

# NUMERICAL INVESTIGATION OF SCREW DESIGN INFLUENCE ON SCREW FEEDING IN A ROLLER COMPACTOR

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**Abstract.** Roller compaction refers to a dry granulation process where fine particulate feed is fed to the counter rotating rolls of a roller compactor to form ribbons which are further milled to produce free flowing agglomerates. For the continuous production of ribbons, there needs to be an adequate supply of powder by the screw to the rolls without any interruptions. In general, screws used in roller compactors are designed to convey powders of all types (cohesive, bulky, compressible, etc.), whereby usage of different screw designs for different powder types may be avoided. However, using such single screw type roller compactors for poor flowing powders may be challenging. On the other hand, the selection of the right screw for a given powder can only be done based on a combination of prior experience and trial-and-error experimentation. Empirical correlations exist to predict the draw down rate of screw feeders depending on their design, however, these correlations assume that there is continuous supply of powder by the screw, which limits its application to free-flowing powders only. To address this, in this study numerical simulations are performed based on discrete element method (DEM) to investigate the impact of screw design on the powder supply to rolls for cohesive and poorly flowing powders.

The geometry considered includes a hopper, horizontal feeding screw below the hopper, and two counter-rotating rolls at the end of the screw. Two different screw designs are investigated where the main difference between them is the pitch length. The influence of scraper speed is investigated. Additionally, the influence of material attribute such as cohesion is studied. For both designs, the simulation results calculated include the rate of powder supply by the screw, velocity of particles in the screw etc. The simulation results of powder supply rate are also compared with results obtained based on empirical correlation. Overall, this simulation approach helps in selecting appropriate screw design for the given cohesive powder.

## 1 INTRODUCTION

Roller compaction is a dry granulation process designed to compact fine powders i.e. densifying the powder blend by application of pressure, to produce ribbons which are further processed to yield granules and pertains to continuous manufacturing procedure [1]. Roller

compaction process has significant effect on flowability, homogeneity, compressibility of active pharmaceutical ingredients and excipients and thus can affect post compression parameters of tablet [2]. Therefore, it is necessary to optimize the process parameters to obtain good quality granules.

A typical roll compactor consists of a hopper connected to a single rotating screw, which feeds the material into the gap between two counter-rotating rolls and cheek plates on the sides to avoid leakage which is represented in Figure 1. Experimental studies on screws have been conducted by Bates [3] to match different screws and material in hopper in order to investigate flow pattern.

It is frequently found that a mechanical discharging apparatus in a roll compactor is virtually essential for handling cohesive powder. One such method is the screw feeder which comprises a helical screw blade or "flight" on a horizontal shaft (Figure 2). The construction of the screw may be of uniform or varied geometry [3].

Theoretical models have also been proposed by Yu and Arnold [4] for a uniform flow pattern based on the pitch characteristic of screws, and Roberts [5] for uniform drawdown used to predict the flow patterns generated in hoppers for a given screw. However, screw shear and power draw can be affected by the forces acting on the screw which varies along the screw length [6].

Moyses and Thompson developed a new 3-D model for solids conveying in a single screw extruder using DEM. The model has been shown to be an excellent tool for studying solids flow within the screw channel [7][8]. Further, Fernandez et al. studied the influence of screw design on the particle mass flow rate, evenness of particle drawdown from the hopper and power consumption [6]. However, in all these studies, the hopper used did not have any scraper or impeller attached to it and it is one of the useful process attributes for handling cohesive material.

In this study, the impact of screw shape on the discharge from hopper on cohesive material is explored. Also, DEM is used to investigate the effect on total mass flow rate out of the screw, mass holdup, velocity of particles inside screw zone. Finally, the results are compared for different cohesion cases. The screws in this study are one of the commonly found designs having variation in screw pitch spacing. Also, the study aims to evaluate the relative performance of screws and to establish the accuracy of the continuum based analytic model. Further, prediction from this study is compared to theoretical study of discharge prediction from Roberts [5][9].

## **2 MATERIAL AND METHODS**

### **2.1 Discrete Element Method (DEM)**

The DEM is a numerical method based on Newton's laws of motion and was introduced by Cundall and Strack (1979) [10]. It is a Lagrangian method i.e. all particles in the computational domain are tracked by explicitly solving their trajectories [11]. The details of modeling using DEM can be found in [12] and various industrial applications of DEM in [13].

