

Round-Robin Exercise on Calibration of DEM Simulations

Introduction

During the IFPRI's roundtable discussion on "Discrete Element Method (DEM)" (Chemical Heritage Foundation, Philadelphia – USA, June 17th 2017), there was broad consensus that DEM techniques have proven successful for a number of industrial applications. However, the success stories for calibration and validation of DEM simulations were limited to the "granular" (>250 μ m) regime, and parameter estimation/calibration methods differed significantly. Hence, it proved difficult to encapsulate exactly why DEM was successful given known gaps in the physical models and methods for setting model parameters. Moreover, it became clear that the inconsistency in methods used amongst industrialists and academics for calibrating DEM simulations against powder characterization tests is a major impediment to progress in the field. In the present "round-robin" exercise, an attempt will be made to examine various DEM parameter estimation/calibration methods that industrialists and academics have adopted with the intention of establishing best-practices and identifying practical gaps and impediments for successful application of DEM at industrial scale. In particular, several issues were identified:

- The calibration approaches are often not shared (amongst industrialists).
- Failures are typically not documented in the literature
- Calibration tends to be system-dependent

Format

It is proposed that Professor Jonathan Seville, assisted by Dr Andy Ingram, of the School of Chemical Engineering at the University of Birmingham, UK, will act as "Project Coordinator", responsible for managing the project, collecting data from the participants, compiling progress reports, and conducting 'reference validation experiments' using Positron Emission Particle Tracking. Figure 1 shows schematically the project map for this exercise:

1. Define the reference materials and experiments
2. Provide reference materials to the Participants
3. Provide the Participants with "generic" information on the reference experiments
4. Participants conduct their own characterization, model selection, and parameter estimation/calibration
5. Coordinator gathers description and outcome of the calibration methods used by individual participants → provide a summary report
6. Coordinator shares the details of the experimental design with the Participants
7. Participants conduct simulations of the reference systems
8. Coordinator runs the validation experiments (in parallel with step 7 above)
9. Coordinator gathers and compares the outcomes of the modeling and experimental efforts

