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Simulation of Compression Molding of Thermoplastics Using CAE Tools: Assessment of Operational Conditions for Mold Design Development

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Abstract. This study aims to develop a simulation-based research to evaluate the influence of primary operational conditions on the efficiency of compression molding in processing thermoplastic parts in a mold design with no air venting. Moldflow Insight has been used to simulate the compression molding process to assess the quality of a range of semi-crystalline and amorphous thermoplastic products, to study the performance efficiency of the said mold. Simulation results were obtained by varying the mold surface temperature, melt temperature, charge geometry and mesh element size during processing thermoplastics like polypropylene, polyethylene, polystyrene, and polycarbonate. The findings showcased air entrapment at the corners of the mold cavity, which lowered the process efficiency when the mold operated with no venting under varied processing conditions. Simulation results indicated a need to introduce air vents on the mold's parting line. The findings revealed that the compression cycle time and waste generation could be diminished when air vents were included in the mold design and optimal operating conditions were used. Hence, a compression molding mold design incorporating air vents in areas of high air entrapment was developed.

Keywords. Compression Molding, Thermoplastics, Air Entrapment, Venting

1. Introduction

Compression molding of thermoplastics is highly discussed in the scope of use for composites but is seldom discussed on an individual basis to determine appropriate processing parameters and temperatures. Other than compression molding there are different methods used for making composites including the Hand Lay-Up, Open molding, resin infusion methods and injection molding, but compression molding is the most used and convenient method as it provide better surface finish, high pressure processability and high final product quality. (1-3) Hence, leading to a potential research gap.

With the advancement in computational simulation technology, engineering projects can ensure high precision in manufacturing compression molds for

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thermoplastics.(4) Computation analysis aided by commercially available software is a widely accepted strategy applied by plastics processing industries before manufacturing compression molds. (5-6) Computer Designing and Computer Simulation can aid in determining the suitability of a mold and product design for mass production upon clearly represents part designs and verifies the stress and deformation values. (7-9) Further, engineers can also work on evaluating alternative materials without physically using any material and compromising the availability of machine time for production. (10) Furthermore, simulations can also be utilized to optimize the processing parameters to produce better quality processing and products.

Henceforth, this study covers the CAE analysis cycle of compression molding of semi-crystalline and amorphous polymers. The following sections cover the methodology and results of the said simulations.

2. Methodology

The methodology for the said study was conducted in two steps. The first step comprised the designing the compression-molded product and the mold used for processing. The second step involved studying the compression molding of semi-crystalline and amorphous polymers using simulation software to identify major areas of air entrapment.

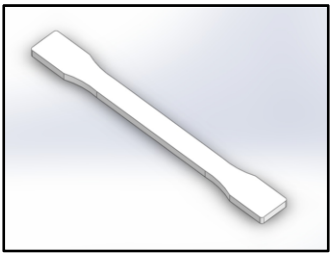
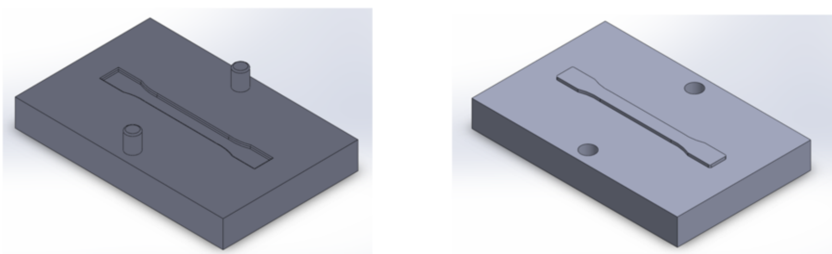


Figure 1. Model of the product design developed in SolidWorks CAD version 2016



(a) (b)

Figure 2. Mold model (a) Cavity and (b) Core developed in SolidWorks CAD version 2016

The simulations were performed for each polymeric sample of the compression-molded product for different operational conditions using the CAE package in Moldflow Insights (version 2019). As per the cavity design in Figure 2a, a three-dimensional compression model was developed to be studied in Moldflow Insight. In the present simulation study, a fill+pack model was used to analyze the behavior of thermoplastics while undergoing compression molding. The polymeric materials were compressed for 100 s during one cycle.

