School of Process, Environmental
& Materials Engineering

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Application of Discrete Element Modelling for the Development of Particulate Processes: linking materials properties to performance

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Linking materials properties (single particles) to performance (bulk behaviour)

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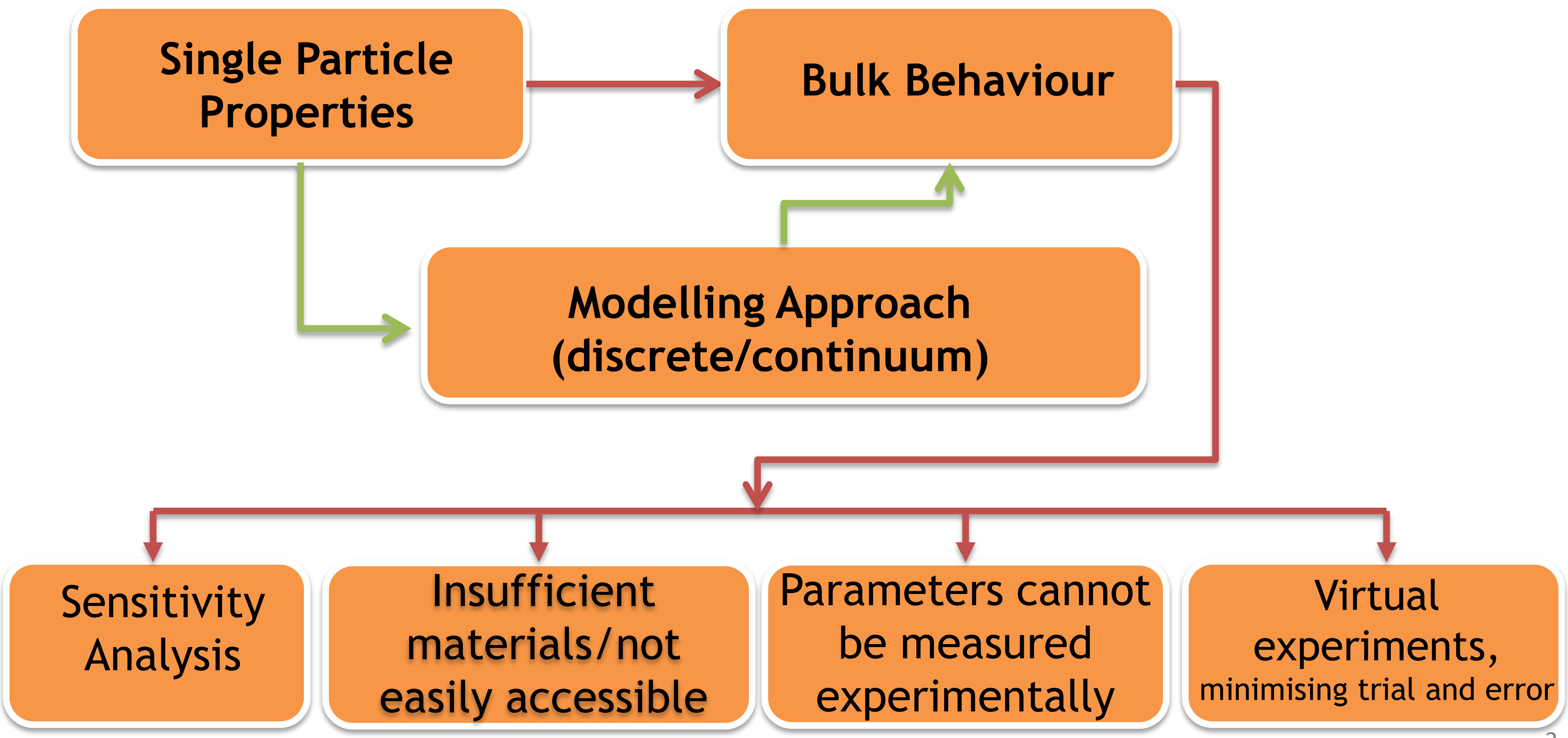
- Characterisation of the bulk behaviour based on single particle properties is of strategic importance in many processes involving particulate solids: e.g. transportation, filling, mixing, compaction, milling and granulation.



Discrete Element Method (DEM)

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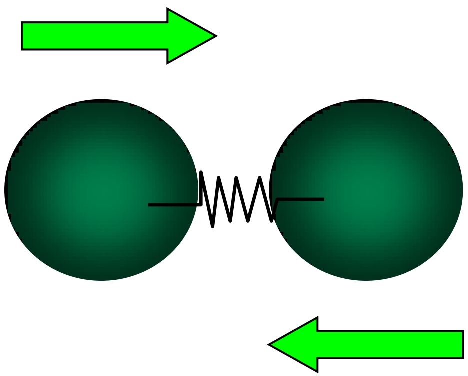
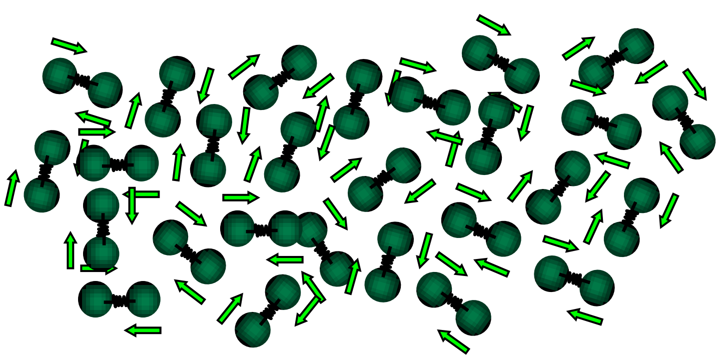
The term Discrete Element Method (DEM) is referred to a family of numerical methods for computing the motion of a large number of particles based on Newtonian laws of motion (Cundall and Strack, 1979).

Solving Newtonian equations of motion particles



$$ma = \sum F$$

$$I\alpha = \sum M$$



Solving Newtonian equations of motion for a large number of particles

Modelling of Bulk Behaviour using Distinct Element Method (DEM)

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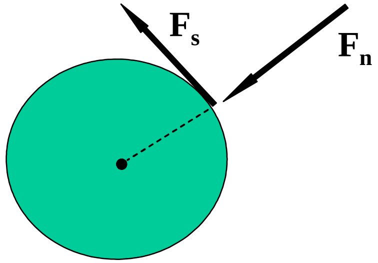
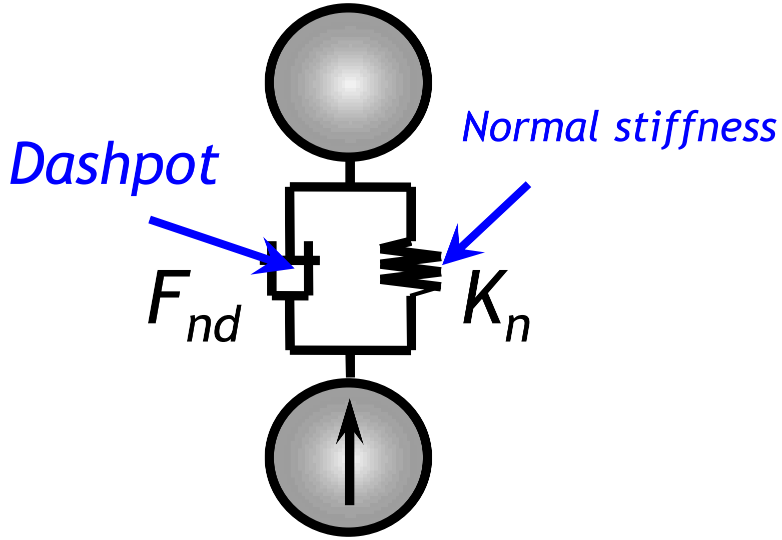
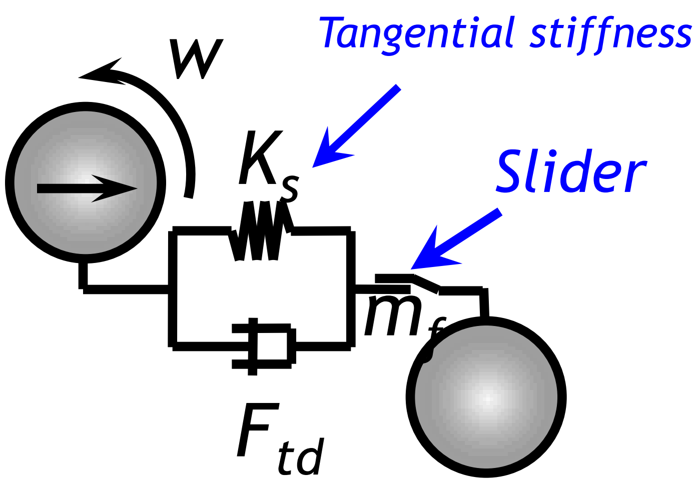
$$ma = \sum F$$

$$I\alpha = \sum M$$





Normal force



Tangential force

Cundall, P.A. and Strack, O.D.L.; *Geotechnique* (1979).

How DEM Modelling Can be Useful..

