Numerical simulation of an impact pin mill with DEM-PBM coupling model

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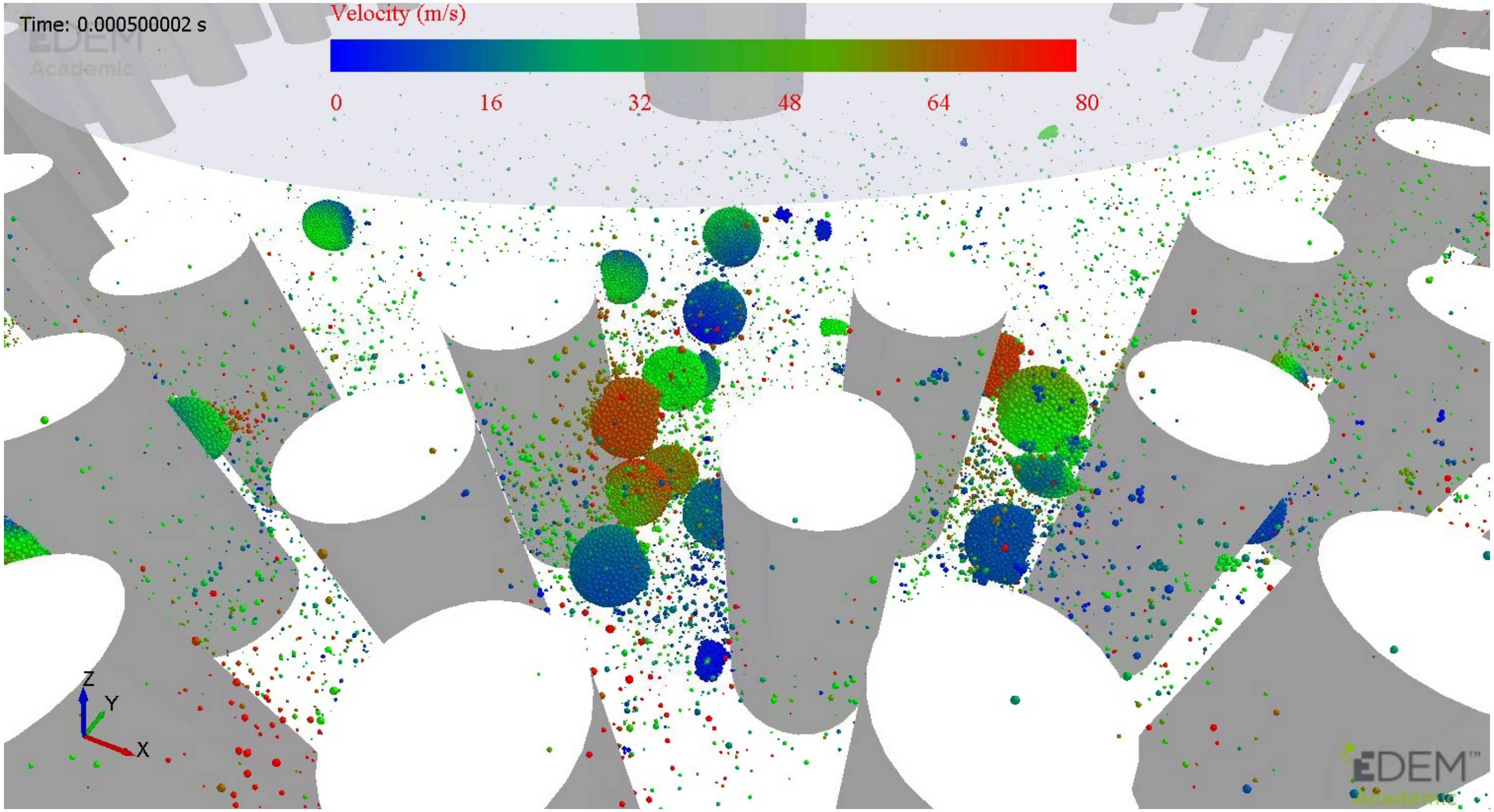
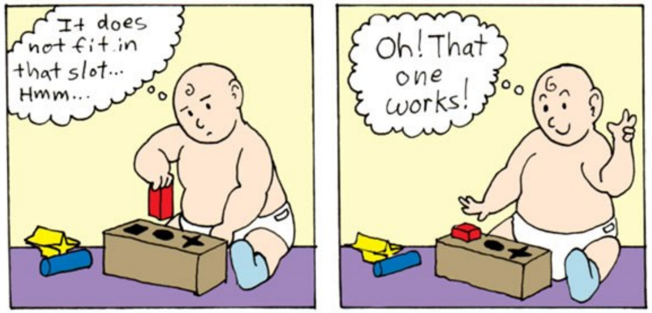


Outline

- Key challenges in milling processes
- DEM simulations of particle dynamics in a pin mill
- Upscaling strategy using DEM-PBM
- Understanding on single particle breakage
- Summary

Challenges in milling processes

- Milling is a common unit operation for size reduction
  - Reduce amount of coarse particle
  - Increase surface area
  - Improve flowability/ ease of use
  - .....
- Energy-intensive and inefficient(less than 10%)
  - Roller mill
  - Impact mill
  - Ball mill
  - ....
- Design and optimization of milling processes
  - Black box
  - Trial and error
  - Empirical scale-up rule



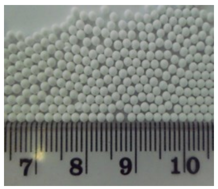
- Fundamental understanding is therefore important

Fluidised bed jet mill by HOSOKAWA MICRON LTD.

Air classifier mill by HOSOKAWA MICRON LTD.

Impact milling test

- Predict the grindablity of different materials
- Predict the grinding efficiency for given mills



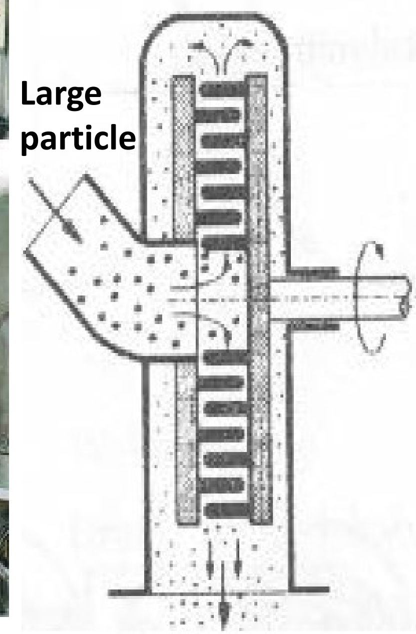
Alumina (Brittle)

Zeolite 4AK (semi-brittle)

Characteristics of the zeolite 4AK and Alumina granules

Producing Place		CWK Chemiewerk Bad Köstritz	Sasol GmbH Hamburg
Parameter	Unit	Zeolite 4AK	Alumina Al_2O_3
Diameter	mm	1.2-2.0; 2.0-2.5	1.0-1.18
Bulk density	g/ml	0.76	0.88
Specific gravity	–	2.18	3.37
Water content	≤ %wt	1.0	0.6
Fracture force	≥ N	24.9	34.49
Strength	MPa	8.34	17.84
Elastic modulus	GPa	2.45	12.23

