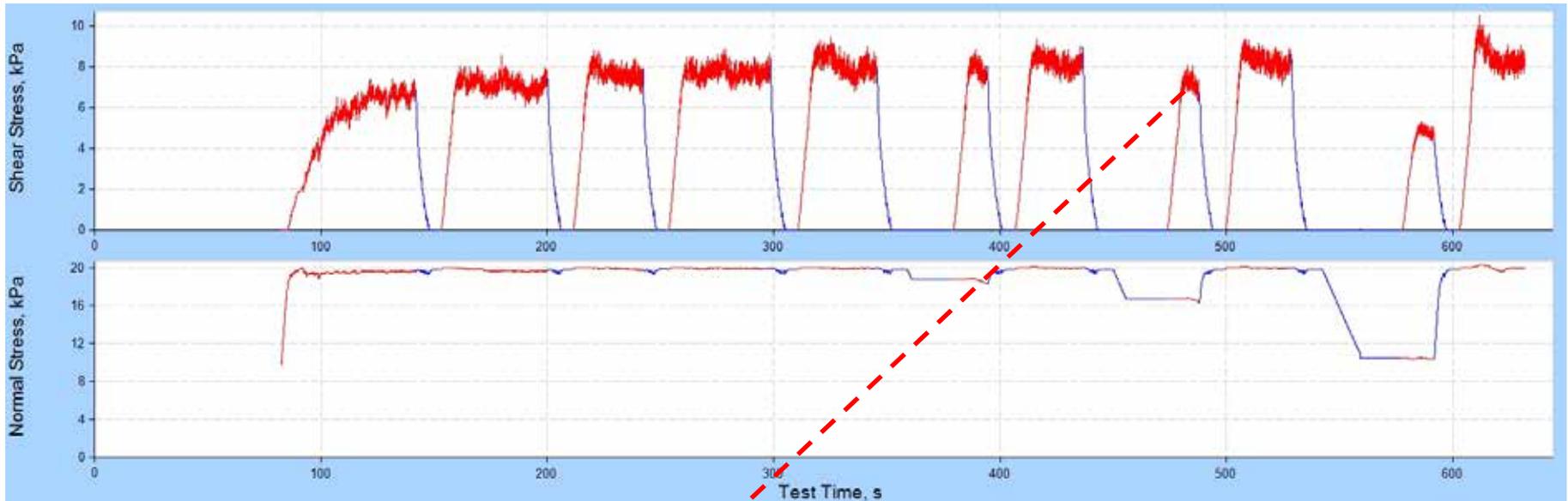
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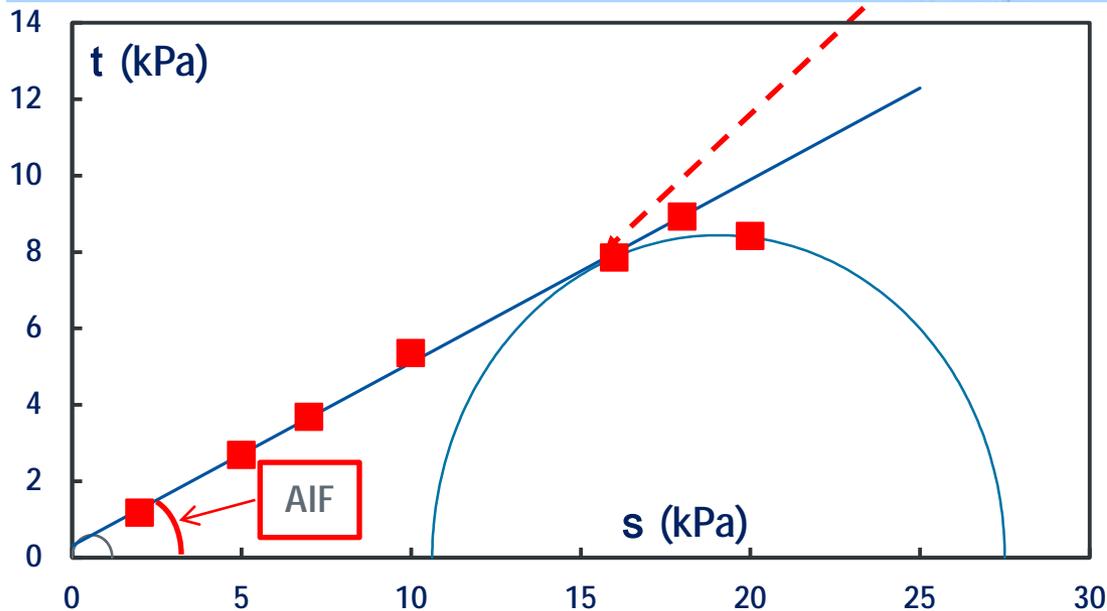
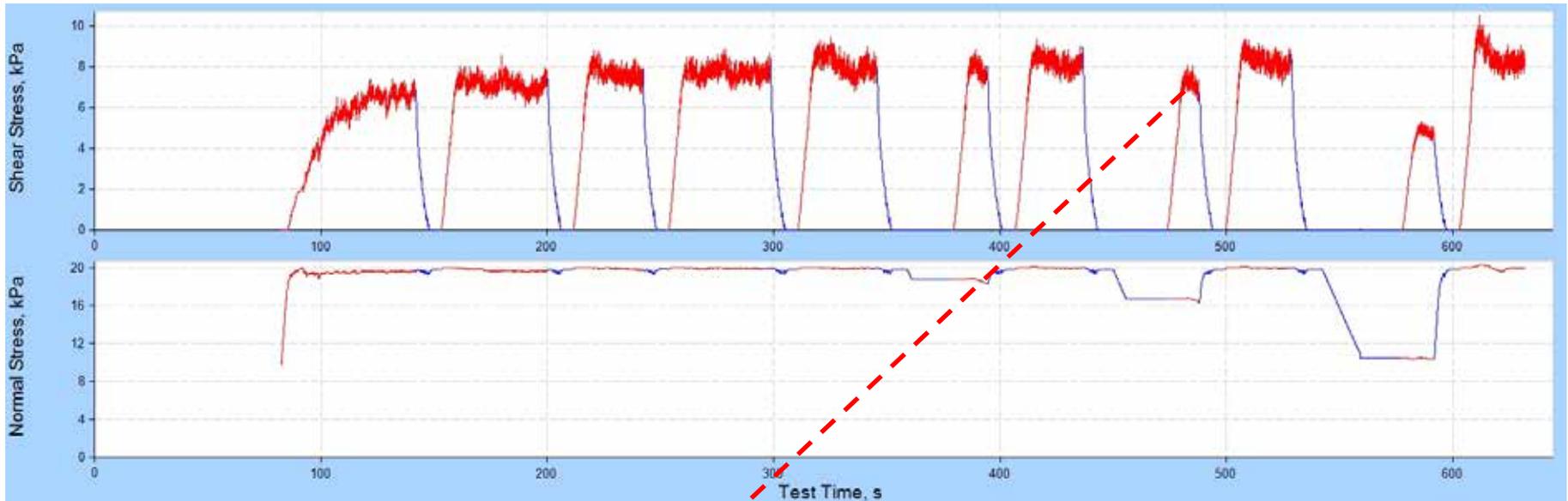
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Shear Test - Experiments

