

USING SIMULATIONS TO DETERMINE OPTIMUM RUN PROCESSING CONDITIONS IN EXTRUSION

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ABSTRACT

For years, simulation tools have been used to predict performance. Often, simulation is used for prediction of output, temperature and pressure. In this paper, it will be used to determine how to effectively run polymer and predict potential difficulties. It will be shown that this simulation tool can be used to pinpoint problems beforehand, eliminating costly mistakes. Two case studies will be examined.

DISCUSSION – FLOW 2000™ SOFTWARE PACKAGE

Before examining the case studies, the simulation software tool needs to be described. This software is called FLOW 2000™ and is manufactured by Compuplast International. The software can be run on a typical computer and does not have any special requirements. This is a package of polymer flow tools with analysis packages for extruders, dies and rheology. The FLOW 2000 Extruder module uses a marching, 2D Finite Difference Method analysis. It is based on the following original work:

Agur, E. E., and Vlachopoulos, J. “Numerical Simulation of a Single-Screw Plasticating Extruder”, Polymer Engineering and Science, 22, 1084, (1982)

It has several improvements to handle Barrier screws, more mixers, improved feeding models and screw heat transfer. The version used for these simulations was 5,0,0,0. Rheology information such as flow curves and specific heat parameters are entered. Feed screws are modeled and different resins and processing conditions can be entered and solved.

DISCUSSION – CASE STUDY 1

BACKGROUND

The first case study involves a novel material and extruder application. It was co-extrusion coating for high barrier packaging. The customer is a major global supplier of high barrier products. They were limited with what they could supply commercially due to high melt quality defects. In addition to needing high quality melt, they wanted good output.

MATERIAL SPECS & PROCESSING

One of the extruders needed to be able to run two particular nylons. One of the nylons was Mitsui MXD6, grade 6011. This is a 2.6 MI semicrystalline polymer with a density of 1.22. The second nylon was a blend of 75% MXD6 with 25% UBE nylon 6, grade 1022C2. The straight MDX6 was more difficult to process; therefore, all simulations were based on the straight MXD6.

Now is a good time to talk about the processibility of this material. This is a very hydroscopic material. It will absorb water quickly. If this material gets too wet or hot, the moisture shows up in the melt curtain as holes and distortions. To demonstrate this moisture problem, Figure 1 shows a graph of the processing temperature versus the saturated moisture content for this material. This material as used out of sealed bags is guaranteed to have no more than 0.09% moisture when exposed to air for 1.5 hours at 81% Relative Humidity. From the graph of Figure 1, the material must be processed at a temperature where the saturated moisture is below the curve. This means that the temperature must be less than 275C (529F) if the material has 0.09% moisture. From the graph, it can be seen that temperature and moisture interact closely to cause product failure. Lower temperature throughout the length of the screw will mean that a higher moisture level can be tolerated.