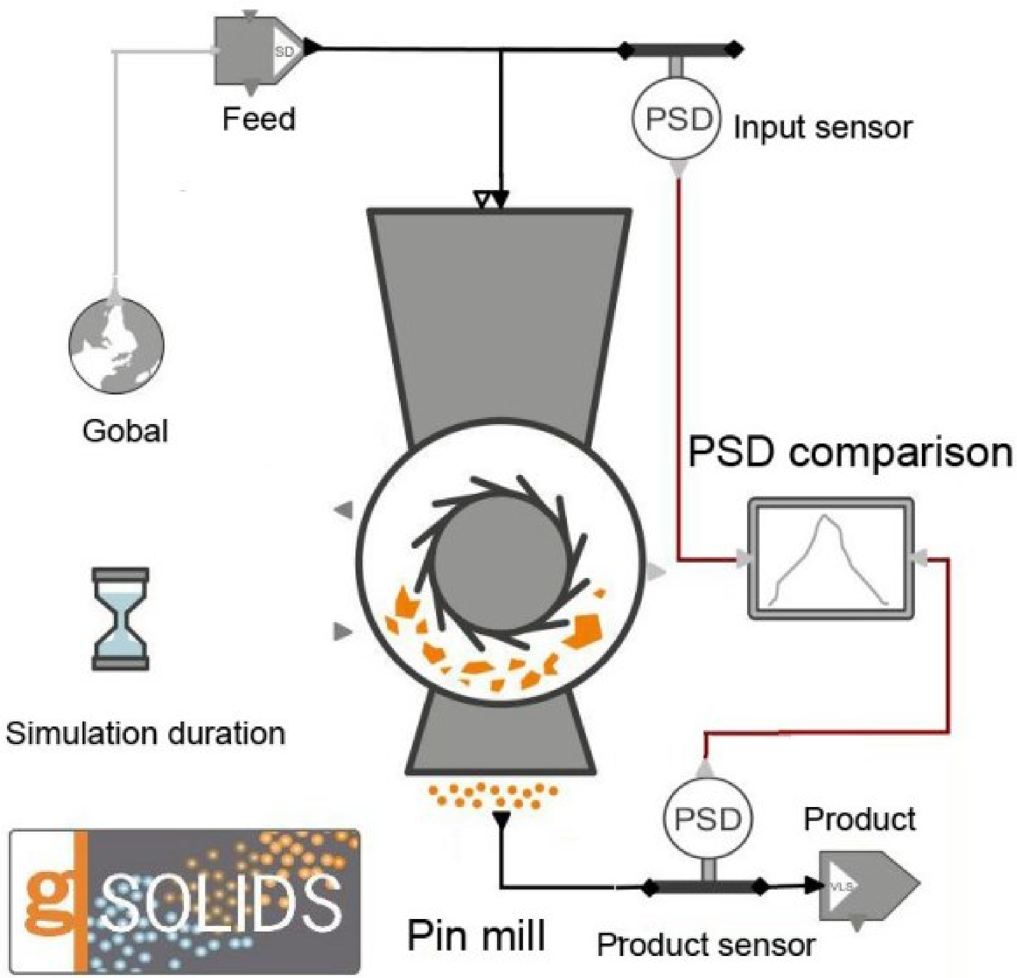
Impact pin mill



High velocity impact UPZ100 mill
by HOSOKAWA MICRON LTD.

Rotatory speeds:
18000 rpm, 12000rpm, 8000 rpm
Feed rates:
24kg/h, 19kg/h, 14kg/h, 9kg/h

gSOLIDS for milling process



Flowsheet simulation of milling process

"With four parameters I can fit an elephant, and with five I can make him wiggle his trunk" -----Attributed to von Neumann by Enrico Fermi

PBM-DEM coupling for milling process

Methodology in gSOLIDS

Population balance model

$$\frac{\partial M_p(x,t)}{\partial t} = -S_M(x)M_p(x,t) + \int_0^x S_M(y)M_p(y,t)b_M(x,y)\,dy$$

Breakage rate Vogel *etal* 2005

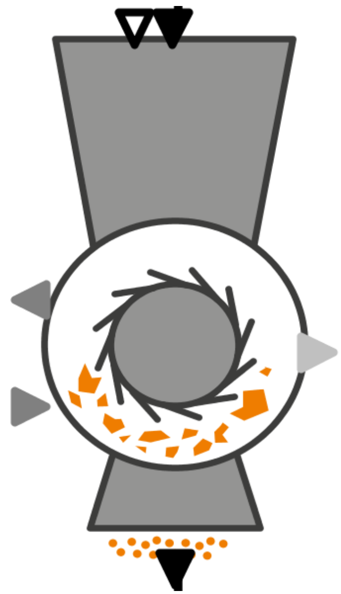
$$S_M(x) = Sc_M\left[1-\exp\left(-f_{mat}x\left(W_{m,kin}-W_{m,\min}\right)\right)\right]$$

Cumulative breakage Distribution

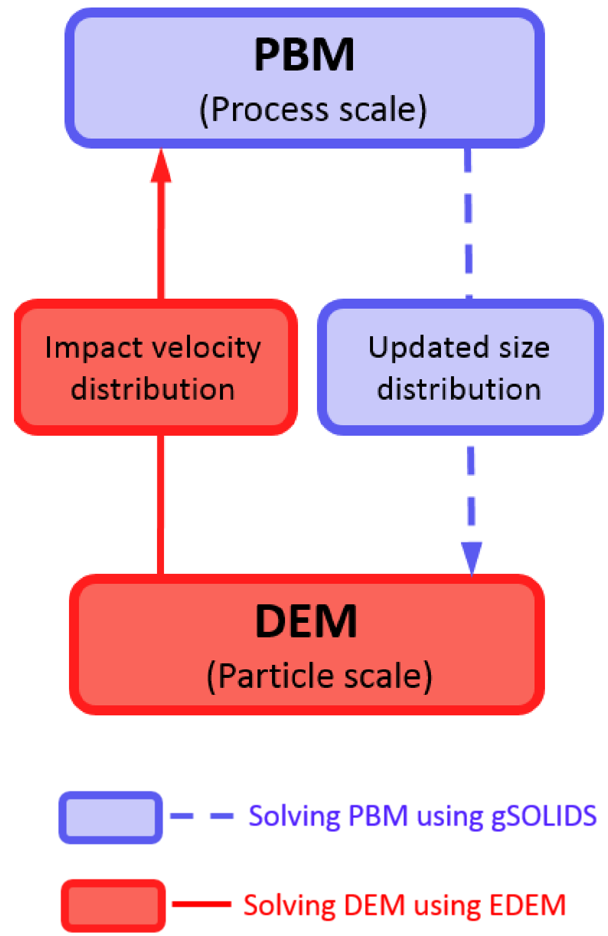
$$B_M(x,y) = \frac{1}{2}\cdot\left(\frac{x}{y}\right)^q\cdot\left(1+\tanh\left(\frac{x-x'}{x'}\right)\right)$$

Blue variables---material dependent
--- from single particle breakage

Red variables---machine dependent
--- from DEM simulation of mill



Multiscale Model



- Calibrate the material dependent properties and use them for different mills

Outline

- Key challenges in milling simulation
- DEM simulations of particle dynamics in a pin mill
- Upscaling strategy using DEM-PBM
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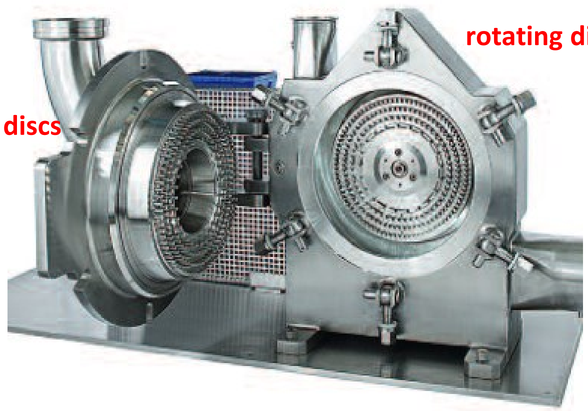
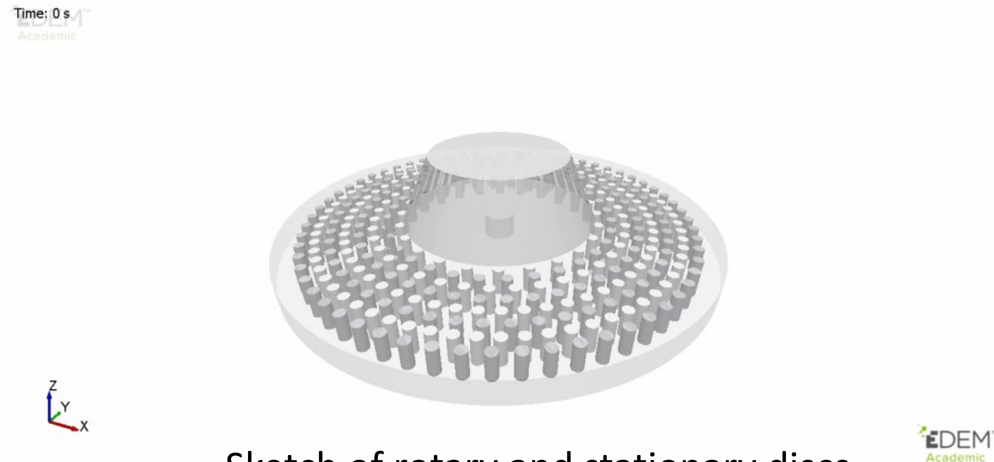
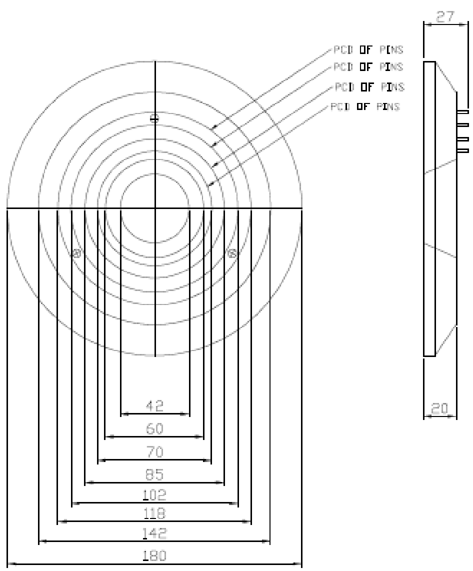
DEM simulation of impact pin milling



