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Impact of roll gap and screen size in the post-compaction dynamics of roller compaction and mill system: a DEM study

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Abstract. In the pharmaceutical industry, managing the flow properties of powder blends is challenging due to their poor flowability. Roller compaction mill, a key granulation technique, enhances the processability of these blends by compressing powders into dense ribbons, which are then milled into granules. This study employs Discrete Element Method (DEM) simulation to analyze the mechanical behavior and post-compaction dynamics of pharmaceutical ribbons, focusing on roll gap and screen size. The simulations reveal that the ribbon expands by up to 20% upon exiting the roller, with significant changes in volume fraction due to variations in roll gap. When the ribbon interacts with the mill impellers, it breaks upon contact, resulting in the formation of smaller clusters of particles as it passes through the screen. This study highlights the critical impact of screen size on particle size distribution (PSD), cluster count, and total volume. Moreover, the effect of roll gap on solid fraction of the ribbon and regional cluster distribution are studied thoroughly. Clearly, adjusting mill-screen design could optimize milling results, emphasizing the importance of controlling mechanical settings for better product uniformity and efficiency in solid dosage form manufacturing.

1. Introduction

The roller compactor is a very important piece of equipment in the pharmaceutical production sector, utilized primarily during tablet making in the process of granulation. The process, called dry granulation, is pivotal in converting primary powder particles into bulky, freely flowing granules, which are subsequently compressed into tablets. The process of granulation plays a significant role in the final product's quality—its homogeneity, dissolution rate, and stability. It is, therefore, crucial to understand and optimize factors affecting roller compaction to ensure better product quality and manufacturing efficiency [1].

Recent technological advances have seen the increasing integration of computational modeling techniques in pharmaceutical process development, which helps in minimizing the extensive resource allocation for experimental trials. Of them, the Discrete Element Method (DEM) [2] has emerged as an extremely efficient technique for simulating particulate systems in minute detail [3]. By mimicking the interaction and motion of discrete particles, DEM allows researchers to see the mechanical response of powder during compaction and milling and provides valuable data on how changes in process conditions influence granule properties [4].

This study employs Discrete Element Method (DEM) simulation to analyze the mechanical behavior and post-compaction dynamics of pharmaceutical ribbons produced via roller compaction. It focuses on the expansion, breakage, and milling of ribbons into smaller clusters of particles as shown in Figure 1. This study highlights the critical impact of roll gap and screen size on particle size distribution (PSD), count of clusters of particles, and total volume of clusters. The findings emphasize the importance of controlling these parameters for better product uniformity and efficiency. The insights gained are crucial for optimizing equipment design and scaling up processes in solid dosage form manufacturing. Also, our findings could be useful for designing new machines and for the optimization of existing ones, with a direct contribution to advancements in pharmaceutical manufacturing technology.

2. Discrete element method (DEM)

The Discrete Element Method (DEM) [2] is extensively used to simulate the behavior and interaction of discrete particles under various physical conditions. In the context of granulation processes, DEM provides valuable insights into particle dynamics, which are crucial for optimizing the manufacturing processes. Below, we detail the DEM simulation parameters and equations utilized in the study. The motion of each particle in DEM is governed by Newton's laws, accounting for translational and rotational dynamics. The fundamental equations [5] are:

$$m_i \frac{d\vec{v}_i}{dt} = m_i \frac{d^2\vec{x}_i}{dt^2} = \Sigma\left(\vec{F}_{c,ij} + \vec{F}_{ext,i}\right) \qquad \ldots(1)$$

$$I_i \frac{d\vec{\omega}_i}{dt} = I_i \frac{d^2\vec{\theta}_i}{dt^2} = \Sigma\vec{M}_{t,ij} \qquad \ldots(2)$$

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where, m_i is the mass, $\vec{v}_i$ the velocity, $\vec{x}_i$ the position, I_i the moment of inertia, $\vec{\omega}_i$ the angular velocity, $\vec{F}_{\mathrm{c,ij}}$ the contact force, $\vec{F}_{\mathrm{ext,i}}$ the external force, and $\vec{\mathrm{M}}_{\mathrm{t,ij}}$ the tangential torque applied on the i-th particle.