For each polymer, simulations were conducted by varying the initial charge geometry, mesh size, melt temperature, and mold temperature (discussed in the subsequent sections), resulting in 400 simulations. Other parameters that affected processing were maintained constant (Table 1). (11) Based on the simulation results, the masses of the different compression-molded products (M_{comp}) were used to derive the average compression-molded masses to evaluate the process variability, keeping into consideration the standard deviations. Here, the expected theoretical ideal mass (M_{Ideal}) obtained for each polymeric sample was used as a standard to indicate any variability in processing results. The efficiency of mold filling (n) was calculated using the simulated and ideal masses in equation mass. Equation 1 can further be used to evaluate the performance efficiency of the process and identify the specific operating conditions under which the mold gets filled completely without the presence of air bubbles. These results helped investigate the process performance under distinct processing conditions using a single parameter associated with each processing condition. Furthermore, the presence of air traps was also studied using the air traps analysis in Moldflow Insight.

$$\eta\% = \frac{\boldsymbol{M\,Ideal}}{\boldsymbol{MComp}} * \mathbf{100} \tag{1}$$

Table 1: Range of the processing parameters utilized in the simulation study

Polymeric Material	Range Variable Parameters			
	Mold temperature (°C)	**Melt temperature (°C)**	**Mesh size (mm)**	**Initial Charge Geometry**
Polypropylene	30,40,50,60,70	200,210,220,230,240	4mm, 2mm	Cuboidal, Cylindrical
Polyethylene	20,30,40,50,60	200,210,220,230,240	4mm, 2mm	Cuboidal, Cylindrical
Polystyrene	30,40,50,60,70	210,220,230,240,250	4mm, 2mm	Cuboidal, Cylindrical
Polycarbonate	80,90,100,110,120	270, 280, 290, 300, 310	4mm, 2mm	Cuboidal, Cylindrical

2.1. Processing Parameters

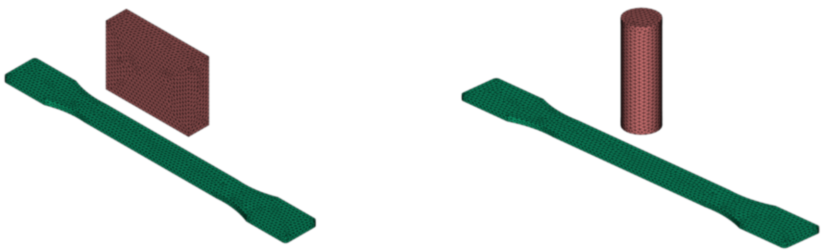
2.1.1. Initial- Charge Geometry

The amount of initial charge used highly impacts the amount of raw material required for a process. Hence, initial charge mass is an important factor that was taken into consideration for the scope of this simulation to determine the cost of the final product for industrial mass production. Equation 2 was used to calculate the initial mass of the charge.

$$i = V\rho + s \tag{2}$$

Where 'i' is the initial mass of the charge, 'V' is the volume of the product, 'ρ' is the density of the polymer and 's' is the percentage shrinkage of the polymer. The percentage shrinkage and required volume of the initial charge of the polymers used. The volumetric shrinkage of polymers under study was taken into account while designing the compression element to ensure that the final volume of the compression-molded product is equivalent to the product volume, i.e., around 7284.24mm^3 after mold filling, cooling, and solidification.

Different charge geometries are known to have different fill times. Hence, for the scope of this study, two types of charge geometry were used; cylindrical and cuboidal. Using the volume derived using equation 2, the dimensions of different charge geometries were calculated. All the charge geometries were designed in Solidworks 2019 and placed above the dumble-shaped product for the scope of the compression molding study (figure 6). The simulation results were then monitored to note the impact of charge geometry on the mold filling efficiency.



