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Analysis of seeded granulation in high shear granulators by discrete element method

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Abstract

In this paper, the process of seeded granulation in a high shear mixer is simulated by the discrete element method (DEM). A 5 litre Cyclomix granulator manufactured by Hosokawa Micron B.V. was simulated at different impeller rotational speeds. It has been observed that the seeded granules form by a continuous growth and reduction in size during the granulation process. Quantitative analysis shows that in general a higher number of seeded granules form at lower impeller rotational speeds; however it is found that for all the seeded granules the seed surface coverage by fines is from 5% to 60%. Further analyses revealed that seeded granules with the seed surface coverage higher than 50% are more frequently formed at high impeller rotational speeds. The work demonstrates the capability of DEM for modelling granulation processes, as a tool to explore the underlying mechanisms of granulation in general and seeded granulation in particular.

Keywords: Dem; Granulation; Seeded granulation; Seeded granules; Granule structure; Cyclomix

1. Introduction

Granulation of fine powders is carried out in many industrial sectors, such as food, detergents, pharmaceuticals and agrochemicals to improve physical and mechanical properties of powders, e.g. size, structure, dissolution rate, flow behaviour and to reduce problems associated with segregation and dust formation [1], [2], [3] and [4]. Considerable amount of research work has been carried out focusing mainly on the granulation regimes and mechanisms, modelling and control of the granulation processes, where granule size is of major concern [5], [6], [7], [8] and [9]. Nevertheless,

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little attention has been paid so far to the internal micro-structure and mechanisms leading to the formation of different internal granule structures. Granule properties depend not only on morphology and size, but also on the internal microstructure, which in turn influences the macroscopic and bulk behaviour such as bulk density, flowability and dissolution rate. Therefore, if the microstructure at the single granule level can be better controlled, the bulk properties of the granules will be more predictable. This is of great importance for industries concerned with the production of granules with good content uniformity, such as food and pharmaceuticals.

Rahmanian et al. [10] described a method of granulation, whereby a large particle of the feed is present at the granule core. They termed this method of granulation "seeded granulation" and showed that the formation of seeded granules was strongly dependent on the impeller tip speed and primary particle size distribution, given binder viscosity and binder to powder mass ratio. In the seeding mechanism, partially wetted primary particles and larger seed particles adhere to each other to form granules composed of a large particle surrounded by fines, as shown in Fig. 1.

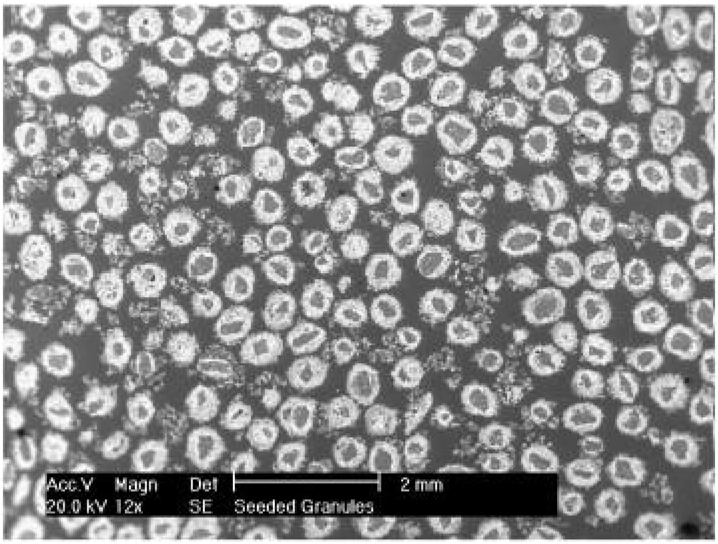

Fig. 1. SEM image of the internal structure of seeded granules.

A simple regime map for the seeded granulation of calcium carbonate powder was proposed [10], based on the Stokes deformation number introduced by Tardos et al. [11] and [12]. Experimental evidence suggested that Stokes deformation numbers above 0.1 favoured seeded granulation. However, it remains to be seen if such regime map can be generalised for other powders. There are uncertainties on the mechanisms of the process at the single particle/granule level which are responsible for seeded granulation, e.g. the effect of shape, surface properties, particle residence time, input energy, geometry of the impellers and type of granulators (batch or continuous) [13]. All

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of these parameters can affect the optimum process conditions and hence the internal microstructure of granules and formation of seeded granules.