The contact interactions between particles are described by the Hertz-Mindlin contact model, which provides realistic contact forces including elastic and damping components:

$$\vec{F}_{c,i} = \vec{F}_{nor,ij} + \vec{F}_{tang,ij} = \left(\kappa_{nor}\,\vec{\delta}_{nor,ij} - \gamma_{nor}\vec{v}_{nor,ij}\right) + \left(\kappa_{tang}\,\vec{\delta}_{tang,ij} - \gamma_{tang}\vec{v}_{tang,ij}\right)$$

where, $\vec{F}_{nor,ij}$ and $\vec{F}_{tang,ij}$ are the normal and tangential components of contact forces on i-th particle. Also, κ_{nor} and κ_{tang} are the normal and tangential elastic constants, γ_{nor} and γ_{tang} are the damping constants. $\vec{\delta}_{nor,ij}$ and $\vec{v}_{nor,ij}$ are the normal overlap and relative normal velocity between i-th and j-th particles, and $\vec{\delta}_{tang,ij}$ and $\vec{v}_{tang,ij}$ are the tangential overlap and relative tangential velocity between i-th and j-th particles. To model the cohesiveness of particles, we have implemented Edinburgh Elasto-Plastic Adhesive (EEPA)[6] model in EDEM software. In the next section, we will discuss about the DEM simulation set up for roller compactor mill system and some results from the simulations.

3. Results and discussion

We employ DEM simulation in this paper to examine roller-compacted pharmaceutical ribbon's post-compaction dynamics and mechanical behavior. Figure 1 presents DEM simulation setup with an illustration of the ribbon formation process and cluster formation through the screen. The primary focus of the investigation is on observation of the expansion and fracture of the ribbon, and subsequent grinding of the fractured ribbons to smaller fragments. DEM simulation helps us visualize the intricate particle-to-particle contact at these processes and develop good insight into material behavior under changing conditions. Two critical parameters are highlighted in this study: roll gap and screen size. The roll gap, or compaction roll gap, is one of the major factors to consider in setting up the density and mechanical strength of the ribbons. A small roll gap will generate more compaction pressure, which leads to denser and stronger ribbons. In contrast, a higher roll gap creates less dense ribbons with weak mechanical strength. Screen size, on the other hand, is a critical aspect of the milling process. It dictates the particle size that passes through the screen during milling. Decreasing screen size results in smaller particles, thereby potentially elevating the rate of dissolution and bioavailability of the drug product. That being said, this increases the likelihood of generating excess fines, therefore reducing the product's flow and compressibility characteristics.

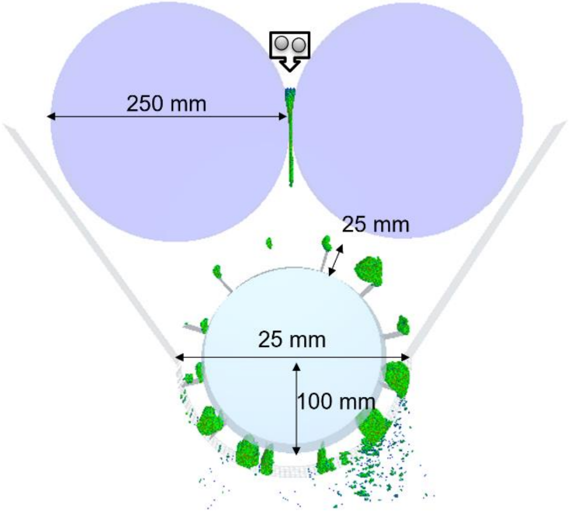


Figure 1: Snapshot of the DEM simulation of roller compaction mill system (with dimensions) at time t = 20 s.

In our DEM study, we have used mono-sized particles of diameter 500 μm. The other particle properties are provide in Table 1. Our simulations show that the ribbon exiting the roller can expand in width by up to 20% as shown in Figure 2. This widening has significant implications for the mechanical property understanding and subsequent processing of the ribbons.

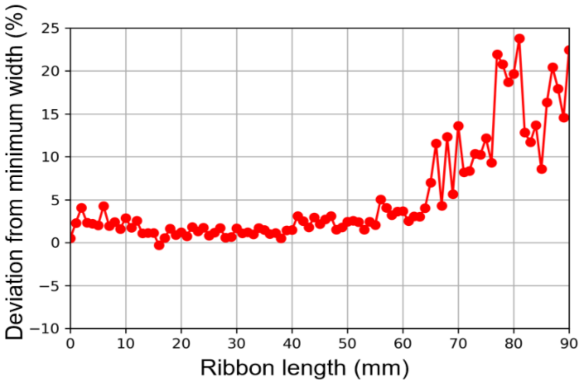


Figure 2: The expansion (in percentage) of the ribbon with respect to the initial width of the ribbon for roll gap 2 mm.

Parameter	Value
Diameter of particle, D_p	500 μm
Young's modulus	10^7N/m^2
Coefficient of Restitution, e	0.4
Coefficient of static friction, μ_s	0.45
Coefficient of static friction, μ_r	0.02
Poisson's ratio	0.2
Surface energy density	0.01 J/m^2
Constant pull-off force	-0.003 N
Density of particles	1500 kg/m^3

Table 1: The parameters of particles.

