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Discrete element method simulation of a twin screw wet granulator

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Abstract. Granulation is a method of particle size enlargement via agglomeration of primary particles to form larger particles. In a Twin Screw Wet Granulator (TSWG), a binder liquid is sprayed onto the surfaces of active pharmaceutical ingredient particles to promote the formation of large granules with specific morphology, flowability, compressibility and other properties. The morphology of granules formed from a TSWG process depends on the material properties of the primary particles and operating conditions applied but mechanistic understanding of the granulation process remains incomplete even today. A large number of experiments are typically performed to determine the operating parameters required for a specific type of primary particles. The Discrete Element Method (DEM) has been applied extensively by researchers for simulations of various types of particulate processes. However, good agreements between DEM simulations of the TSWG and experimental measurements have not been demonstrated in the literature to date. In this study, the DEM was coupled with a capillary liquid bridge model to simulate the granulation process in a TSWG using the EDEM software, and Python programs were applied for data collection and post-processing. Different liquid contents (30%, 45%, 60%), screw speeds (450 rpm, 900 rpm) and solid throughputs (12.5 kg/h, 25 kg/h) were applied to investigate the effects of these parameters on the residence time distribution (RTD) of particles in the TSWG and particle size distribution (PSD) of the granules formed in various regions of the granulator. It was observed that agglomeration of particles occurred in the conveying elements of the TSWG, and large granules were kneaded in the kneading elements to generate new granules with different shapes and sizes. The aspect ratio (AR) was calculated to evaluate the shapes of the granules formed. Comparisons of simulation results with experimental data reported in a previous study were conducted to validate the accuracy of the simulation results.

1 Introduction

Wet granulation is a method of particle size enlargement of primary particles using a liquid binder to form larger particles. It is extensively utilized in the pharmaceutical industry, particularly in the production of tablets and capsules. The granulation process enhances the flowability of the drug powder, improving the processability of the materials. One method of wet granulation is using a twin-screw wet granulator (TSWG), which consists of two counter-rotating screws built using both conveying as well as kneading elements.

The morphology of granules formed from a TSWG process depends on the material properties of the primary particles and operating conditions applied but mechanistic understanding of the granulation process remains incomplete. To address this knowledge gap, both experimental investigations and numerical simulations have been applied to explore the particle behaviors within the granulator. For instance, the granule formation process has been studied using X-ray imaging techniques [1], and through parametric evaluations of the operating space [2-4] to elucidate connections between the process parameters and granule quality. An inability to experimentally evaluate the dynamic changes in particle size as the particles move through the granulator prevents a more detailed investigation into the mechanisms of granulation, although Verstraten and co-workers [5] opened up the granulator at every compartment to isolate granule samples.

On the other hand, modeling investigations allowed a more in-depth investigation of the mechanisms occurring inside the granulator. The techniques of Computational fluid dynamics (CFD), Finite Element Method (FEM) and Population Balance Modeling (PBM) [3, 6, 7] have been applied on the granulator assuming the powder to be a continuum.

However, the ability to capture particle dynamics and changes at the particle level make the Discrete Element Method well-suited to study the twin screw granulator. Zheng and co-workers [8] applied DEM to investigate the residence time distribution in a TSWG, revealing the influence of particle properties and screw speed on particle size changes. Although DEM has been applied extensively by researchers for simulations of various types of particulate processes [3, 8-10], good agreement between DEM simulations of the TSWG and experimental measurements has not been demonstrated in the literature to date. In this study, DEM was used with a capillary liquid bridge model to simulate the granulation process within a TSWG. The capillary force was incorporated as the cohesive force due to its applicability for wet particles. Particle motion within the

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TSWG was numerically analyzed to investigate its effects on particle size distribution (PSD) and aspect ratio (AR) at different granulator regions under various parameters. Finally, the simulation results were compared against the experimental results of Verstraeten and co-workers [5] using the same experimental configurations, providing insights into the underlying mechanisms.

2 Computational Method

The Discrete Element Method (DEM) [11] is used as the method to simulate the particles in the granulator. The Hertz-Mindlin no-slip contact model [12] is used to model the repulsive contact between the particles in the DEM simulation. As the particles are expected to be wet in the granulator, a liquid bridge model [13-16] is used to simulate the attractive force between them.

