

Parametric Simulation of Injection Molding Plastic Composites with Bio-Based Fillers

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Abstract

As the nation continues to demand greater supplies of energy, the fuel ethanol industry is poised to contribute substantial quantities of transportation fuel for the foreseeable future. Ethanol manufacturing from corn grain results in three main products: bioethanol, the primary end product; residual nonfermentable corn kernel components, which are typically sold as animal feed known as “distillers grains”; and carbon dioxide. The sale of distillers grains contributes substantially to the economic viability of each ethanol plant’s operations. This approach to utilization is well established, but must be augmented if it is to retain high-value returns as the generated quantities increase as the industry continues to grow throughout the nation. Thus other novel applications must also be pursued. Based on our laboratory investigations, it appears that these residues have much potential for manufacturing into various bio-based products, especially composites. Before they can be successfully used commercially, the compatibility of thermoplastics and bio-based fillers must first be examined. Additionally, appropriate methods of manufacture must be determined and optimized, because inclusion of biological materials can produce very unique processing conditions and final product behavior. Thus the objective of this study was to simulate the processing behavior of a plastic filled with a biological material, such as distillers grains, when subjected to injection molding. Simulations were conducted to determine the effects of parametrically altering the thermal, rheological, and physical properties of polypropylene, to simulate the inclusion of a biofiller. Injection mold filling, cooling, and final quality were predicted for each of the treatments under investigation. This study represents an initial step in an initiative to utilize biofillers in plastic composites. Thus the information generated here will be essential for further efforts to utilize biological materials, such as distillers grains, in manufactured products, as this utilization avenue has potential for high-value returns which are much greater than currently available as livestock feed alone.

Keywords

Bioplastics, Composites, Fillers, Properties, Simulation

Introduction

Currently corn grain is the primary biological material that can be economically converted into fuel ethanol on an industrial scale in the U.S. The corn-based ethanol industry is poised to produce substantial quantities of biofuels during the coming century as this industry continues its rapid expansion. The number of corn ethanol plants, and their processing capacities, has been markedly increasing in recent years. For example, at the end of 2005, 97 manufacturing plants in the U.S. had an aggregate production capacity of nearly 16.3 billion L/y (4.3 billion gal/y), and exponential growth is predicted for the next several years. More information on the growth of this industry can be found in [1, 2, 3].

Ethanol manufacturing from corn grain results in three main products: fuel ethanol, the primary end product; residual nonfermentable corn kernel components, which are typically marketed as “distillers grains”; and carbon dioxide. Anecdotally, the rule of thumb commonly used in industry states that for each 1 kg of corn processed, approximately 1/3 kg of each of these constituent product streams will be produced. The production process consists of several steps, including grinding, cooking, liquefying, saccharifying, fermenting, and distilling the corn grain. In-depth information on this process can be found in [4, 5, 6, 7], but is beyond the scope of this paper.

The nonfermentable residues (i.e., proteins, fibers, fats, and ash) are removed from the process stream during the distillation stage as whole stillage. They are centrifuged and dried, to ensure a substantial shelf life, and then sold as distillers grains (most commonly as DDGS – “distillers dried grains with solubles”) for feed rations to local livestock producers, or shipped via truck or rail for use by distant customers. The sale of distillers grains as livestock feed contributes substantially to the economic viability of ethanol manufacturing, and is thus a vital component to each plant’s operations. Several studies have thoroughly examined chemical and nutritional properties of these byproduct feeds, including [8, 9, 10, 11]. [12] comprehensively reviewed much of the available chemical, nutritional, and physical property research to date.

As the ethanol industry continues to grow rapidly, however, the increased supply of distillers grains will undoubtedly affect its potential sales price vis-à-vis feed demand, which could severely impact the production economics of the industry in the near future. If estimates of future ethanol production hold true, using these process residues as livestock feed alone may not prove to be sustainable, and thus alternative utilization avenues should be investigated. One potential strategy could be use in manufactured products, especially plastics.

As researchers look for ways to displace petroleum-based components in plastics, filler materials are a logical area to investigate. One objective of the displacement is to attempt to achieve comparable physical properties for various molded products. If possible, it is desirable for the filler to also contribute structural advantages, such as strength and toughness. Basically, the combination of two or more distinct materials yields a composite material [13]. One potential method to displace petroleum based products involves using DDGS as a biofiller in the injection molding process. Traditional injection molding was first conceptualized in 1868 by John Wesley Hyatt to make a billiard ball from a cellulose formulation. In 1946, James Hendry marketed his screw injection machine, which replaced the plunger system. Screw machines are the

predominate injection molding machine used today [14]. Basically, molten plastic is forced into a closed cavity of a specific, desired geometry.

Various processing parameters influence molding success. These keys include melt temperature, mold temperature, injection pressure, injection time, dwell time, freeze time, and dead time [15]. The inclusion of a filler, however, will alter material properties, which will thus affect processing behavior and final product quality. These altered properties will include thermal conductivity, specific heat, and rheological behavior. Rheological properties include viscosity, and the parameters which are used to quantify the effects of shear rate and temperature.

Computer-aided engineering (CAE) software provides powerful analysis of product designs and manufacturing parameters. Three dimensional (3-D) computer-aided designs (CAD) solid models provide a starting point to evaluate heat transfer and structural integrity. Flow analysis is a member of the CAE software family. Injection mold analysis can either be 2-D or 3-D. The 3-D flow analysis, while more computationally intense, performs better for most injection mold cavity studies [14]. As an input, these software programs use part geometry, processing parameters, thermal properties, and material flow characteristics. Most software programs break the model into small entities, and each of these small units is studied in relation to its neighbors. This technique is called finite element analysis (FEA). The output of these programs includes knit lines, fill patterns, fill time, sink marks, etc. [15]. There are a plethora of studies where authors use these computational flow analysis programs [16-23]. With a mathematical model, the researcher can attempt to optimize the parameters for desired results. Several authors suggest methods for optimization [24]. Taguchi methods [25, 26] have been used, as well as neural networks [27, 28, 29]. Others have studied composite injection molding with dedicated flow analysis software [30, 31, 32]. Little work, however, has been pursued examining use of fillers.

Therefore, as a first step toward investigating the feasibility of using DDGS as a biofiller, the objective of this study was to simulate the processing behavior of a plastic filled with a biological material when subjected to injection molding, by parametrically altering the rheological and thermal properties of the plastic, and examining processing behavior and final product quality.