Impact pin mill



Sketch of rotary and stationary discs

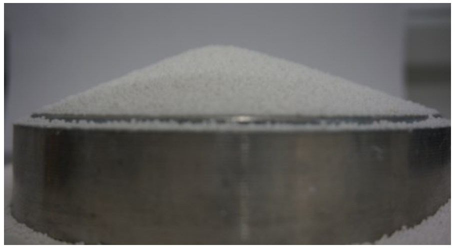


Sketch of impact pin mill

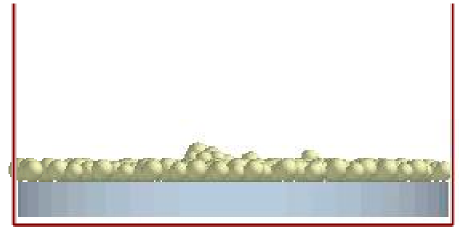
DEM simulation parameters for Alumina particle

Parameters	Value
Particle density (kg/m^3)	3370
Particle diameter (mm)	1.1
Particle Poisson's ratio	0.3
Particle Young's modulus (GPa)	15
Coefficient of restitution	0.82
Coefficient of static friction	0.37
Coefficient of Rolling friction	0.1
Pin density (kg/m^3)	7850
Pin Poisson's ratio	0.25
Pin Young's modulus (GPa)	81

