

Parametric evaluation for powder flowability using a Freeman rheometer: a discrete element method study

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ABSTRACT

Discrete element method (DEM) based on the description of the microscopic contacts between a number of discrete particles is widely used to predict bulk powder behaviour from single particles. However, input particle parameter calibration is still a challenging concern for a precise DEM modelling [1]. In previous work it has been demonstrated that a statistical methodology can be used to understand the impact of DEM input parameters where the link between these parameters and output responses were considered at 3 levels, i.e., empirical, semi-empirical and mechanistic [2]. In the present study, we apply a similar statistical methodology by simulating a Freeman FT4 powder flow tester (Freeman Tech., Malvern, UK).

In a Freeman FT4 tester the flowability of a powder is reflected by the force and torque necessary to drive the impeller upwards and downwards during standard test cycles [3]. The objective of the current work is: (1) to understand the influence of input single particle properties on bulk powder responses; and (2) to explore the possibility of using the FT4 for DEM model calibration purposes.

In this work, the flow energy tests with FT4 were modelled using LIGGGHTS Open source DEM code [4]. A Hertz-Mindlin model was employed to model inter-particle contacts, and the Johnson-Kendall-Roberts model was incorporated to account for the particle cohesion. A parametric study on the impact of the input particle properties (namely: Young's modulus E , restitution coefficient ε , cohesion energy density k and inter-particle static/rolling friction coefficients μ_s/μ_r) on the flowability of monosized spherical particles ($d = 2$ mm) was carried out first using a Design of Experiments (DoE) approach. In this approach a full, half and quarter factorial DoE was used, to ascertain the extent of simulations that need be carried out to gain a good understanding of key system parameters. These designs contained 35, 18 and 10 simulations respectively, and the merits of each are evaluated in this paper.

It is shown that both force and torque responses are highly sensitive to variation in inter-particle static friction coefficient, and to a lesser extent, rolling friction coefficient. The restitution coefficient is insignificant. When the Young's modulus is at a high value the cohesion energy density is insignificant; when it has a lower value the cohesion energy density can have a very significant effect, showing an interaction between the two parameters.

Effect of particle size and shape of the particles is being investigated while holding other input particle properties constant. Irregular shaped particles are represented using a multisphere (clump) approach which is implemented in LIGGGHTS.

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