Materials and Methods

The addition of fillers to thermoplastics can substantially alter the physical properties of these combined materials, which will impact subsequent behavior during the injection molding process, and thus final product quality and performance. Using polypropylene as a benchmark material, a 3D model of a typical “dog-bone” specimen (Figure 1) was constructed according to ASTM Method D790 [33], and was used in a series of injection molding simulations.

To simulate the effects of adding biofillers, several physical parameters were systematically altered in this study. Thermal properties included thermal conductivity and specific heat. For the base polypropylene, the values of thermal conductivity and specific heat were, respectively, 0.164 (W/m°C) and 2740 (J/kg°C). Rheological properties altered in this study included various parameters used to define the viscosity relationship. For thermoplastics, which are classified as shear-thinning materials, viscosity can be defined using the Cross-WLF model:

$$\eta = \frac{\eta_0}{1 + \left(\frac{\eta_0 \gamma}{\tau^*} \right)^{1-n}}$$

where:

$$\eta_0 = D1 \exp \left[\frac{-A1(T - T^*)}{A2 + (T - T^*)} \right]$$

where: η is the viscosity (Pa's), γ is the shear rate (1/s), T is the temperature (K), T^* is $D2+D3P$ (K), P is the pressure (Pa), $A2$ is $A2^*+D3P$ (K), while n , τ^* , $D1$, $D2$, $D3$, $A1$, and $A2^*$ are regression coefficients based on empirical data. For the base polypropylene used in this study, the values of these coefficients were, respectively, 0.2751 (-), 24200 (Pa's), 4.66×10^{12} (Pa's), 263.15 (K), 0 (K/Pa), 26.12 (-), and 51.6 (K).

Using polypropylene as the baseline, a formal experiment was designed to include five factors (thermal conductivity, specific heat, τ^* , $D1$, and n), each at two levels (+/- 25% from the base values). This resulted in a 2^5 experiment (32 treatments), which was implemented factorially. Additionally, a center point (i.e., the base polypropylene) was also included. This resulted in 33 total treatment combinations. The coded experimental design that was used is provided in Table 1, while the experimental design with actual variable values is given in Table 2.

Simulations of the injection molding process were conducted with Moldflow Part Advisor (version 7.2) software, using a mold temperature of 40°C, a maximum injection pressure of 180 MPa, and a shot volume of 8.57 cm³. Processing conditions determined via the simulations included fill time (s), injection pressure (Pa), pressure drop (Pa), flow front temperature (C), surface temperature (C), freeze time (s), confidence of mold fill (-), required clamping force (tonnes), and total cycle time (s). Final quality of the molded products included cooling quality, quality prediction, locations of weld lines, locations of air traps, locations of sink marks, and skin orientations.

Results and Discussions

Because polypropylene was the baseline material used for this study, an examination of the simulation results for this benchmark, as a prelude to all the results from the various treatment combinations, is useful. The resulting processing conditions for the polypropylene were quite good. Fill time of the specimen (Figure 2) was 1.68 s. Injection pressure (Figure 3) varied from 0 to 3.88 MPa, depending on location within the sample. The pressure drop (which is the inverse of injection pressure) was also determined (Figure 4), which also varied from 0 to 3.88 MPa. Temperature of the flow front (Figure 5) varied from 239.24 to 240.00°C, depending on location within the sample. The flow temperature during processing was high throughout the sample, but was slightly cooler near the ends of the mold. Variations in surface temperature (Figure 6), on the other hand, ranged from -5.67 to 2.54°C. Throughout the specimen, temperature variation was most at the center and least at the edges and ends. Variations in freeze time (Figure 7)

ranged from -0.28 to 0.14 s, and was least near the edges throughout, and at the center. Confidence of mold fill (Figure 8) was good throughout the extent of the mold.

Considering all quality parameters calculated, the final molded polypropylene specimen was determined to be very good. Cooling quality was good throughout (Figure 9), and overall predicted quality was also excellent (Figure 10). No weld lines were present in the specimen (Figure 11), and neither were air traps (Figure 12). No sink marks were present throughout the product either (Figure 13). Skin orientation results illustrate the flow lines throughout the product, which radiate from the injection (i.e., center) point (Figure 14).

Comparing the results from all simulation runs, it becomes apparent that the graphical results appeared very similar for all treatment combinations (data not shown). In-depth examination of the numerical results, however, provides several interesting insights. Altering the rheological and thermal properties produced definite changes in processing conditions and final product properties. In order to see where specific differences occurred, treatment combination effects (i.e., results from each specific run) were compared (Table 3). Some treatment combinations produced either increased or decreased values compared to the unaltered polypropylene. Moreover, some factor levels had a more drastic effect than others, as evidenced by the calculated change (%) versus the unaltered polypropylene for each combination. Pure polypropylene had an injection time of 1.68 s, and a cycle time of 25.15 s. Those treatments with a low thermal conductivity and a high specific heat produced greater injection and cycle times. On the other hand, those treatments with high thermal conductivity and low specific heat produced decreased injection and cycle times as compared to polypropylene. The required injection pressure for pure polypropylene was 3.88 MPa. Most treatment combinations resulted in a decreased pressure, although some factor combinations did require greater pressure. A few, however, resulted in a minimal change. The clamping force required for polypropylene was 0.58 tonnes. The results show that most of the treatment combinations required less force, although a few did require an increase. Ultimately, these observed behaviors were due to the trade-off between the thermal and rheological properties of the plastic during molding.

Considering only the main treatment effects (i.e., not the treatment combination effects) produced “pseudo-replications” for each main factor ($n=16$ for each main effect) because the independent variable had two levels each. Results of this analysis are provided in Table 4. As shown, various trends were evident. As thermal conductivity and specific heat increased, injection time increased. On the other hand, as the rheological parameters increased, it appeared that no trends for injection time were evident. Injection pressure increased as each of the factors increased. Clamping force did not show any trends as each of the factors was increased, though. Cycle time decreased as thermal conductivity increased, but increased as specific heat increased.

Even though the actual addition of fillers was not incorporated into the models used in this study, the range of potential bulk property changes that were considered should, at least as a starting point, provide a range of potential variations that could be expected when actually adding various fillers. Thus, the next step in our ongoing research efforts is to conduct experimental trials where biological materials, including distillers grains, will be used as fillers. These will be combined with various thermoplastics, subjected to injection molding, and tested extensively, not only for product quality, but also for resultant mechanical strength.