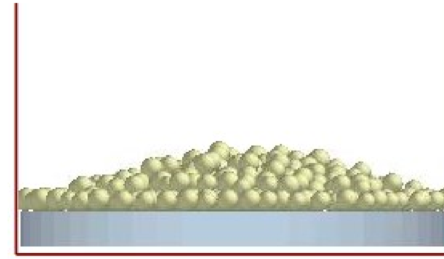
DEM parameters calibration



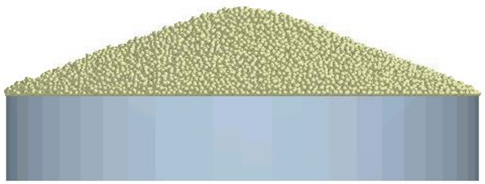
Alumina

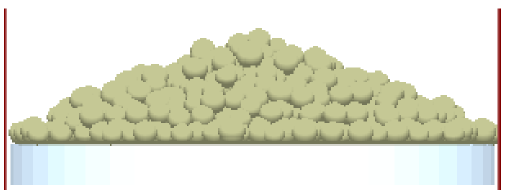


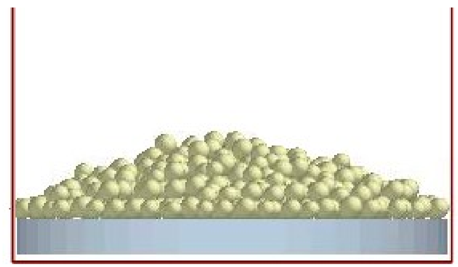
$\mu_{rf} = 0.01$



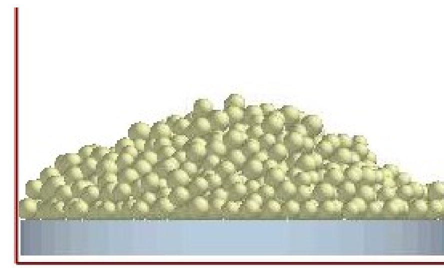
$\mu_{rf} = 0.05$



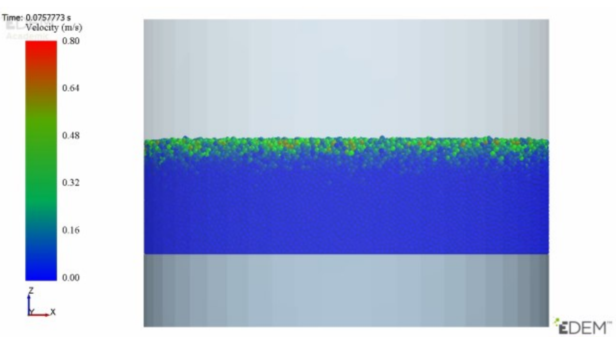


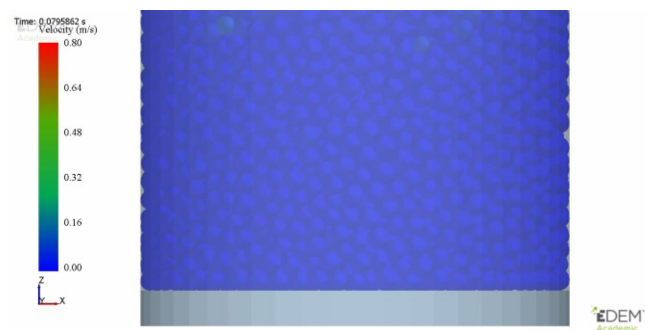


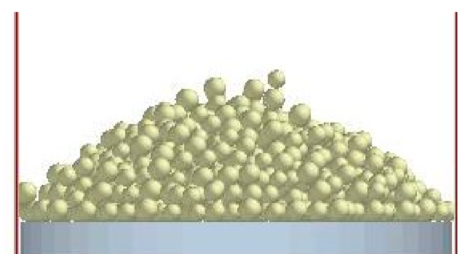
$\mu_{rf} = 0.1$



$\mu_{rf} = 0.2$

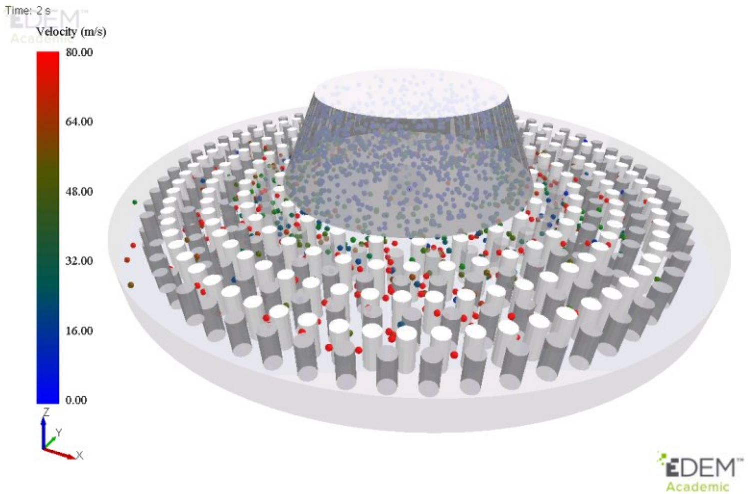




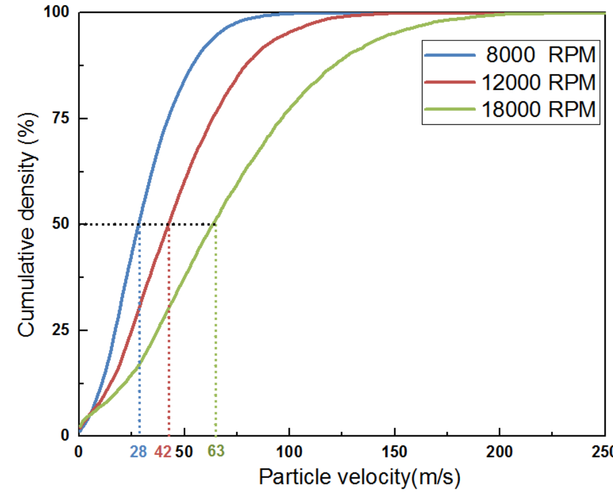


$\mu_{rf} = 0.3$

Velocity and residence time distribution

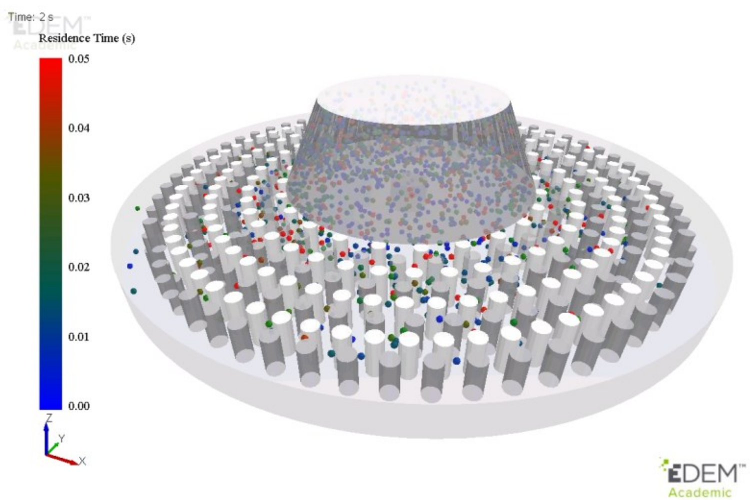


Particle velocity distribution inside the pin mill

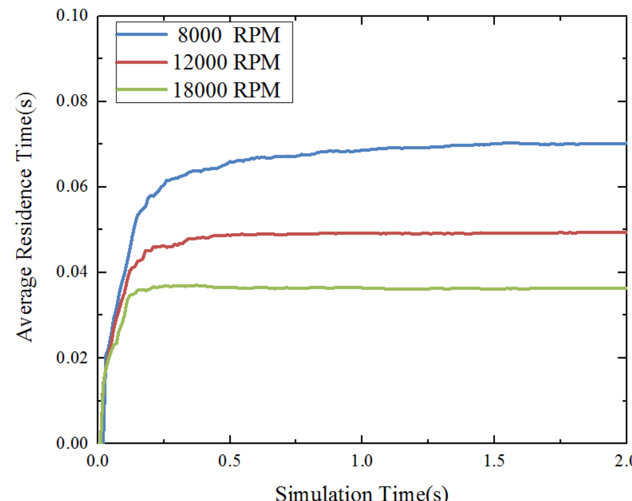


Particle velocity cumulative distribution

➢ Average particle velocity increases with increasing of pin rotating speed



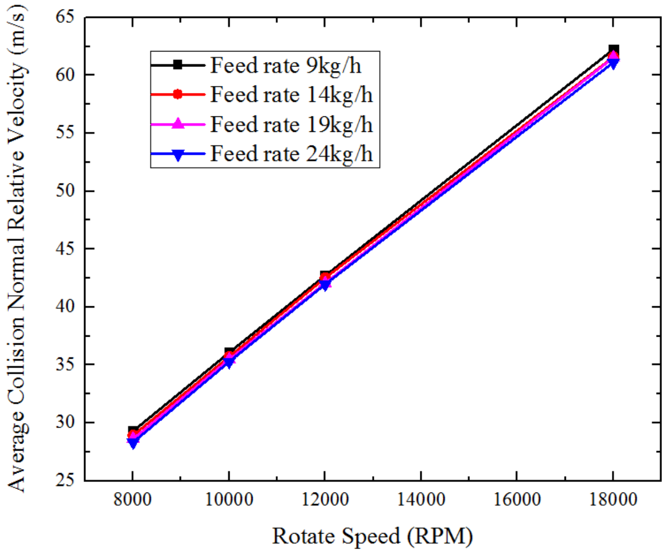
Particle residence time distribution inside the pin mill



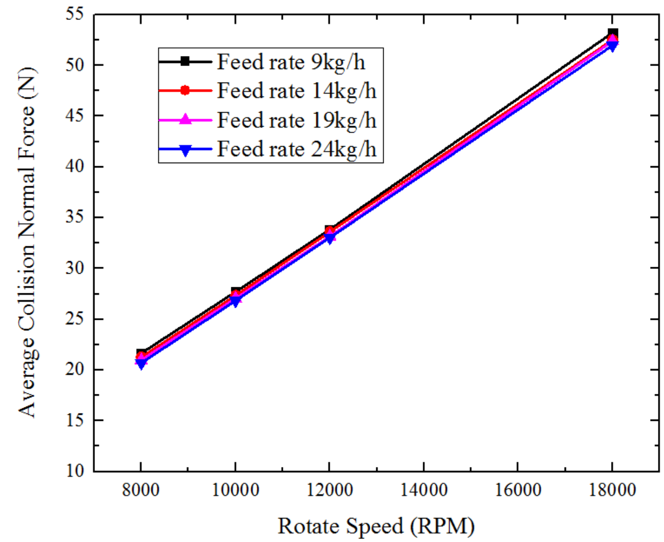
Average particle residence time

➢ Average particle residence time decreases with increasing pin rotating speed

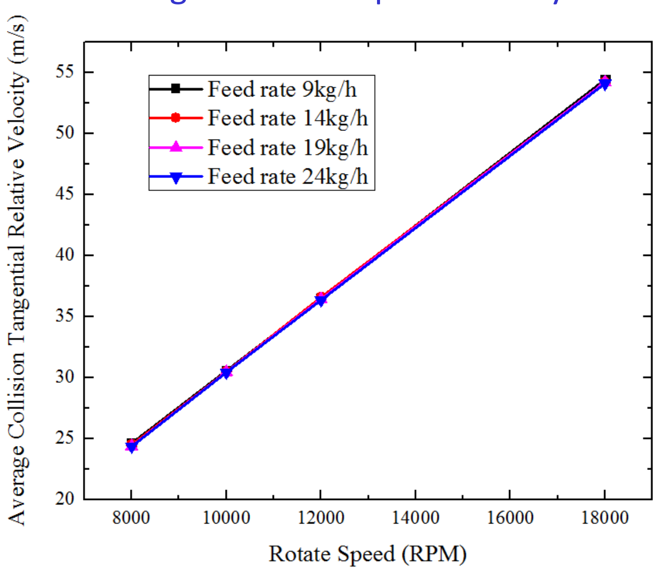
Impact statistics: effect of rpm and feed rate



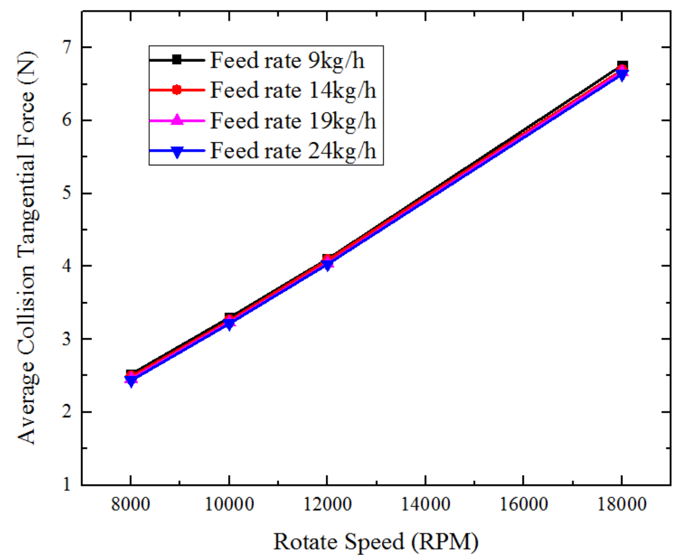
Average Normal impact velocity



Average Normal impact force



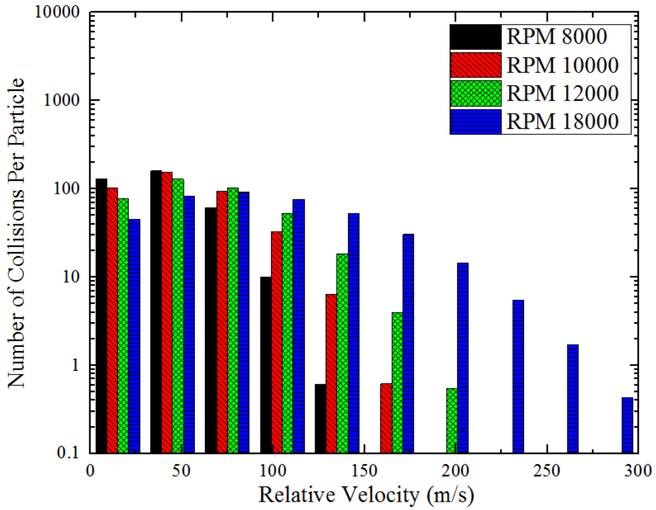
Average Tang. impact velocity



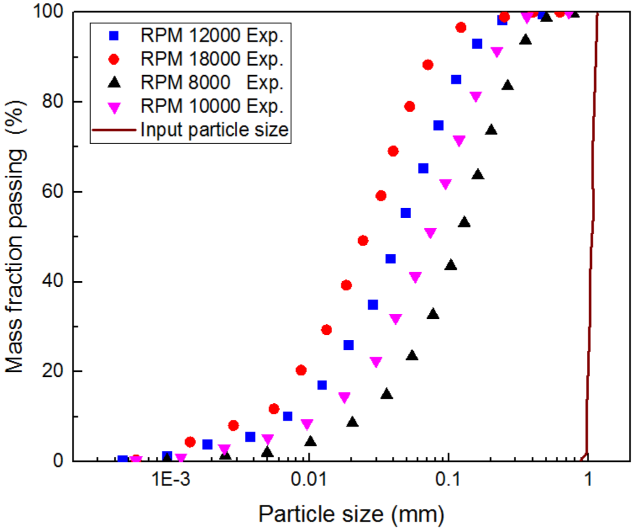
Average Tang. impact force

- Although tangential velocity is large, tangential force can be relatively small – friction mobilisation

