Modelling of segregation during injection moulding

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Abstract. The goal of this study is to establish a proper simulation model of segregation, a phenomenon which causes inhomogeneity in filled polymer products. We did preliminary research, in which we calcinated injection moulded specimens of 80 mm x 80 mm x 2 mm, with 75 µm, 125 µm and 250 µm glass beads with 10 m%, 25 m% and 40 m% filler rates. According to preliminary simulations, the boundary conditions were set and an EDEM model was created.

1. Introduction
Since the second half of the 20th-century, polymer products have been conquering the industry. Injection moulding is one of the most productive and most widely used polymer processing technologies, which allows engineers to design virtually any kind of product while guaranteeing fast and cost-effective manufacturing. The versatility of injection moulding is also used to create complex manufacturing procedures, like when combined with 3D printing technologies [1]. Even though primarily injection moulding is a technology of polymer manufacturing, processing metal [2] and foam [3] are also possible, demonstrating the endless potential of the subject.

Homogeneity is essential to produce products which meet the needs of the market. Unfortunately, homogeneity might be difficult to accomplish, especially when fillers are added to the product. In this case, more fillers will be located at the end of the path of the melt flow and closer to the surface of the mould, in the so-called frozen layer. This phenomenon is called segregation. Perhaps the most common example to this is using masterbatch colouring, for in this case, the segregation of the colouring pellets causes unevenly coloured lines across the surface [4]. Depending on the type of the filler, the effect of segregation also differs. According to some investigation, the phenomenon at the end of the flow path is nearly neglectable in case of using reinforcing fibres, while observing spherical fillers like beads, the segregation across the flow path is significant [5]. Further research confirmed, that regarding beads, different sizes induce different degree of segregation, and in this case shrinkage is also a problem that must be considered [6]. Another important issue when it comes to fibre fillers is their orientation, which is a widely researched subject [7].

In the design phase, FEM simulation software is used by engineers to predict and prevent errors that may occur during the actual process of injection moulding. This way, more complex tasks can be optimised, which saves precious time [8]. However, simulating segregation is difficult. Despite this fact, quite few research was made in this field. Even though continuum modelling is often used in polymer manufacturing simulation software [9, 10], this technique cannot model segregation. A discrete element method can analyse the behaviour of the particles one by one, therefore it may be better for this purpose than the finite element method [11, 12].
According to the literature review, segregation occurring during injection moulding can significantly alter the distribution of the fillers, resulting in degrading properties. Since DEM can be used to simulate the segregation of distinct particles, the aim of this study was to investigate, whether FEM-DEM simulations are capable of modelling segregation during injection moulding.

2. Materials, machinery and methods
We injection moulded glass bead-filled specimens. The matrix material was TIPPLEN H 145 F polypropylene, as it has remarkable processability. Based on the literature, we used three different sizes (<75 µm, 70–125 µm, 150–250 µm) of glass beads. First we sieved the Cerablast G120, G100 and G50 glass beads to sort them according to size. Then we compounded the beads into the polypropylene with an LTE 25-30/C simple screw extruder, creating 6 mm long pellets, and injection moulded the 80 mm x 80 mm x 2 mm specimens using an Arburg Allrounder 370 S 700 290 machine. It is a servo-hydraulic machine with a maximum clamping force of 70 tons. Its maximum injection pressure is above 2000 bars and it is equipped with a 30 mm diameter position-regulated screw, so the settings during procedure remain unchanged and the reproducibility of the products is assured. We determined the glass bead content of the specimen by calcination, using a Denkal 6B furnace.

3. Experiments
We performed several tests on the specimens, then compared the data to the segregation simulation results.

3.1. Preliminary experiments
Before creating the specimens, we ran simulations in Moldflow 2018, in order to determine the ideal injection speed. We found that injection speed affects the frozen layer, which is a determining factor in segregation. The simulations showed that injection speeds between 20 cm³/s and 80 cm³/s result in a significantly thinner frozen layer. After the simulations, we injection moulded the specimens (Figure 1).

3.2. Segregation
In order to observe segregation across the flow path, we divided a specimen into four sections (Figure 1), in which we examined the distribution of the glass beads by calcination. According to the ISO 3451-1 standard, calcination lasted for four hours, at 600 °C. After all the polypropylene matrix material burnt, the mass of the leftover material was weighed. In order to see how the size and quantity of the beads affect segregation, we performed the tests using 75 µm, 125 µm and 250 µm fillers with 10 m%, 25 m% and 40 m% glass bead contents each. There was no significant change in density at 10 m% from the mass differences in the case of smaller beads. However, the density of 250 µm fillers increased by 2–5% at the end of the flow path. We found, that the larger the filler, the more inhomogeneous the system is, since at the end of the flow path the glass beads tend to pile up. With 40% content of the 125 µm glass beads, the maximum difference in distribution was 8%, while with 250 µm this number was over 12%. This phenomenon may be a result of the drag force, since the larger surface is affected by greater forces in the melt flow. Moreover, the larger beads are also more likely to collide with each other.