In the present work an attempt is made to investigate the process conditions which lead to the formation and breakage of seeded granules by the use of the discrete element method (DEM). Full information on the particle flow pattern both at microscopic and macroscopic levels may be obtained [7] and [14], hence providing a better understanding of control and optimisation of the mechanisms of granulation processes through sensitivity analyses.

2. Methodology

DEM simulations of the granulation process were conducted using EDEM® software provided by DEM Solutions, Edinburgh, UK. The Hertz–Mindlin contact model was used for the elastic behaviour of the particles. In wet granulation, bonding forces are the results of the surface tension and viscous forces. In this paper, due to the limitation of the computer code, we only consider the surface tension forces and implementation of viscous forces will be carried out in future studies. A low value of coefficient of restitution is used in order to account for viscous dissipation. A linear cohesion model was used to simulate the interparticle cohesion force (F) based on the following equation:

$$F = kA \tag{1}$$

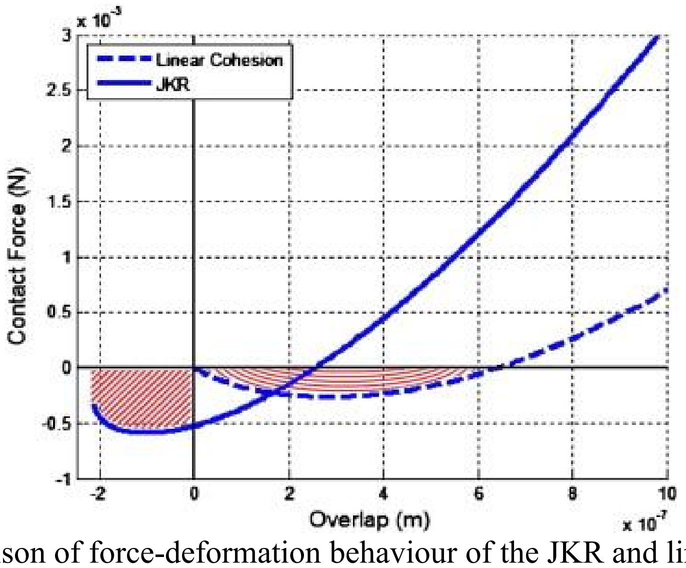

Fig. 2. Comparison of force-deformation behaviour of the JKR and linear cohesion contact models.

where A is the contact area between the particles and k is the cohesion energy density with the unit Jm^{-3}. The value k is calculated based on a surface energy from the JKR model [15], where the tensile work of the linear model (Eq. (1)) is equated with work of cohesion in JKR [15] (two shaded

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areas in Fig. 2). The material properties used in the simulations are summarised in Table 1.

Table 1. Material properties used in the simulations.

Property	**Particles**	**Surfaces**
Density (kg m^{-3})	800	7800
Poisson's ratio	0.2	0.29
Young's modulus (GPa)	0.24	200
Interface energy (J m^{-2})	1.5	–

The particle system for the simulation consists of 1460 8-mm in diameter particles and 146,000 2-mm in diameter particles representing seed and fine particles respectively. The size ratio between the seeds and fine particles is selected based on the minimum size ratio from the regime map suggested by Rahmanian et al. [10]. The interaction properties used in the simulations are summarised in Table 2. In these simulations all particles are cohesive, resembling the case where the binder is uniformly distributed among seeds as well as fine particles. Furthermore, as larger particles are simulated as compared to the experiments, the interface energies are adjusted such that the ratio of kinetic energies during collision to the tensile work of cohesion is roughly in line with that of experimental work.

Table 2. Interaction properties used in the simulations.

Property → ↓Interaction	**Coefficient of restitution**	**Coefficient of static friction**	**Coefficient of rolling friction**
Particle–particle	0.2	0.5	0.1
Particle–wall	0.2	0.3	0.1

A 5 litre Cyclomix high-shear mixer granulator, manufactured by Hosokawa Micron B.V. was selected for the simulation, and its 3D CAD geometry was imported into the DEM software as shown in Fig. 3. The granulator consists of an impeller with four sets of blades and a pair of knives. The impeller is enclosed in a bowl shaped in a frustum of a cone. The granulator knives cut/break the loose granules formed in the granulator.