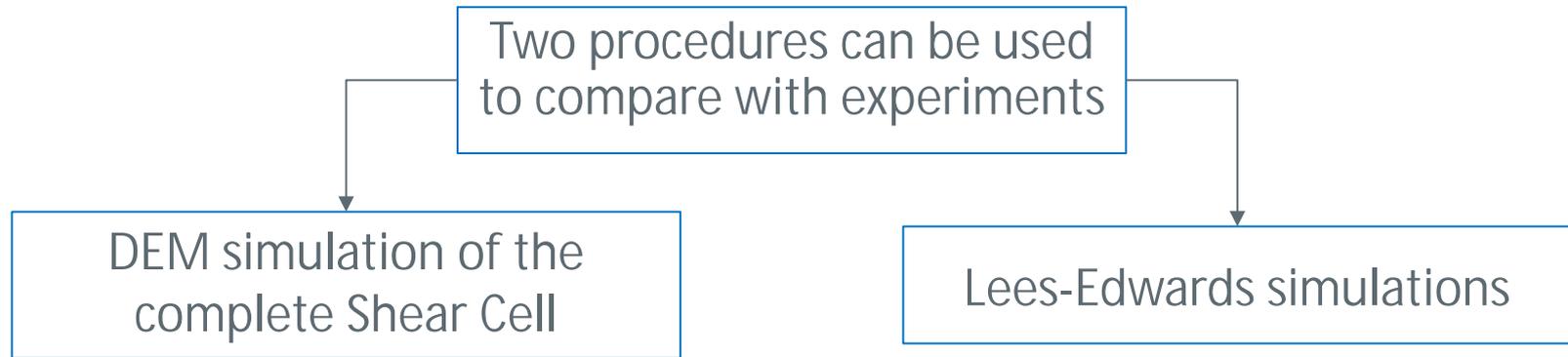
0.5mm diameter dry glass beads



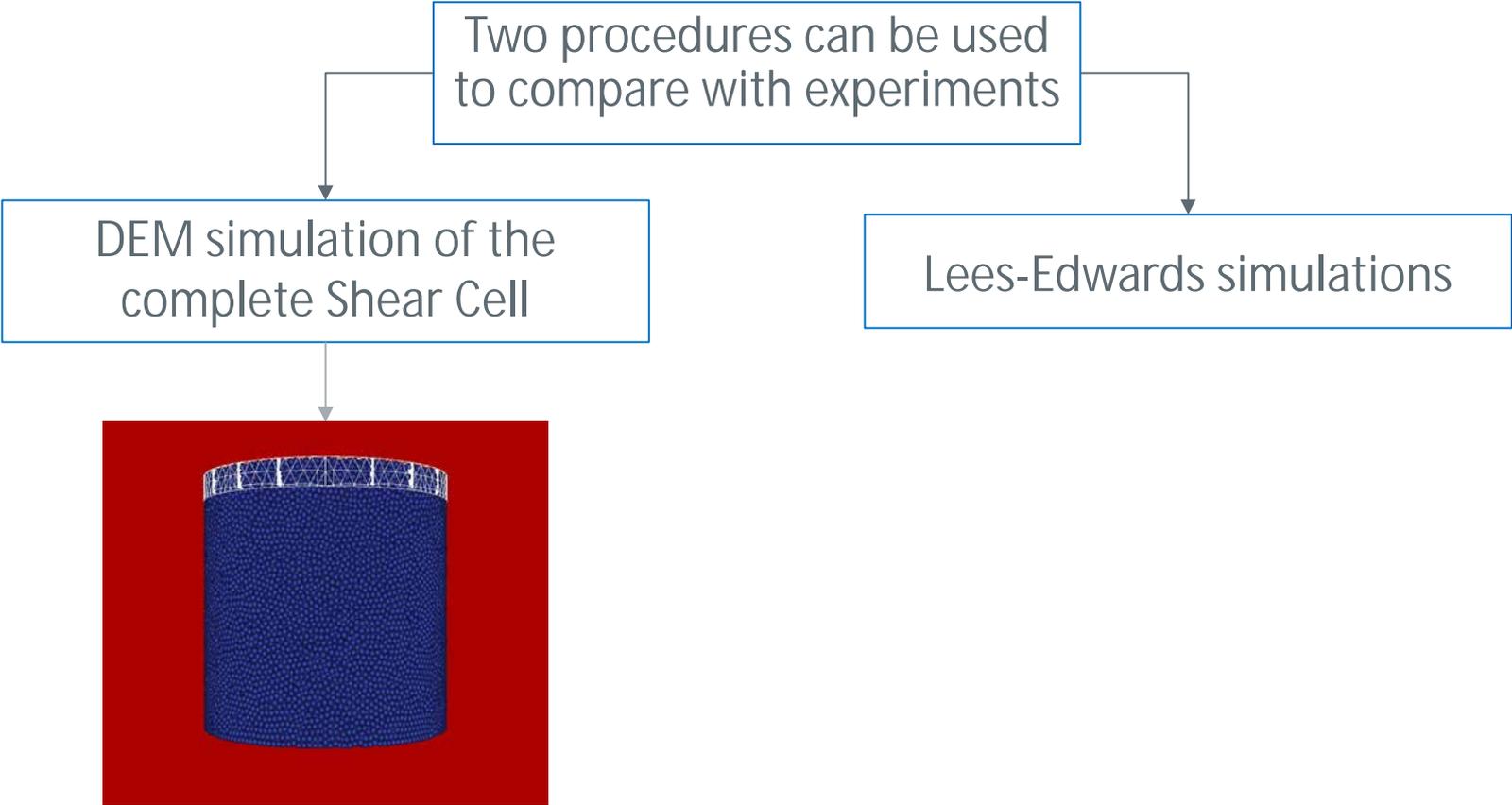
New experimental results:

- Study the **influence** of the **number of pre-shear** on:
 - The initial state of the powder bed before a shear test
