Effect of coarse-graining on simulated powder flow properties

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Abstract— Among experimental devices, the Anton Paar Powder Rheometer is a tool for evaluating the bulk flow behavior of powder in dynamic conditions. This device measures the required torque for the rotation of the impeller inside the powder bed. The obtained experimental data can help to calibrate discrete element method (DEM) parameters. In order to speed up, larger, coarse-graining particles with proper scaling rules have to be applied. Some up-scaled simulations could produce a qualitatively similar trend to the experiment in one-tenth of the computing time. However, the applied coarse-graining scaling rules could not generate quantitatively the same results. In other words, the torque is not conserved by up-scaling stiffness alone, which to understand is ongoing work.

Keywords: DEM; Anton Paar Powder Rheometer; coarse-graining, bulk flow property;

1. Introduction

Powders are widely used in many industrial applications, such as pharmaceutical, chemical, food, cosmetic, and metallurgical. They are used in mixing, granulation, and reaction [1]. They consist of many small particles which interact with each other, and also with the surroundings. They behave differently under different conditions; moreover, they are considerably away from simple solids or fluids [2, 3].

The discrete element method (DEM) is a powerful tool for simulating granular materials. DEM can track each particle (microscale) and can predict the bulk property of a system (macroscale). Due to the high accuracy of DEM simulations, it uses lots of resources [4] to track each particle, and from a numerical experiment to identify the bulk properties of solids. As one way to overcome this bottleneck, the coarse grain method is introduced [5].

The coarse-grain discrete element method (CG-DEM) is a method to speed up DEM simulation. It utilizes an up-scaled collection of particles, as compared to the real, primary particles. Sakai and Koshizuka showed that a particular scaling rule for contact and drag force should be considered when the up-scaled particles are used [5]. Several studies confirmed that the DEM parameters should be changed when particle size is changed [1, 6, 7].

A precisely tuned set of input DEM parameters is required to simulate a practical condition for a given material. In order to have precise inputs, simulations need to be calibrated with experiments [8]. In this study, we use the Anton Paar Powder rheometer, and afterward, coarse-graining scaling rules are applied in the simulations.

2. Experimental procedure

2.1. Anton Paar Powder Rheometer

The Anton Paar Powder Rheometer is a device that operates in dynamic conditions. It consists of a concave grooved impeller and a cylindrical container. It measures the torque required for the rotation of the impeller within a bed of powder. In fact, the torque is the result of shear stress applied by the rotation of the impeller to the powder. In this study, the rotation speed of the impeller was set to 600 rpm. Fig 2 shows the whole experimental setup.

Figure 1. Anton Paar Powder Rheometer setup [9].

2.2. Powder properties

High density polyethylene (HDPE) has been used as powder in the rheometer cell. This free-flowing powder has a 214.6 μm median size. Before the experiment, the powder sample was dried in an oven. Subsequently, 43.6 g of the dried powder was poured into the cell.

3. DEM simulation

DEM is a tool that consists of a large number of discrete elements (particles). These particles can have arbitrary shapes. In DEM, each solid particle interacts with the surrounding medium (particle-particle, particle-fluid and particle-wall interactions). Based on the formulation of particle interactions, particles are assumed hard-sphere (event-driven) or soft-sphere (time-driven). In most granular flows, a particle may have contact with multiple other particles; therefore, we used the soft-sphere formulation. Newton's second law of motion describes the translational motion of each particle and, Euler's second law, its angular/rotational motion [4]:

$$m_i \frac{d\vec{v}_i}{dt} = m_i \frac{d^2\vec{x}_i}{dt^2} = \sum_{j\epsilon CL_i} \vec{F}_{ij} + m_i\vec{g} \quad (1)$$

$$I_i \frac{d\vec{\omega}_i}{dt} = \sum_{j\epsilon CL_i} (\vec{M}_{ij}^{t} + \vec{M}_{ij}^{r}) \quad (2)$$

where m_i, I_i, $\vec{x}_i$, $\vec{v}_i$ and $\vec{\omega}_i$ are respectively mass, moment of inertia, displacement vector, velocity vector, and rotational speed vector of particle *i*. The sum $\sum_{j\epsilon CL_i} \vec{F}_{ij}$ involves the forces due to other particles *j* with particle *i*, $m_i\vec{g}$ is the gravity force as an external force, and the sum $\sum_{j\epsilon CL_i}(\vec{M}_{ij}^{t} + \vec{M}_{ij}^{r})$ involves the tangential forces that generate torques, or rolling resistance torques, of other particles *j* with particle *i* [4].