(a) **(b)**

Figure 3: (a) Rectangular Charge Geometry (b) Cylindrical Charge Geometry

2.1.2. Meshing

Moldflow Insight generates a two-dimensional or three-dimensional mesh to divide and annotate the domains in a mold or part design in the pre-processing stage. (12-14) In the study, the CAD models of the product and initial charge were converted into tetrahedral solid meshes before performing the required analysis. (15) Different mesh sizes i.e., 4mm and 2mm, were used to obtain results across different processing parameters as indicated in figure 5. The resulting geometry was divided into different numbers of elements which increased with a decrease in mesh size. The simulation results were then used to study the process efficiency, time taken for simulations, and change in output.

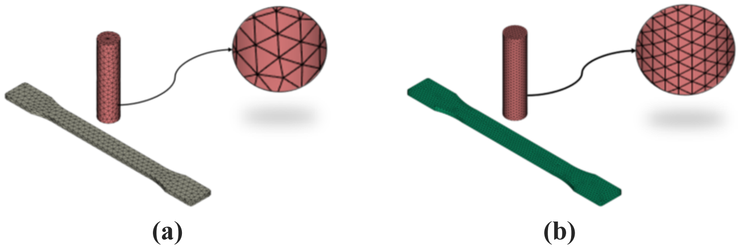


Figure 4. Different sizes of mesh element (a) 4 mm (b) 2 mm

2.1.3. Melt Temperature and Mold Surface Temperature

In this study, a range of mold and melt temperatures were studied to obtain the optimal range of processing. Furthermore, the impact of mold and melt temperature on process efficiency was also studied.

As per the simulations, the mass of the dumble-shaped products was used to evaluate the efficiency of the compression molding process with respect to the expected ideal mass of the product (as per density calculations) The compression-molded mass (M_{ccomp}) estimated in the simulations was compared with the expected ideal mass (M_{ideal}) of the product and the deviations between the data (δ) were calculated using equation 3. This was used to obtain the accuracy of the simulation results to obtain optimal processing conditions.

$$\delta\,\% = \{(\frac{Mideal}{M\,comp})\text{- }1\} * 100 \quad (3)$$

3. Results

3.1. Effect of Processing Parameters

3.1.1. Initial Charge Geometry

In the simulation study, it was observed that cuboidal geometries required less material to completely fill the mold to avoid short shots, but the outputs indicated lower mold filling efficiency and higher degree of deviation from ideal expected product mass. On the other hand, cylindrical geometries offered higher degree of mold filling efficiency and less deviation from ideal expected product mass. Hence, becoming a more favorable initial charge geometry, as observed in figure 5 and figure 6. Further, semi-crystalline polymers (Polypropylene, Polyethylene) showcased higher level of deviations (30-40%) and low mold filling efficiencies than amorphous polymers (Polystyrene, Polycarbonate- 10-20%) when subjected to similar processing conditions and charge geometries. Small air traps were observed around the ends of the product geometry (Figure 7). Here, higher mold filling efficiencies indicate better utilization of raw materials, less energy consumption, better mechanical properties of product, and smaller air traps.