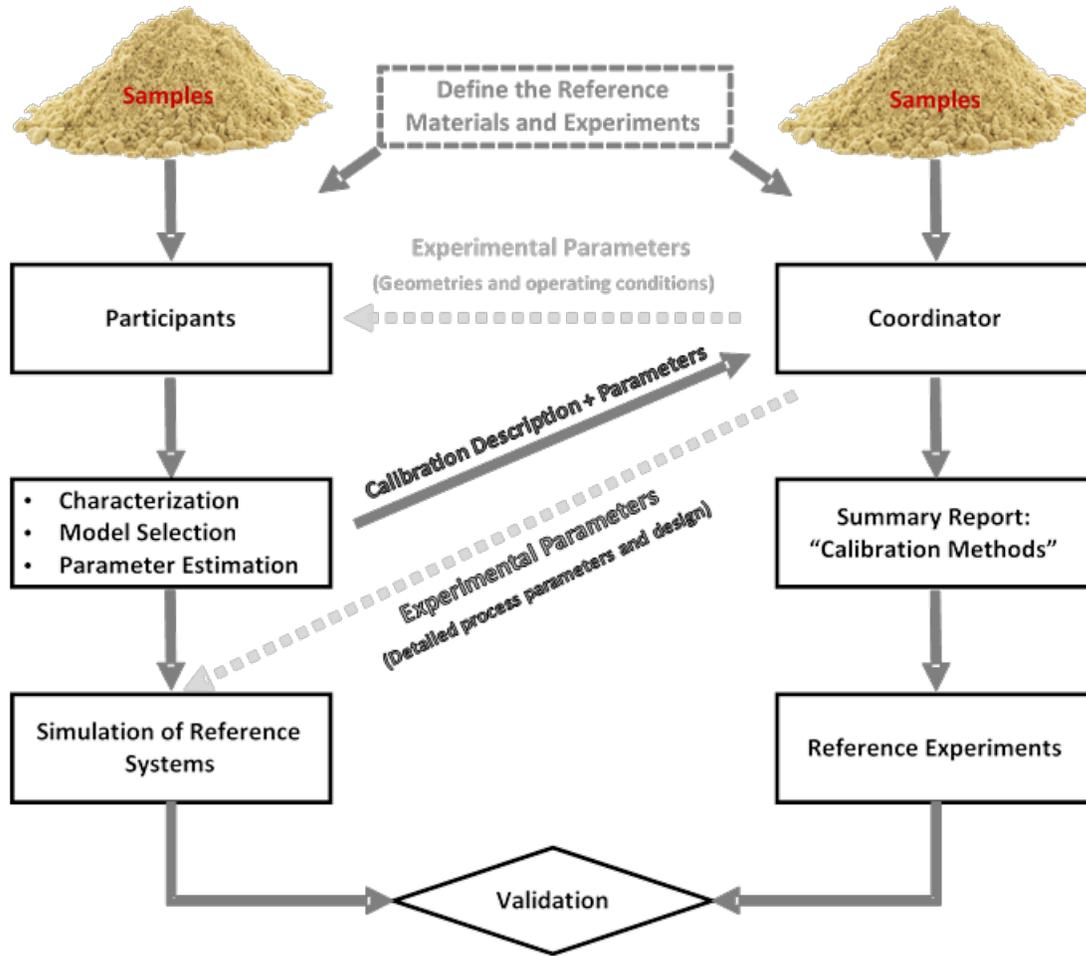


Fig. 1: Project map

Material and Process Selection

We propose to use two test materials for the study: alumina (>300 μm with narrow size distribution) and limestone (<100μm). For processes, we propose the following:

1. A rotating drum, of diameter 240mm and without internals, in both batch (horizontal) and continuous (inclined) mode

This geometry has been extensively studied by the Birmingham team using PEPT (Figure 2), revealing detailed tracer motion in the axial direction and the transverse plane and the existence of, and exchange between, the dense contact-dominated “passive” zone, moving in solid body rotation, and the less-dense higher-speed surface region. From the point of view of this DEM validation study, the rotating drum is therefore a good test because of the co-existence of the two regions in one experiment.

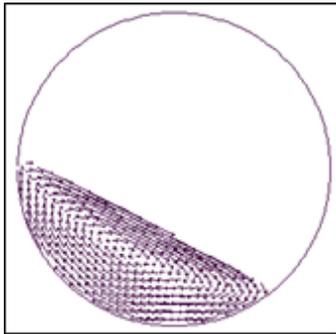


Fig. 2(a): Motion in transverse layer, showing average velocity arrows (binary mixture of 20% 1.5mm and 80% 3.0mm glass beads in a 240 mm drum at 9.6 rpm; 3.0mm)

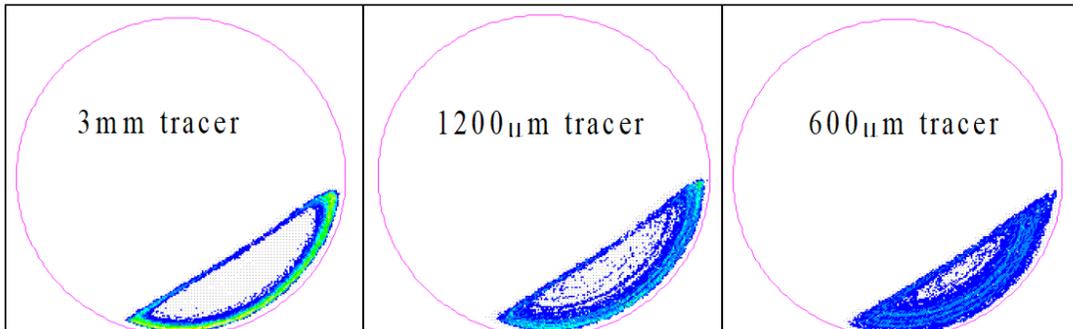


Fig.2(b): Transaxial PEPT occupancy plots (fraction of run time spent at each location) for three different sizes of tracer particle in a bed containing a wide range of particle sizes, showing segregation.

A further useful aspect of rotating drums in this study is that change of speed of rotation takes the solids motion through a wide range of behaviour (Figure 3) from low-speed slipping/slumping to high-speed cascading/cateracting.