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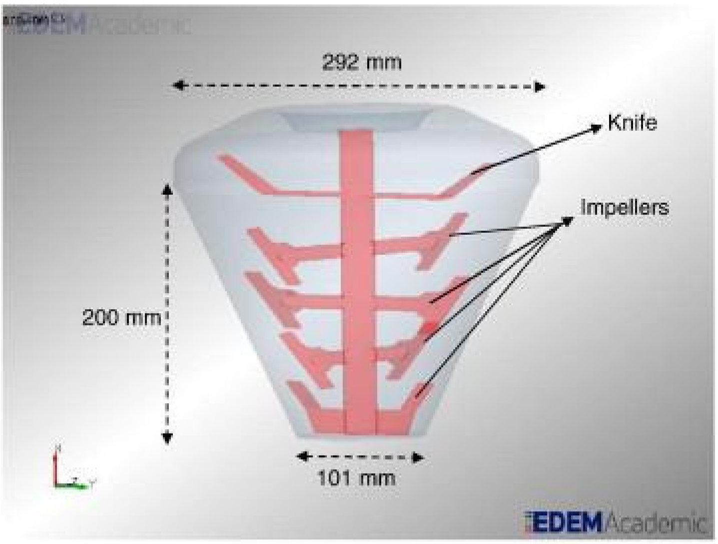

Fig. 3. Imported geometry of Cyclomix granulator.

3. Results and discussion

The particulate system was created by introducing a random mixture of seed and fine particles from a surface above the knives. The particles were then let to settle under the gravitational forces. The filling was carried out while the impellers were stationary. The simulation was then carried out for 10 s of real time at four different impeller rotational speeds; 150, 200, 287, 345 rpm.

Fig. 4 shows a snapshot of the velocity field inside the granulator for a representative rotational speed (287 rpm), revealing a relatively high shear region near the top impeller. This is in agreement with the previous work [8]. It should also be noted that the concentration of particles at the bottom of the granulator is lower than that of upper part.

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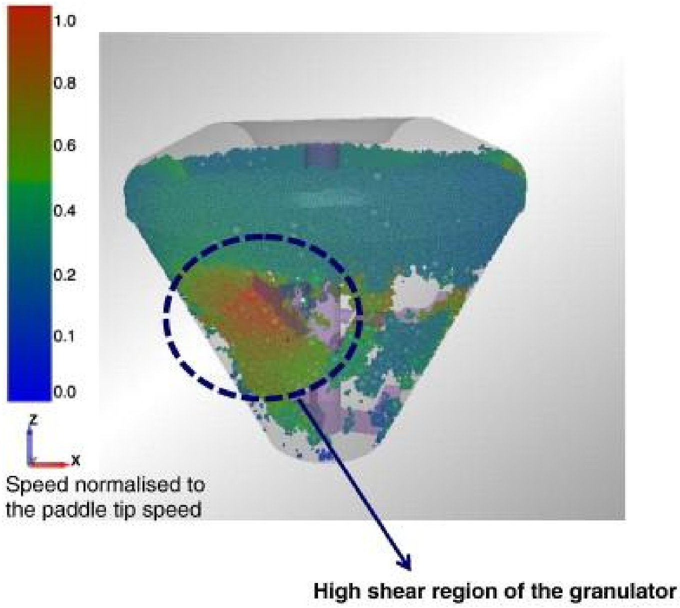

Fig. 4. The schematic flow field inside the granulator simulated by DEM, colours correspond to particle normalised velocity.

During the agitation the motion of particles and in particular those of the seeds affects the particle concentration in various regions of the granulator. The concentration of the seeds in different regions of the granulator (Fig. 5) for different impeller rotational speeds is shown in Fig. 6. It can be seen that as the rotational speeds are increased, the concentration of seeds increases at the top part of the granulator. It can also be seen that the seed concentration at the bottom for the rotational speeds of 287 and 345 rpm is lower than those of 150 and 200 rpm. This is due to the fact that more particles are lifted up at high impeller rotational speeds.