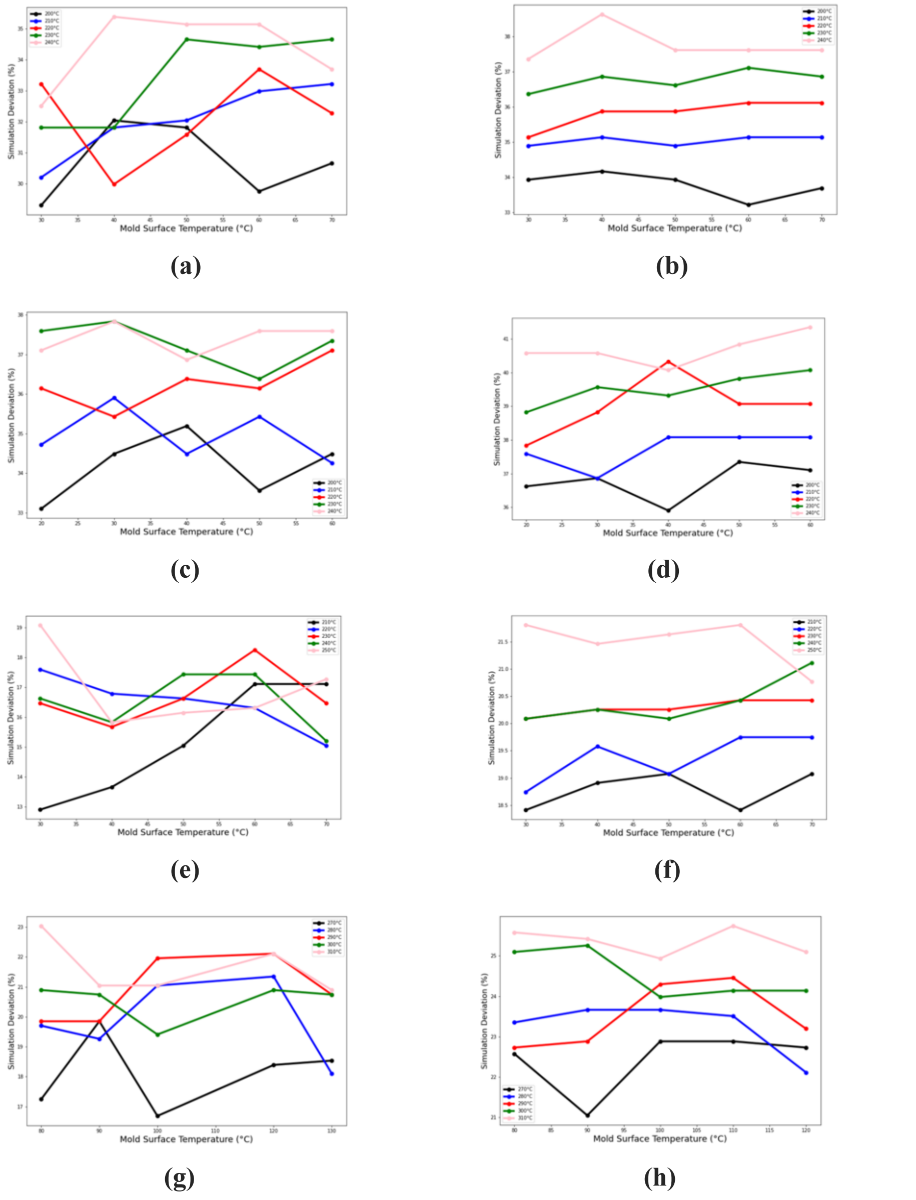


Figure 5: Simulation deviation with varying mold surface temperature and melt temperature with 4mm mesh size for studied polymers using cylindrical charge geometry (a) PP (c) PE (e) PS (g) PC and rectangular charge geometry (b) PP (d) PE (f) PS (h) PC