Conclusions

The goal of this study was to conduct a series of simulations to determine the effects of parametrically altering the thermal and rheological properties of polypropylene, in order to simulate the inclusion of a biofiller. It is clear that changes in the bulk properties of thermoplastics affect their processing behavior during injection molding, which in turn impact ultimate product quality. These simulation results provide key feedback, and will be a useful reference base from which to work, but there is definitely a need to experimentally examine the compatibility of various fillers with specific plastics, such as polypropylene, and to optimize processing conditions for specific processing operations, such as injection molding. Even though initial groundwork has been accomplished, much work remains in order to develop novel bio-based composites that can effectively utilize biofillers, including distillers grains.

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BIOGRAPHICAL INFORMATION

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Appendix 1: Tables

Table 1. Factorial experimental design with coded variables.^a

RUN	Variables				
	Tau*	D1	n	Thermal Conductivity	Specific Heat
1	-1	-1	-1	-1	-1
2	-1	-1	-1	-1	1
3	-1	-1	-1	1	-1
4	-1	-1	-1	1	1
5	-1	-1	1	-1	-1
6	-1	-1	1	-1	1
7	-1	-1	1	1	-1
8	-1	-1	1	1	1
9	-1	1	-1	-1	-1
10	-1	1	-1	-1	1
11	-1	1	-1	1	-1
12	-1	1	-1	1	1
13	-1	1	1	-1	-1
14	-1	1	1	-1	1
15	-1	1	1	1	-1
16	-1	1	1	1	1
17	1	-1	-1	-1	-1
18	1	-1	-1	-1	1
19	1	-1	-1	1	-1
20	1	-1	-1	1	1
21	1	-1	1	-1	-1
22	1	-1	1	-1	1
23	1	-1	1	1	-1
24	1	-1	1	1	1
25	1	1	-1	-1	-1
26	1	1	-1	-1	1
27	1	1	-1	1	-1
28	1	1	-1	1	1
29	1	1	1	-1	-1
30	1	1	1	-1	1
31	1	1	1	1	-1
32	1	1	1	1	1
33	0	0	0	0	0

^a Where τ^* , D1, n are empirical regression coefficients used to define viscosity.

Table 2. Factorial experimental design with actual variable values.^a

RUN	Variables				
	Tau*	D1	n	Thermal Conductivity	Specific Heat
1	3.495E+12	18150	0.2063	0.123	2055
2	3.495E+12	18150	0.2063	0.123	3425
3	3.495E+12	18150	0.2063	0.205	2055
4	3.495E+12	18150	0.2063	0.205	3425
5	3.495E+12	18150	0.3439	0.123	2055
6	3.495E+12	18150	0.3439	0.123	3425
7	3.495E+12	18150	0.3439	0.205	2055
8	3.495E+12	18150	0.3439	0.205	3425
9	3.495E+12	30250	0.2063	0.123	2055
10	3.495E+12	30250	0.2063	0.123	3425
11	3.495E+12	30250	0.2063	0.205	2055
12	3.495E+12	30250	0.2063	0.205	3425
13	3.495E+12	30250	0.3439	0.123	2055
14	3.495E+12	30250	0.3439	0.123	3425
15	3.495E+12	30250	0.3439	0.205	2055
16	3.495E+12	30250	0.3439	0.205	3425
17	5.825E+12	18150	0.2063	0.123	2055
18	5.825E+12	18150	0.2063	0.123	3425
19	5.825E+12	18150	0.2063	0.205	2055
20	5.825E+12	18150	0.2063	0.205	3425
21	5.825E+12	18150	0.3439	0.123	2055
22	5.825E+12	18150	0.3439	0.123	3425
23	5.825E+12	18150	0.3439	0.205	2055
24	5.825E+12	18150	0.3439	0.205	3425
25	5.825E+12	30250	0.2063	0.123	2055
26	5.825E+12	30250	0.2063	0.123	3425
27	5.825E+12	30250	0.2063	0.205	2055
28	5.825E+12	30250	0.2063	0.205	3425
29	5.825E+12	30250	0.3439	0.123	2055
30	5.825E+12	30250	0.3439	0.123	3425
31	5.825E+12	30250	0.3439	0.205	2055
32	5.825E+12	30250	0.3439	0.205	3425
33	4.660E+12	24200	0.2751	0.164	2740

^a Where τ^* , D1, n are empirical regression coefficients used to define viscosity.

Table 3. Treatment combination effects for all injection molding process conditions.

Run	Injection Time		Injection Pressure		Clamping Force		Cycle Time	
	(s)	Change (%)	(MPa)	Change (%)	(tonnes)	Change (%)	(s)	Change (%)
1	1.55	-7.74	2.25	-42.01	0.26	-55.17	24.78	-1.47
2	2.61	55.36	1.94	-50.00	0.26	-55.17	37.80	50.30
3	0.93	-44.64	2.57	-33.76	0.30	-48.28	17.17	-31.73
4	1.56	-7.14	2.25	-42.01	0.26	-55.17	25.04	-0.44
5	1.66	-1.19	3.16	-18.56	0.35	-39.66	24.89	-1.03
6	2.58	53.57	2.56	-34.02	0.28	-51.72	38.05	51.29
7	1.04	-38.10	3.88	0.00	0.44	-24.14	17.28	-31.29
8	1.56	-7.14	3.22	-17.01	0.36	-37.93	25.04	-0.44
9	1.66	-1.19	3.18	-18.04	0.36	-37.93	24.89	-1.03
10	2.59	54.17	2.71	-30.15	0.31	-46.55	38.05	51.29
11	1.04	-38.10	3.68	-5.15	0.42	-27.59	17.28	-31.29
12	1.56	-7.14	3.22	-17.01	0.37	-36.21	25.04	-0.44
13	1.66	-1.19	4.14	6.70	0.46	-20.69	24.89	-1.03
14	2.69	60.12	3.29	-15.21	0.36	-37.93	38.16	51.73
15	1.04	-38.10	5.15	32.73	0.57	-1.72	17.28	-31.29
16	1.56	-7.14	4.22	8.76	0.47	-18.97	25.04	-0.44
17	1.66	-1.19	2.57	-33.76	0.30	-48.28	24.89	-1.03
18	2.59	54.17	2.27	-41.49	0.26	-55.17	38.06	51.33
19	0.93	-44.64	2.91	-25.00	0.34	-41.38	17.17	-31.73
20	1.56	-7.14	2.58	-33.51	0.30	-48.28	25.04	-0.44
21	1.65	-1.79	3.93	1.29	0.44	-24.14	24.89	-1.03
22	2.70	60.71	3.20	-17.53	0.36	-37.93	37.91	50.74
23	1.04	-38.10	4.76	22.68	0.54	-6.90	17.28	-31.29
24	1.56	-7.14	3.98	2.58	0.44	-24.14	25.04	-0.44
25	1.67	-0.60	3.72	-4.12	0.47	-18.97	24.89	-1.03
26	2.70	60.71	3.21	-17.27	0.37	-36.21	38.16	51.73
27	1.04	-38.10	4.22	8.76	0.49	-15.52	17.28	-31.29
28	1.56	-7.14	3.74	-3.61	0.43	-25.86	25.04	-0.44
29	1.79	6.55	5.19	33.76	0.74	27.59	26.25	4.37
30	2.73	62.50	4.23	9.02	0.61	5.17	38.17	51.77
31	1.06	-36.90	6.47	66.75	0.89	53.45	17.28	-31.29
32	1.69	0.60	5.60	44.33	0.82	41.38	25.15	0.00
33	1.68	-	3.88	-	0.58	-	25.15	-