The linear-viscoelastic force-displacement model was used to calculate the normal contact forces between particles, while also simple tangential forces and torques are used [10]. An open-source software, MercuryDPM, was used for the simulations, with the code implemented in modern C++.

3.1. *Simulation condition*

The cylindrical container is 50 mm in diameter and 100 mm in height. Particles are filled in the container to have the same mass as in the experiment. For the base case simulation, the impeller rotation speed was fixed at 600 rpm. Table 1 lists the parameters that were used in the DEM simulations. Upscaled particles with scale factor 5 (relative to the primary particles) were used in the base case simulation, which is considered as CG=1.

3.2. *Coarse-graining*

The coarse-graining scaling rules were used to adjust the force for the larger particles. In these cases, the coarse-graining factors were CG=1.6 and 2. The stiffness of the system has been scaled based on the coarse-graining factor:

$$k_{cg}=n\,k_{original} \quad (3)$$

where $k_{original}$, n and k_{cg} are the normal stiffness of the base case, the coarse-graining scale factor, and the normal stiffness for the coarse-grained case. This is a preliminary set of simulations, without a detailed calibration carried out yet.

TABLE I. SIMULATION CONDITION FOR THE BASE CASE.

Parameter	***Value***	***Unit***
Normal stiffness	1000	N/m
Coefficient of restitution	0.8	-
Dynamic friction	0.55	-
Rolling friction	0.3	-
Particle density	950	kg/m^3
Time step	3.6×10^{-6}	s

4. Results and discussion

Fig. 2 shows the bulk response in the experiment and simulations, with the impeller torque plotted against time. The experimental result shows that the torque response of the powder reaches its peak at 20 s and decreases until reaching a steady state after 80 s. The simulations produce a similar trend in the result, they reach a peak and then decrease to a steady state level. While the experimental time scale is 100 s, the simulation needs only 10 s to produce similar results.

The base case simulation results (CG=1) closely match the experimental results. In contrast, the CG=1.6 and CG=2 produce a larger torque. An increase in coarse-graining scale also leads to higher fluctuations in the torque. The torque response of the coarse-grained cases (CG=1.6 and 2) could not generate the same results, even though the accepted stiffness scaling rule was applied, seemingly insufficient for the torque. This indicates that also other input parameters should be scaled, which is our ongoing research.

5. Conclusion

The bulk response of a non-cohesive HDPE powder was measured in the Anton Paar Powder Rheometer. The base case DEM simulation was performed to find reasonably matching DEM input parameters, and then scaling rules were applied for two cases (CG= 1.6 and 2). The DEM results produced a similar trend as the experiment but on a shorter time scale. The base case DEM simulation torque agreed well with the experimental results, while applied coarse-grained rules could not generate the same results. To understand and correct this discrepancy is ongoing research, as well as calibrating other powder materials.

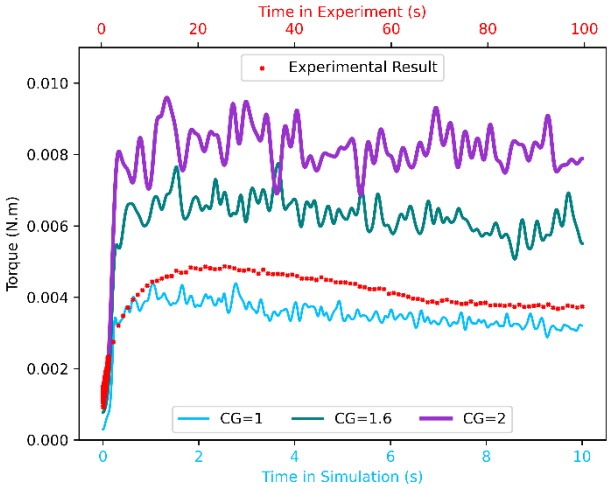

Figure 2. Bulk (torque) response in experiment and simulation.

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