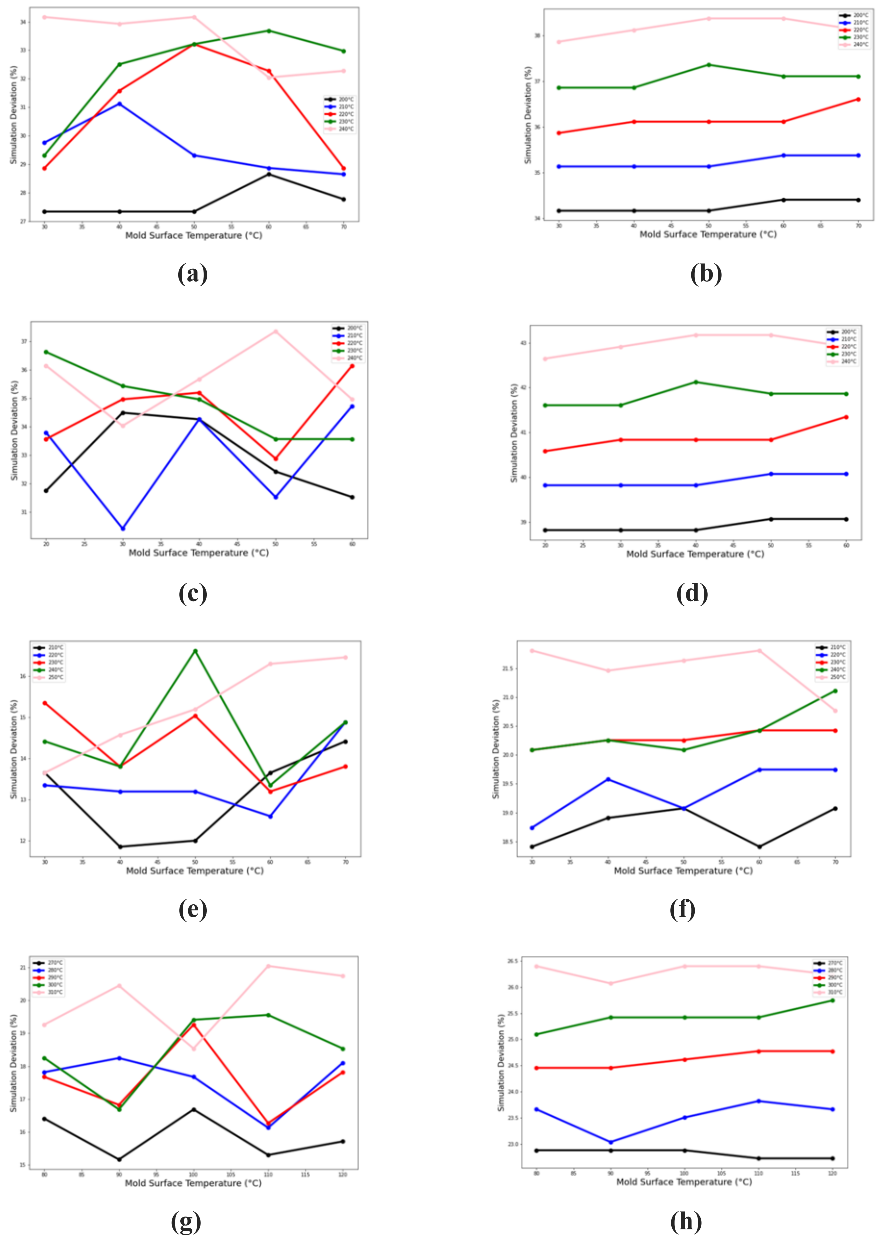


Figure 6: Simulation deviation with varying mold surface temperature and melt temperature with 2mm mesh size for studied polymers using cylindrical charge geometry (a) PP (c) PE (e) PS (g) PC and rectangular charge geometry (b) PP (d) PE (f) PS (h) PC