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- Effect of single particle properties and process variables on bulk behaviour in particular processes needs to be understood...... sensitivity analysis
- In a number of applications there is insufficient material for testing or material is not easily accessible, e.g. pharmaceutical and nuclear industries
- Some parameters can not be measured or quantified in the - experiments, e.g. internal particle flow and stresses
- Scale-up: moving from lab scale to pilot plant and industrial scales requires extensive trial and error….
- Modelling is a mean to interpret experimental results

Analysis of Segregation of Mixtures:
Sensitivity analysis

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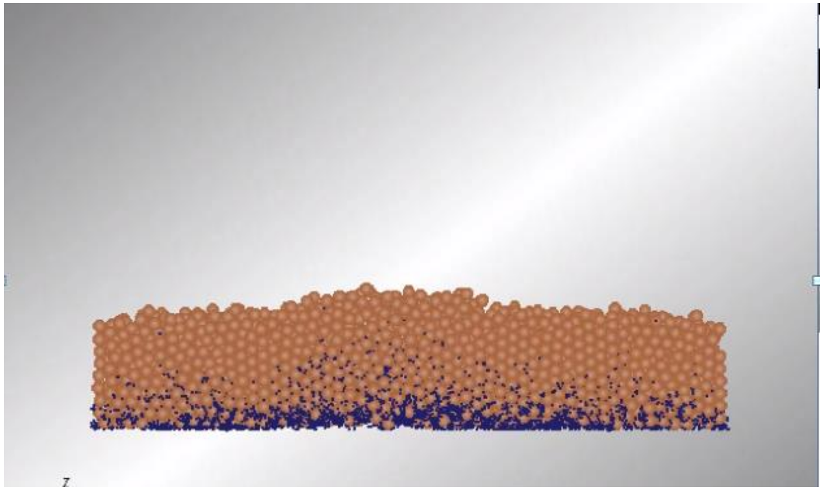
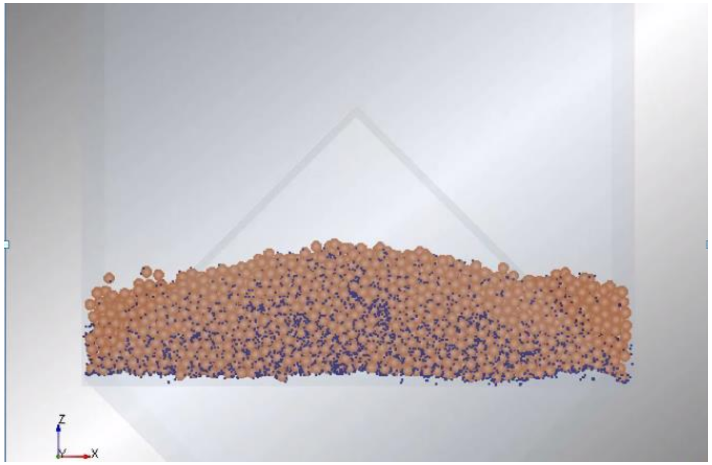
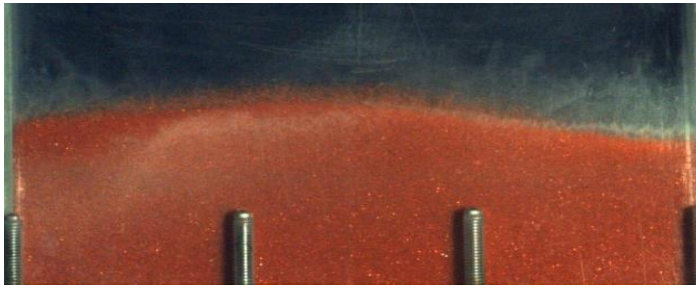
How to avoid segregation of light fine particles from dense course particles?

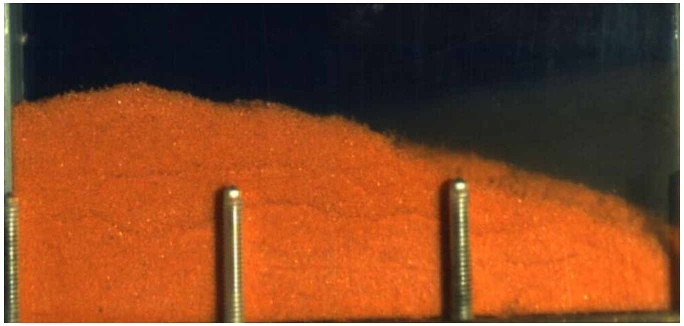


Both beads free-flowing



Dense Coarse Beads Cohesive
Surface Energy (Γ) = 0.5 J/m^2





Segregation during Heap formation

- Interpretation of Experimental Results
- Sensitivity Analysis

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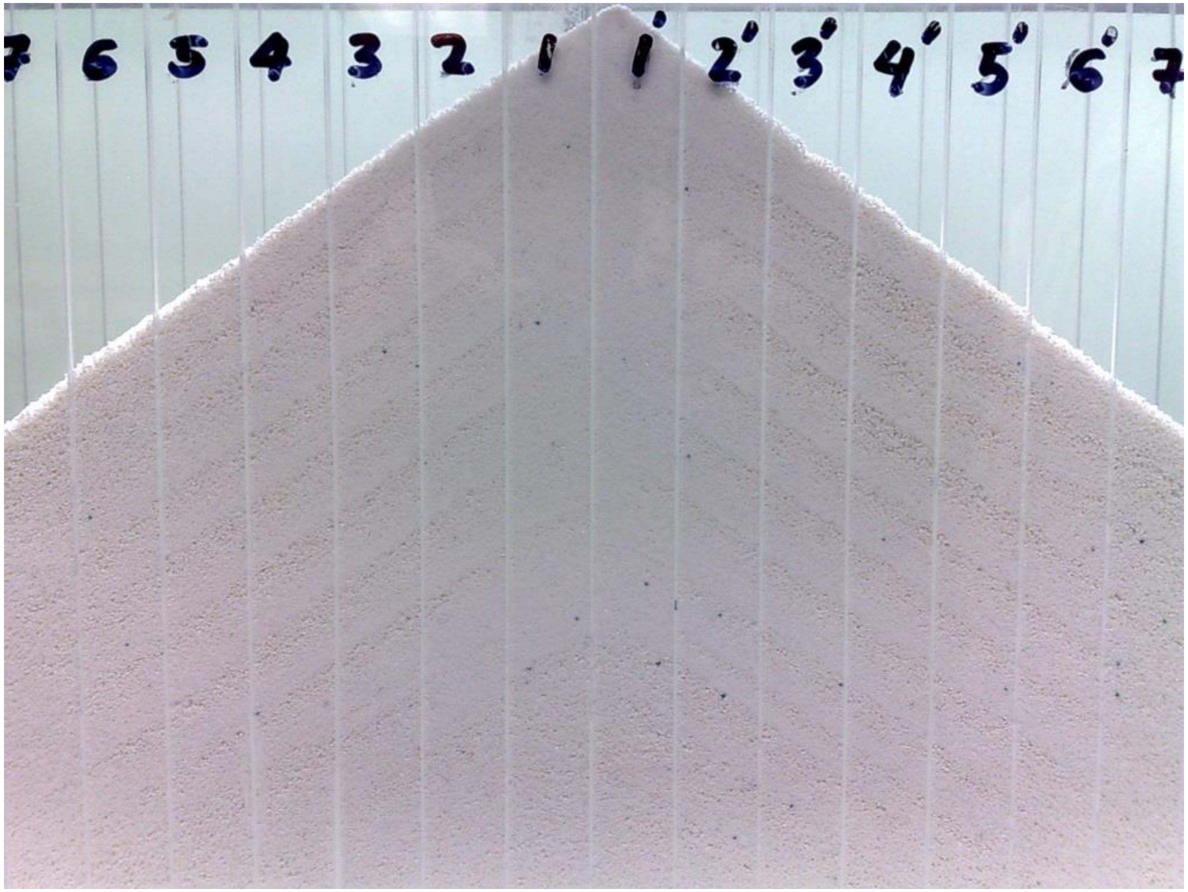
➢ Understanding the cause of segregation during heap formation



DEM Modelling of Segregation during Heap Formation: effect of cohesion on segregation

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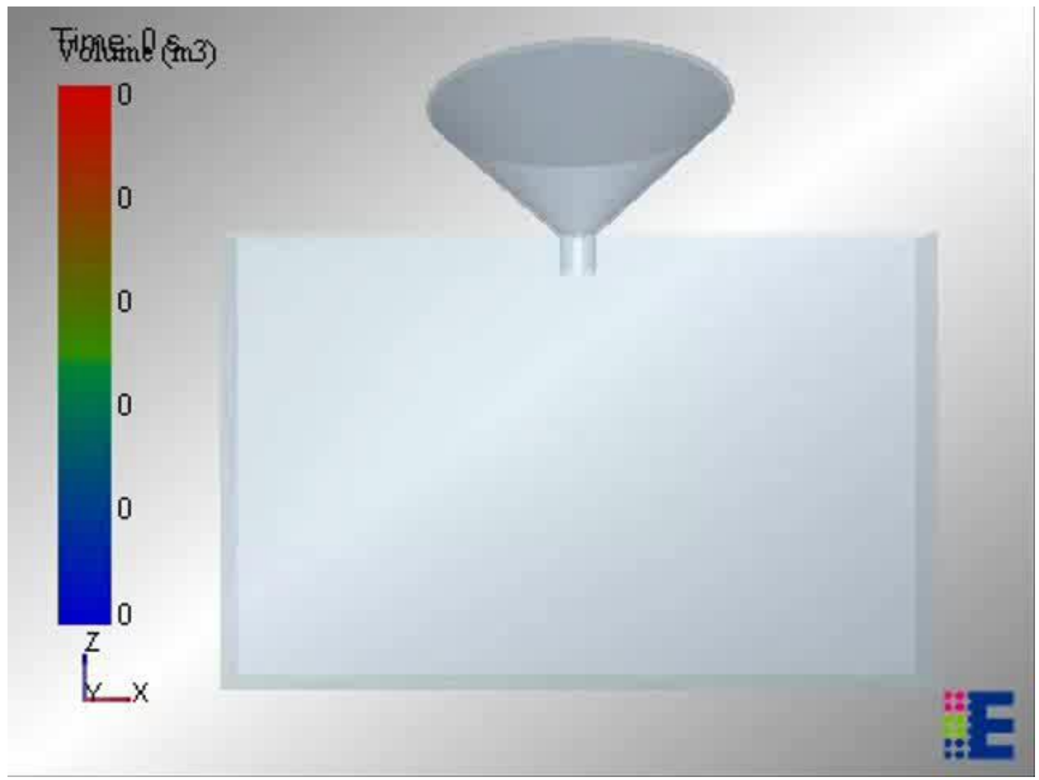
- Initial packing of sample: a randomly mixed system
- Colours represent volume (related to size) of particles



DEM Modelling of Segregation during Heap Formation: effect of cohesion on segregation