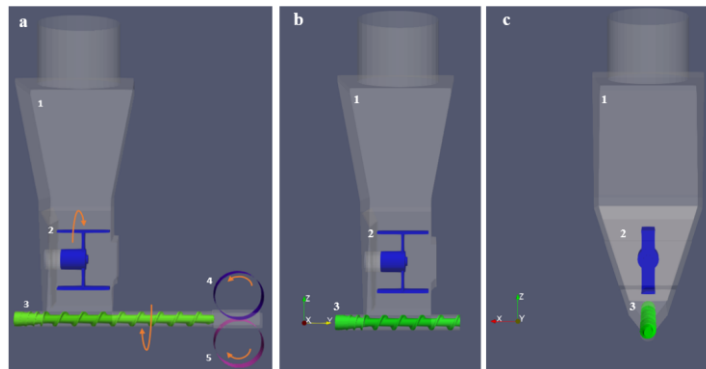
In this work all the computations were performed using the open source DEM software known as LIGGGHTS [17]. LIGGGHTS stands for LAMMPS improved for general granular and granular heat transfer simulations. It is a parallel C++ DEM code based on the Molecular Dynamics (MD) code LAMMPS [14] distributed by the developers via the GNU public license [11] and in this study LIGGGHTS version 3.7 is used. The models chosen in this study include Hertz and Mindlin & Deresiewicz theories for the calculation of normal and tangential forces,

respectively [15]. The cohesion is included through the simplified Johnson-Kendall-Roberts model [16] which adds an additional normal force contribution and this is successfully implemented in our previous study [17]. The other non-contact force considered includes gravity.

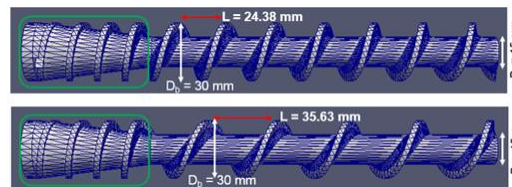
The current study aims at using the well-developed models of DEM to capture the particle flow in the hopper of a roller compactor under different material and process attributes.

## 2.2 Geometry

The hopper design including scraper, screw and rolls are shown in Figure 1. Two different geometries of same design are used in this paper for performing simulations. Figure 1a shows the complete roll compactor geometry, Figure 1b shows the same geometry but only half of the screw is considered for simulations (to optimize simulation time and discharge behavior of the particles) and Figure 1c is the x-z plane view of the same geometry as shown in Figure 1b.



**Figure 1** Roll compactor geometry (a) including rolls (b) no rolls included, y-z plane view and (c) no rolls included, x-z plane view



**Figure 2** Screw designs

The hopper is marked as 1 in the Figure 1. Here, the hopper is selected such that the walls are steep enough and have friction low enough to let the material slide in a mass flow manner to the screw zone. Location 2 is the scraper used inside the hopper, one of the reason is to handle cohesive powder so that the powder is continuously fed to the screw zone. Location 3 is the screw, 4 and 5 are the upper roll and lower roll respectively. The roll gap can be adjusted according to required final ribbon density in addition to the force applied by the rolls on the material and screw speed.

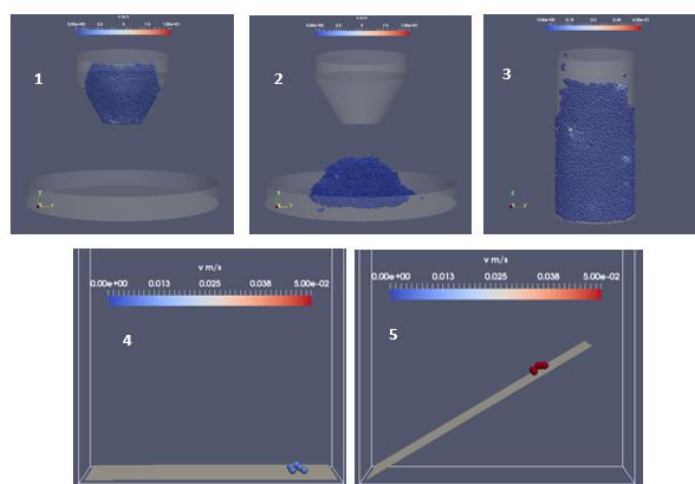
The screws are one of the basic types of feeders used in roller compaction process. They play an important role in particle feeding to the rollers. With different screw types, the consolidation of particles in the compaction zone might differ. The main difference between

the two screws is the pitch. Screw 1 has lower pitch with 24.38 mm as compared to screw 2 with 35.63 mm.