2.1 Simulation conditions

A digital model of the Consigma^{TM}-25 (GEA Pharma system, Collette, Wommelgem, Belgium) is used along with the same experimental configuration of Verstraeten and co-workers [13]. The TSWG features two co-rotating screws with a diameter and length-to-diameter ratio according to that of the Consigma-25, as shown in Fig. 1. The entire granulator is shown with material entering and exiting in Fig. 1 (a), while the conveying element is shown in Fig. 1 (b), kneading element is shown in Fig. 1 (c) and final chopping element at the end of the granulator is shown in Fig. 1 (d). The different numbered compartments are shown in the schematic diagram on Fig. 1 (e). To simplify the simulation, hydrochlorothiazide (HCT), the primary API used in the experiments [5] was directly applied as the simulation spherical particle, and the particle size was fixed at 134 µm, the D_{50} in the experimental particle size distribution.

As both the particle size and liquid content were fixed in the simulation, the liquid bridge shape adopts the form of a pendular bridge between two equally sized spheres. The rupture distance and the bridge volume between the two spheres are calculated using the model equations.

The process parameters were varied systematically to both validate the simulations as well as explore the operating space. Different Liquid/Solid ratios, screw speeds and material throughputs were simulated

Particle positions were analyzed to determine various quality attributes associated with granule formation.

3 Results and Discussions

The simulation allowed the determination of particle behavior in each compartment of the twin screw granulator. Particle size distributions were evaluated at the end of each compartment and compared with the corresponding experimental result as obtained by Verstraeten and co-workers [5].

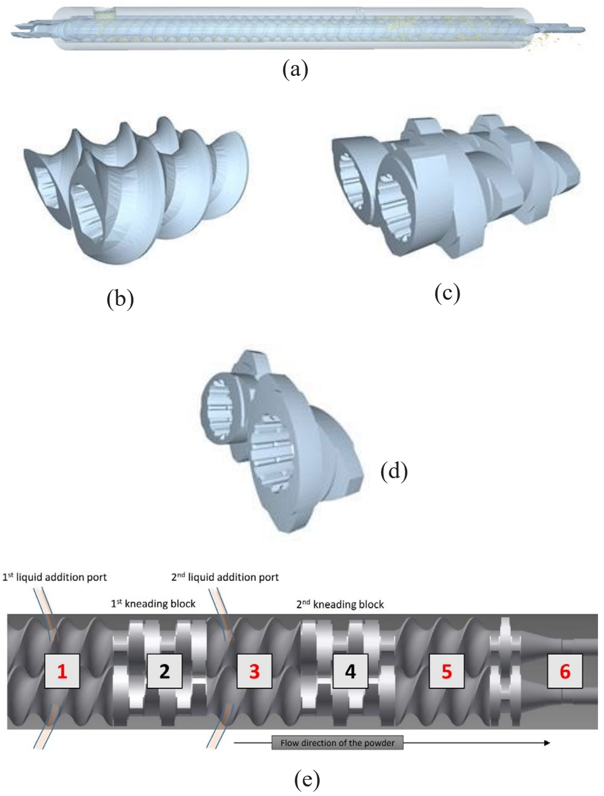

Fig. 1. Snapshot of the Consigma-25 twin screw granulator used in the DEM simulations: (a) Entire granulator with material entering and leaving at entry and exit, respectively; (b) Conveying element; (c) Kneading element; (d) Final chopping element at the exit of the granulator; (e) schematic diagram pointing out the different elements along the length of the granulator.

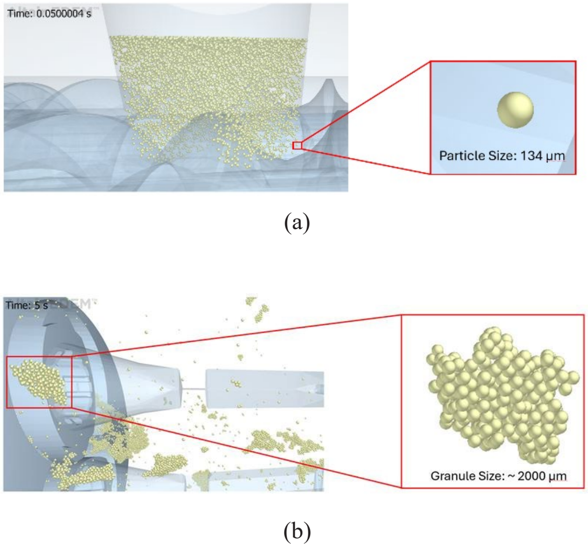

Fig. 2. Size differences between particles entering and leaving the granulator: (a) Particles are sized at 134 µm while entering the granulator; (b) Particles grow to ~2000 µm at the exit of the granulator.