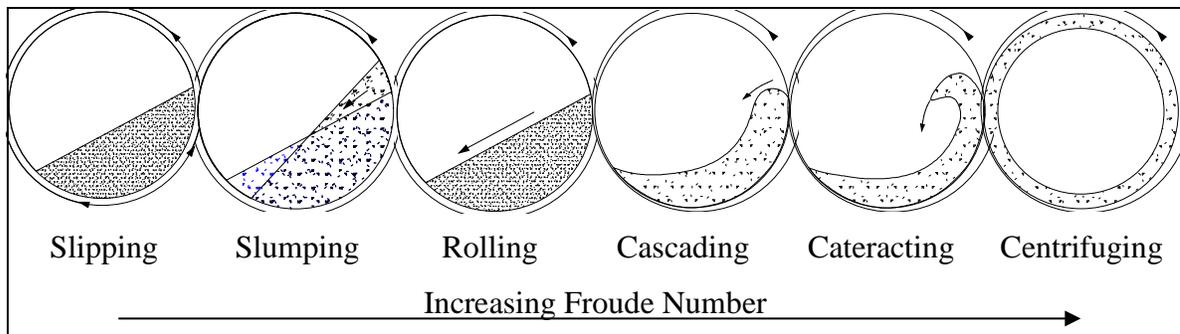


Fig. 3: Changes in rotating drum motion with Froude number (Ingram *et al.*, 2005)

There are numerous opportunities for numerical comparison between DEM simulations and PEPT, including:

- The shape of the active/passive interface
- The exchange rate between the two layers
- The transaxial and axial velocity profiles
- The rotation speed at which the slumping/rolling transition occurs
- (in continuous mode) the residence time distribution
- (in continuous mode) the axial profile of the bed depth

Some of these are also amenable to theoretical derivation, as in Ding *et al.* (2001, 2002) and Ingram *et al.* (2005).

For a fixed drum geometry and particulate material, process variables include rotation speed and fill level and in continuous mode, angle of inclination, exit geometry and feed rate. We would recommend varying only speed and in continuous mode, feed rate, since these are the most interesting variables.

2. A high-shear mixer (true cylinder of diameter 0.16m, vertical shaft), with a selection of blades, from discs and blunt-faced to sharp edged, so able to cover the range from friction-dominated to inertia-dominated blade interactions.

This is a purpose-built device, with torque measurement, and the blades are relatively simple in geometry, as shown for example in Figure 3. Change in speed again takes the motion through low-speed friction-dominated behaviour to high-speed toroidal flow (Figure 4), and different blade shapes give interestingly different torque-speed relationships (Figure 5).

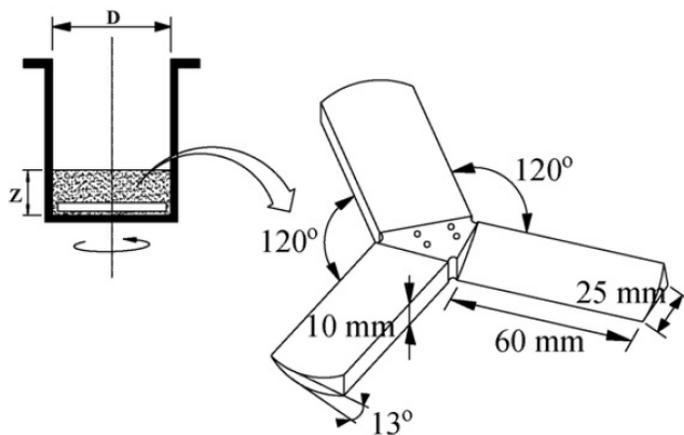


Fig. 4: High shear mixer with example blade (Tu *et al.*, 2009)

