Coarse-grained DEM modelling of wet granulation drum process

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***Abstract*— Discrete Element model (DEM) is a reliable tool for obtaining useful micro- and macro-scale data about particulate processes, including wet particle systems. However, it is computationally expensive when it comes to industrial scale systems with millions of particles. Coarse-graining (CG) is an upscaling approach in which groups of particles are represented by larger meso-particles, resulting in a significant improvement of DEM efficiency. It is important to consider appropriate scaling rules that account for the underlying physics of the system.**

We compare two different scaling approaches for wet particle systems in a rotating drum namely Weber (We)-based and Bond (Bo)-based scaling. The results suggest that the We-based scaling can better reproduce the system's flow behaviour.

Using We-based scaling, we investigate the impact of coarse-graining on granulation, focusing particularly on the granule size distribution (GSD). Subsequently, we analyse and compare the granule size distributions across coarse-grained discrete element method (CG-DEM) simulations. The results suggest that the size distribution of the granules in the original particle system could be potentially predicted from the size distribution of an upscaled CG system.

Keywords: Coarse graining; Discrete Element Model (DEM); Wet particles; Granule size distribution (GSD)

1. Introduction

Wet granulation is an important process in various industries due to the enhancement of properties, including bulk flowability and particle strength [1]. In this process, liquid binder is added to the powder under shear, and the wet particles start to cluster into granules. Material and process parameters influence the micro-scale phenomena underlying wet granulation, and, in turn, the final characteristics of the granules. Experimental investigation of granulation across multiple scales is important though extremely challenging [2].

DEM [3] is widely used for the simulation of granular systems. However, high computational cost is a major drawback. To increase the efficiency of the simulations, it is possible to use coarse-grained (CG) particles which have *n*-times larger diameter than the original ones. This approach has a bifold effect on the computation, namely the number of particles reduces a lot, and the numerical time-step increases [4,5]. However, appropriate scaling rules should be considered in the CG model in order to reproduce the behaviour of the original particle systems accurately.

To upscale wet systems, Chan and Washino [6] proposed a quadratic scaling (n^2) of the inter-particle particle forces in a vertical mixer and showed the validity of the CG-model for predicting the mixing behaviour. Four different scaling strategies for cohesive wet powders within a gas-solid fluidized bed were evaluated by Tausendschön et al. [7]. These strategies include dimensionless overlap-based, stress-based, and coefficient of restitution-based scaling (all resulting in n^2 scaling of interparticle forces), as well as Bond number-based scaling, which leads to n^3 scaling of interparticle forces, so that the Bond number-based scaling results in an over-prediction of the cohesive force. Jarray et al. [8] validated the Weber-based scaling (n^2) experimentally by using different size glass beads and tunable capillary forces.

To our knowledge, the effect of CG-DEM modelling on the granule size distribution has not been sufficiently investigated. In this study, firstly, scaling rules based on Weber and Bond numbers are compared. Then, using the appropriate Bo-based scaling, as resulting from the comparison, the applicability of the CG modelling for the prediction of granule sizes and their distribution is studied.

2. Modelling

YADE open-source DEM modelling framework [9] is used for the simulations in a drum granulator with *0.2* m diameter and 0.06 m length, with a periodic boundary in axial direction.

To compare the We- and Bo-based scaling rules, *360000* monodisperse particles with diameter *0.001* m are used as original (primary) particles. *48* lifters (baffles) of *0.001* m height are added to drum to avoid wall slip. To avoid ordering effects and to investigate the effect of CG on the size distribution of the formed granules, polydisperse spherical particles are used, with *80*% of the particles having *0.001* m diameter (d) and *20*% having $0.001 < d < 0.004$ m, and the geometry of the drum is varied in terms of the number and height of the baffles.

Furthermore, graph analysis is adopted to identify the granules, via the "Networkx" library in Python [10]. Following the study by Dong et al. [11], the particle contacts are filtered based on criteria related to the cohesive force and the angle between the velocity vectors of the colliding and contacting particles. Using a Breadth-First Search (BFS) algorithm for the filtered contacts, the granules are identified, and their volumes are reported.

3. Results

3.1. Comparing We and Bo-based scaling

Initially the scaling approaches based on constant Weber number (We) and constant Bond number (Bo) are compared. The former is given by the ratio between the inertial and capillary forces, as

$$\mathrm{We} = \frac{\rho_p R v^2}{\gamma \cos\theta}, \tag{1}$$

where R is the particle radius, ρ_p is the particle density, v is the estimated velocity of the flowing particles, γ is the liquid surface tension, and θ is the solid-liquid contact angle. On the other hand, the Bond number is the ratio between cohesion and gravity forces:

$$\mathrm{Bo} = \frac{3\gamma \cos\theta}{2R^2\, g\, \rho_p}\ . \tag{2}$$

Based on such non-dimensional numbers, interparticle contact and liquid bridge forces can be upscaled in the CG simulation to maintain flow properties consistent with the original unscaled system [12], where We and Bo lead to the quadratic (n^2) and cubic (n^3) force scaling, respectively.