### 2.3 Particle size selection

Three-dimensional simulations done with DEM are recognized to be extremely CPU-intensive, requiring from a few hours to several days in the case of systems involving a large number of particles. The current hopper system has a volume of about 3000 cm<sup>3</sup>. In this volume, a typical pharmaceutical dry granulation blend having about 200 µm particle diameter, could contain about  $3 \times 10^9$  particles. To address this, typical procedure is to consider enlarged particle size in simulation but keeping the bulk behavior of powder closer to reality. In this study, particles with radius of 2.0 mm were selected and considered for simulations which has in total particles of about 170,000 within the hopper.

### 2.4 Material property calibration



**Figure 3** Calibration screenshots (1) Angle of repose at filled state (2) Angle of repose at final state (3) Bulk density for particles filled inside the cylinder (4) Angle to start flow filled state (only 5 particles are used) (5) Angle to start flow final state i.e. angle at which the particles start to roll from the surface.

After the particle size is selected, different microscopic particle properties which enter as input parameters in DEM simulations are calibrated based on bulk properties available through experimental data. This results in increased accuracy and validity of the discrete element modeling work. The different material properties calibrated include cohesion energy density, rolling friction and particle density using the angle of repose, initiation of flow over an inclined plate and bulk density, respectively. The standard calibration procedure is followed as described e.g. by Jensen et al. [18] and by Coetzee and Els [19], which is also depicted in Figure 3.

The rationale for calibrating the particle density, rolling friction and cohesion energy density is due to the observation that these properties influence the powder flow behavior in hoppers [20], [21]. The measured data of bulk density, angle of repose and initiation angle of particles to slide on inclined plate for the considered powder blend are 0.24 g/mL, 57° and 30°, respectively. The final calibrated values of particle density, cohesion energy density and rolling

friction for particle size 2 mm is given in Table 1. The other microscopic particle properties which are not calibrated, however taken from literature [17].

**Table 1** Final values of particle properties after calibration

Property (DEM input parameter)	Particle radius of 2.0 mm	Property used for calibration
Particle density / g/mL	0.613	Bulk density
Cohesion (particle-particle) / J/m <sup>3</sup>	90000	Angle of repose
Cohesion (particle-wall) / J/m <sup>3</sup>	6000	Angle of repose
Rolling friction (particle-wall) / -	0.54	Angle to start flow

## 2.5 Initialization of simulations

With the finalized values of DEM input parameters after calibration, simulation of hopper with screw conveying is performed with the selected particle sizes of 2 mm. The typical simulation procedure is that for the selected particle size, using the particle properties defined in Table 1, the particles are filled into the hopper during which the scraper and the screw is idle. Once complete filling of particles and their subsequent settling is achieved, which is observed through the total particle kinetic energy and rotational kinetic energy, the filling is said to be complete. With this filled state, the process parameters such as screw speed and scraper speed are set and simulations as per the plan given in Table 2 is started.

## 3. RESULTS AND DISCUSSION

At first, a base case is considered to define basic result that are studied in this paper to evaluate the differences. The results are then organized at first to find the differences in screw type considering different process parameter such as scraper speed. Following which the impact of cohesion on the discharge rate is studied.

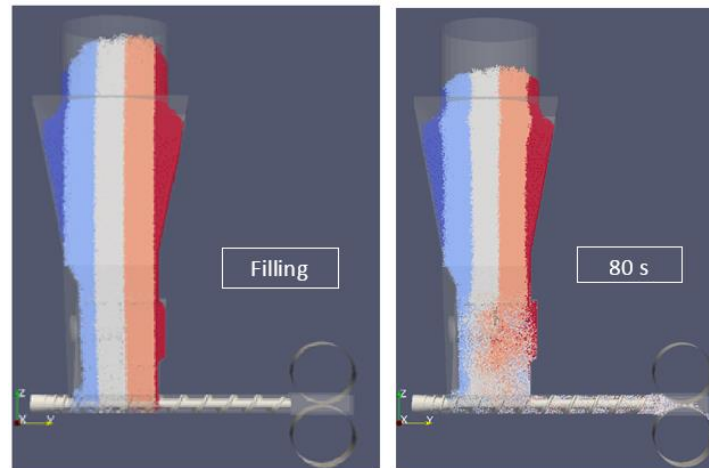
### 3.1 Base case

The calibrated value of material properties for 2 mm particle size is taken to describe the basic results extracted from the details generated by the DEM simulation for all the particles at every time step.