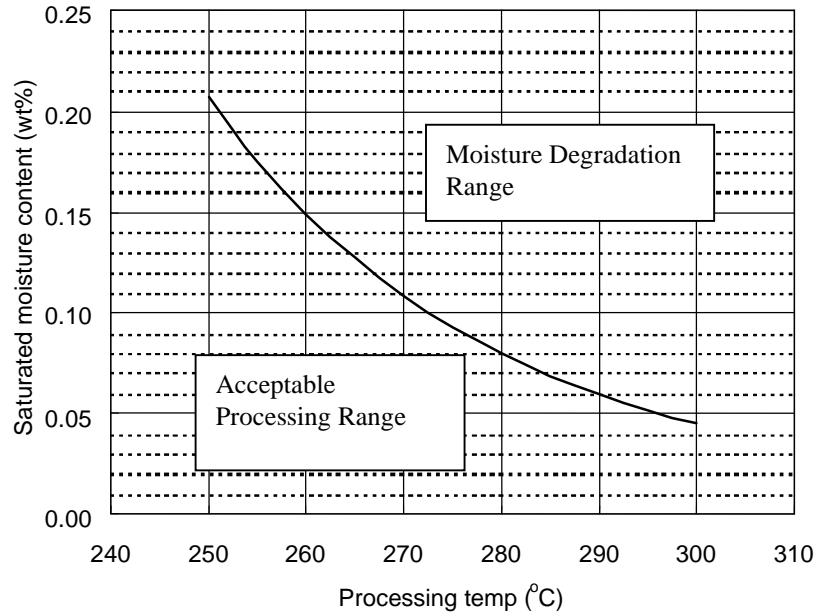


Figure 1: Saturated moisture content of N-MXD6 at processing temperature

This material also starts melting at 240C (464F). In addition to the shear heat that the screw generates, the material itself generates heat because it is very viscous at lower temperatures. The hotter the melt temperature gets, the more moisture will show up in the melt curtain. If this polymer is exposed to high temperature with moisture entrained, it will actually depolymerize. This means that the moisture breaks the polymer chain and terminates the end group, dropping the viscosity. All of these factors make processing this material very difficult. If there is too much shear in the screw, the material will overheat and moisture problems or gels will appear. If there is not enough shear in the screw, the material will not completely melt. The goal for this screw is to produce a wider, more forgiving operating window by providing a screw that would completely melt the nylon at the lowest temperature possible.

SIMULATIONS

A preliminary design was developed using FLOW 2000. The proposed screw was a single flighted screw with a twisted spiral mixer about two feet from the end of the screw. This design was sent to the customer. They were afraid that the design would put too much shear heat into the Nylon. The customer had many bad experiences with previous screw designs. They were reluctant to have any type of mixer due to shear heat concerns. Alternatives were discussed with pros and cons of each. Three removable ends were proposed for the screw. Figure 2 shows the three mixer tips. Tip #1 had no an exchange flight mixer. The

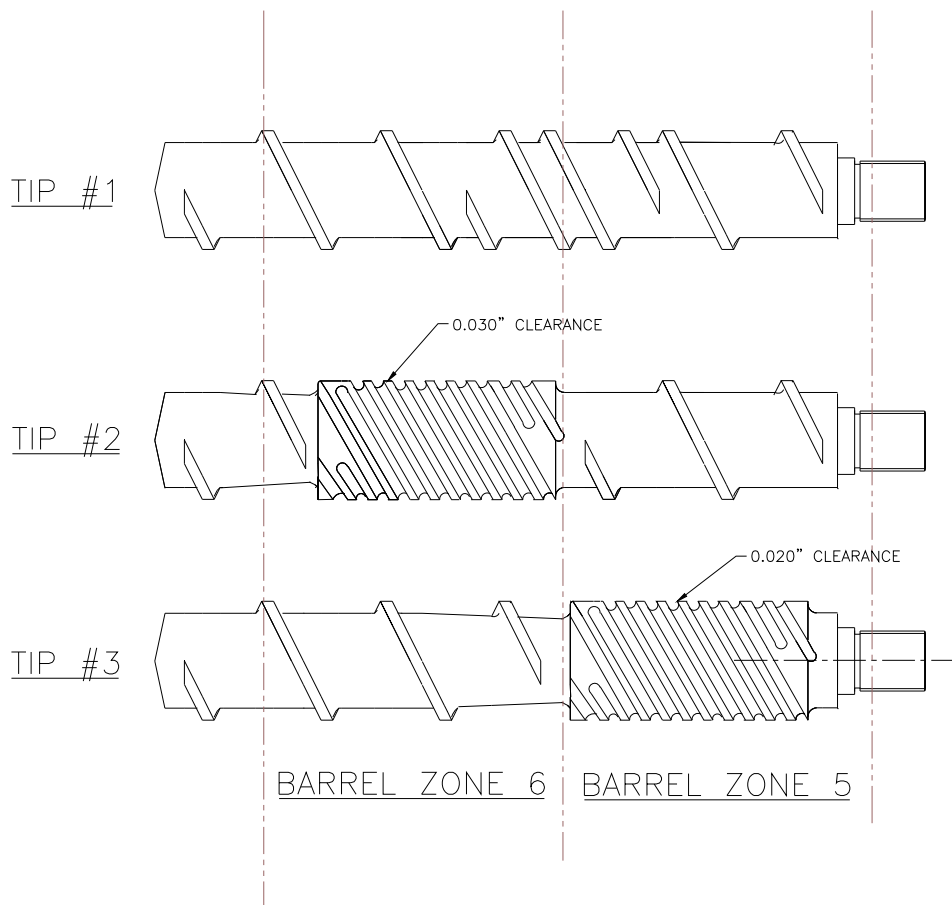


FIGURE 2

primary flight ends and a secondary flight splits the channel. This is the lowest type of mixing available. Tip #2 had a twisted mixer near the end of the screw. This mixer had 0.76 mm (0.03 inches) of clearance. Tip #3 had a twisted mixer with 0.5 mm (0.02 inches) clearance located in barrel zone 5 of the extruder. The reason for putting this mixer so far back from the end of the screw was to complete melting and send the nylon as gently as possible through the system. All simulations were run with the same set up conditions for temperature, pressure, etc. unless noted.