Table 4. Main effects for injection molding process conditions.

Parameter	Injection Time (s)			Injection Pressure (MPa)			Clamping Force (tonnes)			Cycle Time (s)		
	Mean	Change (%)	St. Dev.	Mean	Change (%)	St. Dev.	Mean	Change (%)	St. Dev.	Mean	Change (%)	St. Dev.
Tau* (Pa's)												
3.495E+12	1.71	1.53	0.60	3.21	-17.17	0.85	0.36	-37.18	0.09	26.29	4.54	7.71
4.660E+12	1.68	-	-	3.88	-	-	0.58	-	-	25.15	-	-
5.825E+12	1.74	3.68	0.60	3.91	0.76	1.13	0.49	-15.01	0.18	26.33	4.70	7.48
D1 (Pa)												
18150	1.70	1.12	0.61	3.00	-22.63	0.79	0.34	-40.84	0.08	26.27	4.46	7.69
24200	1.68	-	-	3.88	-	-	0.58	-	-	25.15	-	-
30250	1.75	4.06	0.59	4.11	5.90	0.99	0.51	-11.56	0.17	26.35	4.78	7.50
n (-)												
0.2063	1.70	1.23	0.61	2.94	-24.26	0.66	0.34	-40.73	0.08	26.29	4.52	7.72
0.2751	1.68	-	-	3.88	-	-	0.58	-	-	25.15	-	-
0.3439	1.75	3.96	0.59	4.17	7.43	1.01	0.51	-11.66	0.17	26.34	4.72	7.47
Thermal Conductivity (W/m°C)												
0.123	2.16	28.31	0.51	3.22	-16.96	0.86	0.39	-33.30	0.13	31.55	25.43	6.72
0.164	1.68	-	-	3.88	-	-	0.58	-	-	25.15	-	-
0.205	1.32	-21.53	0.30	3.90	0.56	1.12	0.47	-18.66	0.17	21.39	-14.96	4.02
Specific Heat (J/kg°C)												
2055	1.34	-20.31	0.34	3.86	-0.48	1.13	0.46	-20.58	0.17	21.15	-15.91	4.04
2740	1.68	-	-	3.88	-	-	0.58	-	-	25.15	-	-
3425	2.09	24.23	0.55	3.30	-14.95	0.92	0.40	-30.63	0.15	31.17	23.95	6.68

Appendix 2: Figures

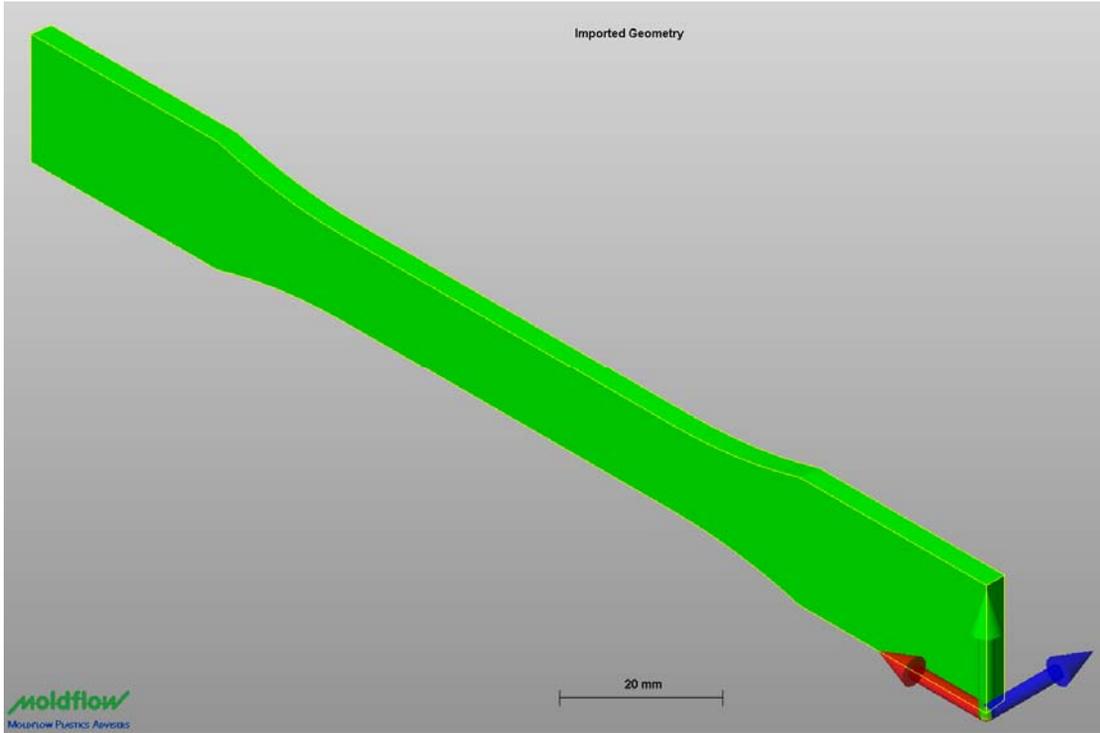


Figure 1. Standard “dog-bone” solid model used for all simulations.