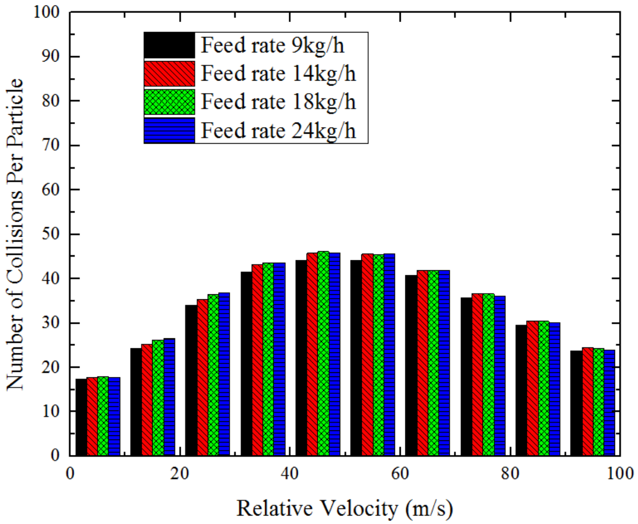
Impact velocity: effect of rpm and feed rate



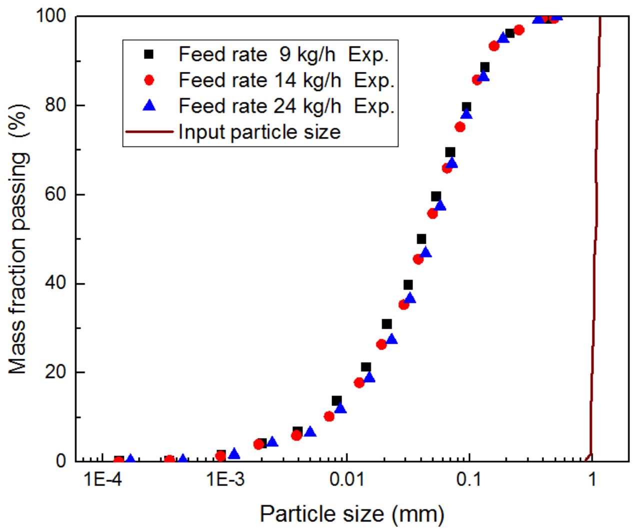
DEM simulation: different rotation speed



Exp. results: different rotation speed



DEM simulation: different feed rates



Exp. results: different feed rate

- ➢ DEM simulation results are qualitatively consistent with experimental observations

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PBM prediction using gSOLIDS

Breakage rate

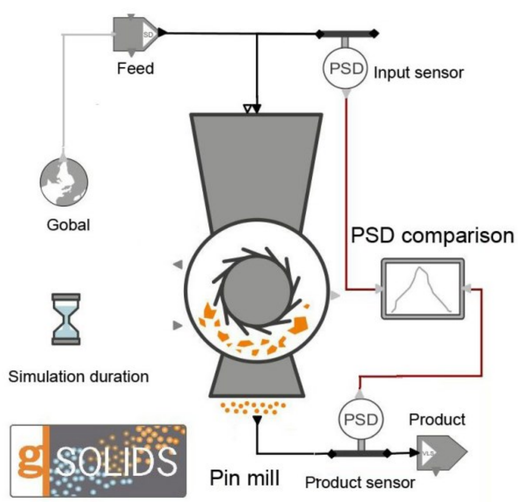
$$S_M(x) = Sc_M\left[1-\exp\left(-f_{mat}\,x\left(W_{m,kin}-W_{m,\min}\right)\right)\right]$$

Cumulative breakage Distribution

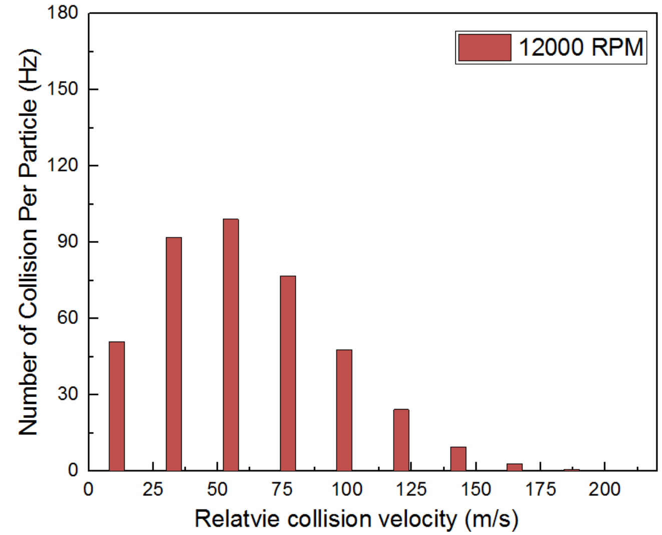
$$B_M(x,y) = \frac{1}{2}\cdot\left(\frac{x}{y}\right)^{q}\cdot\left(1+\tanh\left(\frac{x-x'}{x'}\right)\right)$$

Red variables---machine dependent
--- from DEM simulation of mill

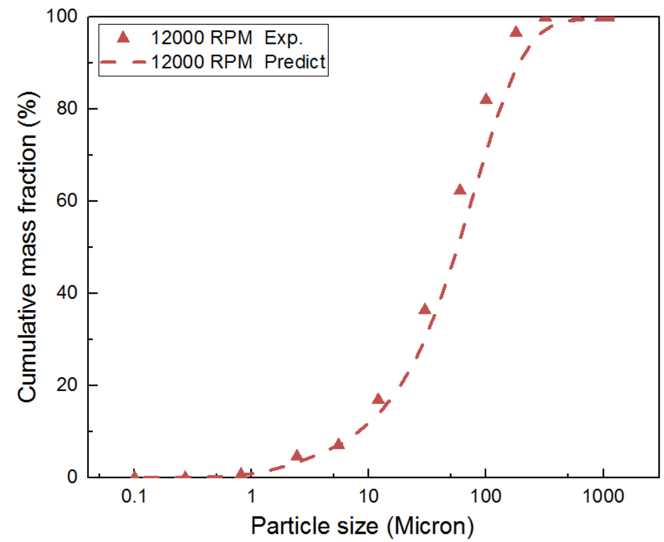
Blue variables---material dependent
--- Estimated from experimental data



Flowsheet simulation of milling process



Impact velocity distribution from DEM



Product particle size distribution predictions

PBM prediction using gSOLIDS

Breakage rate

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Cumulative breakage Distribution

$$B_M(x,y) = \frac{1}{2}\cdot\left(\frac{x}{y}\right)^q\cdot\left(1+\tanh\left(\frac{x-x'}{x'}\right)\right)$$