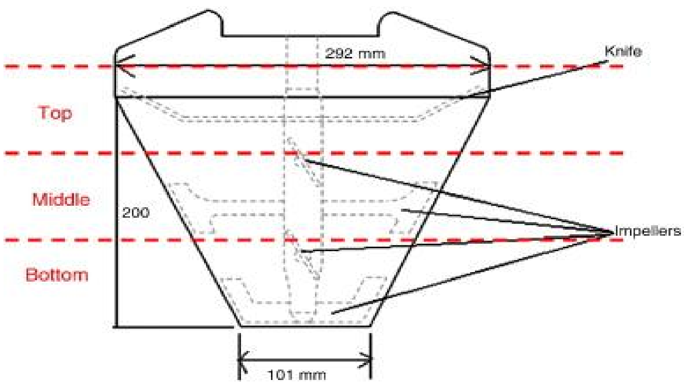

Fig. 5. Measurement regions considered for analysis.

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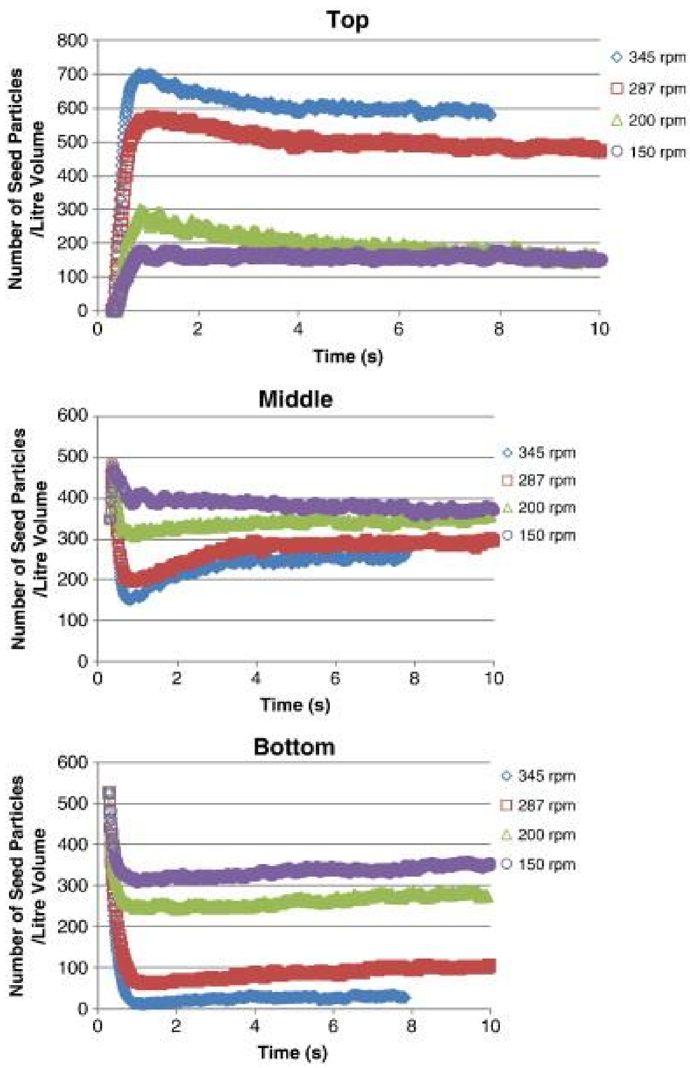

Fig. 6. Concentration of seeds at various regions of the granulator at different rpms.

A snapshot of the internal view from the granulator is shown in Fig. 7, where the formation of agglomerates can be observed qualitatively. It can be seen that the agglomerates have formed in both seeded and non-seeded forms. A closer observation reveals that the formation of seeded granules involves continuous reduction and growth in size (Fig. 8; this is best viewed by video observations). Five of the seeded granules are visualised in Fig. 8 (other particles are not displayed for clarity) at different sequential times. The seeded granules in Fig. 8a grow in size as granulation proceeds to the stage in Fig. 8d. As it can be seen from Fig. 8f these granules are now breaking. This phenomenon goes on continuously during the granulation process and causes the seeded granules to grow by adhesion forces and to reduce in size by breaking under shear deformation, giving rise to different sizes and coordination numbers.