To further our study, we also expand the investigation to examine the ribbon-mill impeller interaction. Upon contact with the impellers, the ribbon is broken into pieces. In this part of the study, we hold the gap between two rollers constant (2 mm) to decouple the effects of screen size and roll gap on the resulting particulate clusters. We have used sieve sizes as 2, 3 and 4 mm for three different simulations. Our findings indicate that screen size plays a vital role in the control of particle size distribution (PSD), number of clusters, and total volume of the milled product. The fluctuation of these parameters is highly dependent on the screen size, which influences not only the final product characteristics but also reveals important material properties after milling. Figure **3** shows the effect of sieve size in PSD of clusters which are coming through the sieve. To quantify these effects, we conduct a 'regional analysis' by collecting and comparing clusters from different regions of the screen. In doing this, we quantify differences in volume, number of particles, and PSD, illustrating the profound impact of screen size on these parameters. Through regional analysis, we have also observed that middle part of the screen produces most of the clusters.

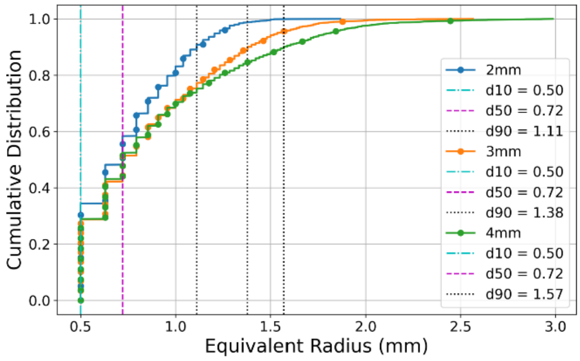
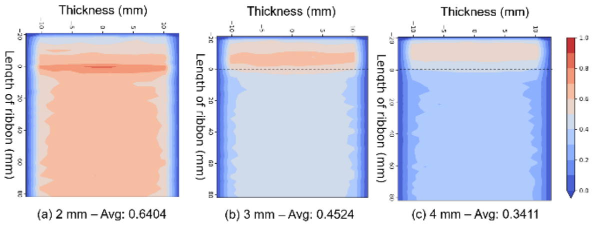


Figure 3: Comparison of PSD of clusters for different sieve size.

In this study, we have also conducted a test case to examine the impact of variable gap between rolls, as compared to that with a fixed gap. We kept roll gaps as 2, 3 and 4 mm to check the effect of roll gap in ribbon solid fraction and cluster PSD. It is observed that solid fraction of ribbon decreases as we increase the roll gap as shown in Figure 4. Similarly, the roll gap has a significant role in influencing the regional distribution of particulate clusters. The findings suggest the potential for optimizing milling results through adjustment of mill-screen design. Changing the gap caused substantial variation in cluster distribution and cluster type. This indicates that tight control of mechanical parameters, such as the roll gap, is critical for the optimal function of roller compaction and milling processes. Precise fine-tuning of such parameters can lead to enhanced uniformity of product and enhanced efficiency in the process.



(a) 2 mm – Avg: 0.6404 (b) 3 mm – Avg: 0.4524 (c) 4 mm – Avg: 0.3411

Figure 4: Comparison of solid fraction of ribbons for different roll gaps

The findings of these observations have broad and significant implications for equipment design and process scale-up in the production of solid dosage forms. Knowledge of the effect of the roll gap allows more logical design and equipment optimization. The information can particularly be utilized in scaling up processes to guarantee desired product quality and uniformity are maintained at high levels of production. Overall, this study highlights the importance of mechanical setting control in compaction and milling operations. Adjustment of settings such as the roll gap facilitates the production of more consistent products, with enhanced efficiency and overall quality. These findings can improve feedstock design in additive manufacturing, enhancing powder flow. The results are beneficial in improving pharmaceutical manufacturing processes and can be a foundation for more efficient and trustworthy production of solid dosage forms.

4. Conclusions:

This paper emphasizes the relevance of roller compaction to enhance the powder blends' flow behavior in the pharmaceutical industry. Based on the use of DEM simulations, we have illuminated the mechanical response and post-compaction flow of ribbons of pharmaceuticals, the roll gap and screen size having been demonstrated as relevant parameters on crucial quality characteristics such as PSD, number of clusters, and overall volume. The results indicate that the volume fraction and expansion of the ribbon are highly sensitive to the roll gap, while the screen size significantly influences the PSD after milling. The regional analysis of the different screen areas has quantitatively approximated the extensive variation due to screen size, indicating its importance in milling. Through optimization of mechanical properties such as roll gap and screen size, the pharmaceutical industry is able to achieve higher consistency and efficiency in the manufacturing process, leading to a better-quality final dosage forms.

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