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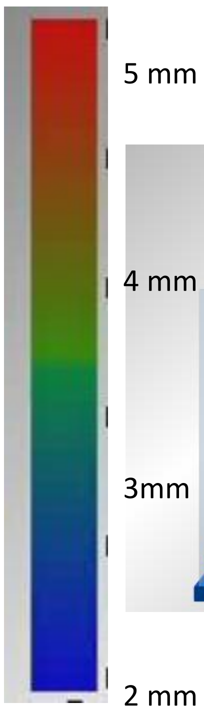
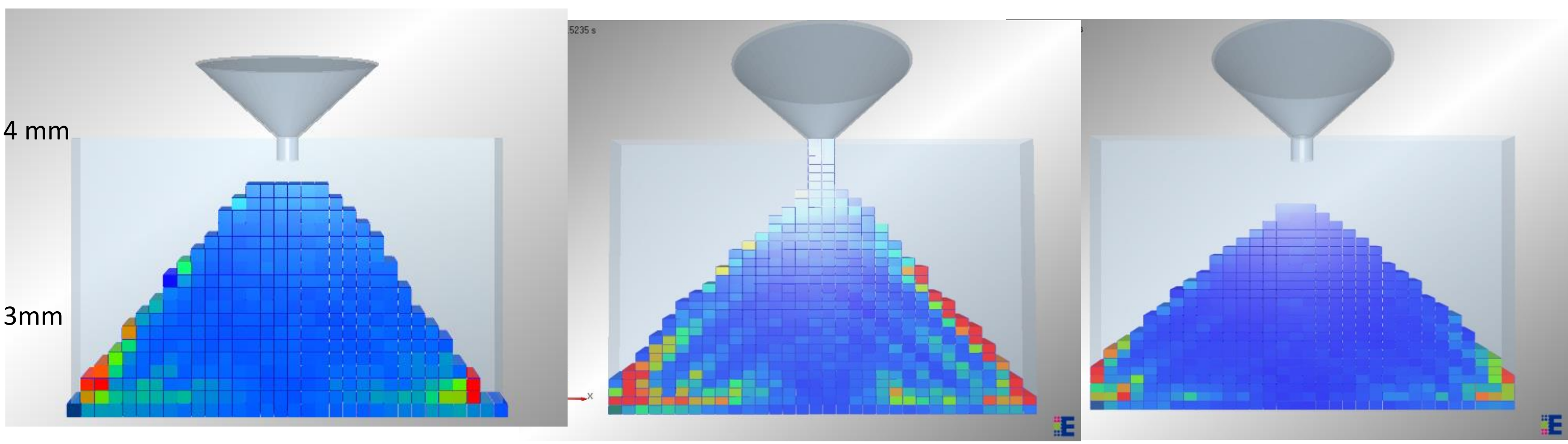
- Colours represent average size of particles in each bin

All particles are cohesive

Fine particles are cohesive

All particles are free flowing





Formation of Seeded Granules in Cyclomix High Shear Mixer:
Interpretation of Experimental Results

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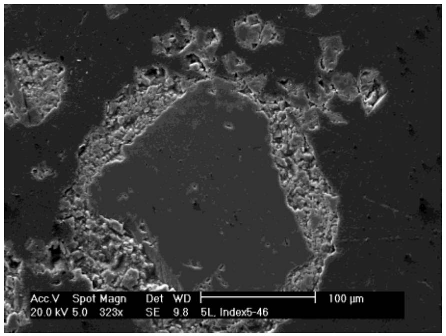

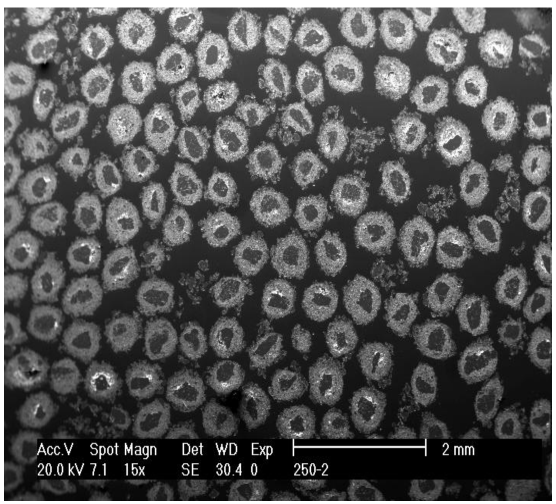

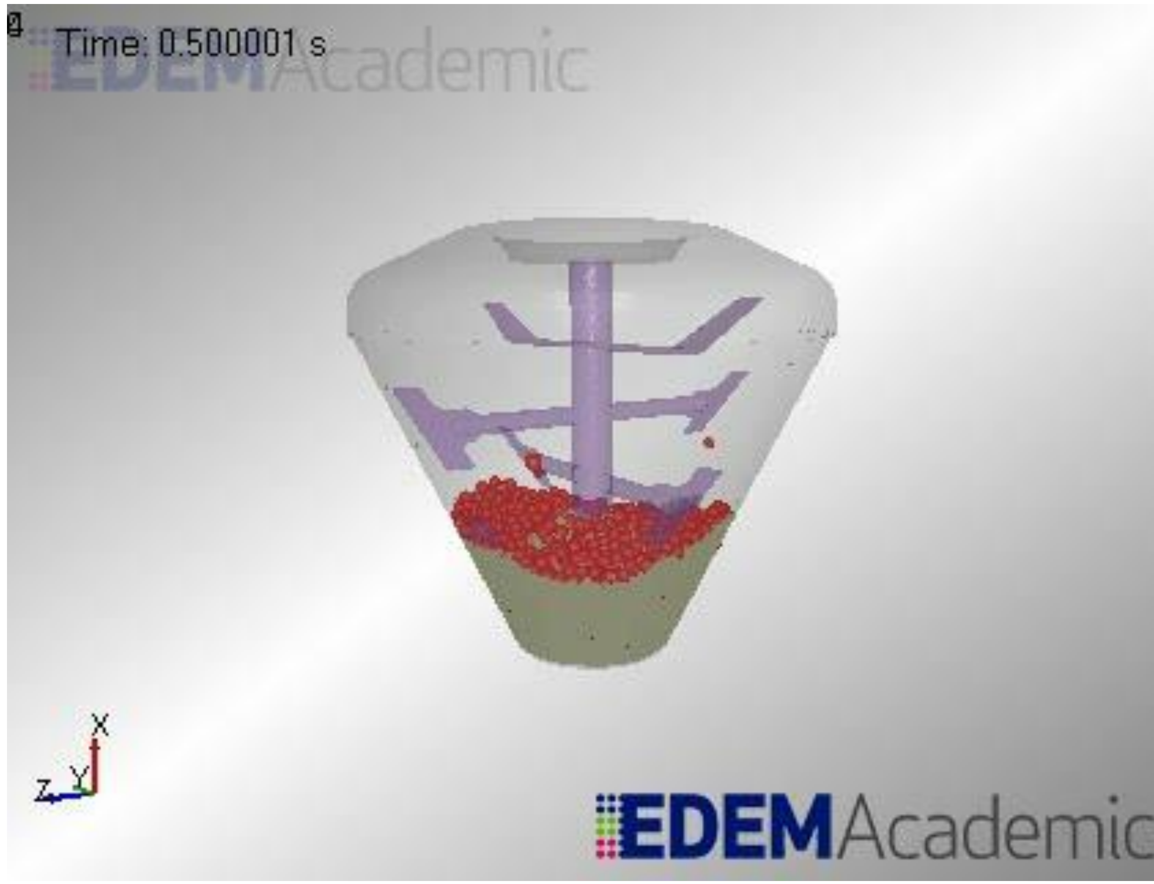

Seeded granules occur in Cyclomix high shear mixer under certain operating conditions

DEM Simulation of Granulation in Cyclomix

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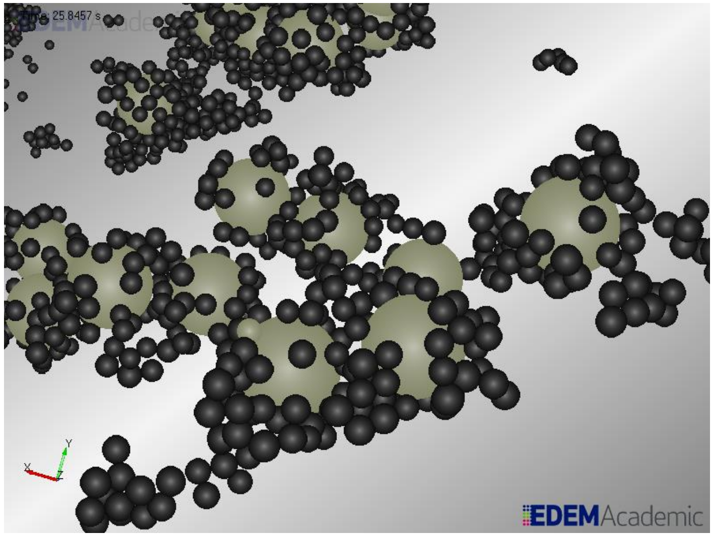