An example of particle size differences at the inlet and the outlet of the granulator are shown in Fig. 2. The particle size at the entrance is 134 μm, with final granule sizes reaching 2000 μm at the exit of the granulator.

Particle size distributions are determined at the outlet of the granulator with change in L/S ratio (Fig. 3), change in screw speed (Fig. 4) and change in throughput (Fig. 5). The three figures show that increased amounts of fluid, and sufficient contact of particles with the fluid and with other wet particles all contribute towards increasing the particle size.

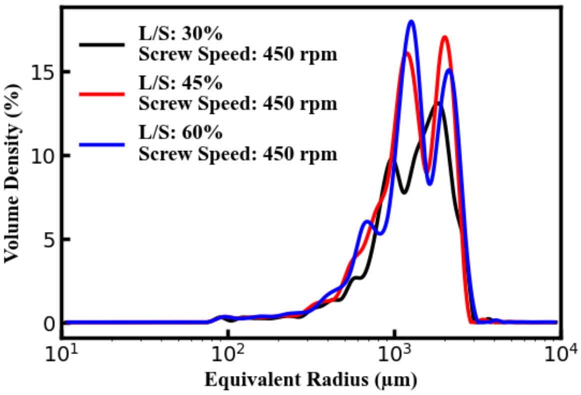

Fig. 3. Particle size distributions of granules obtained at the end of the granulator as a function of L/S ratio at fixed screw speed and throughput of 12.5 kg/h.

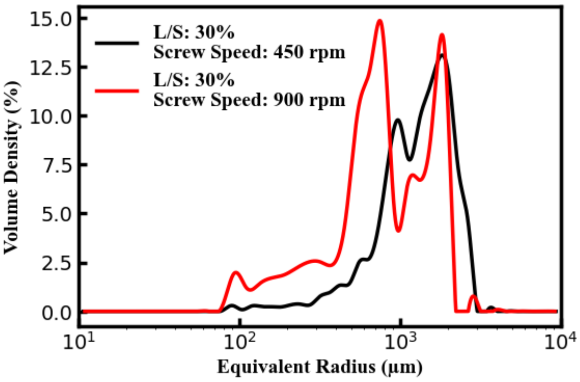

Fig. 4. Particle size distributions obtained at the end of the granulator as a function of screw speed at fixed L/S ratio and throughput of 12.5 kg/h

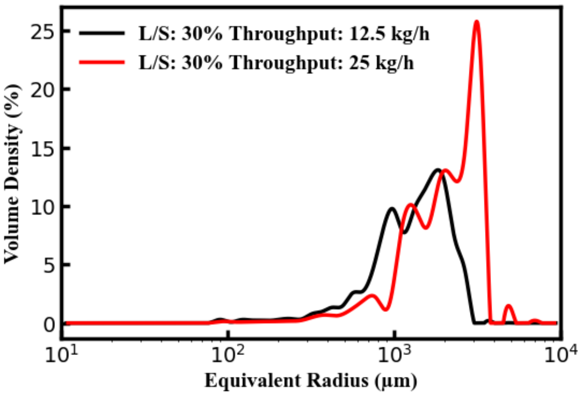

Fig. 5. Particle size distributions obtained at the end of the granulator as a function of throughput at fixed L/S ratio and screw speed of 45 RPM.