 - The Angle of Internal Friction (AIF)

Shear Test – DEM Simulation



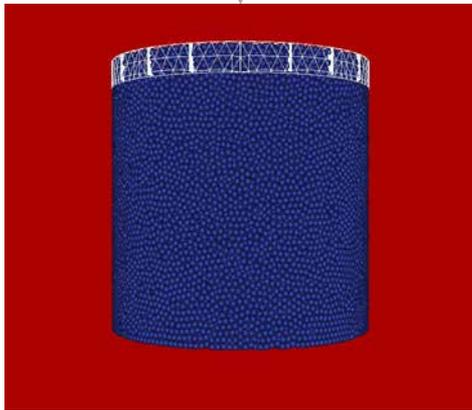
Shear Test – DEM Simulation



Shear Test – DEM Simulation

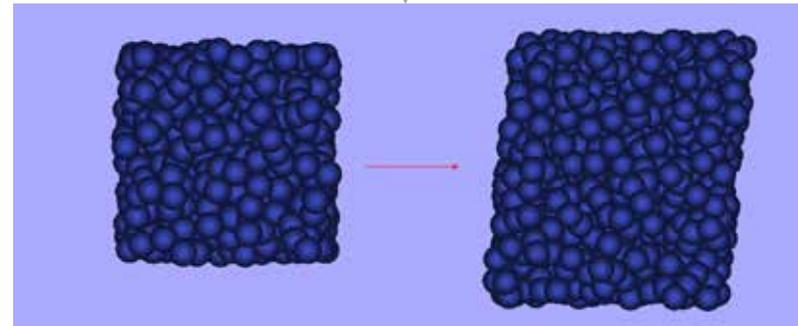
Two procedures can be used to compare with experiments