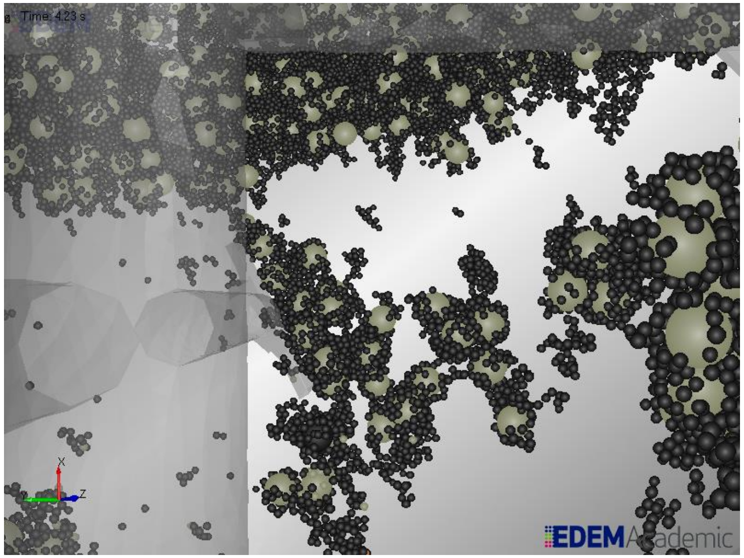

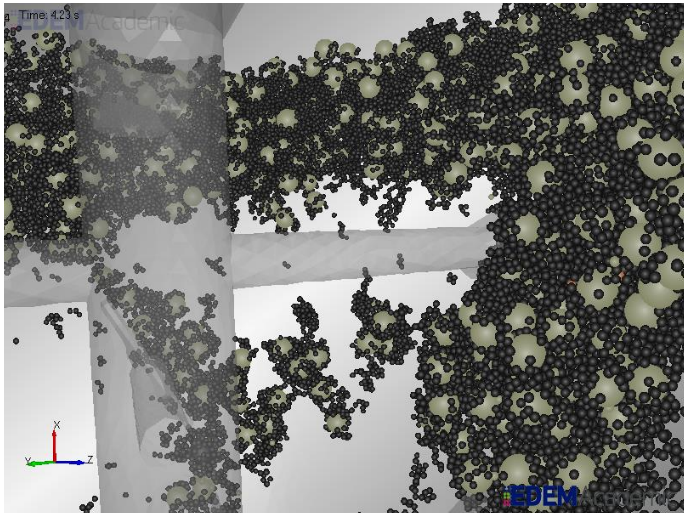

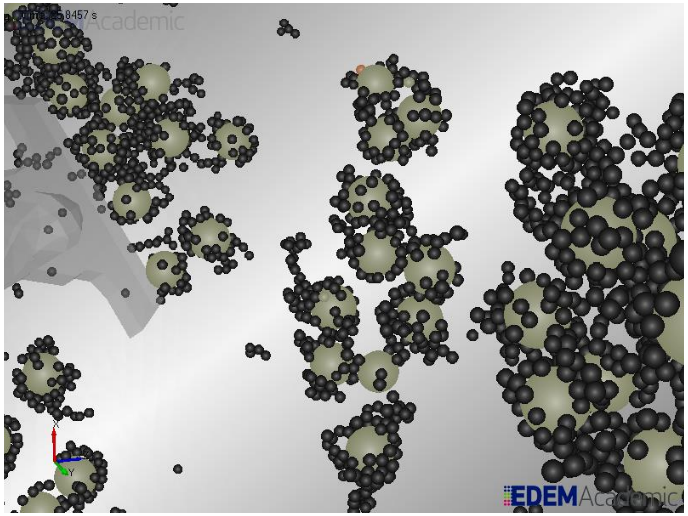

DEM Simulation of Granulation in Cyclomix: formation of seeded granules

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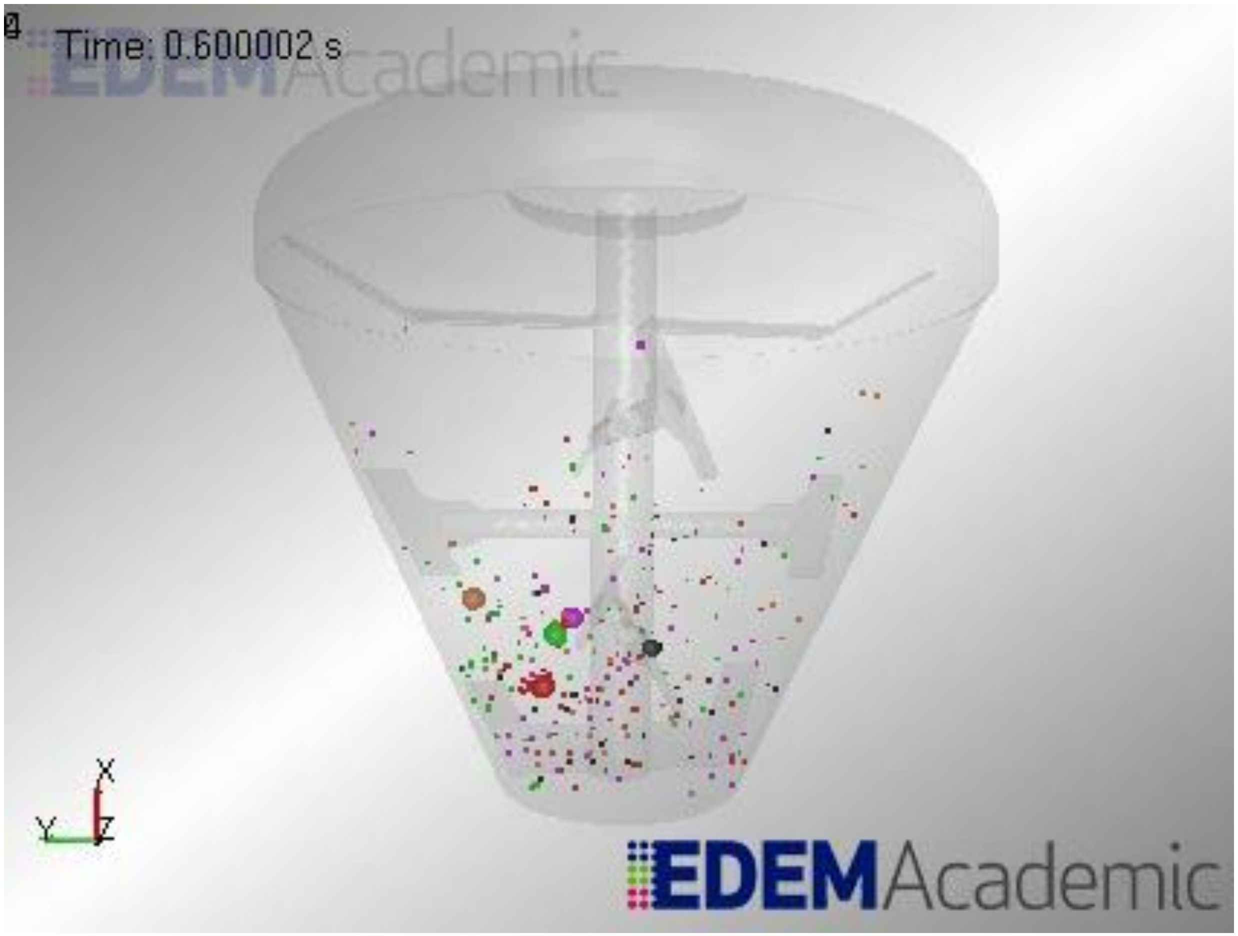

Seeded granules are quickly formed in the high shear region (middle part) and break as soon as they approach the top part

Predicting Breakage of Granules, Compacts

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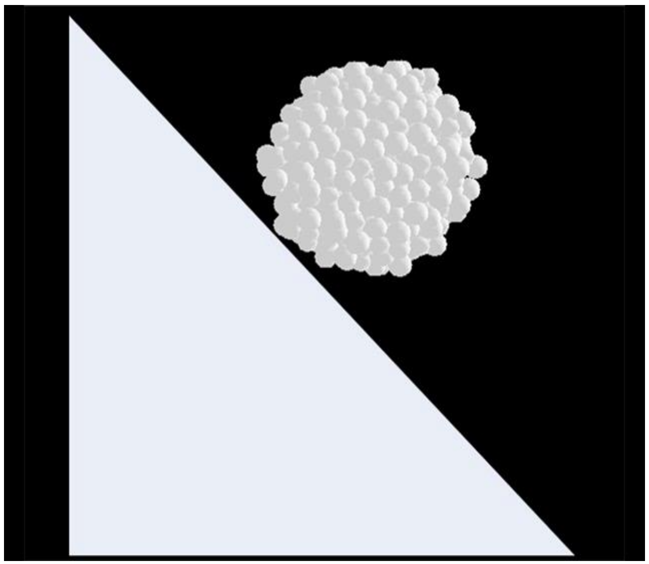
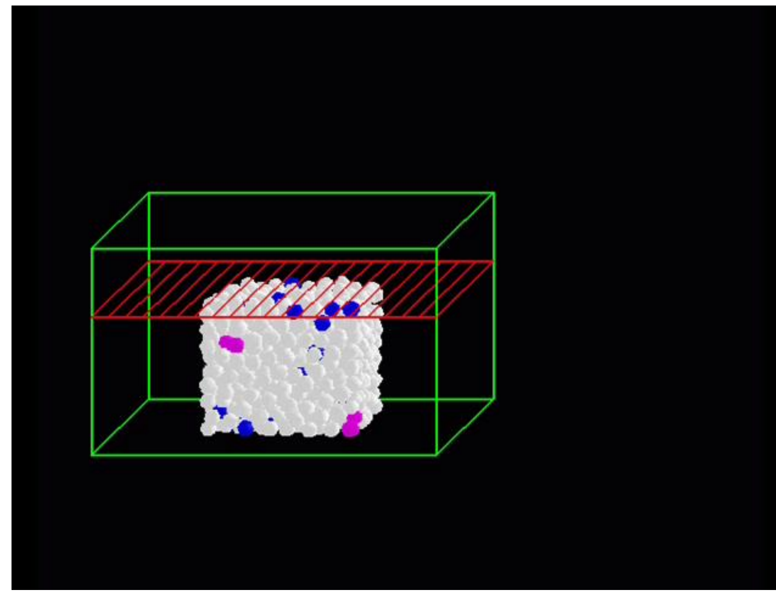
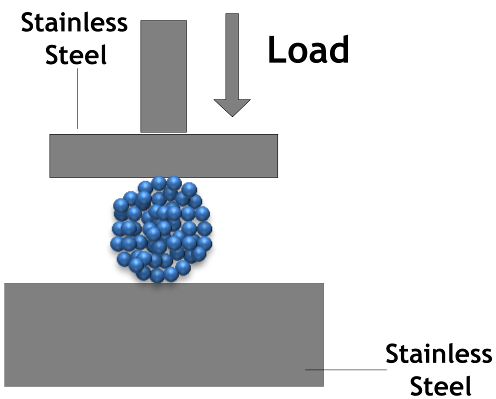
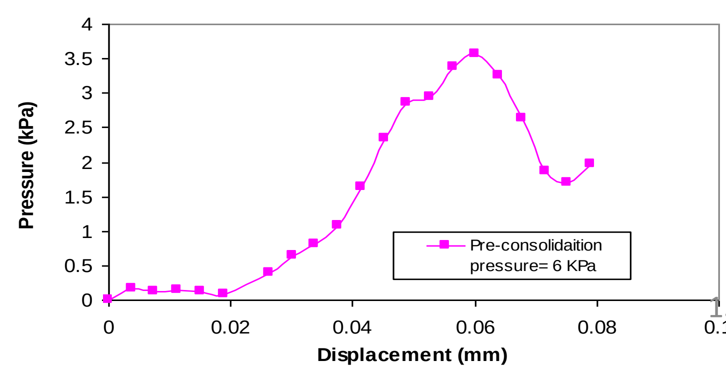
❑ Modelling the agglomerate and compact breakage









DEM of Mixing of Particulate Solids:

Minimising Trial and Errors; Insufficient Available Materials; Parameters Difficult to Measure

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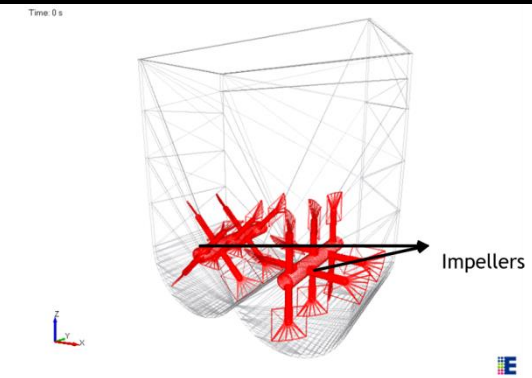
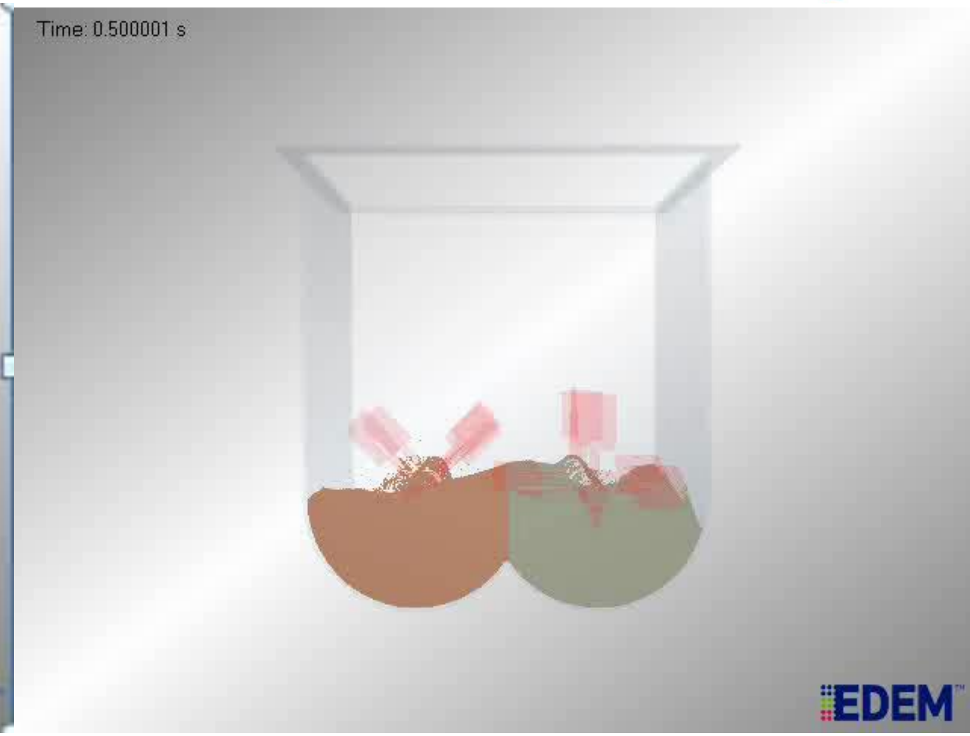
Particle motion analysis in a paddle mixer





Experimental Measurement using (Position Emission Particle Tracing (PEPT)

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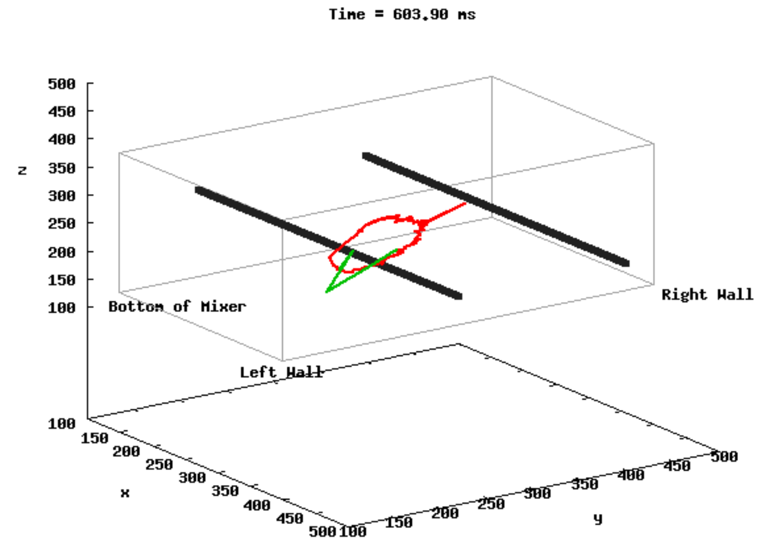
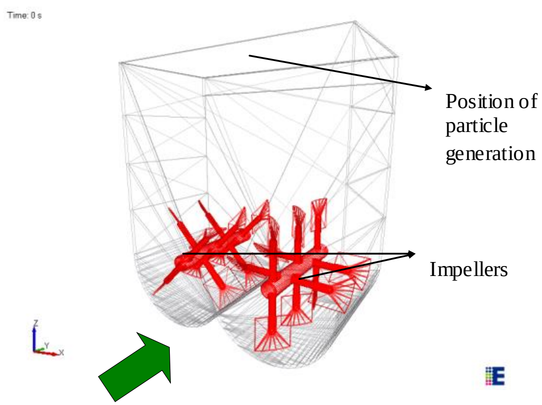
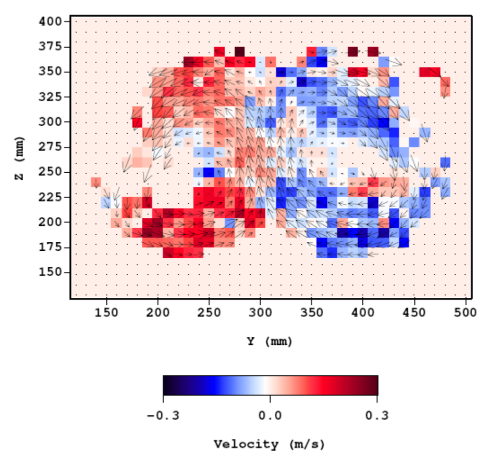
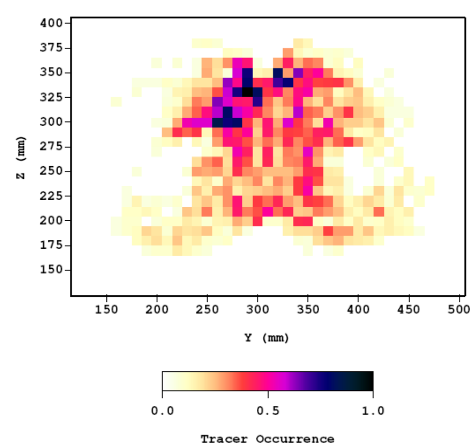
- 6l paddle mixer was seeded with a positron charged tracer particle.
- The mixer was run at various condition over a period of time (usually 20-30 min).
- Position of the tracer is continuously recorded against time.
- Bulk flow properties per trial is analysed from the temporal velocity and occurrence frequency of the tracer.



Boon Ho Ng (2007)







Quantitative Comparison of Powder Flow between DEM and PEPT

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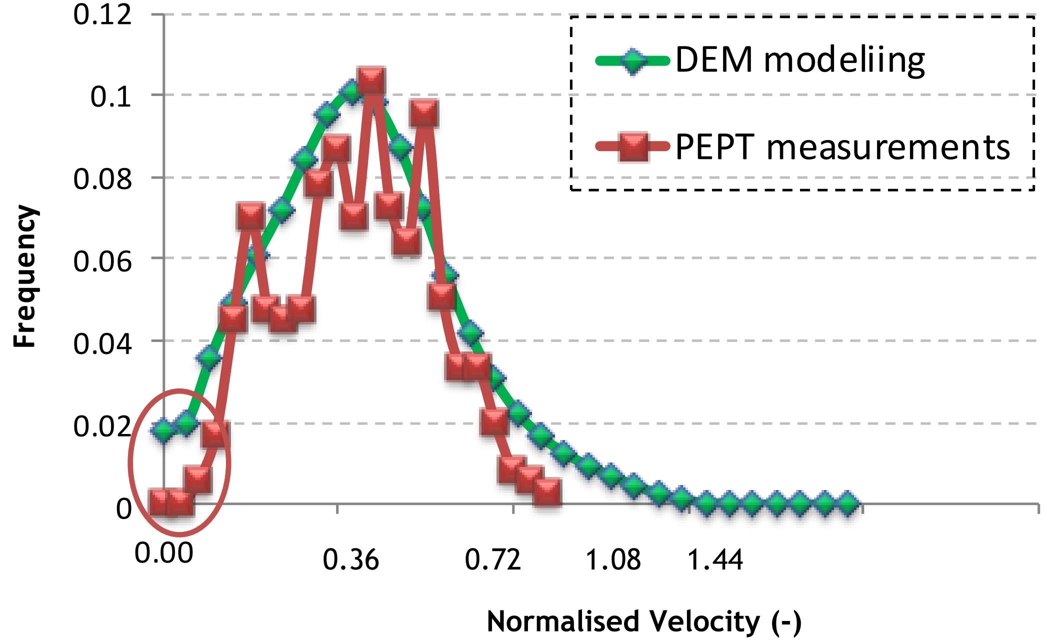

Average normalised velocity from PEPT: 0.43

Average normalised velocity from DEM: 0.41

- **DEM: data on all particles**
- **PEPT: the time averaged data for one tracer but over a long period of running time (excess of 10 minutes)**