Differences are observed between particle sizes as they change in the different compartments of the granulator. The particle size distributions from compartments 1, 3 and 5 of the simulated granulator at an L/S ratio of 60%, throughput of 12.5 kg/h and screw speed of 450 RPM are compared to the experimental distributions obtained at the same conditions [5] in Fig. 6 (a) and (b). The leftward shift of both particle size distributions shows the effect of the two kneading elements (compartments 2 and 4), which cause the particle sizes to reduce as a result of increased shear. To determine the shapes of granules, the obtained aspect ratios of granules in the wetting compartment are compared to the experimental aspect ratios for the same compartment at various L/S ratios in Fig. 7. The simulated aspect ratios are biased to purely large granules due to the uniformity of liquid-solid contact across the height of the granulator arising from the liquid bridge model. The experimental system has a liquid spray at the top of the granulator, which likely leaves the bottom of the granulator less exposed to liquid, leading to the existence of fine-sized granules in the experiment. As can be seen from the particle size distributions and aspect ratios, there is qualitative agreement of the simulated results with the experimental measurements. These results were used to validate the simulation method and the DEM contact model parameters. The results will be discussed in detail by Yu and co-workers [17].

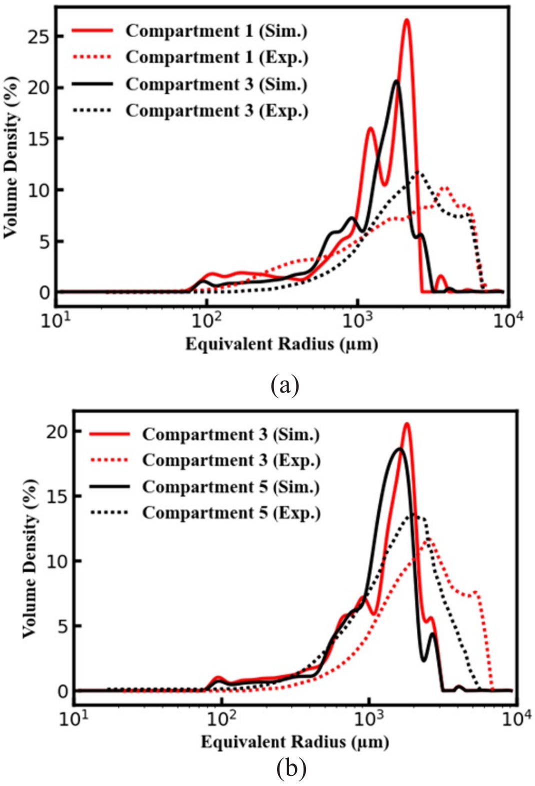

Fig. 6. Granule size distributions compared between Compartments 1, 3 and 5 as obtained from simulations and experiments conducted by Verstraeten and co-workers [5] for L/S ratio of 60%, throughput of 12.5 kg/h and screw speed of 450 RPM: (a) Between compartments 1 and 3 particles reduce in size as seen in both simulations and experiments; (b) Between compartments 3 and 5 particles reduce in size once again due to compaction and restructuring under shear forces in the kneading element.

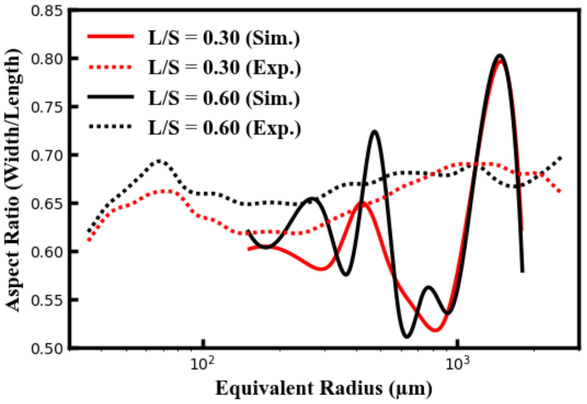

Fig. 7. Aspect ratio distributions of granules compared to experimental aspect ratios under different L/S ratios in the wetting compartment. The simulated aspect ratios are biased to purely large granules due to the uniformity of liquid-solid contact across the granulator arising from the liquid bridge model. The experimental system has a liquid spray at the top of the granulator, which likely leaves the bottom of the granulator less exposed to liquid, leading to the existence of fine-sized granules in the experiment.

This paves the way for the use of DEM to probe the granulation process in the twin-screw granulator and draw further insights using more modeling advancements. Furthermore, this opens up the possibility of using DEM to run digitally evaluate the operating space prior to running resource-internsive experiments for both process understanding and scale-up.

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