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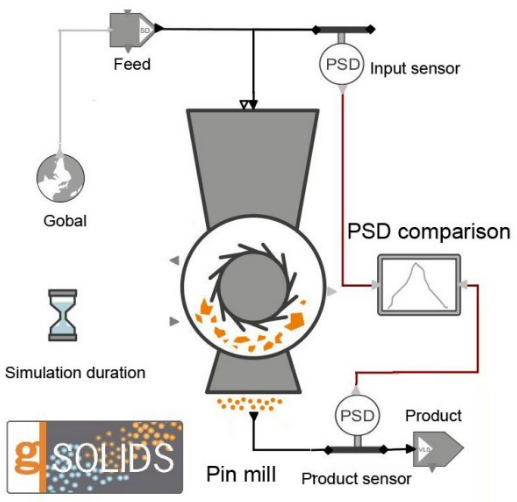
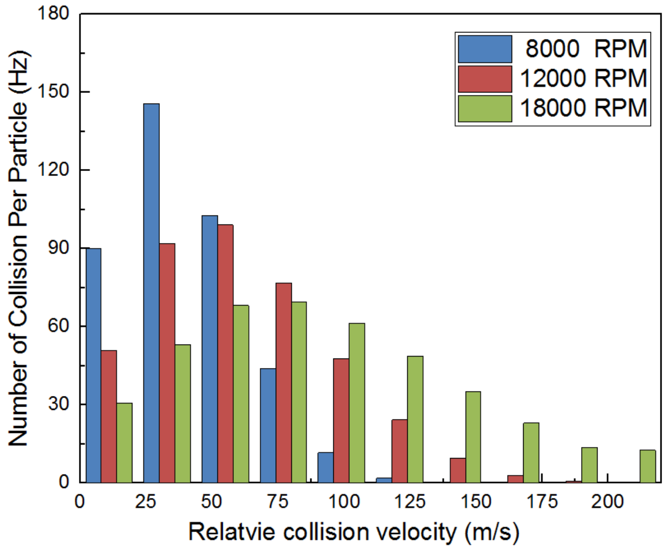
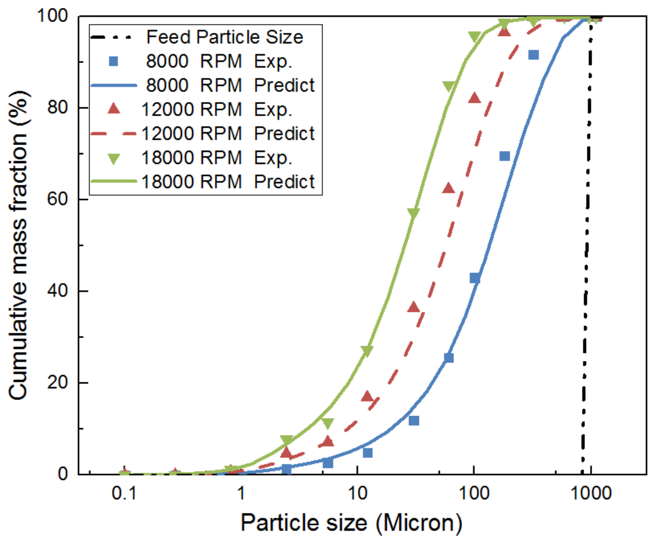


Flowsheet simulation of milling process



Impact velocity distribution from DEM



Product particle size distribution predictions

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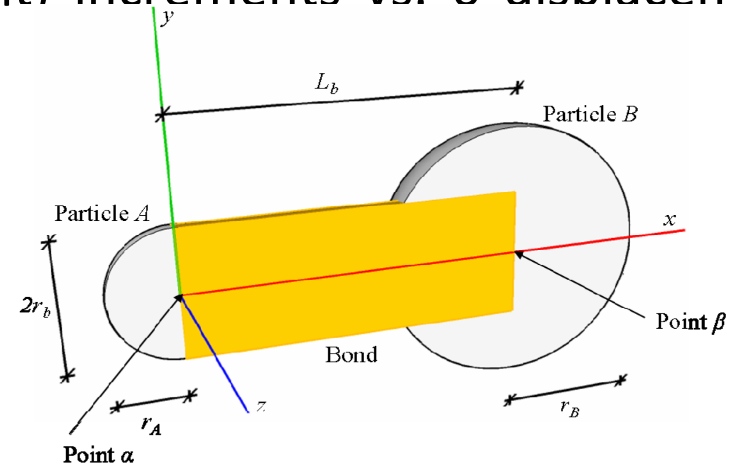
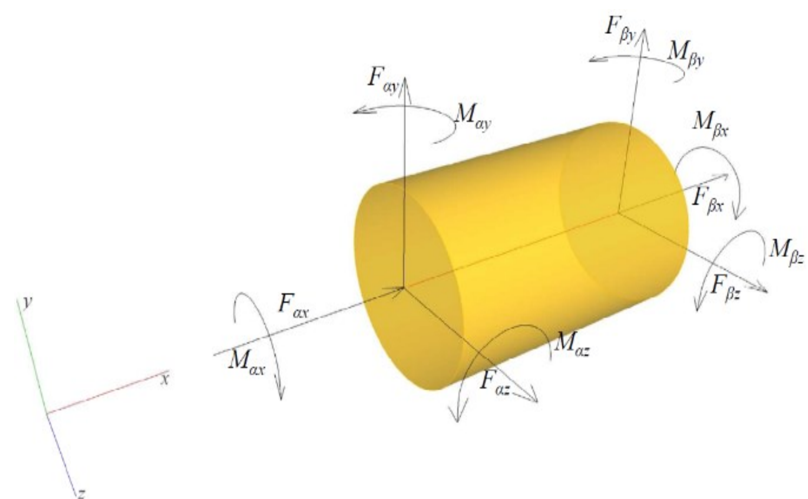
Single particle scale: bonded DEM simulation

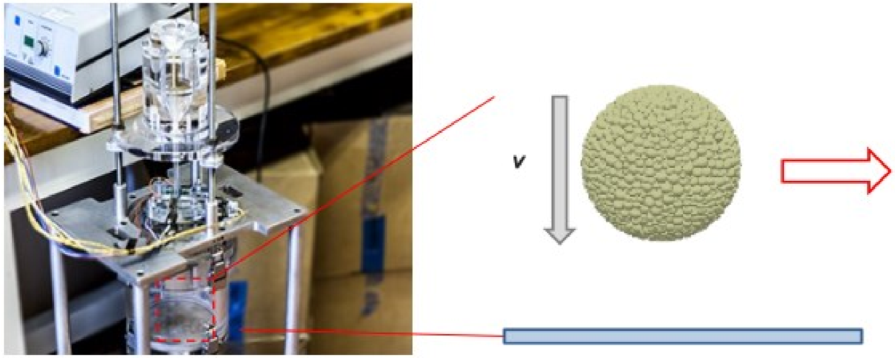
- A bonded particle model based on Timoshenko beam theory has been developed in Edinburgh (Brown et al. 2014)
- The model considers 6 forces (moment) increments vs. 6 displacement (rotation) increments at two bond ends

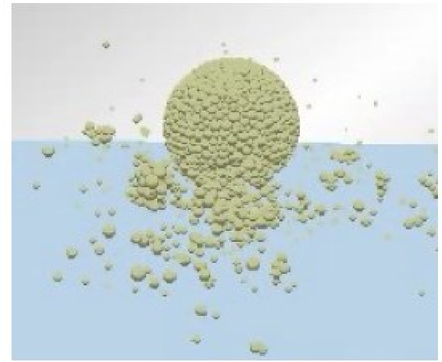
$$\begin{Bmatrix} \Delta F_{\alpha x} \\ \Delta F_{\alpha y} \\ \Delta F_{\alpha z} \\ \Delta M_{\alpha x} \\ \Delta M_{\alpha y} \\ \Delta M_{\alpha z} \\ \Delta F_{\beta x} \\ \Delta F_{\beta y} \\ \Delta F_{\beta z} \\ \Delta M_{\beta x} \\ \Delta M_{\beta y} \\ \Delta M_{\beta z} \end{Bmatrix} = [K] \begin{Bmatrix} \Delta d_{\alpha x} \\ \Delta d_{\alpha y} \\ \Delta d_{\alpha z} \\ \Delta \theta_{\alpha x} \\ \Delta \theta_{\alpha y} \\ \Delta \theta_{\alpha z} \\ \Delta d_{\beta x} \\ \Delta d_{\beta y} \\ \Delta d_{\beta z} \\ \Delta \theta_{\beta x} \\ \Delta \theta_{\beta y} \\ \Delta \theta_{\beta z} \end{Bmatrix}$$