The particle size of 2.0 mm is filled inside the hopper every 0.5 second till 20 s to achieve uniform filling. Appropriate time is allotted to particles after insertion so that the particles are settled inside the hopper aptly. During the filling, scraper, screw and rolls are idle. Once the filling is done, the particles are colored in the direction of positive y axis as can be seen in Figure 4.

**Table 2** Simulation details including process parameters

Run.	Geometry	Screw type	Particle radius	Cohesion (J/m <sup>3</sup> )		Scraper Speed (rpm)	Screw Speed (rpm)
				Particle - particle	Particle-wall		
1	Full	Screw 2	2.0 mm	90000	6000	15	90
2	Half	Screw 2	2.0 mm	120000	1200	5	90
3	Half	Screw 1	2.0 mm	120000	1200	5	90
4	Half	Screw 2	2.0 mm	120000	1200	20	90
5	Half	Screw 1	2.0 mm	120000	1200	20	90
6	Half	Screw 2	2.0 mm	120000	1200	15	90
7	Half	Screw 1	2.0 mm	120000	1200	15	90



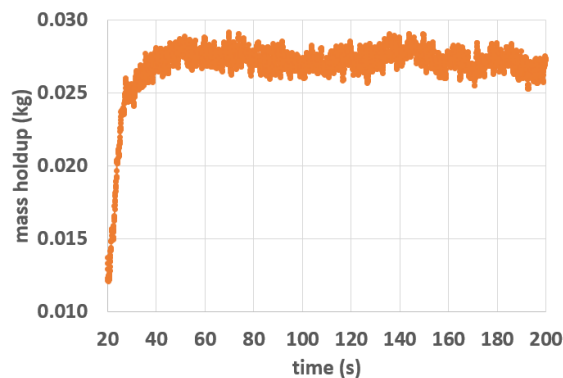
**Figure 4** Geometry of screenshot at filling state and 80 s of discharge

After filling is complete, the scraper, screw and rolls are rotated at the speed of 15 rpm, 90 rpm and 10 rpm respectively. Figure 4 shows the flow state at filling and 80 s of discharge. The mixing of particles in the scraper zone can be seen at 80 s. Also, the particles are seen to be

completely filled in the screw zone as the rolls rotate and discharge takes place. However, mass flow behavior is observed i.e. the powder seems to discharge smoothly without any obstruction in flow. Following this, various aspects such as mass holdup, throughput and velocity of particles in screw zone is studied to observe the particles behavior.

### 3.1.1 Mass holdup in screw zone

Mass holdup refers to the weight of particles in kilograms inside the screw zone. The achievement of steady state is explained through the mass holdup inside the screw zone. As the screw rotates, the particles are drawn from the hopper, inside the screw zone and is conveyed through the screw towards the rolls.



**Figure 5** Mass holdup inside the screw zone

Figure 5 shows the escalation of mass of powder inside the screw zone. It can be seen from Figure 4, filling state that there is already presence of some particles inside the screw zone, therefore, the ordinate in Figure 5 starts from value other than 0 at 20 seconds. As the time progresses, the mass holdup inside the screw zone increases and reaches a constantly fluctuating value signifying the steady state achievement and the average mass holdup inside the screw zone is 0.027 kg. However, the mass holdup might vary if the screw speed is changed from 90 rpm to other value.

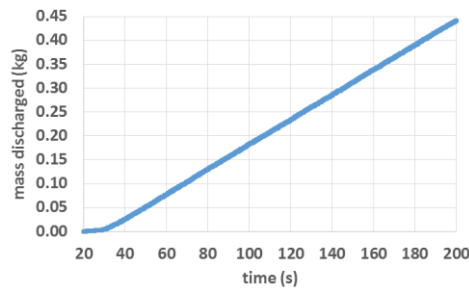
### 3.1.2 Discharge behavior study

To study the discharge behavior of particles, factors such as throughput and velocity acting on particles in the screw zone are studied.

#### Throughput

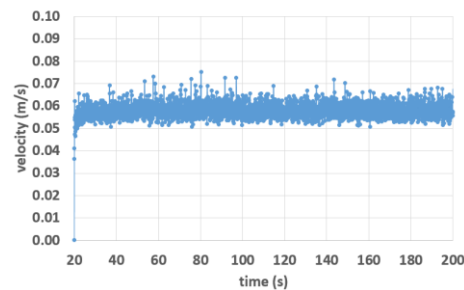
Throughput is defined as the mass of powder coming out of the system considered per unit time. Figure 6 represents the throughput of the system. While looking at the abscissa, it can be observed that initially, the mass discharge is almost zero. This is the time frame that particles took to travel from outlet of the hopper to the point where particles come out of the system. After which, the graph follows linearly increasing trend which represents achievement of constant throughput. Here, the slope of the graph represents the throughput which is around

0.0026 kg/s and 9.35 kg/h corresponds to packing fraction of 0.26 in screw zone (explained in next section based on calculation from equation 1 from Roberts [5]).



