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

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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.
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).

\[
ma = \sum F \\
I\alpha = \sum M
\]
Modelling of Bulk Behaviour using Distinct Element Method (DEM)

\[ ma = \sum F \]
\[ I\alpha = \sum M \]

Normal force

Dashpot

Normal stiffness

Tangential stiffness

Slider

\[ F_{nd} \]

\[ K_n \]

\[ F_s \]

\[ F_n \]

\[ F_{td} \]

\[ m_f \]

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

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

Both beads free-flowing

Dense Coarse Beads Cohesive
Surface Energy ($\Gamma$) = 0.5 J/m$^2$
Segregation during Heap formation
• Interpretation of Experimental Results
• Sensitivity Analysis

➢ Understanding the cause of segregation during heap formation
DEM Modelling of Segregation during Heap Formation: effect of cohesion on segregation

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

Colours represent average size of particles in each bin

All particles are cohesive

Fine particles are cohesive

All particles are free flowing
Seeded granules occur in Cyclomix high shear mixer under certain operating conditions.
DEM Simulation of Granulation in Cyclomix
Seeded granules are quickly formed in the high shear region (middle part) and break as soon as they approach the top part.
Modelling the agglomerate and compact breakage
DEM of Mixing of Particulate Solids: Minimising Trial and Errors; Insufficient Available Materials; Parameters Difficult to Measure

Particle motion analysis in a paddle mixer
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.
Quantitative Comparison of Powder Flow between DEM and PEPT

- **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)

Average normalised velocity from PEPT: 0.43
Average normalised velocity from DEM: 0.41
DEM Modelling of Cyclomix High Shear Mixer Granulators: Scale-up

Scale-up \[ \frac{\omega_2}{\omega_1} = (\frac{d_1}{d_2})^n \]
n = 1 \quad \text{Tip speed constant}
n = 0.5 \quad \text{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
The coefficient of variation of shear stress decreases as the impeller tip speed is increased.
Modelling of Particle Milling:

1. Minimising Trial and Errors
2. Insufficient Available Materials

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

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

Milling Rate Constant, $K_p$ (s$^{-1}$)

- MCC-18 Hz
- MCC-25 Hz
- αLM-25 Hz
- Starch-25 Hz
- Sucrose-12 Hz
- Sucrose+Aerosil-25 Hz

$K_p = 0.1218 P_n \alpha H / K_c^2$

$R^2 = 0.9826$

Milling Power

$P_n \alpha H / K_c^2$ (m$^2$ s$^{-1}$)

Material property group
Solid-fluid flow modelling

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

Dispersion

Fluidization

Sedimentation/re-suspension
Solid-fluid Flow Modelling: DEM-CFD coupling

Pneumatic conveying, powder dispersion and fluid diffusion

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

- $0.2 \text{ J/m}^2$
- $0.6 \text{ J/m}^2$
- $1.0 \text{ J/m}^2$

$t = 1 \times 10^{-4} \text{s}$
$t = 2 \times 10^{-4} \text{s}$
$t = 3 \times 10^{-4} \text{s}$
$t = 4 \times 10^{-4} \text{s}$

Solid-fluid Flow Modelling: agglomerate dispersion
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.
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)

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