DEM Modelling of Cyclomix High Shear Mixer Granulators: Scale-up

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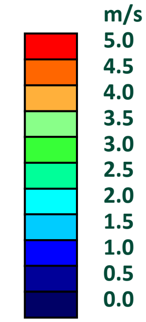
Scale-up $\omega_2/\omega_1=(d_1/d_2)^n$

n = 1 Tip speed constant

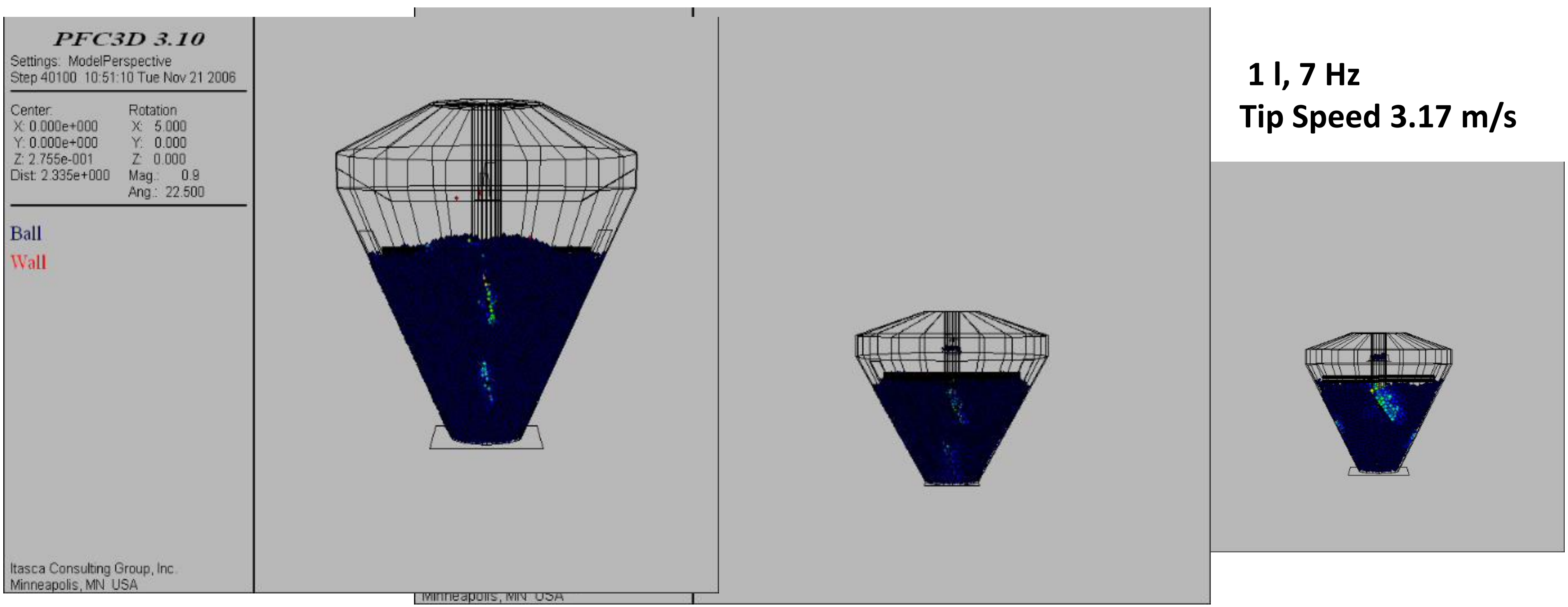
n = 0.5 Froude number constant



50 l, 2 Hz
Tip Speed 4.13 m/s

5 l, 5 Hz
Tip Speed 3.52 m/s

1 l, 7 Hz
Tip Speed 3.17 m/s



DEM Modelling of Cyclomix High Shear Mixer Granulators: Scale-up

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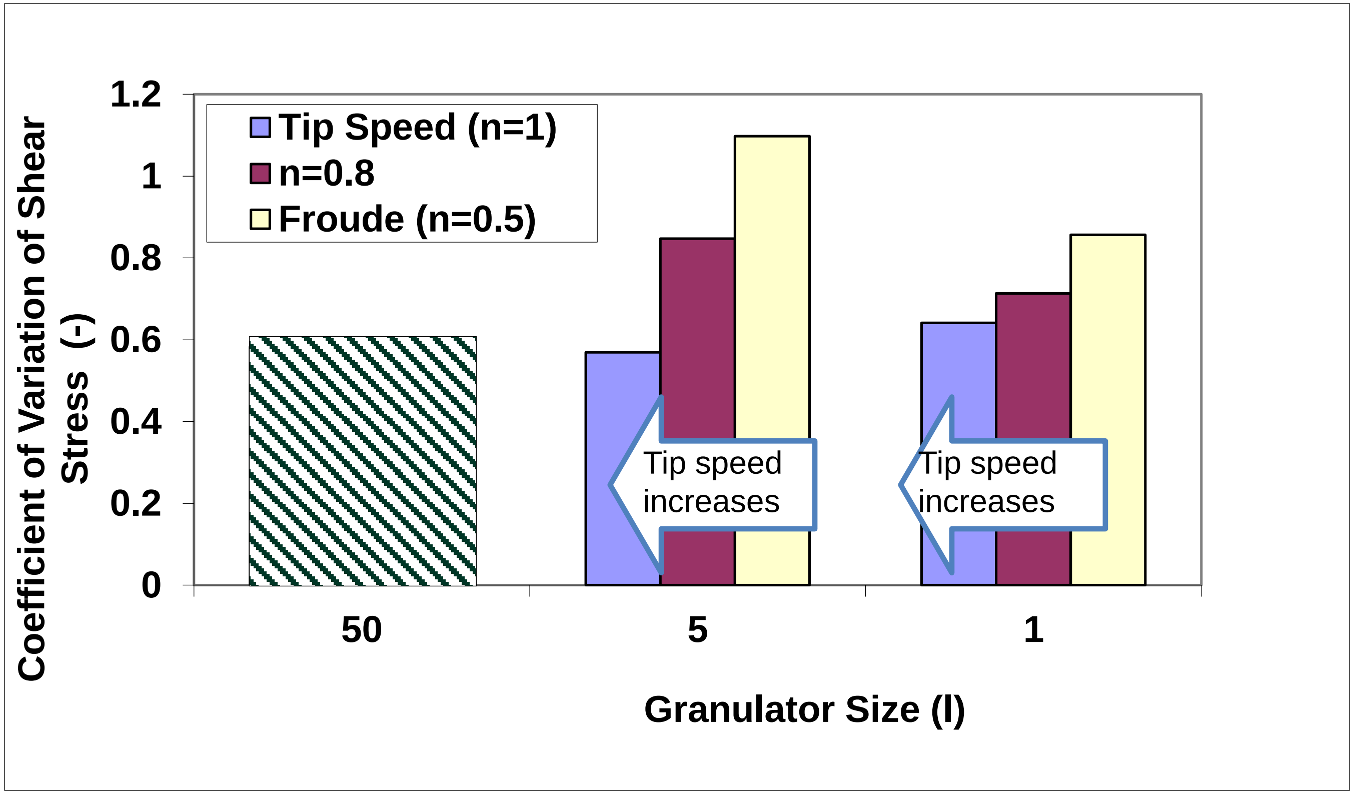

The coefficient of variation of shear stress decreases as the impeller tip speed is increased.

Modelling of Particle Milling:

- Minimising Trial and Errors
- Insufficient Available Materials

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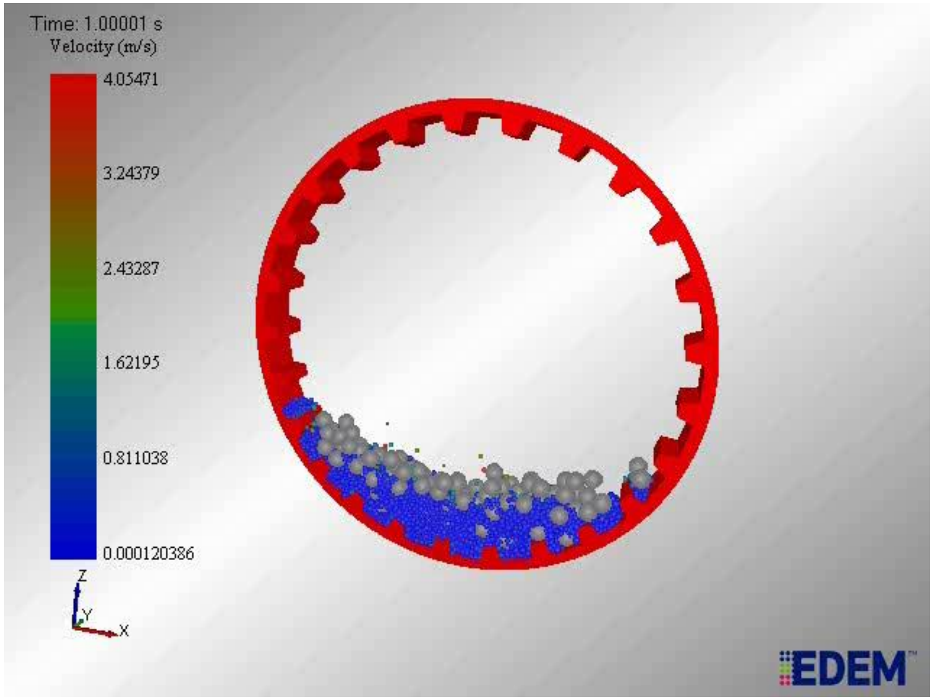

1- Modelling particle breakage: particle made of agglomerates, clusters of smaller elements bond

Computationally very expensive, difficult to model full scale mill

2- Predicting the mill performance: collisional energy, stress magnitude and distribution

Modelling of Ball Milling

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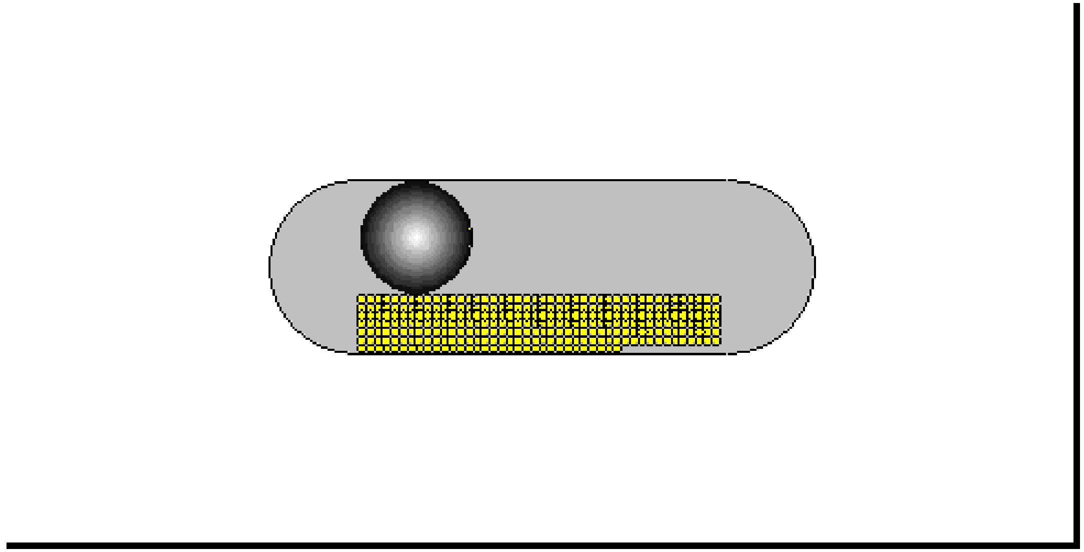
DEM simulation at 25 Hz of milling frequency in the single ball mill