**Figure 6** Throughput of the process

### Velocity of particles inside screw zone



**Figure 7** Velocity of particles inside the screw zone

Velocity of particles inside the screw zone is shown in Figure 7 will help to analyze the cohesive behavior of powder particles inside the screw zone. A cuboidal box is considered to mark the x, y and z bound in the region belonging to screw zone and velocity of particles at every 0.05 seconds is calculated. For the particle size of 2 mm, the average velocity of particles inside the screw zone is 0.058 m/s. The rotational speed of screw is 90 rpm, which is 0.137 in linear velocity. The velocity of particles is lower than the tip speed of screw which can be attributed to the presence of a lot of particles inside the screw zone, where only limited number of particles near to the screw surface are in contact with the screw. This result would help to compare the behavior of cohesive particles in different process conditions and material properties.

### 3.2 Comparison of screw design

For comparing screw designs, the half geometry as shown in Figure 1b and 1c is considered in order to reduce the overall simulation time. The two screw geometries considered are shown in Figure 2. The particle size of 2 mm with higher particle-particle cohesion and lower particle wall cohesion is considered to observe how the cohesive blend would behave to the change in process parameter such as scraper speed (5 rpm, 15 rpm and 20 rpm). Also, the mass discharged from the screw is calculated over time.



Table 3 shows the respective throughput and mass holdup data in the screw zone for different screw type and scraper speed. The throughput for comparing the two screw designs with scraper speed of 5 rpm, 15 rpm and 20 rpm are as shown below in Table 3:

**Table 3** Study of screw 1 and screw 2 design on mass discharge and mass holdup in screw zone

Run	Screw type	Scraper speed (rpm)	Throughput (kg/h)	Mass holdup in screw ( kg)
2	2	5	11.5	0.012
3	1	5	10.5	0.013
4	2	15	12.6	0.014
5	1	15	11.2	0.015
6	2	20	12.6	0.014
7	1	20	11.1	0.015

It is interesting to observe that the mass discharge rate out of the hopper is higher for the cases with screw 2 as compared to screw 1. This observation can also be compared to the theoretically calculated throughput from the equation 1 from Roberts [5], [9] as following:

$$m = \pi\rho\varphi\omega L(D_b^2 - D_s^2)/4 \quad (1)$$

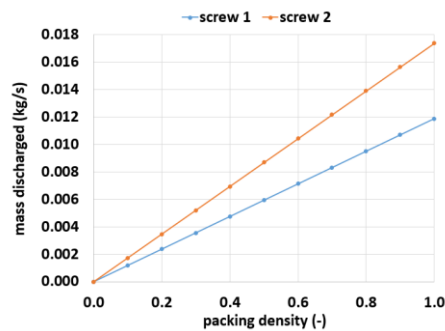
Where,  $m$  is the throughput in kg/s,  $\rho$  is the bulk density in kg/m<sup>3</sup>,  $\varphi$  is the packing density in screw,  $\omega$  is the screw speed in round per second (rps),  $L$  is the screw pitch in meter,  $D_b$  is the blade diameter in meter and  $D_s$  is the shaft diameter in meter.

The Figure 8 is prepared from equation 1 for the two different screws 1 and 2 respectively differing in screw pitch. It can be perceived that with changing packing density of particles inside the screw zone, the flow rate increases and is higher for screw 2 as compared to screw 1. This observation is well in agreement with the DEM simulation observation where screw 2 shows higher discharge in all the coupled cases of different scraper speed.

### Mass holdup in screw zone

The packing fraction of particles inside the screw zone is 0.24 and the volume of empty space to be filled with particle inside the screw zone is 83 ml which gives the volume of particles inside the screw zone to be ~ 20 ml. The maximum consolidation inside the screw should be 60 % of available empty space which is ~50 ml (packing fraction is 0.6). Therefore, the particles inside the screw zone is in safe operation mode to move freely and interact with the surrounding

particles and wall. The mass holdup in screw column of Table 3 shows the respective mass holdup in the screw zone for respective cases.