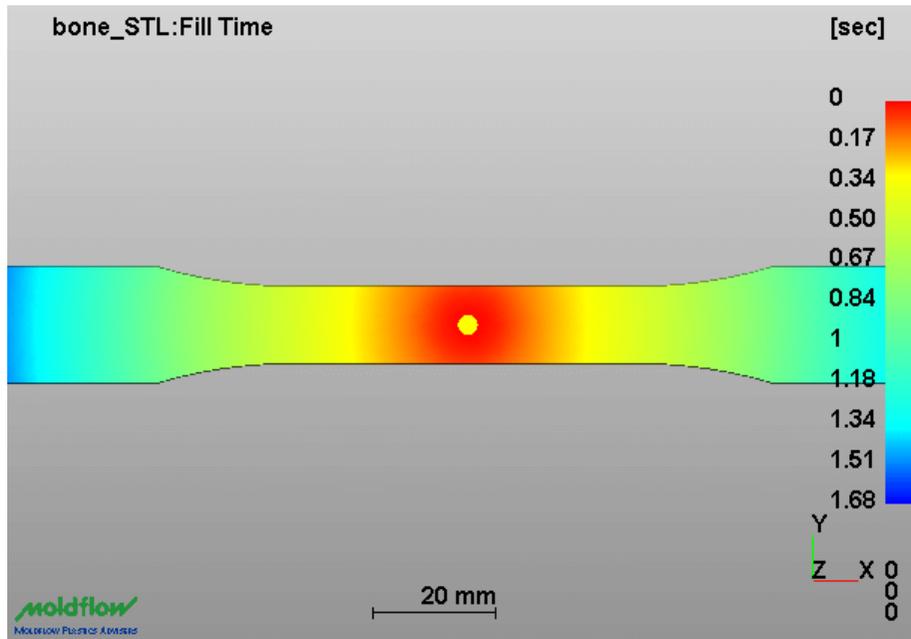


Figure 2. Fill time results for pure polypropylene (Treatment 33).

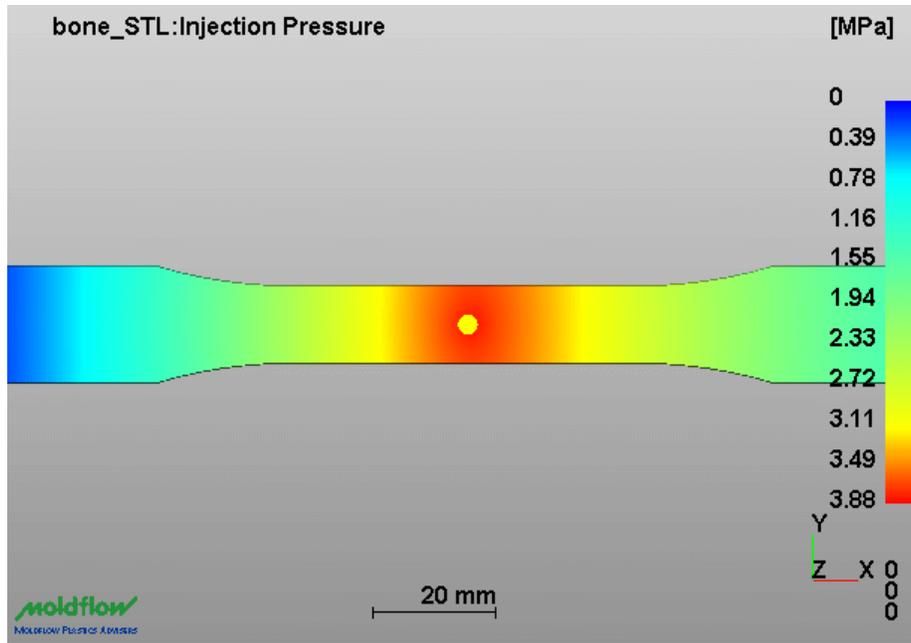


Figure 3. Injection pressure results for pure polypropylene (Treatment 33).

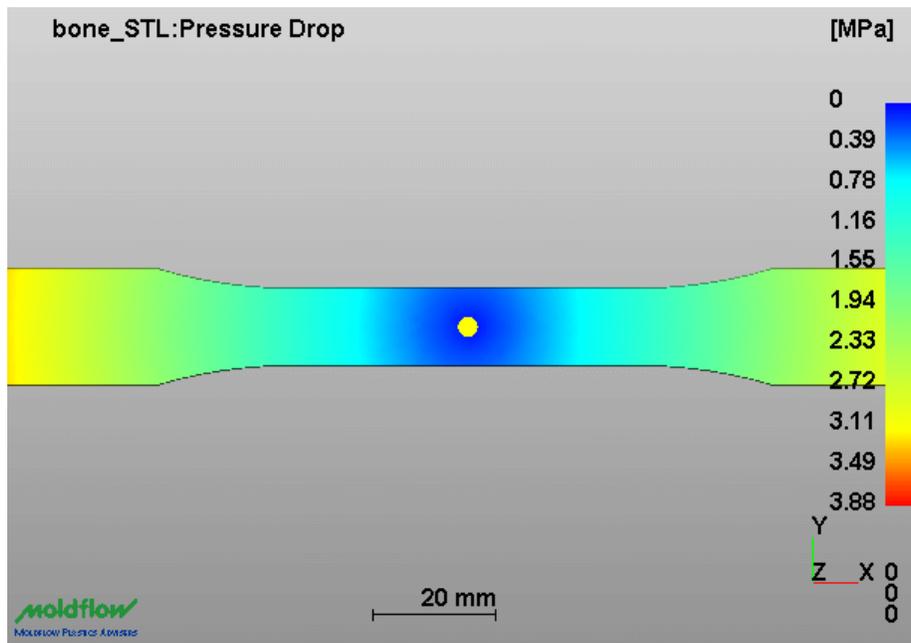


Figure 4. Pressure drop results for pure polypropylene (Treatment 33).