- ***Milling energy*** **(E_n) is deduced from the relative velocity (v) and reduced mass (m^*) of the two objects in contact by:**

$$E_n = \sum_{j=1}^{n} \frac{1}{2} m^* v_j^2$$

- ***Milling power*** **(P_n) is deduced from:** $P_n = \frac{E_n}{t}$

Unification of Results

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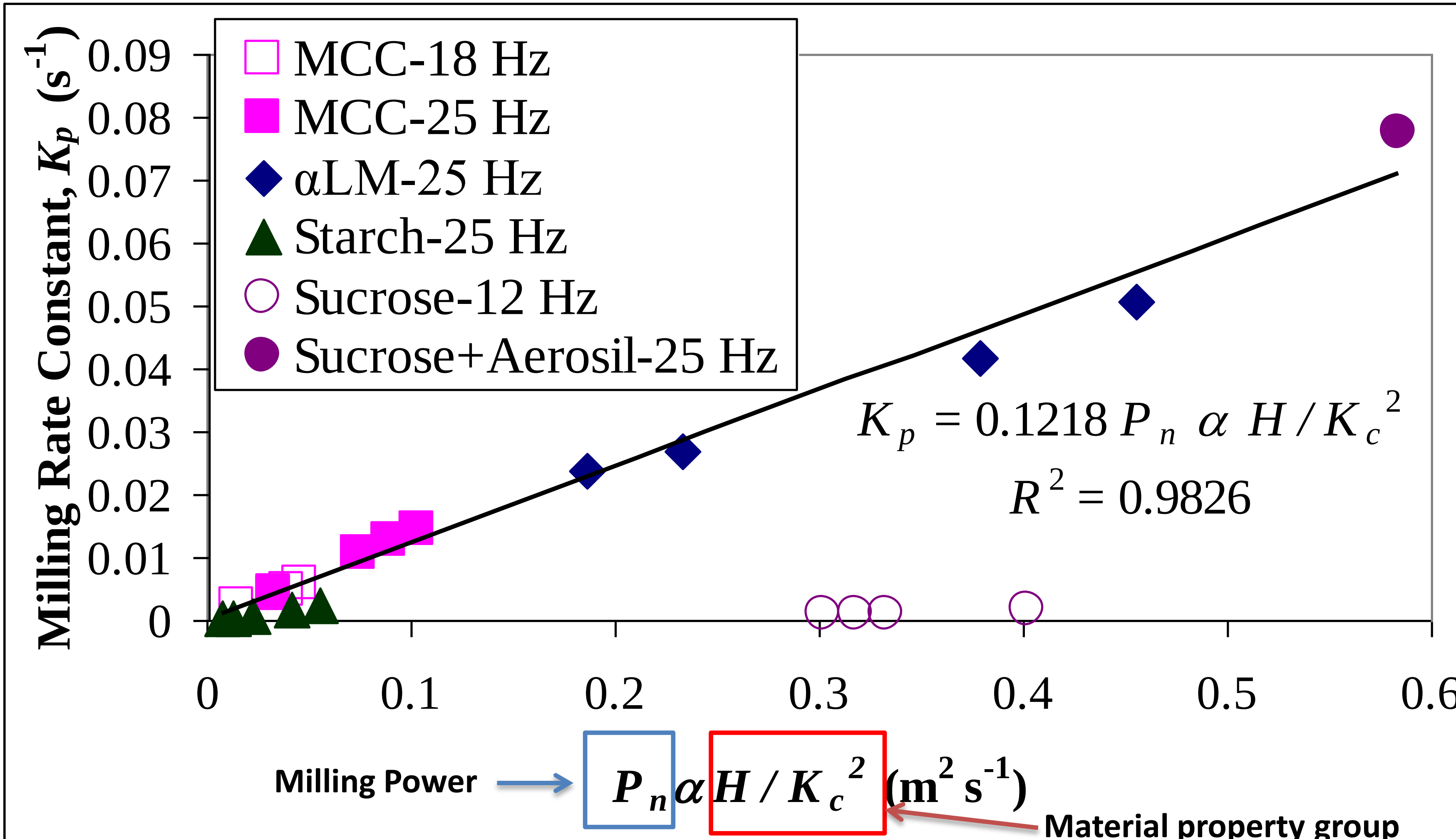

Solid-fluid flow modelling

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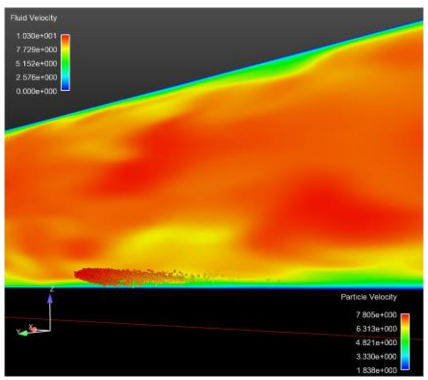
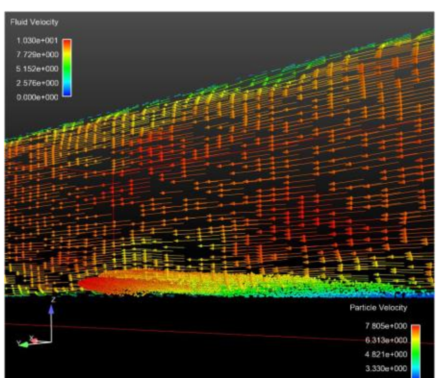
Solid/fluid interaction

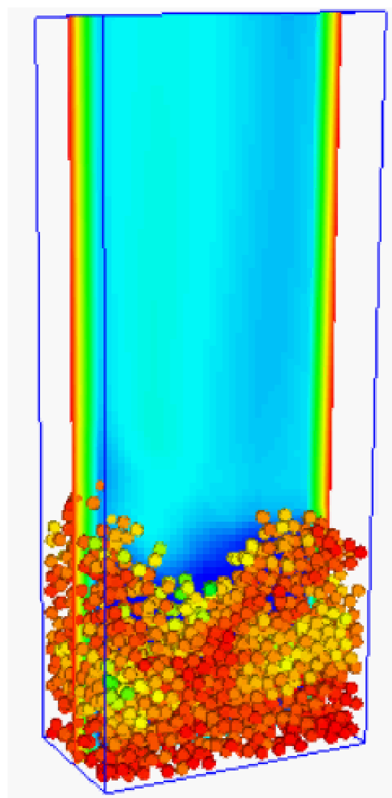
DEM + Continuum Method (CFD); Full Fluid-Solid coupling

Dispersion

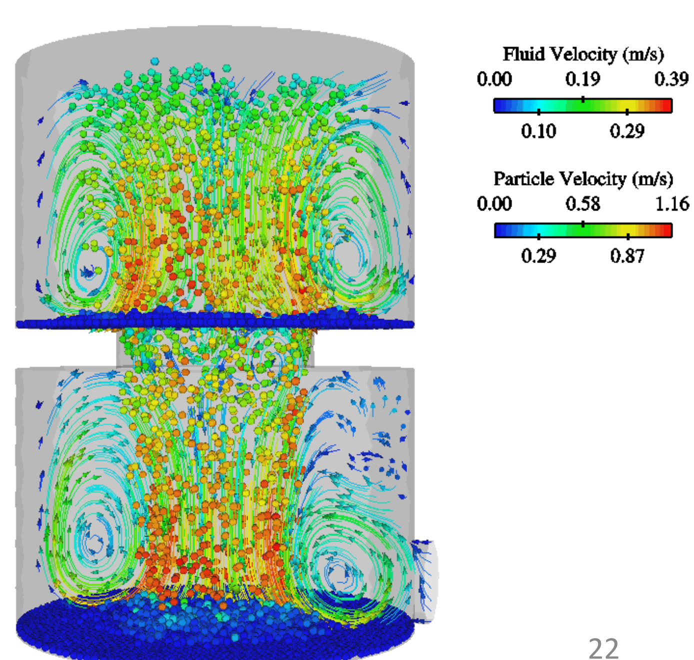




Fluidization



Sedimentation/ re-suspension



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Solid-fluid Flow Modelling: DEM-CFD coupling

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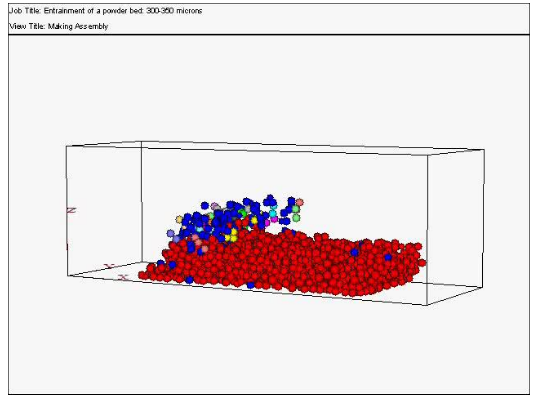
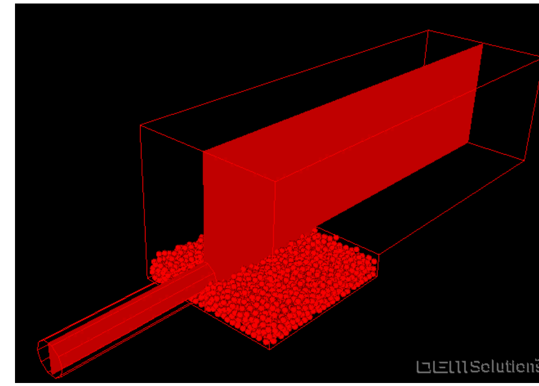
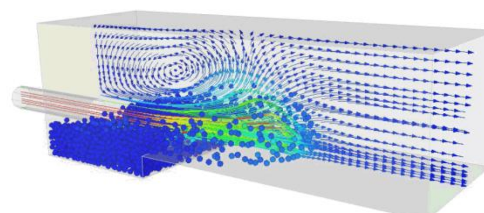
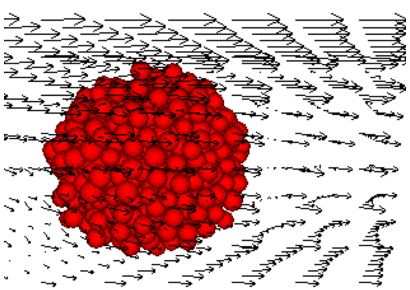
Pneumatic conveying, powder dispersion and fluid diffusion