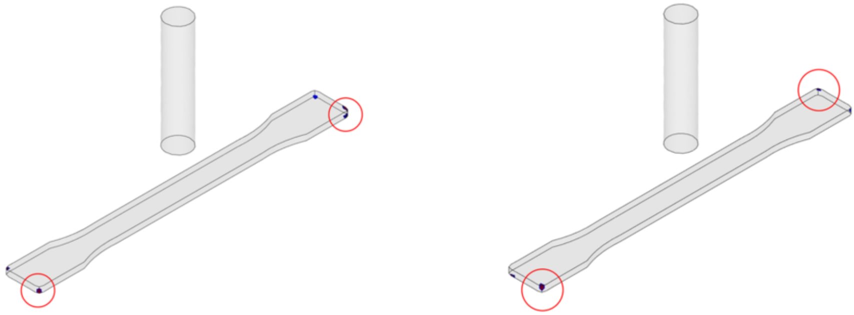


Figure 7: Air entrapments observed during simulation

3.1.2. Mesh Size

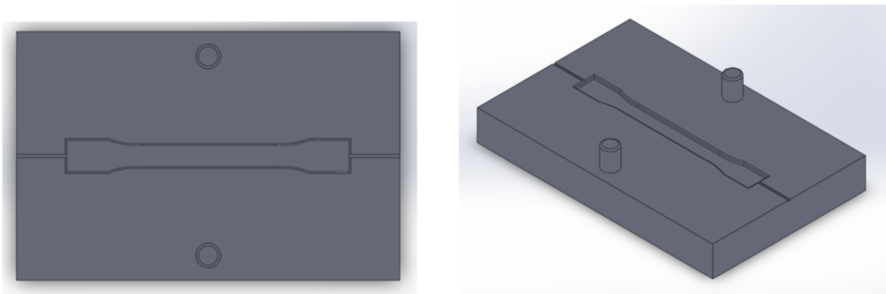
The simulation studies indicated that a tetrahedral geometry is able to obtain 97.1 % node refinement in complex geometries, but fails to refine nodes across corners and edges. It was observed that the level of mesh refinement or mesh density only has a very low impact (2-3%) on increasing mold filling efficiency for both semi-crystalline and amorphous polymers (Figure 5). In the cases studied, the mesh with highest level of refinement or highest mesh density was associated with the longest time for computation. Even as the accuracy of results increased slightly with mesh refinement, the time taken computation increased manifolds hence, increasing the processing time for the simulation. It was further observed that higher mesh refinement showcased more warnings during processing due to issues in node refinement across the edges of the products. Upon processing, the presence of air traps was more pronounced in lower mesh densities.

3.1.3. Melt Temperature and Mold Surface Temperature

In the study, it was observed that an increase in melt temperature of polymers around the processing range, increased the deviation percentage (5-10%) from ideal expected product mass (Figure 5 and figure 6). This increase in deviation percentage could be attributed to inferior mold filling efficiencies and increased air traps. It was observed that at lower temperatures, higher masses of samples were obtained, leading to higher average molecular weight in molded parts, which translates well into increase in impact resistance, shorter cycle time, lower energy consumption, and reduced air traps.

Further, the impact of increase in mold temperature was not very profound on mold filling efficiency and process deviation. In the simulations, it was observed that increase in mold surface temperatures in amorphous polymers showcased lower degrees of molded-in stress, which could produce better crack-resistance and fatigue performance. While in semi-crystalline polymers, no significant observations on molded-in were observed.

A mold designs without air vents (venting system) was evaluated in the study to determine an appropriate location for a venting system. Based on the simulation results on air trap analysis, air traps are concentrations on the corners of the compression molded product, making it a region of concern. To prevent mold degradation which can lead to additional cost of processing and material wastage, a second mold design is presented that accounts for the presence of a venting system which is composed of channels (air vents). These channels are distributed along the end of the mold (female cavity). The virtual project of the air vents of the mold can be visualized in Figure 8. The vents were introduced into the mold with 29.65 mm length, 2 mm width, and 1 mm depth on Solidworks 2016. The design has been developed keeping in mind air trap analysis, mold filling efficiency, and process deviation percentages of semi-crystalline and amorphous thermoplastics. The model predicts that the new mold design with air vents could significantly increase the mold filling efficiency and reduce the presence of air vents.



(a) **(b)**

Figure 8: Mold cavity with air vent developed in SolidWorks CAD version 2016 (a) Top view (b) Isometric view

4. Conclusion

This simulation study through computational analysis has evaluated the effect of various processing parameters on the efficiency of the compression molding process for thermoplastics. Furthermore, the study analyzed the distribution of air traps across the product using Moldflow Insight 2019. As the simulation package in Moldflow Insight successfully located a region of concentration for the presence of air vents, mold modifications were presented to result in higher mold filling efficiency. The impact of charge geometry on ensuring proper raw material utilization was indicated via the simulation results. It was concluded that a cylindrical initial charge geometry offered higher mold filling efficiency with less raw material requirements in comparison to a cuboidal initial charge geometry. The simulations further showcased how higher mesh refinement could increase the mold filling efficiencies but also increase the computation time. The inadequacy of a tetrahedral mesh design along the edges of the product design was observed. The results indicated an decrease in mold filling efficiencies with increase in elt temperature which resulted in partial filling of the mold. Whereas, the impact of increase in mold surface temperature on melt temperature was not very significant. It was observed that all temperature and pressure combinations showed some degree of air entrapment. Using these results and the air traps analysis a new mold design was developed. The mathematical model used by

Moldflow Insight showcased great caliber in predicting the behavior of various polymers undergoing compression molding. Based on the results obtained, it can be possible to optimize the compression cycle and reduce material wastage by introducing a venting system in the mold design and appropriate processing parameters. The findings illustrated that computational simulations can be a powerful tool to aid decision-making and process optimization to be applied in compression molding processes.

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