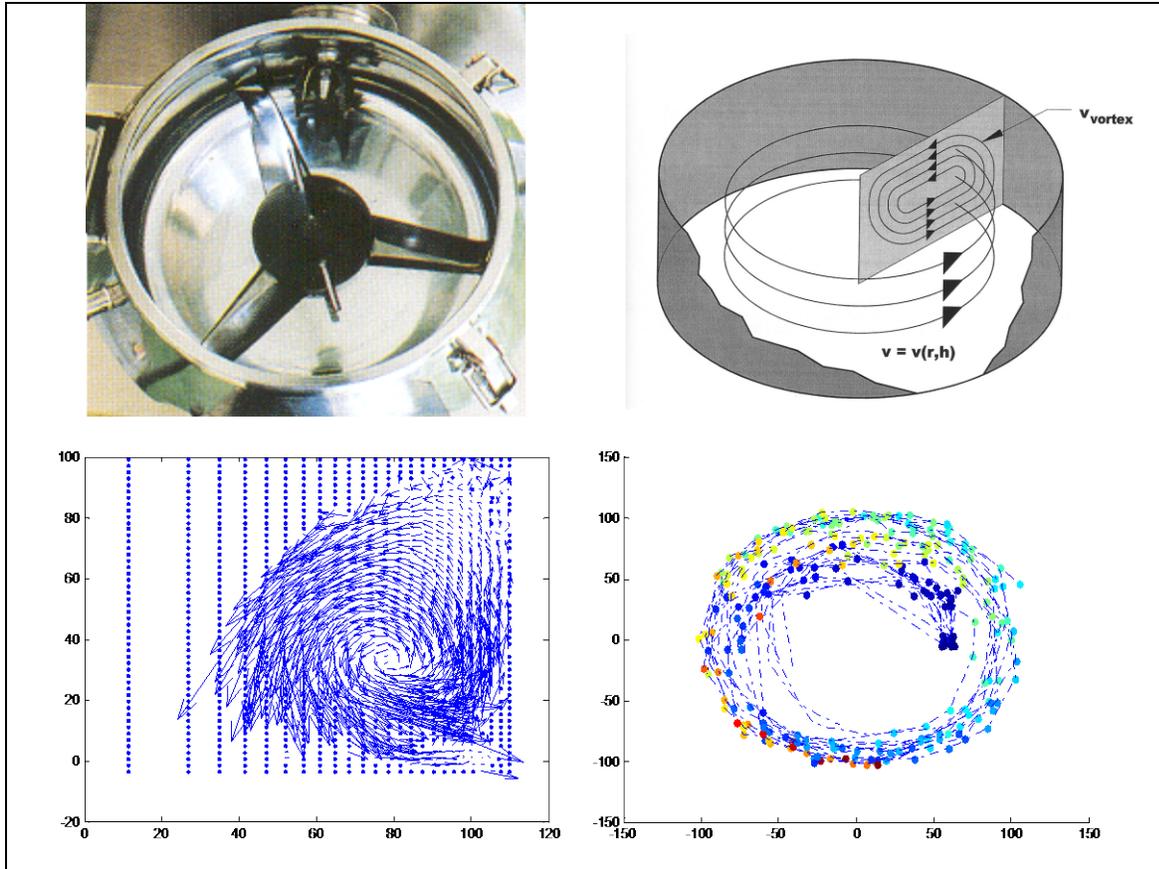


Fig. 5: Examples of PEPT measurements in a high-shear mixer: mixer top view (top left); measurement geometry (top right); time-averaged and azimuthally-averaged velocity profile (bottom left; bed axis passes through origin); and single particle trajectories, showing dispersion from same starting point.

Given a mixer geometry and particulate material, the operating parameters are again rotation speed and fill level, in addition to blade shape. It is suggested to keep fill level constant and vary speed. Outputs for comparison between DEM and PEPT would again include bed shape, averaged and instantaneous velocities and measures of dispersion and/or mixing derived from trajectories such as those shown in Figure 5. A useful non-PEPT output is torque, as shown in Figure 6.

Funding

The managerial and administrative efforts of the academic coordinator are estimated to be equivalent to those for conducting an IFPRI Review (i.e. ~\$8.5k). The efforts on setting up the experimental setup and conducting the experiments was estimated to be ~80% of one year of a typical IFPRI Project (i.e. ~\$30.5k).

| Coordination & Management Activities | |
|--|--------------|
| Managing the program (data collection, email communications, follow-ups) | \$8.5k |
| Writing summary of "calibration methods and results" | |
| Writing summary of "validation and experimental results" | |
| Writing the final report | |
| The efforts equivalent to an IFPRI Review (i.e. \$8.5k) | |
| Validation Experiments | |
| Distribution of samples | \$30.5k |
| Experimental Setup | |
| Conducting experiments | |
| Comparing participants results | |
| The efforts equivalent to 80% of one year of an IFPRI Project | |
| TOTAL | \$39k |

References:

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