Figure 1. The specimen and the four different sections for the examination of segregation
3.3. Preliminary simulations

We ran preliminary simulations in Autodesk CFD 2018 and Moldflow 2018 to set the boundary conditions of the behaviour of the polypropylene and glass beads. These boundary conditions are necessary for the discrete element method.

3.3.1. The torque limit required to tear out a glass bead

The torque limit above which a glass bead is torn out is a crucial boundary condition. As the mechanical model suggests, this torque is related to how much the filler is embedded into the frozen layer. Whether the bead stays still or is dragged out by the flow depends on the balance of the torques applied to point “A” (Figure 2). The moments balancing each other are derived from the flowing material and the vacuum between the frozen layer and the embedded bead. There is vacuum in the system due to the fact, that when a bead is torn out, there is a small gap between the frozen layer and the bead, which the viscous melt cannot flow into immediately. In the simulations, we examined different rates of embedment—half, a quarter and an eighth of the bead. Preliminary studies suggest that examining a higher rate of embedment than half is unnecessary, since in that case the bead stays in place as it is self-locking by shape. The cross-section of the flow was set to be five times the diameter of a bead and a p=0 Pa boundary condition was set at the end of the flow path (Figure 3).

We found that with an injection speed of 5 cm³/s, the 250 µm glass beads are torn out when the contact surface of the filler and the melt is below 70%, while in the case 75 µm beads this is 75. Higher injection speeds decrease this limit, but it never went below 50%. Thus, it is probably true that if a bead is embedded at least 50%, it will not be torn out by the flow. However, a bead may stay immobile even if far less than half of it is embedded, especially in the case of smaller beads and slower injection speeds.
3.3.2. Determining injection moulding parameters for EDEM 2018.2 simulations. The two essential parameters are filling time and the velocity profile in the cavities. For the three sizes of the fillers, we used three different, reduced-sized models in the simulations. The Moldflow simulations showed that the velocity of the melt in the frozen layer is 0 and it increases towards the middle of the section, where it reaches its maximum. Along the flow path, melt velocity decreases, and reaches its minimum at the end of the flow path (Figure 4). Naturally, these phenomena cannot be neglected in EDEM simulations.

![Figure 4. The velocity profile in Moldflow 2018](image)

3.4. Modelling segregation in EDEM 2018.2 software

Modelling segregation is a rather complex problem, for several factors must be considered. For this reason, EDEM simulation would seem to be ideal to perform this task. Software packages using a discrete element method do not consider complex, multi-element systems as continuums. This enables the observation of the behaviour of the glass beads one by one. Considering the velocity and the viscosity results of the Moldflow simulations, drag force model was used. The particles’ collision with each other or the wall was handled as a linear spring contact model. The data of the system gathered from the previous preliminary simulations were handled with the use of C++. Establishing such a complex simulation did pose some difficulties. In the end, we ran 2D simulations based on the velocity profile according to the values in the middle line, disregarding the effect the mould’s surface might have on the velocity towards it (Figure 4). These profiles were chosen according to the right time step from Moldflow. Since we did the procedure manually, we considered only 10 time steps in a simulation. The established model consisted of four parts (Figure 5):

- the factory, which emits the glass beads modelling particles according to filling time, m%, and the size of the beads,
- the shear flow, which describes the characteristics before the melt front, according to the velocity profile,
- the overall dimension of a 2 mm x 10 mm x 80 mm geometry
- and the fountain flow which describes the behaviour of the melt front itself.
4. Results
In this section we present the results of the simulations.

4.1. The results of the simulations
The first obvious phenomenon of the model is the increase of density of the beads across the x axis in the frozen layer (Figure 6). This is due to the characteristics of discrete element modelling, for the generated ten velocity profiles of the ten time steps mean ten differently characterised fountain flows. Since there are velocity components in the y axis, the beads located in the melt front gain velocity in the y direction, getting stuck in the frozen layer, and having their speed reduced to 0. Regarding the frozen...
layer, the results are satisfying, as the effect of injection speed can be observed quite well, according to the expected tendency (Figure 7). However, a great error of the model is that it does not consider the frozen layer as a physical wall, rather a layer whose speed is 0. This results in the anomaly that a glass bead can be embedded into it, regardless of the fact that it is already in the solid state (Figure 8). Another rather unrealistic anomaly is that at the beginning of the flow path at the top and the bottom of the geometry, beads are stuck in the frozen layer (Figure 9), even though it is not even formed at that time. This increase in density is in contrast to results in the literature and what happens in practice, as the beginning of the path is the very last place where the melt solidifies. The anomaly is somewhat connected to the other error demonstrated in Figure 8 and probably occurs due to the fact that several beads are located at the beginning of the flow path, and the possibility of collision is very high, therefore more beads are pushed into and embedded in the frozen layer.