It was decided that all three screw tips be made for this screw. Before each tip was tested, Flow 2000 was used to determine optimum running conditions and to see if there would be any problems. The first tip run was the no mixer end (Tip #1). This one showed an immediate problem. Figure 3 shows that there will be unmelt problems. This graphic demonstrates the relative unmelted amount along the length of the screw. Each left hand corner of the simulation graphic shows the basic information. The screw diameter, screw RPM, mass flow rate, pressure at the end of the screw and when melting is completed. As can be seen in Figure 3, the material is unmelted. How much of the polymer is unmelted? According to the simulation, the material is 2.8% unmelted. The graphic shows in color how much melting occurs along the length of the screw.

There are several other interesting results from this particular screw design. Figure 4 shows the temperature profile along the entire screw. The bulk temperature of the resin is 301C (574F). This clearly shows how easily the material heats up. The optimal heat profile in the barrel for the resin was 232/288/288/274/274/274C (450/550/550/525/525/525F). This profile gave the best result for temperature uniformity (cross channel), melting and pressure. Although this was optimum, the result from this screw design can be considered unacceptable.

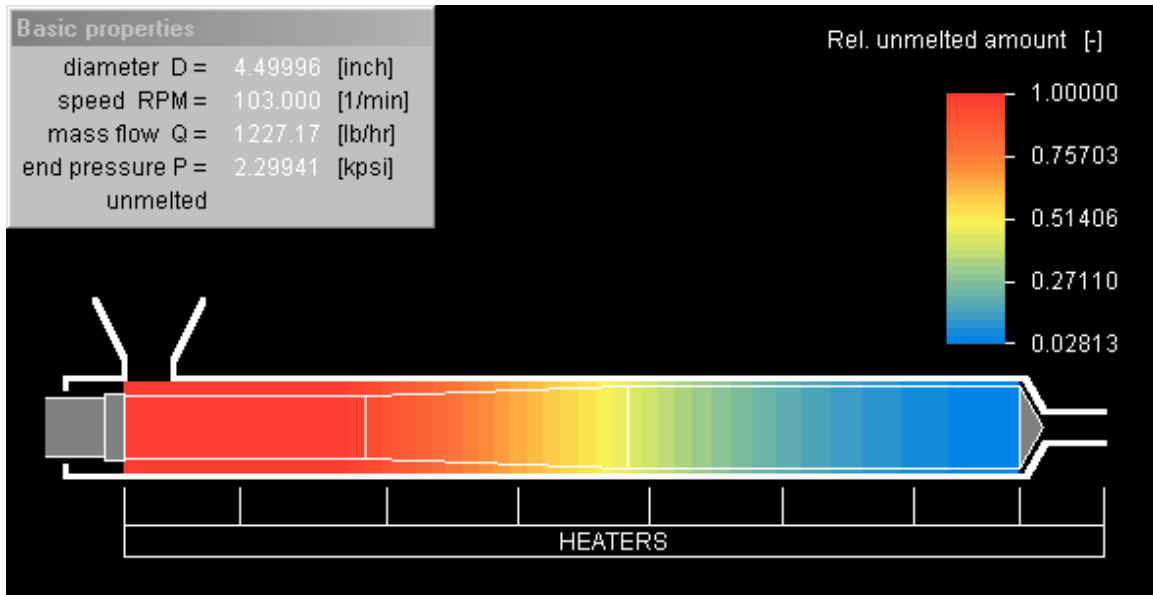


FIGURE 3

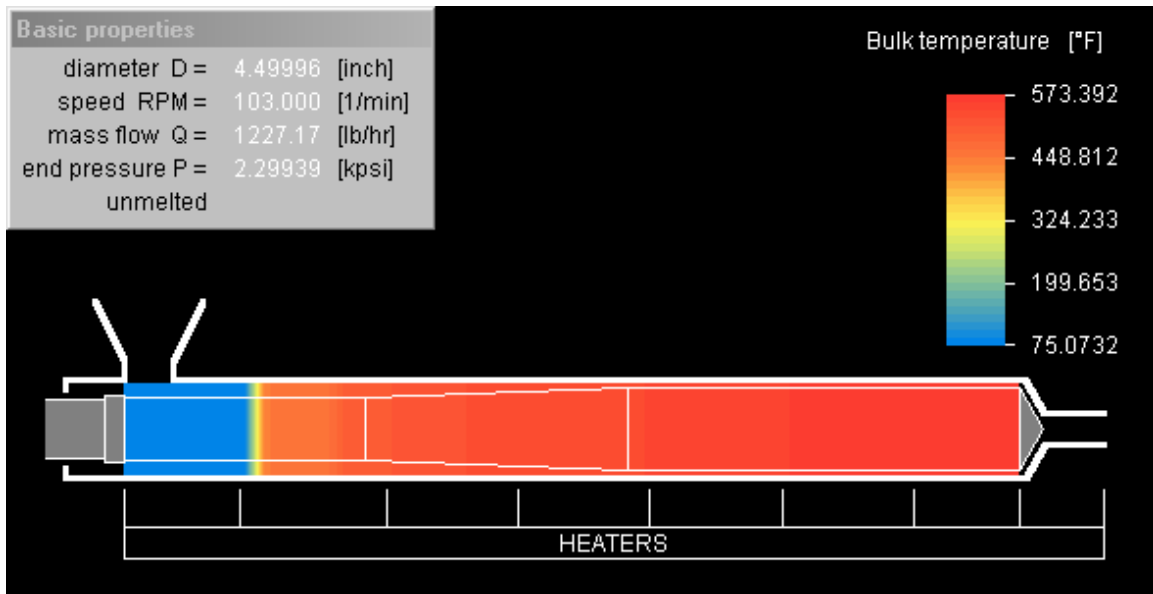


FIGURE 4

This design does not melt the resin completely, keep the resin from overheating or have good cross channel temperature uniformity. Figure 5 shows the difference in temperature from the screw root to the barrel wall. The graph has the screw root as position 0 and barrel wall as position 1 on the X axis. The temperature is on the Y axis. As can be seen from this plot, the temperature varies from 274C (525F) to 317C (603F). This large of a variation can cause flow problems through the die. Also, as was mentioned earlier, this material will show evidence of moisture in the melt curtain more readily the hotter it gets.

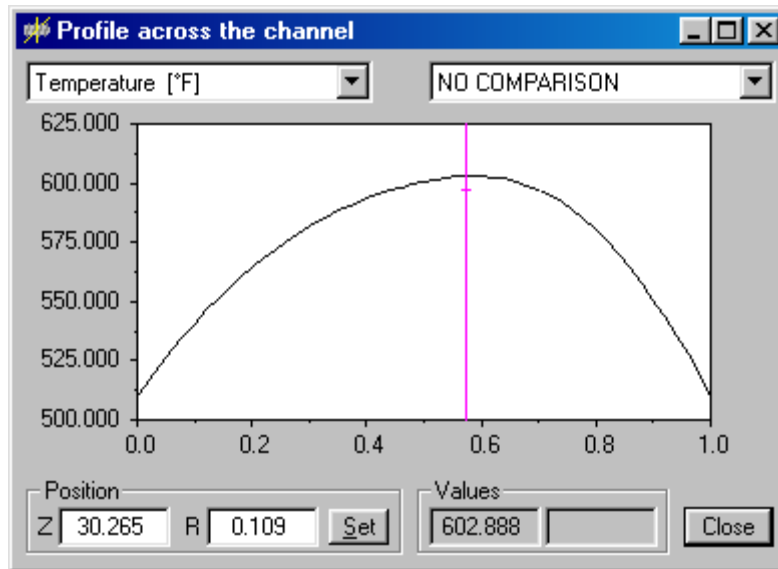


FIGURE 5

The next step was to try the lower shear-mixing tip (Tip #2) on the end of the screw. The concern in using this tip was that the mixer would overshear the nylon. Once again, this will cause moisture to migrate to the high shear zones.