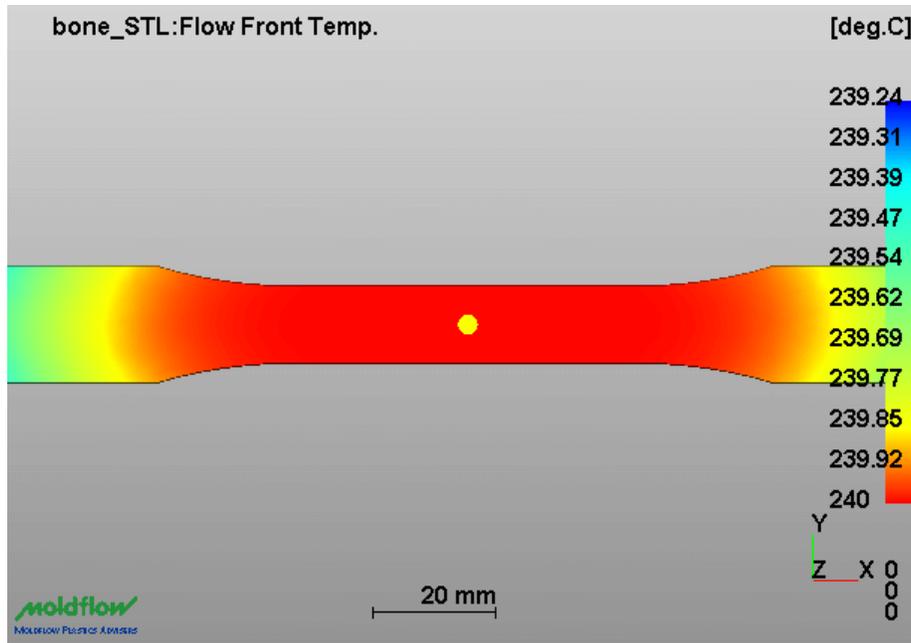


Figure 5. Flow front temperature results for pure polypropylene (Treatment 33).

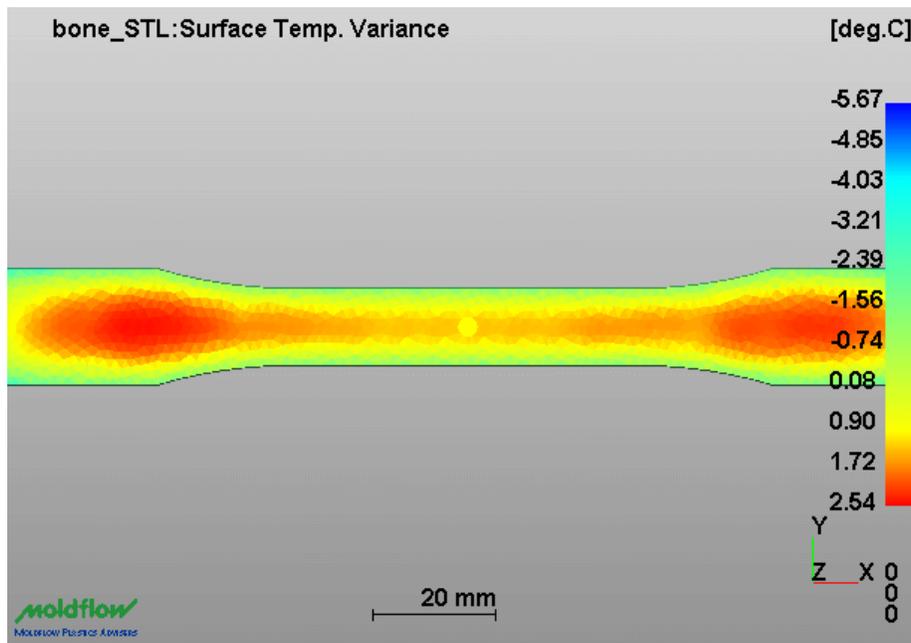


Figure 6. Surface temperature variance results for pure polypropylene (Treatment 33).

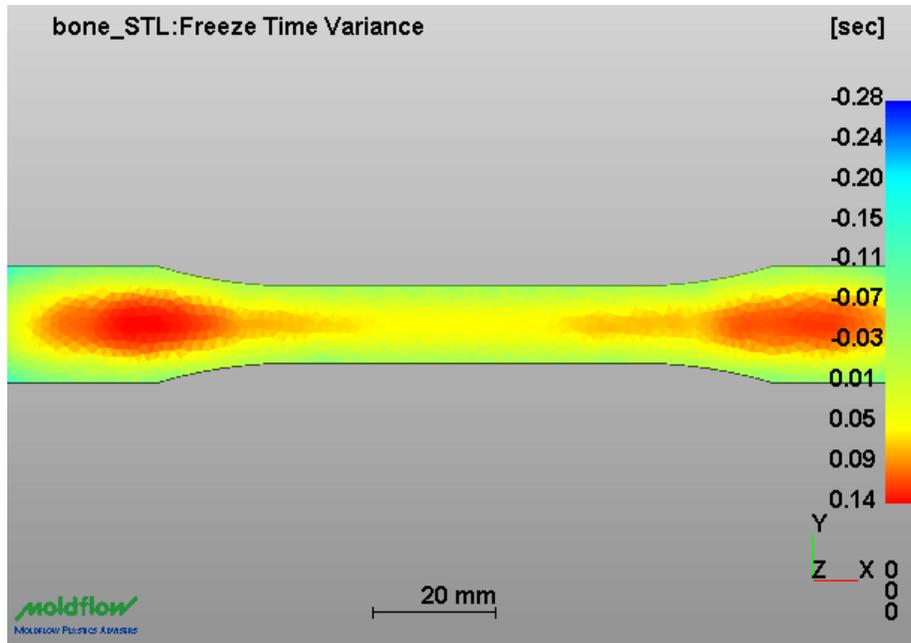


Figure 7. Freeze time variance results for pure polypropylene (Treatment 33).