**Figure 7.** The effect of injection speed on the frozen layer

![Figure 7](image)

**Figure 8.** The anomaly of the filler particles in the model

![Figure 8](image)

4.2. The distribution of the glass beads

The numbers of beads according to the EDEM simulation were placed into histograms with 2 mm-wide domains. These histograms were converted to a diagram (Figure 10). The anomaly of increasing density at the beginning of the flow path can be observed in general, but more significantly in the case of the injection speed of 5 cm³/s. Even though the distribution is quite uniform, at the end of the flow path, there is an expected peak of density. In this respect, the EDEM model worked well, but it is not precise enough, therefore it needs further research and development.
5. Conclusion
In this section we summarise the results of the research and provide some ideas for further development.

5.1. Summary of the results
Comparing the results of the EDEM simulations to the preliminary experiments, it can be stated that the model is promising regarding the frozen layer, as it shows similar tendencies in the thickness of the frozen layer when the injection speed is altered. The simulations could also indicate that the glass beads pile up at the end of the flow path. However, several rather unrealistic anomalies occurred, which need to be corrected. Considering these, using EDEM simulation is promising and the model could be able to simulate segregation after improvement.

5.2. Ideas for further development
As already mentioned before, the boundary condition of 50% embedment may be too much on the safe side, thus finding a more accurate limit might be beneficial. The increase of density across the x axis could be reduced with the use of more than ten time steps, since the error of numerical instability can be eliminated this way. To solve the problem of the 0-speed frozen layer, mobile walls could be used in the model, which would function as a physical obstacle to the filler particles. However, these walls must enable the beads to be freely embedded and perhaps get dragged out by the flow itself or get pushed out by other beads. These walls should also be able to simulate the thickening of the frozen layer. Another way to reduce error is to use a dynamic factory, which adapts to the continuously altering frozen layer. Even though only mono-disperse systems were examined, it might also be beneficial to observe poly-disperse systems, for they are more common in practice.

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References
[1] Boros R, Kannan Rajamani P and Kovács J G 2019 Combination of 3D printing and injection molding: Overmolding and overprinting Express Polymer Letters 13 889-897
[2] Ammosova L, Mönkönnen K and Suvanto M 2020 Precise fabrication of microtextured stainless steel surfaces using metal injection moulding Precision Engineering 62 89-94
[3] Wu H, Zhao G, Wang J, Wang G and Zhang M 2019 A kind of special weld lines with high specific strength and elongation obtained by core-back chemical foam injection molding Express Polymer Letters 13 1041-1056
[4] Zsiros L and Kovács J G 2018 Surface homogeneity of injection molded parts Periodica Polytechnica Mechanical Engineering 62 284-291
[5] Hegler R P and Mennig G 1985 Phase separation effects in processing of glass-bead- and glass-fiber-filled thermoplastics by injection molding Polymer Engineering and Science 25 395–405
[6] Kovács J G 2011 Shrinkage alteration induced by segregation of glass beads in injection molded PA6 Experimental analysis and modeling Polymer Engineering & Science 51 2517–2525
[7] Albrecht K, Baur E, Endres H-J, Gente R, Graupner N, Koch M and Müssig J 2016 Measuring fibre orientation in sisal fibre-reinforced, injection moulded polypropylene – Pros and cons of the experimental methods to validate injection moulding simulation Composites Part A: Applied Science and Manufacturing 95 54–64
[8] Wang M-V, Fatahul A and Vu V-H 2019 The Study of Optimal Molding of a LED Lens with Grey Relational Analysis and Molding Simulation Periodica Polytechnica Mechanical Engineering 63 278-294
[9] Ingber M S, Graham A L, Mondy L A and Fang Z 2009 An improved constitutive model for concentrated suspensions accounting for shear-induced particle migration rate dependence on particle radius International Journal of Multiphase Flow 35 270–276
[10] Nott P R and Brady J F 1994 Pressure-driven flow of suspensions: simulation and theory Journal of Fluid Mechanics 275 doi:10.1017/s0022112094002326
[11] Liu G, Yu F, Wang S, Liao P, Zhang W, Han B and Lu H 2017 Investigation of interstitial fluid effect on the hydrodynamics of granular in liquid-solid fluidized beds with CFD-DEM Powder Technology 322 353-368
[12] Yu H, Cheng W, Wu L, Wang H and Xie Y 2017 Mechanisms of dust diffuse pollution under forced-exhaust ventilation in fully-mechanized excavation faces by CFD-DEM Powder Technology 317 31-47