The first difference in the performance of the two screws is that the material is fully melted for tip 2. Figure 6 shows that the material becomes fully melted as it goes through the mixer.

The next concern is the temperature of the resin. From the graph in Figure 1, we would like to keep the resin at 276C (529F) or less. As can be seen in Figure 6, the maximum temperature is 300C (572F). This would mean that the material would have to have less than 0.04% moisture content. It should be noted that the material directly from bag has moisture content of 0.02%. This would be a very risky design to successfully process this material. If this tip were used, the material would probably run acceptably on dry days but not on humid days.

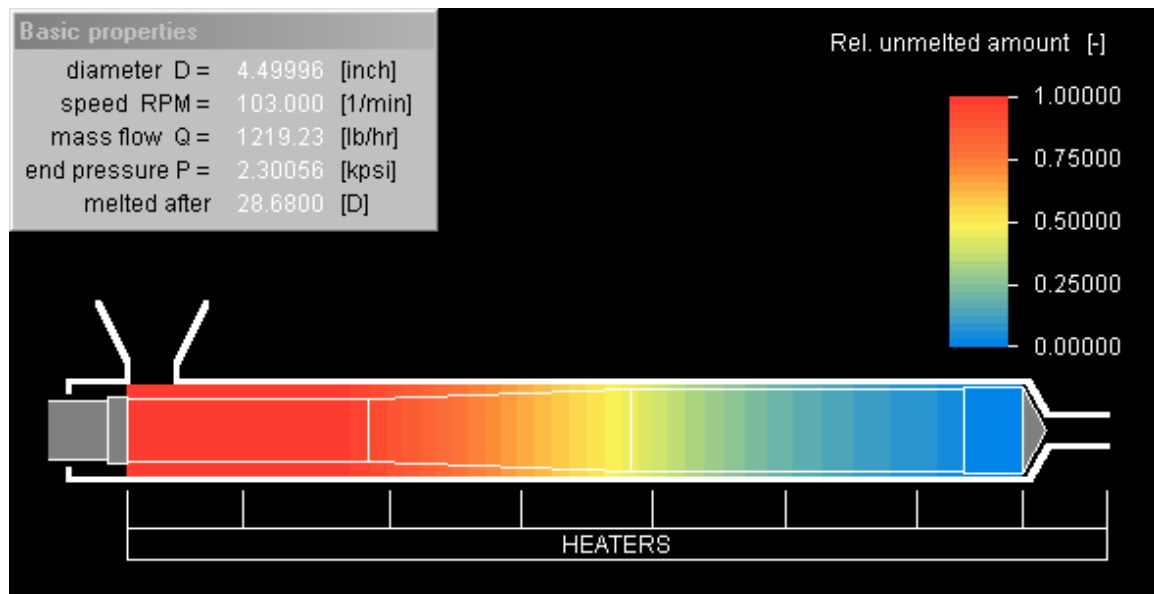


FIGURE 6

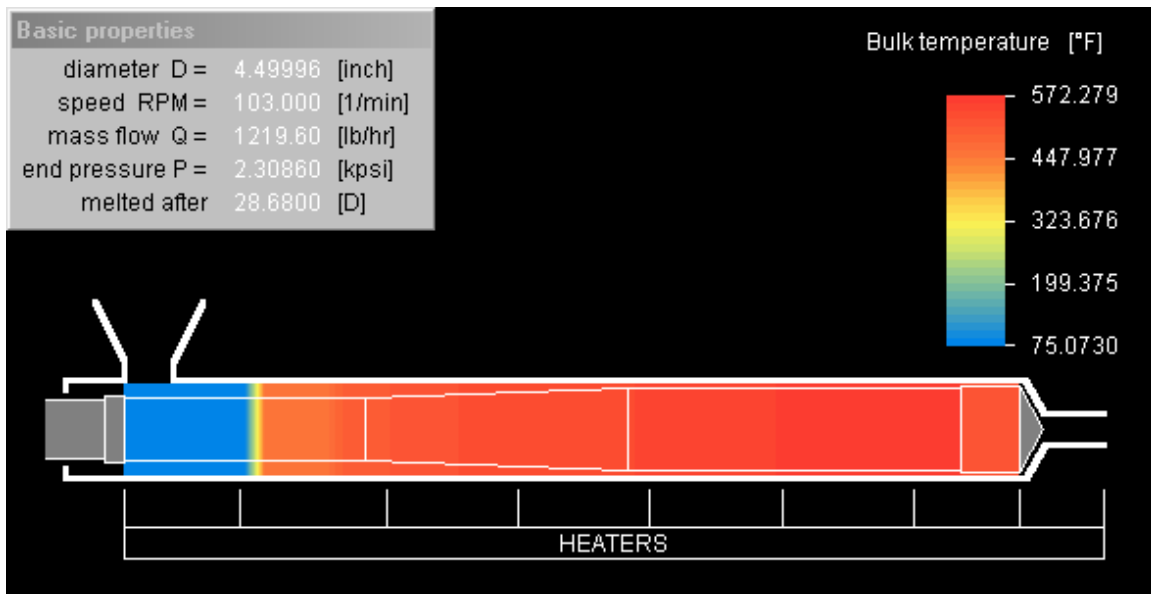


FIGURE 7

The preferred (recommended) tip (Tip #3) had the mixer positioned farther from the end of the screw. The premise behind this design was to melt the nylon quickly without putting too much heat into the material. The metering depth of this screw was deeper after the mixing