Figure 1 shows a comparison between the granular flow in the rotating drum for the original particles and two cases with particles upscaled to CG3, i.e., particle radius three times larger, based on We and Bo scaling. As shown, the bed flow behaviour does not show a good agreement when the Bo-based scaling is used. In fact, the n^3 scaling of the inter-particle forces leads to overly large attractive forces and the formation of one big cluster in the drum. On the other hand, We-based scaling, properly reproduces the flow behaviour as well as the velocity profile of the particles (data not shown here, see [12]). Therefore, We-based upscaling is adopted in the following.

For a more detailed comparison of the rheological behaviour of the We-based CG and the original particle systems, involving several continuum fields, the reader is referred to [12].

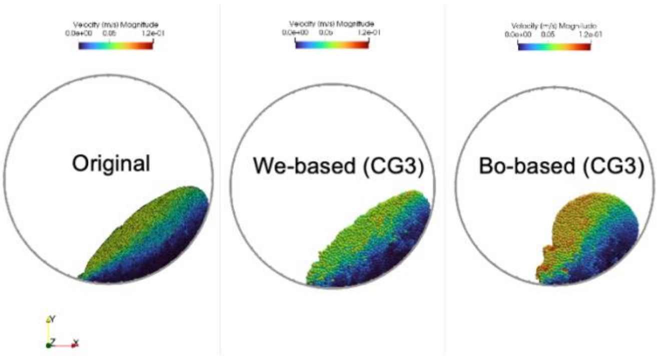

Figure 1. Comparing the We and Bo-based scaling in a rotating drum.

3.2. *Effect of CG on the GSD*

To investigate the effect of CG modelling on the size distribution of the granules, the Same Statistic Weight (SSW) approach is used for the poly-disperse system, in which the shape of the particle size distribution (PSD) of the CG particles remains identical to that of the original particles [13].

Figure 2 presents a snapshot of the CG1 (original particles) and We-based CG2, i.e., particles twice larger than the original ones and forces scaled with n^2 in the drum granulator. As shown, the flow behaviours of the granulated system as well as the particle velocities (colour code) seem to be well captured in the CG2 system.

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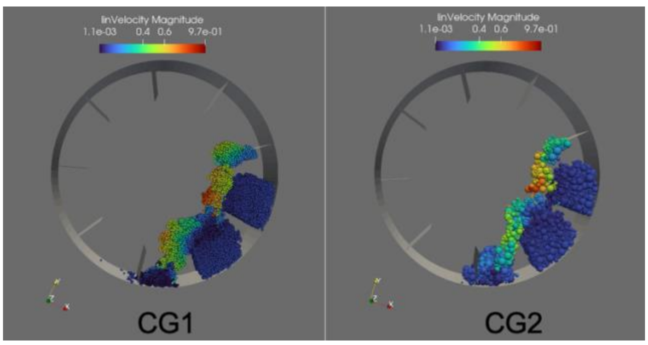

Figure 2. Snapshots of the drum granulator with CG1 and CG2 particles.

Using the granule identification approach [10], the GSD of the CG1 and CG2 systems are compared [12]. The results suggest that for the granules smaller than a limit of 1.4×10^{-7} m^3, via scaling down the size of the formed granules in CG2 system by n^3 times, the GSD of the original particles can be estimated (with an error $<15\%$). However, for granules larger than this limit, the size distribution of the CG2 granules does not reproduce the size distribution of the CG1 granules appropriately (error $>30\%$), possibly due to an insufficient number of particles in the CG2 systems, and loss of information and poor statistics as a result.

4. Conclusion

We studied wet particles flow and granulation in a rotating drum using coarse grain DEM. Upscaling based on the We number corresponds to a quadratic scaling of the interparticle forces, and could reproduce the flow behaviour of the particles, whereas Bo-number based scaling could not. When using appropriate scaling rules for the physics in the system, CG-DEM is a good compromise between the accuracy and the computational efficiency of the DEM simulation.

Moreover, by using the appropriate We-based scaling, as preliminary result, the GSD of granulated particles under shear could be reproduced in the CG2 system for the granules smaller than a limit, above which statistics is too poor. The prediction of the full GSD could be possibly improved by assuring sufficient statistics, i.e., sufficient CG particles or ensembles, in the upscaled system, which is the subject of our future studies.

Acknowledgement

This research is part of the project TUSAIL (Training in Upscaling Particle Systems: Advancing Industry across Length-scales, https://tusail.eu) and has received funding from the European Horizon2020 Framework Programme for research, technological development and demonstration under grant agreement ID 955661.

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