**Figure 8** Mass discharged vs time based on correlation proposed by Robert

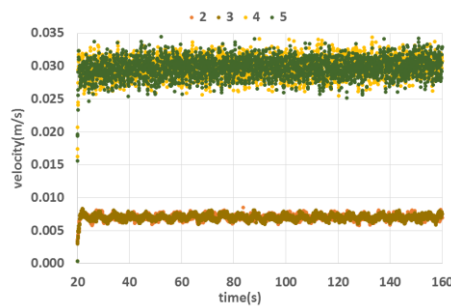
It is interesting to observe that the mass holdup in case of screw 2 is lower as compared to the screw 1. This effect can be attributed to the smaller pitch in screw 1 which can consolidate higher number of particles therefore, larger mass. Furthermore, the effect of scraper speed can also be observed in mass holdup inside the screw zone. It can be compared that the higher scraper speed of 15 rpm and 20 rpm shows higher mass holdup in the screw zone as compared to lower scraper speed of 5 rpm. The same mass holdup in screw zone for 15 rpm and 20 rpm scraper speed can be another reason for the similar discharge rate out of the screw. The mass holdup during the discharge time zone is constant all over for all the cases but differs in magnitude which can be attributed to scraper speed.

### Velocity of particles in screw zone

The average velocity of particles for the case of screw 2 is 0.049 m/s in the screw zone and that for screw 1 is 0.039 m/s. The speed of screw is 90 rpm in both the screw geometries which is 0.137 m/s when converted to linear velocity. Higher velocity of particles in screw 2 case can be attributed to lower mass holdup in screw 2 as compared to screw 1.

### Comparison of scraper speed

When the scraper speed is kept constant, the discharge is merely dependent on the screw shape (or pitch) see Table 3. The reason being the similar supply of powder from the scraper zone to the screw zone in both the cases i.e. different screw shape. However, as the scraper speed is increased, the flow rate is also seen to increase. This could happen because more number of particles per unit time are loosened with the scraper and are forced towards the screw zone. Further, when the scraper speed is increased from 15 rpm to 20 rpm, almost no increase in mass discharge rate is observed for both the screw cases. One reason could be the threshold of powder loosening is achieved in the scraper zone so that there is no further increase in powder mass flow rate from scraper zone to the screw zone. The other reason is the screw speed which is constant at 90 rpm, which would impact the throughput if changed.



**Figure 8** Velocity of particles in scraper zone

Figure 8 shows the velocity of particles in the scraper zone. The velocity of scraper is 5 and 20 rpm for cases 1, 2 and 3, 4 respectively. It can be observed in the Figure 8 that the average velocity of particles is 0.007 m/s for the case 1 and 2 (there is only difference in screw type and the scraper speed is kept at 5 rpm). Similarly, the average velocity of particles for case 3, 4 in the scraper zone are also same at 0.029 m/s. The velocity of particles in scraper zone are not influenced by the change in screw type. Also, with four times increase in scraper speed, average velocity in scraper zone is also increased by four times for both the screws signifying similar loosening of blend.

### 3.3 Impact of cohesion on flow pattern

This simulation was performed with screw 2. The cohesion energy density (reflecting cohesion in  $J/m^3$ ) value of particle-particle interaction is increased from 90000 (case 1) to 120000 (case 6) and particle-wall interaction is decreased from 6000 (case 1) to 1200 (case 6). The influence is the change in average particle velocity in the screw zone i.e. from 0.058 m/s to 0.066 m/s (see Figure 12). There is a little but not significant change in particle velocity in this zone, as on one side, the particle-particle cohesion increase restricts the particles to move freely with respect to each other whereas, decrease of particle wall cohesion tends the particles to move freely and not stick to the wall.

### Mass discharge out of the hopper

The mass discharge rate for case 6 and case 1 are compared and it is observed that the mass discharge for case 6 is 8.02 kg/h and for case 1 is 9.35 kg/h which is expected as the particle - particle cohesion is lower in case 1 as compared to case 6 which leads to lower interaction in between particles and hence higher discharge rate out of the screw.

## 4. CONCLUSION

A comparison of flow from two different type of screws are performed with DEM simulations. The mass discharge rate calculated from theoretical equations are compared to the simulations and are found to be well in agreement suggesting screw 2 to be better than screw 1. Further, impact of scraper speed is also investigated for the throughput. Overall, a vision is emerged to investigate different screw designs. Further, the impact of particle size, particle shape and process parameters change can be applied in order to evaluate its influence on the

flow. The findings are useful for comparing the screw designs and operation of screw feeders for handling cohesive powder.

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