DEM simulation single particle breakage

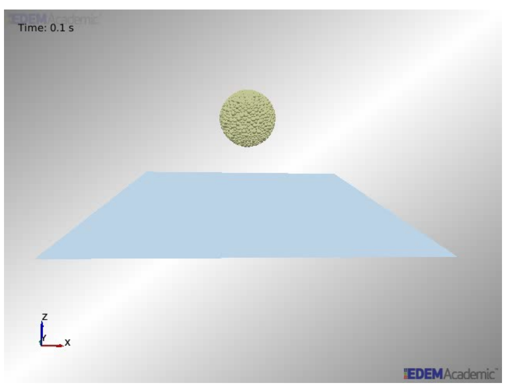




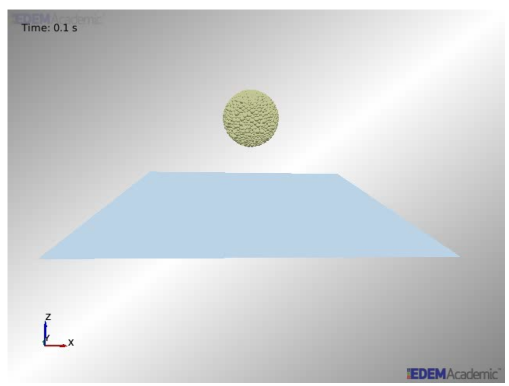
3687 constituent particles for a bonded particle

Single particle impact tester (courtesy from Leeds University)

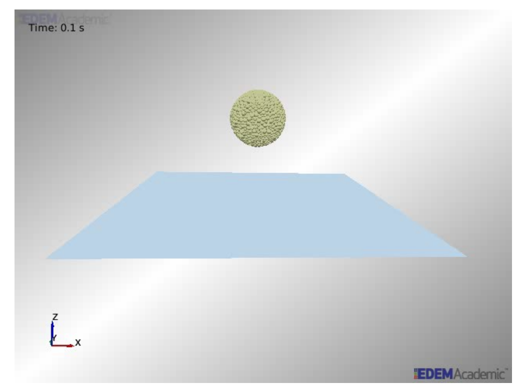
Edinburgh Bonded Particle Model simulation



10 m/s



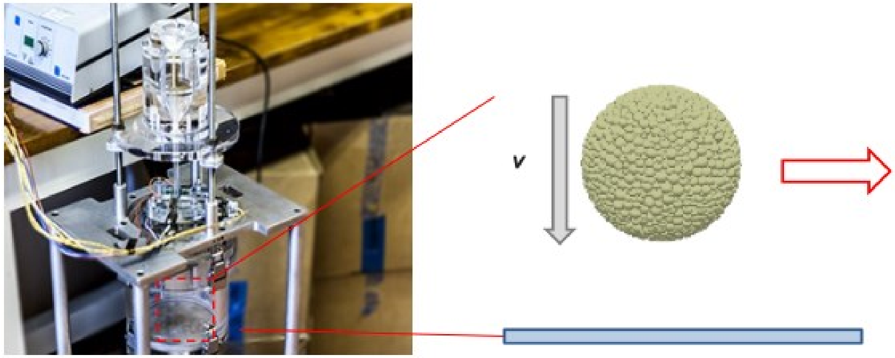
18 m/s



26 m/s

- Breakage pattern is transferred from chipping to fragmentation

Using DEM to get the breakage ratio



Single particle impact tester
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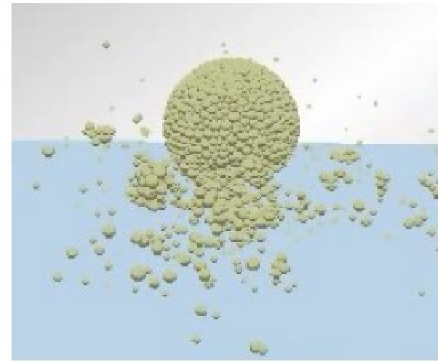
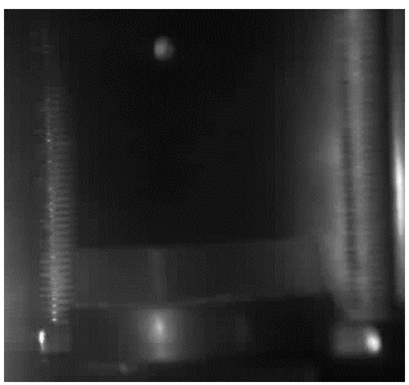
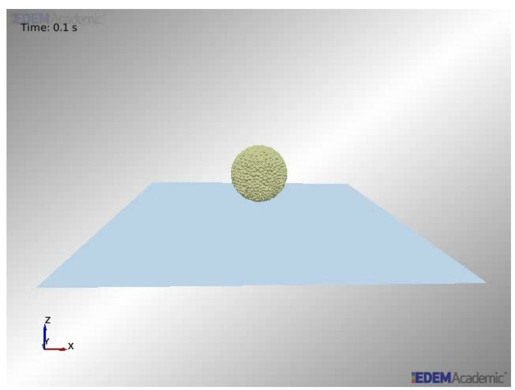


3687 constituent particles for a bonded particle

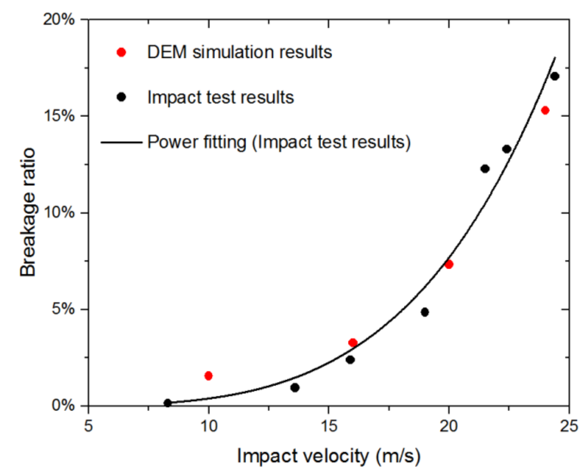
Edinburgh Bonded Particle Model simulation



30 m/s

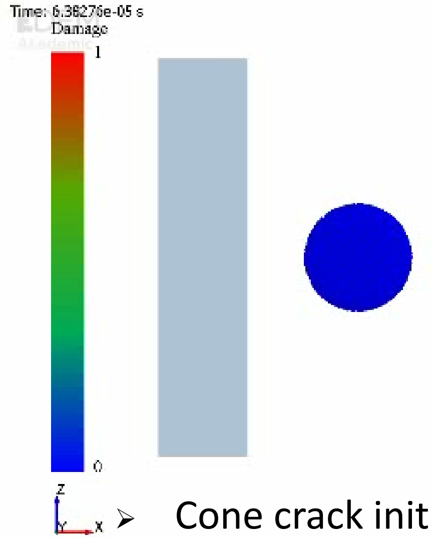


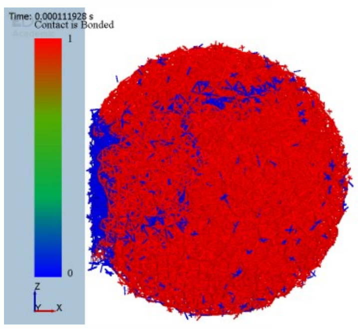
30 m/s

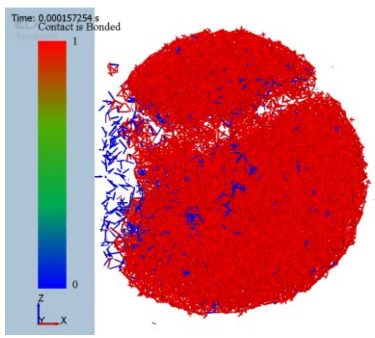


Good qualitative and quantitative agreement with experiment; 2.0 mm zeolite particle