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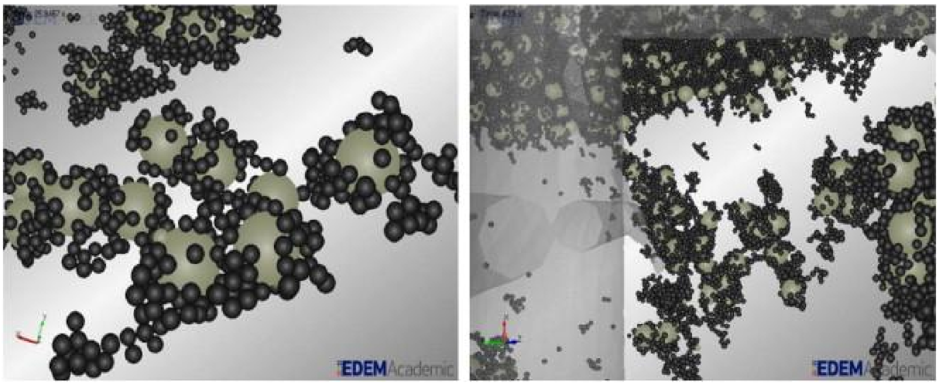

Fig. 7. An internal view from simulated granulator showing seeded and non-seeded granules.