DEM simulation of the complete Shear Cell



Lees-Edwards simulations

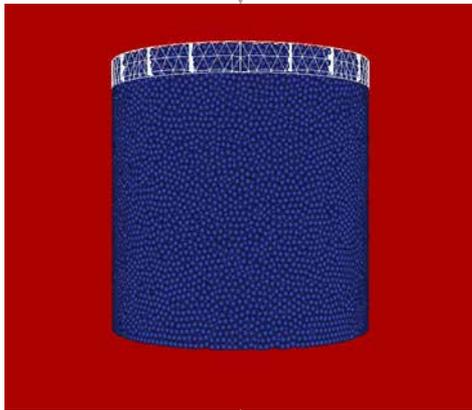
Simulation of the shear zone in a periodic domain by applying Lees Edwards contour conditions



Shear Test – DEM Simulation

Two procedures can be used to compare with experiments

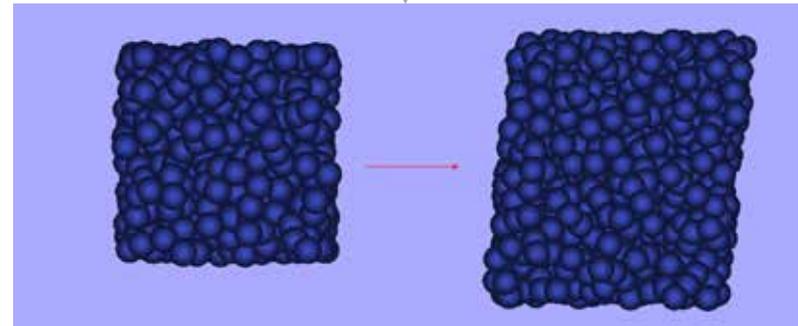
DEM simulation of the complete Shear Cell



- Heavy computational load
- + Information on every particle inside the domain

Lees-Edwards simulations

Simulation of the shear zone in a periodic domain by applying Lees Edwards contour conditions



- Only the shearing zone is simulated
- + Very small particle number

Future Work

```
graph TD; A[Future Work] --- B[DEM Simulations]; A --- C[Experiments];
```

The diagram is a simple tree structure. At the top is a blue-bordered box containing the text 'Future Work'. A vertical line descends from the bottom center of this box to a horizontal line. From the left end of this horizontal line, a vertical line goes down to a green-bordered box containing the text 'DEM Simulations'. From the right end of the horizontal line, a vertical line goes down to a purple-bordered box containing the text 'Experiments'.

DEM Simulations

Experiments

Future Work

```
graph TD; A[Future Work] --> B[DEM Simulations]; A --> C[Experiments]; C --> D["Variable particle-size distributions and shape"]; D --> E[Moisture component];
```

The diagram is a flowchart starting with a central box labeled 'Future Work'. A horizontal line extends from the bottom of this box, with two vertical lines branching downwards to 'DEM Simulations' on the left and 'Experiments' on the right. From 'Experiments', a vertical line leads down to a box containing 'Variable particle-size distributions and shape'. A downward-pointing arrow then connects this box to the final box, 'Moisture component'.

DEM Simulations

Experiments

Variable particle-size
distributions and shape

Moisture component

Future Work

```
graph TD; FW[Future Work] --> DEM[DEM Simulations]; FW --> EXP[Experiments]; DEM --> PC[Parameter calibration]; PC --> MC1[Moisture component]; EXP --> VPSD[Variable particle-size distributions and shape]; VPSD --> MC2[Moisture component];
```

The diagram is a flowchart titled "Future Work". It branches into two main paths: "DEM Simulations" and "Experiments". The "DEM Simulations" path includes "Parameter calibration" and "Moisture component". The "Experiments" path includes "Variable particle-size distributions and shape" and "Moisture component".

DEM Simulations

Parameter
calibration

Moisture component

Experiments

Variable particle-size
distributions and shape

Moisture component

Future Work

DEM Simulations

Parameter
calibration

Moisture component

Experiments

Variable particle-size
distributions and shape

Moisture component

Comparison

**Constitutive Models
for Particles Stresses**



Thank you for your attention!

Acknowledgement:

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