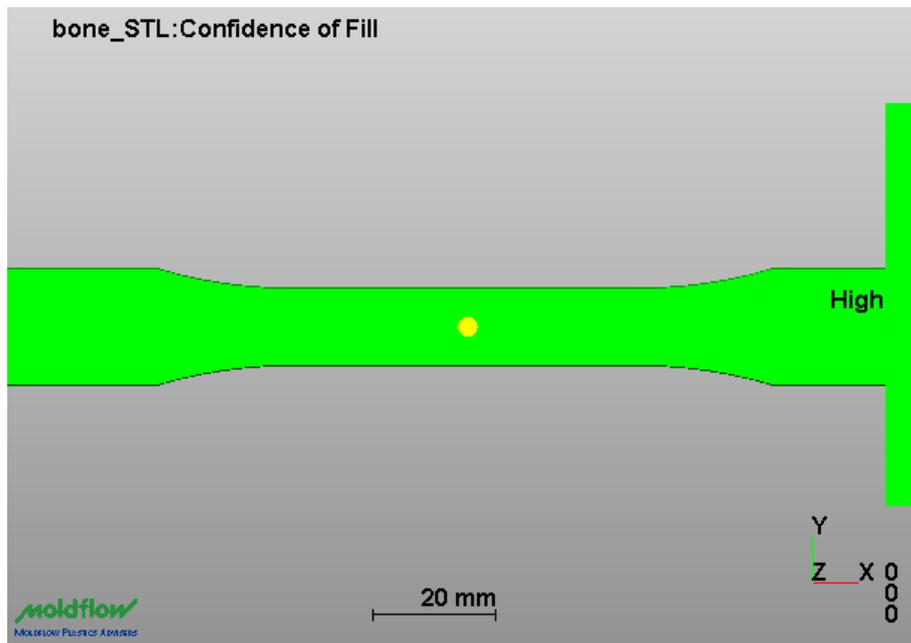


Figure 8. Confidence of fill results for pure polypropylene (Treatment 33).

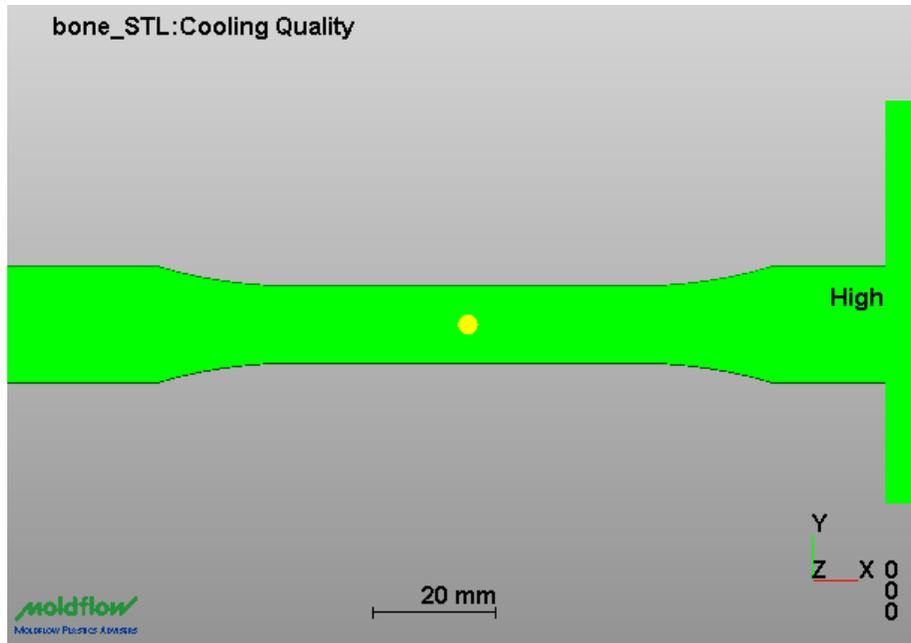


Figure 9. Cooling quality results for pure polypropylene (Treatment 33).

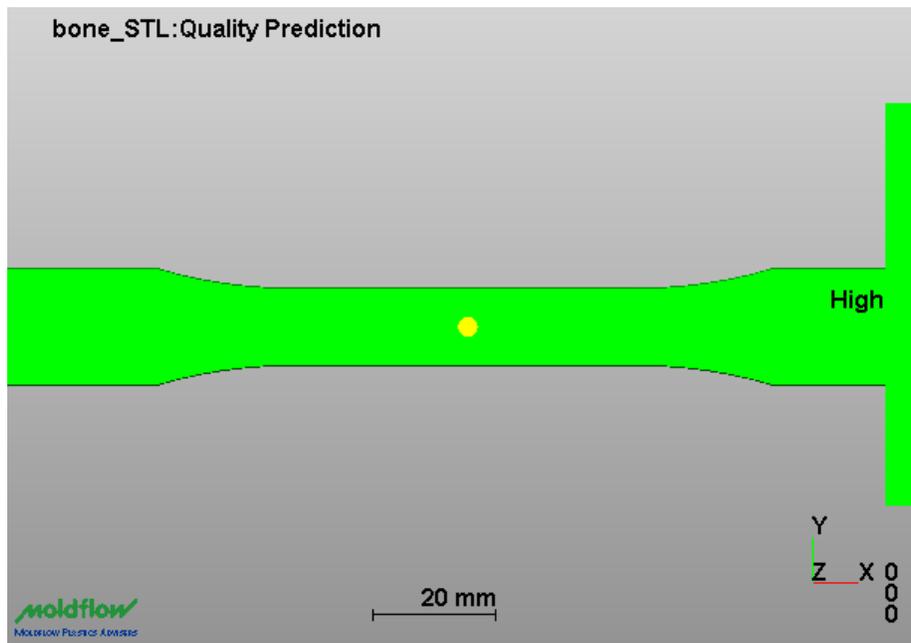


Figure 10. Quality prediction results for pure polypropylene (Treatment 33).

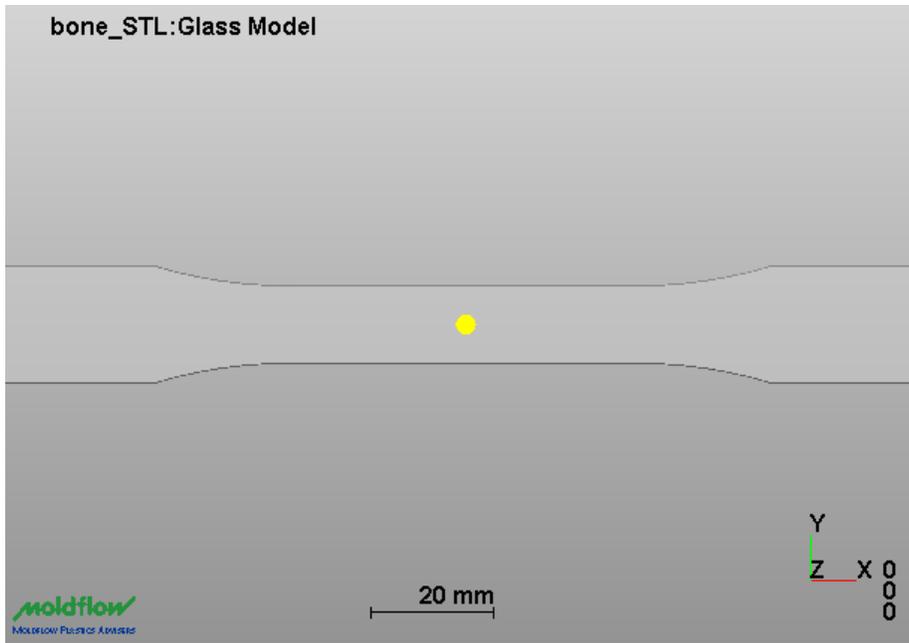


Figure 11. Weld lines results for pure polypropylene (Treatment 33).