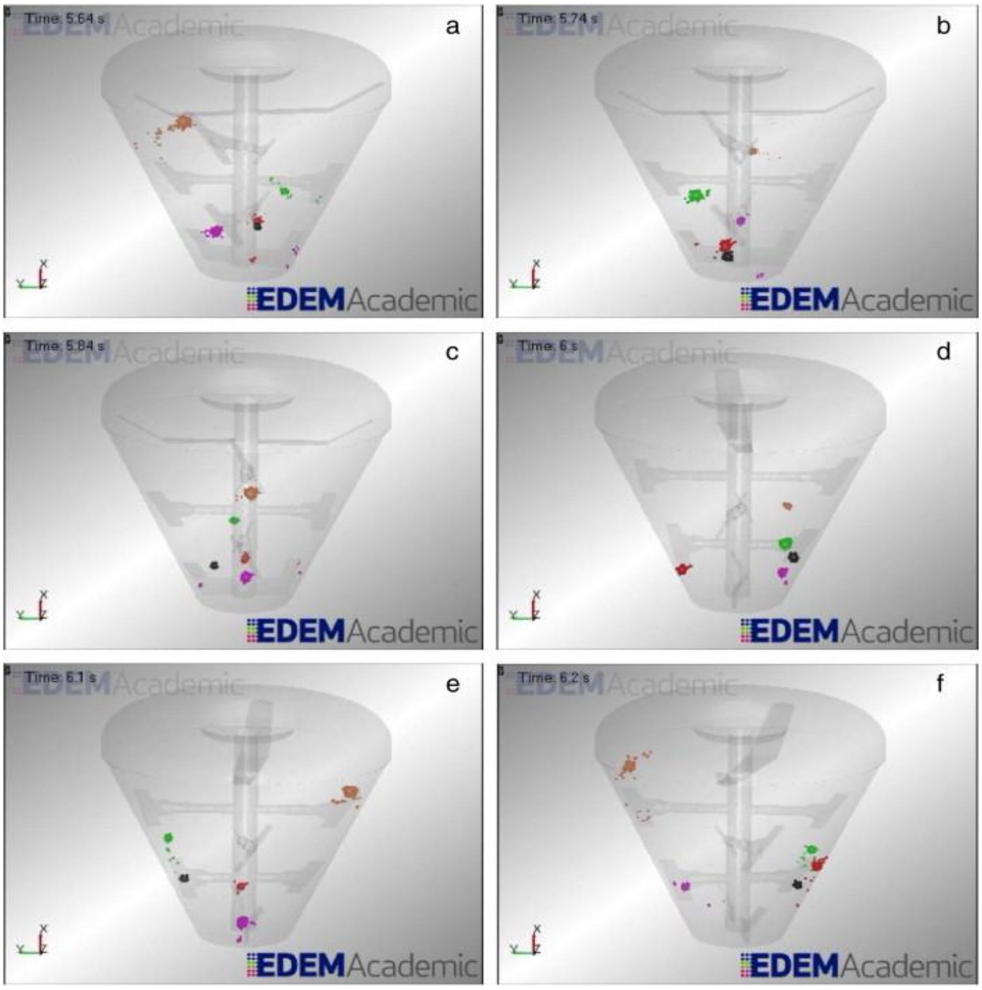

Fig. 8. Simulation of reduction and growth of seeded granules. Snapshots are taken at different sequential times.

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The formation of seeded granules is quantitatively analysed for different impeller rotational speeds. Fig. 9 shows the number of produced seeded granules in the granulator for all rotational speeds. It can be seen that a significantly higher number of seeded granules are produced at 150 and 200 rpm as compared to those of 287 and 345 rpm. The results in Fig. 9 are not in agreement with the findings of Rahmanian et al. [10], who have shown that seeded granules are formed with a higher probability at higher rotational speeds under specific operation conditions. However it should be noted that for the results in Fig. 9, the seeded granules are taken as those which have a seed particle that is bonded with fines, regardless of the number of fines. This means that a seeded granule could be identified by the computer algorithm even when the surface coverage of fine particles is sparse and the coordination number of the fines is small. Further refinement of the results in Fig. 9 is required to provide a more realistic criterion for defining a seeded granule.

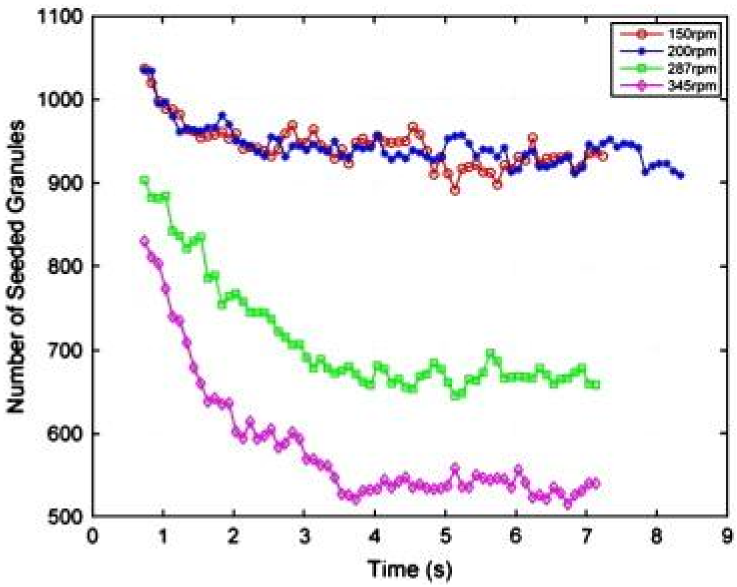

Fig. 9. Seeded granules for different impeller rotational speeds.

In principle, a properly seeded granule should have the seed fully covered with at least one layer of fines. Based on the size ratio of seed to fines (d_{seed}/d_{fine} = 4) analysed in this work, a seed should be in contact with approximately 50 fine particles to get full coverage. However, additional quantitative analyses show that seeded granules in Fig. 9 are formed with a seed surface coverage ranging from 5% to a maximum of 60% of full coverage. This was also qualitatively observed in Fig. 7, where no seeded granule could be seen with the full seed coverage. Further quantitative analysis in Fig. 10 shows the number of seeded granules with a minimum of 40% of surface coverage at different impeller rotational speeds. As it can be seen,

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the results are closer for the impeller rotational speeds as compared to Fig. 7. The trend is reversed when granules with a minimum of 50% coverage are taken into account, as shown in Fig. 11. In this case seeded granules are in fact more frequently seen at higher rotational speeds, i.e. 345 and 287 rpm. It should be noted that the experimental work reported by Rahmanian et al. [10] showed that all analysed seeded granules had their seeds fully covered by fines. A few possible reasons could have contributed to the discrepancies in the surface coverage observed between the simulations and previous experimental work [10]. One reason could be that the granulation experiments [10] were carried out for a few minutes, while the current simulations are only carried out for 10 s of real time due to the computing limitations. Another reason could be due to differences in particle number (so that a good statistical reliability could be obtained), shape and size distribution between the simulations and experiments [10]. Yet another possible reason could be the effect of binder viscosity and level of interface energy. Further investigations of the aforementioned reasons could be the topics of future work.