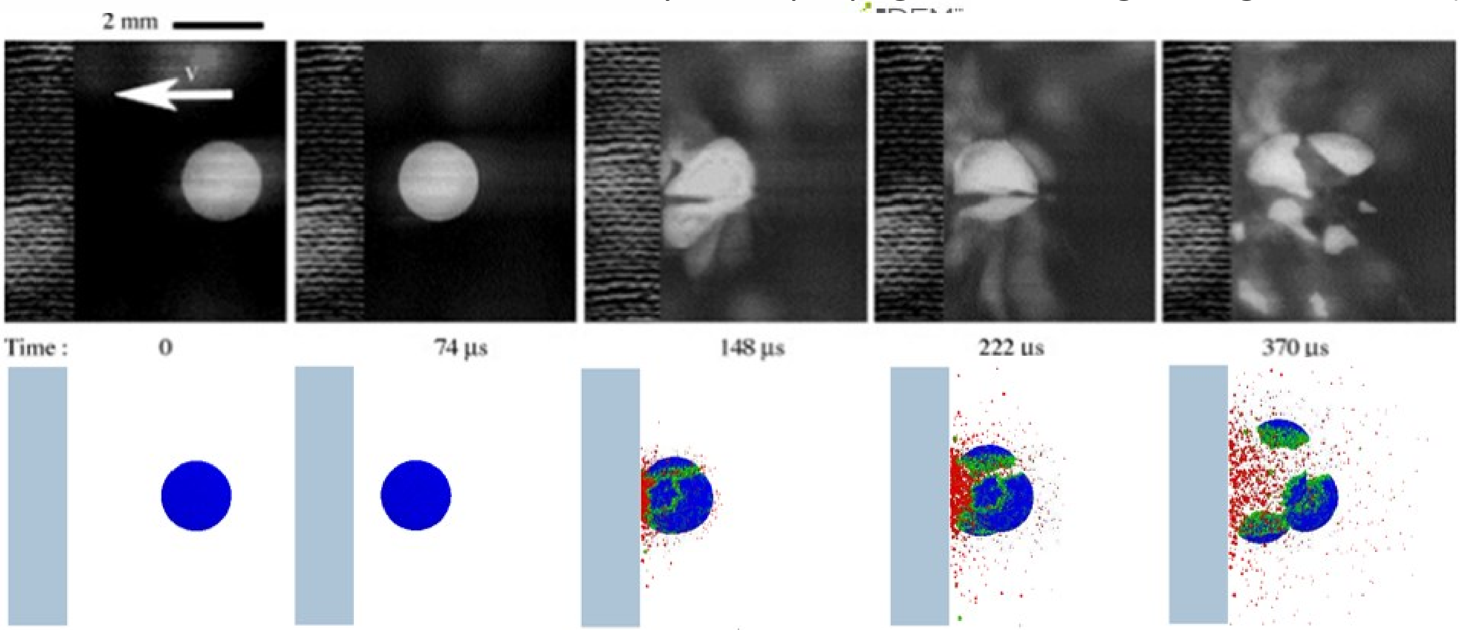
Understanding breakage pattern: Alumina







- Cone crack initiated with secondary crack propagation leading to fragmentation (**23 m/s**)



- Comparisons between the simulation and the experiment of Antonyuk *etal* 2006

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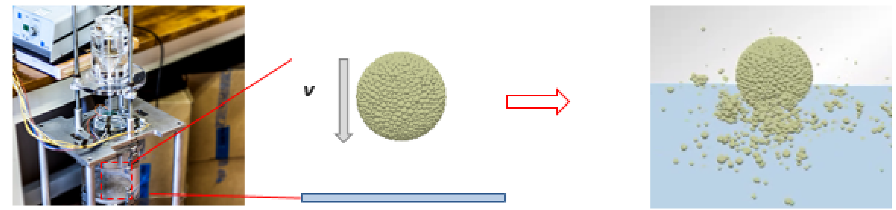
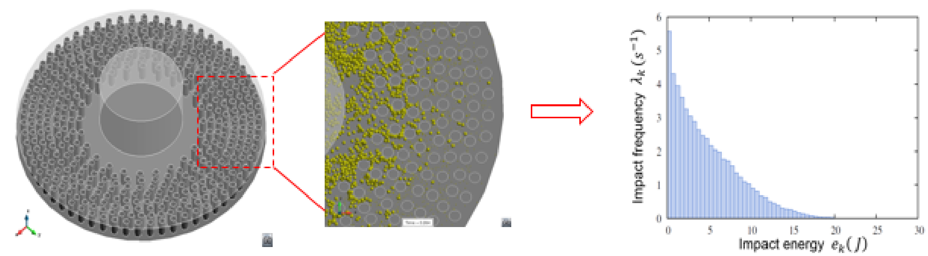
Summary

- Both experiment and DEM simulation were carried out to understand breakage mechanics at single particle scale.
- DEM simulations of particle dynamics in a pin mill with varying operational conditions.
- DEM-PBM coupling upscaling strategy could get a reasonable prediction on the product size distribution.
- Two-way coupling strategy and further improvements are on progress.

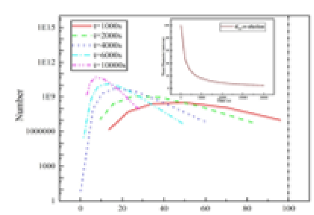


a) Single particle breakage: Use experiment measurement to calibrate DEM
- **Output:** Impact energy e_k with breakage probability P_k and distribution b_{ij}



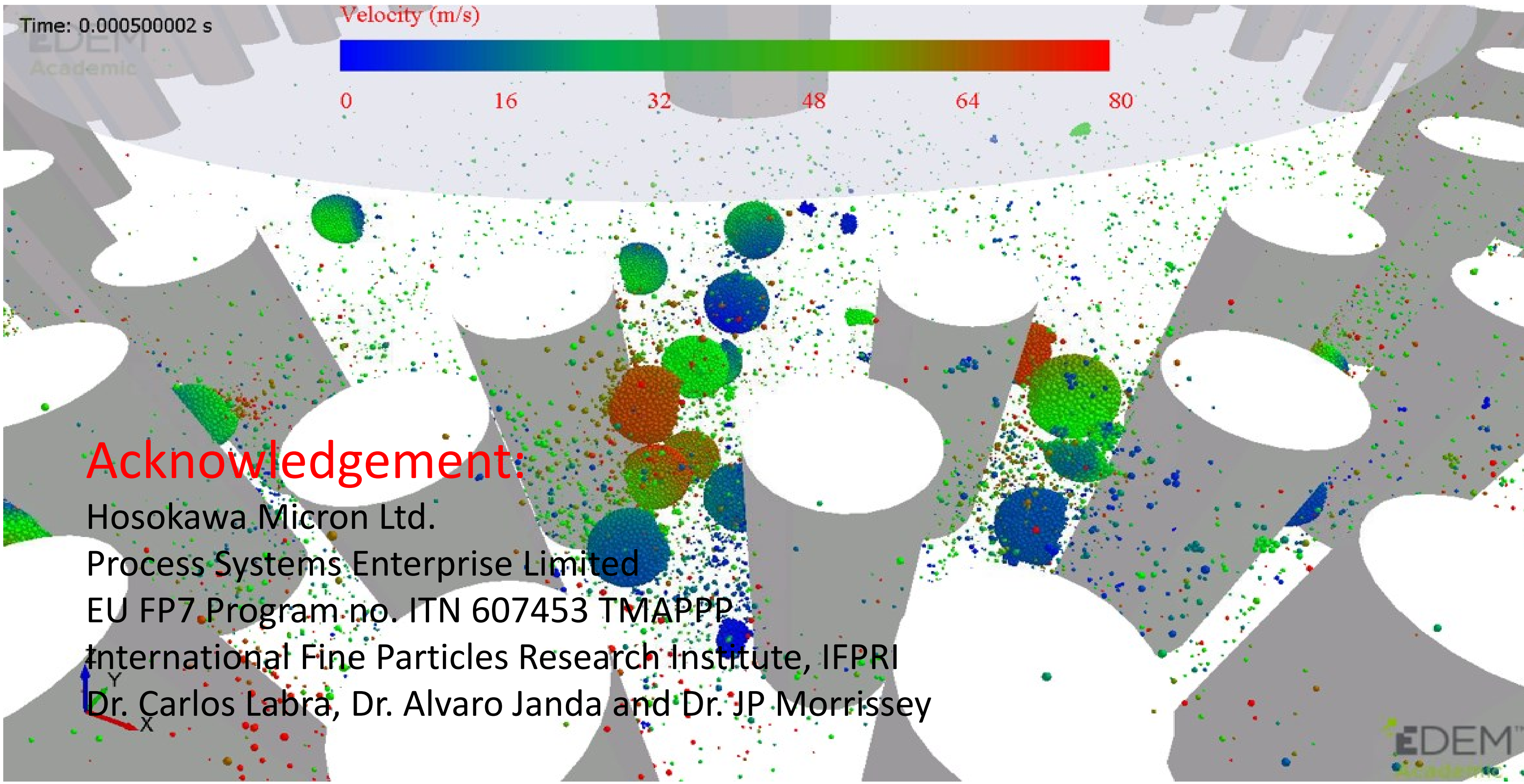
b) Impact mill DEM simulation: Coarse-graining the key parameters
- **Output:** Impact frequency λ_k with energy e_k distribution

$$\frac{dM_i(t)}{dt} = -S_i M_i(t) + \sum_{j=1}^{i-1} S_j b_{ij} M_j(t), \quad S_i = \sum_{k=1}^{N} \lambda_k P_k$$



c) PBM prediction: Integration the outputs of the previous two processes
- **Output:** Time evolution of particles size distribution at system scale

Thank you!



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