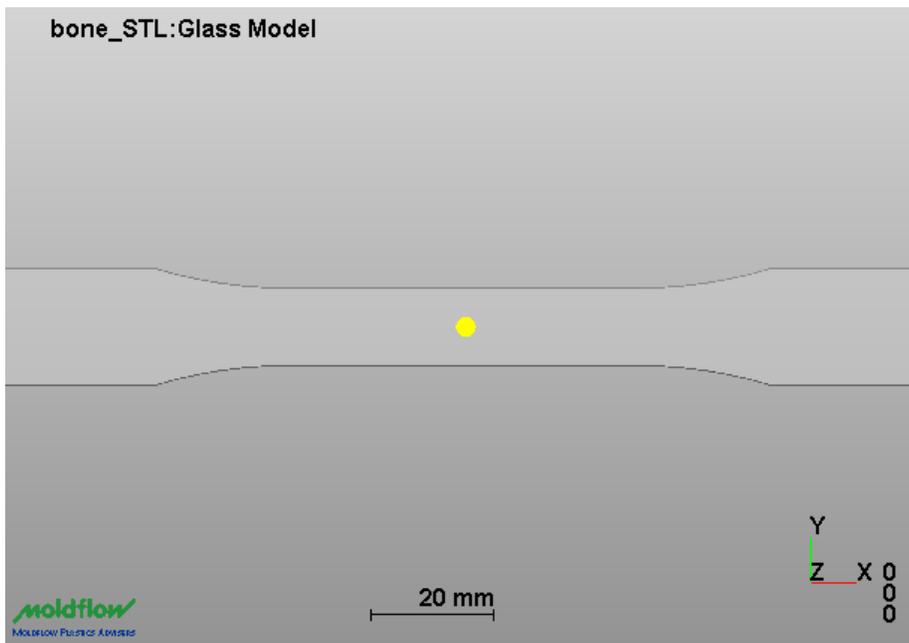


Figure 12. Air traps results for pure polypropylene (Treatment 33).

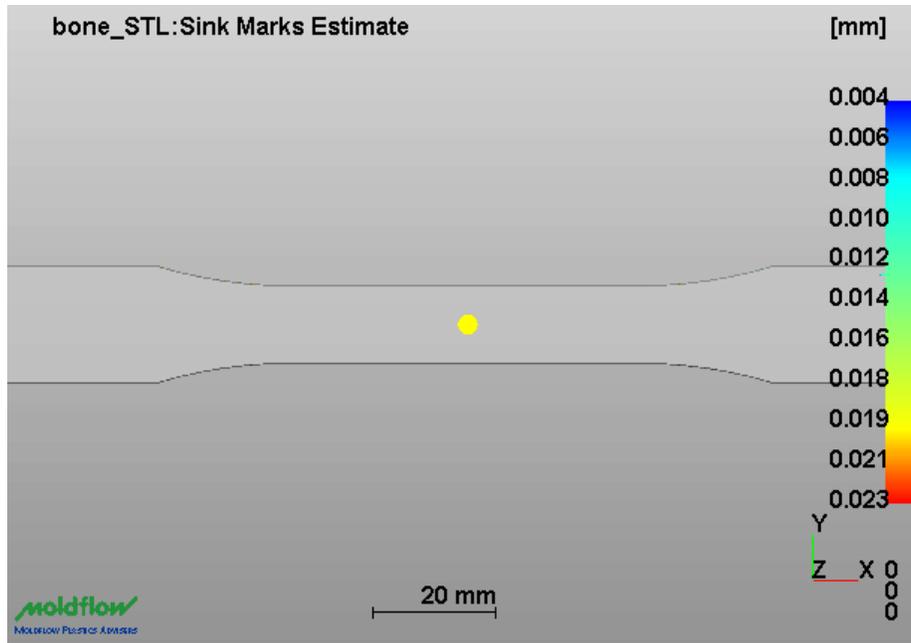


Figure 13. Sink marks estimate results for pure polypropylene (Treatment 33).

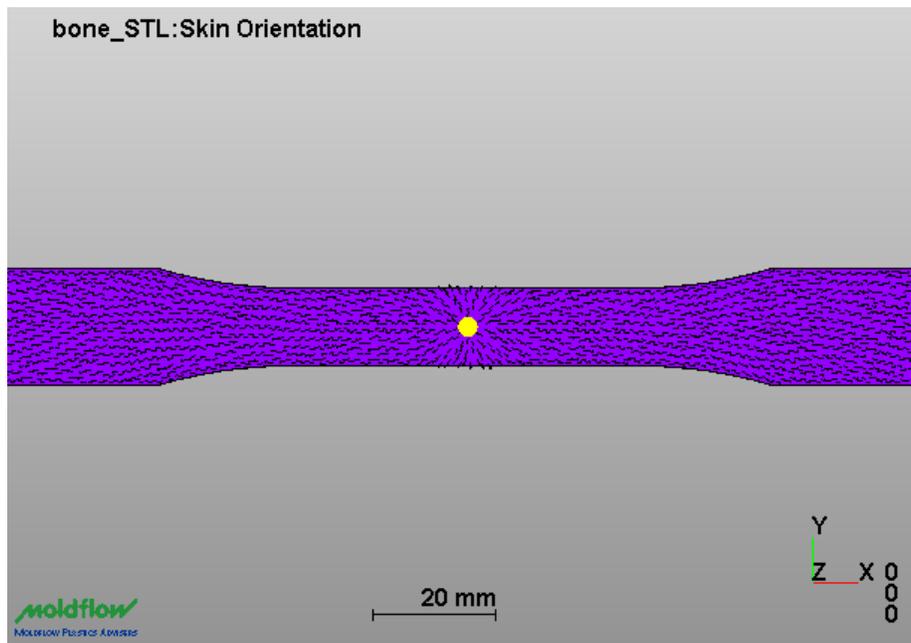


Figure 14. Skin orientation results for pure polypropylene (Treatment 33).