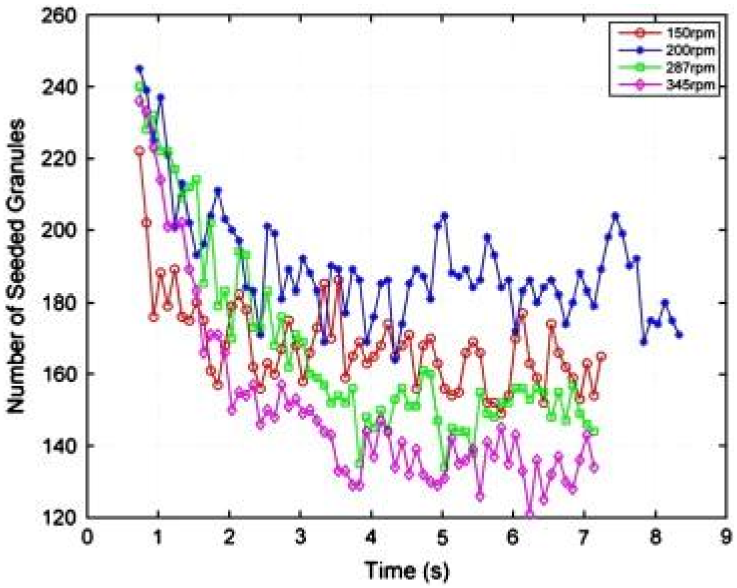

Fig. 10. Seeded granules (minimum 40% of the seed surface covered) at different impeller rotational speeds.

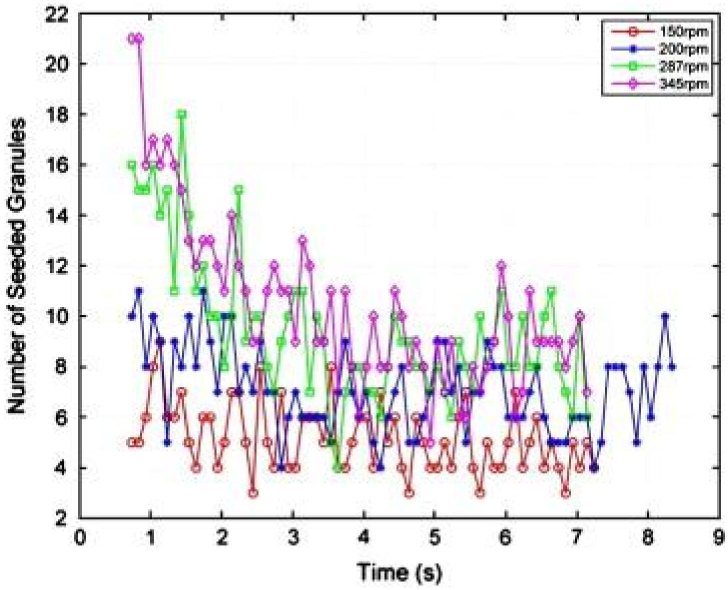

Fig. 11. Seeded granules (minimum 50% of the seed surface covered) at different impeller rotational speeds.

4. Conclusions

The process of seeded granulation in a 5 litre Cyclomix high shear granulator has been simulated by DEM. The results show that during granulation process the seeded granule formation involves a continuous growth and reduction of granule size. The simulation results show that all seeded granules have 5 to 60% surface coverage of the seeds. Further quantitative analyses show that the seeded granules with high surface coverage are present more frequently at high rotational speeds. Further work is needed to quantify the critical conditions, such as the Stokes number representing the conditions that are needed for enhancing seeded granulation; nevertheless, the work has demonstrated the capability of DEM for modelling granulation processes, to investigate the underlying mechanisms of granulation in general and seeded granulation in particular.

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