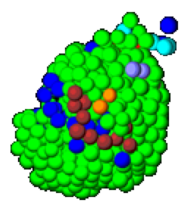


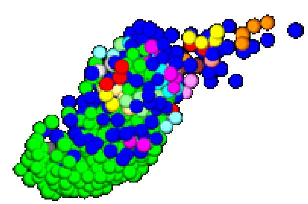


Agglomerate dispersion









Solid-fluid Flow Modelling: agglomerate dispersion

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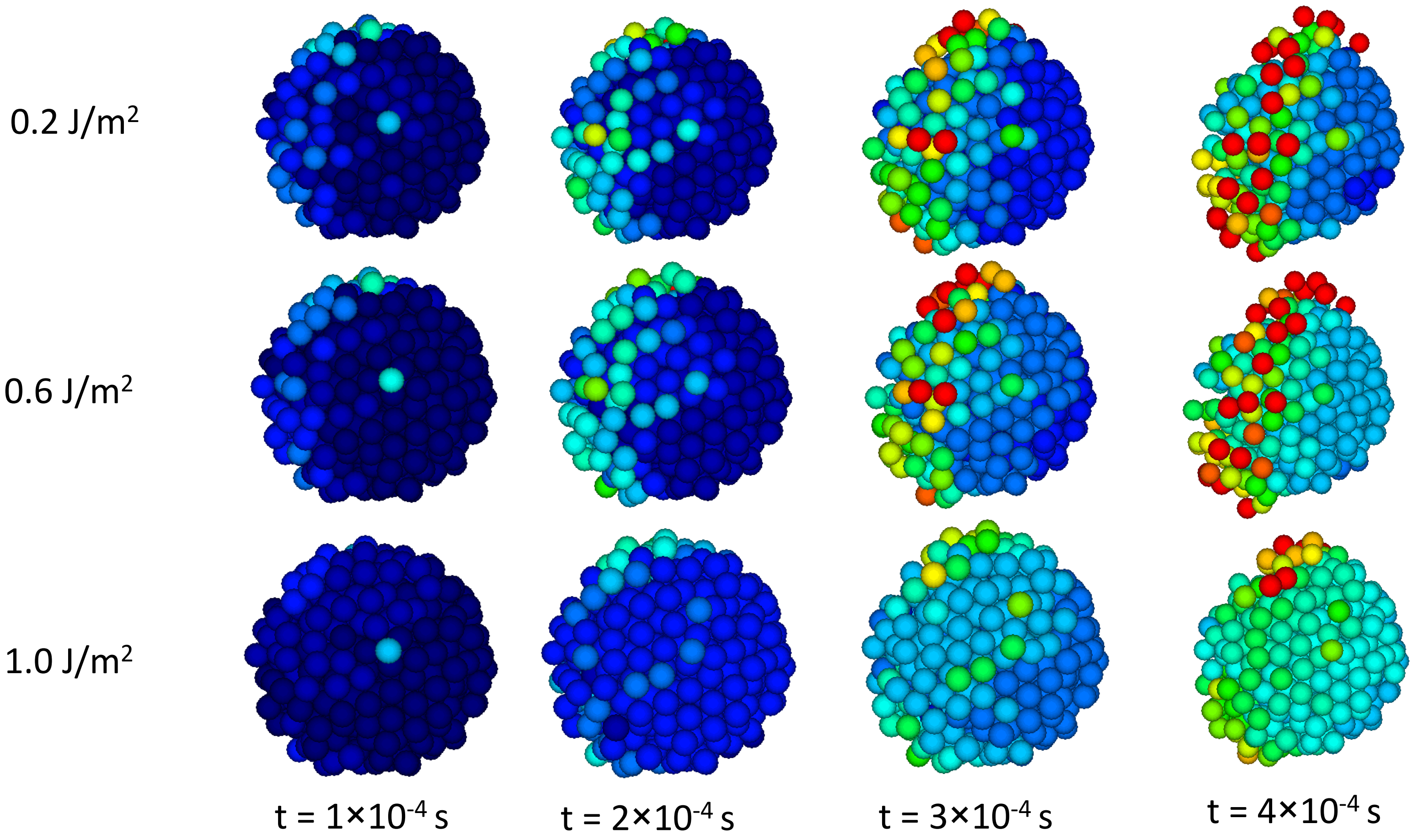
- With an increase in bonding interface energy it becomes increasingly difficult to disintegrate particle clusters.



Solid-fluid Flow Modelling: agglomerate dispersion

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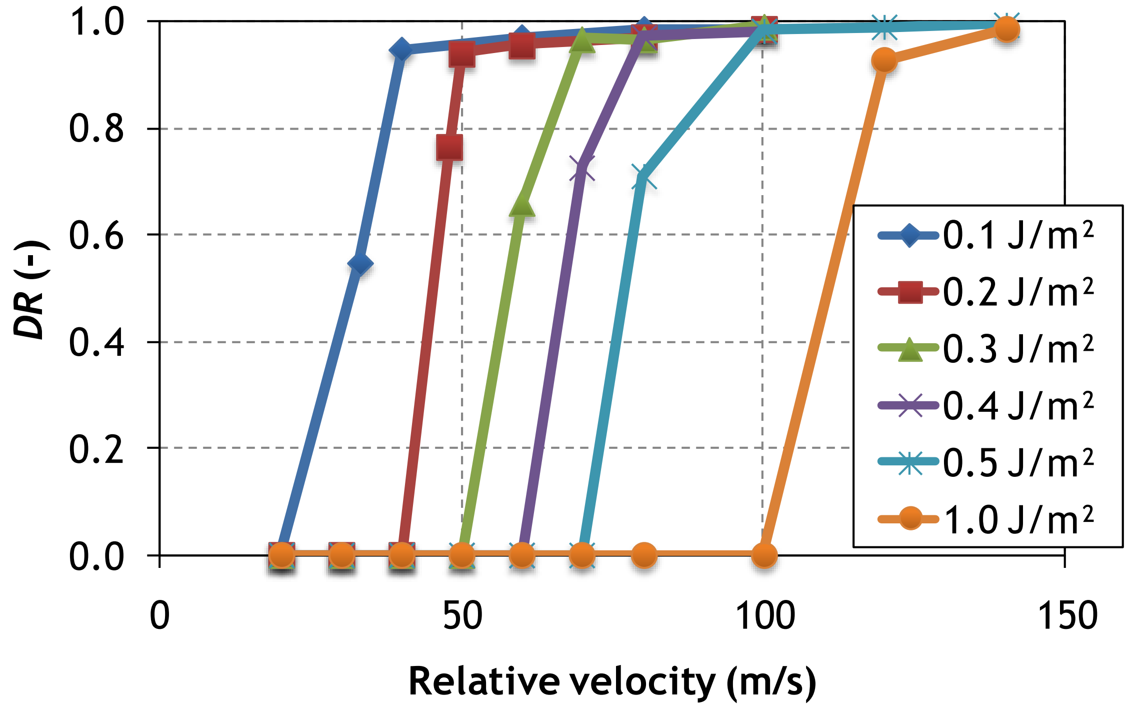
The dispersion ratio (DR); i.e. ratio of the number of broken bonds to the initial number of bonds, (DR = 1 means all bonds are broken)

$$DR = \frac{N_0 - N_t}{N_0}$$

DR shown as a function of relative velocity between the fluid and particles.



Concluding Remarks

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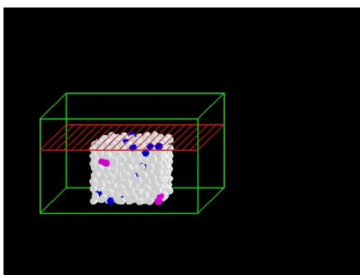
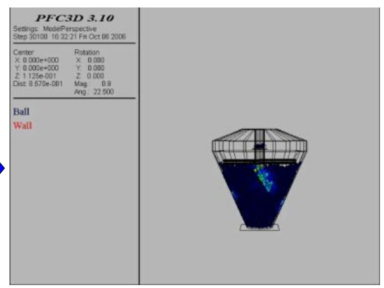
- DEM provides useful information in understanding particulate processes and obtaining parameters difficult to measure by experiment.
- DEM analysis shows good capabilities of interpretation of experimental data
- Numerical modelling capabilities can enable virtual experiments instead of extensive trial and errors:
  - Particulate Process Development
  - Process Optimisation
  - Process Scale-up

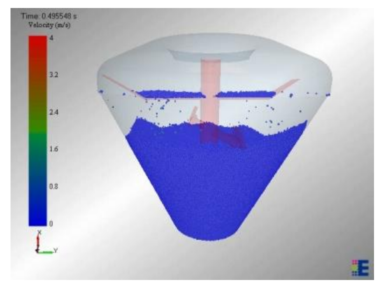
Challenges and Opportunities

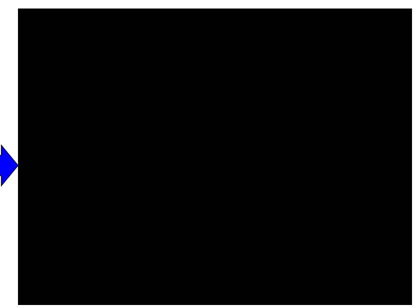
- ✓ Realistic and Complex Models
- ✓ High Performance Computing (CPU&GPU)
- ✓ Model Calibration

Development of Modelling Capabilities (Desktop Workstation)









2002 (5,000)

2005 (40,000)

2008 (500,000)

2012 (10 million)

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Malvern National Nuclear Laboratory P&G Pfizer Sellafield Ltd

Thank you for your attention !