section, again to keep the temperature down. While running this simulation, it was noticed that the output of this design was 15% greater than of the other two. This makes sense due to the fact that this tip has a deeper metering section. To compensate for the output differences, the simulation was run at 88 rpm instead of the 103 rpm of the previous screws. This would again be better for running the material, as the slower screw speed would generate less viscous heating.

Figure 8 shows the completeness of melting. As can be seen, the material is completely melted. This melting occurs rapidly in the mixing section of the screw. It should be mentioned that the clearance on this mixer is 0.51mm (0.02”) versus the 0.76mm (0.03”) clearance of the previous tip.

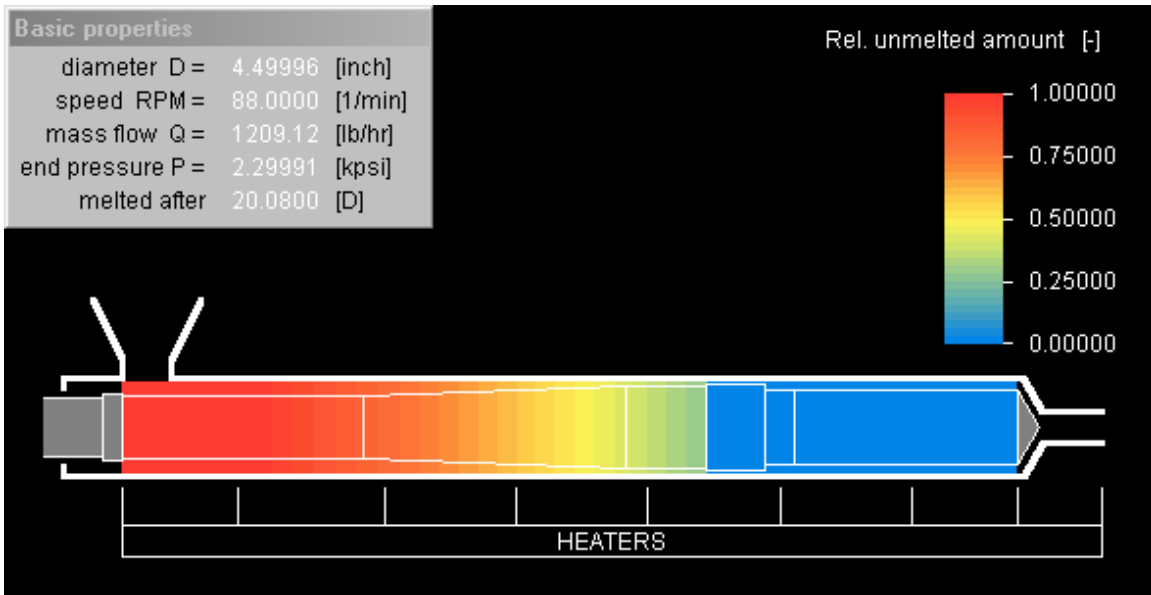


FIGURE 8

The material gets melted but does it get too hot? The 273C (525F) maximum temperature in Figure 9 is within the acceptable moisture processing range. The only concern with this screw design is how even is the temperature going to be cross channel from the root to the barrel wall at the end of the screw?

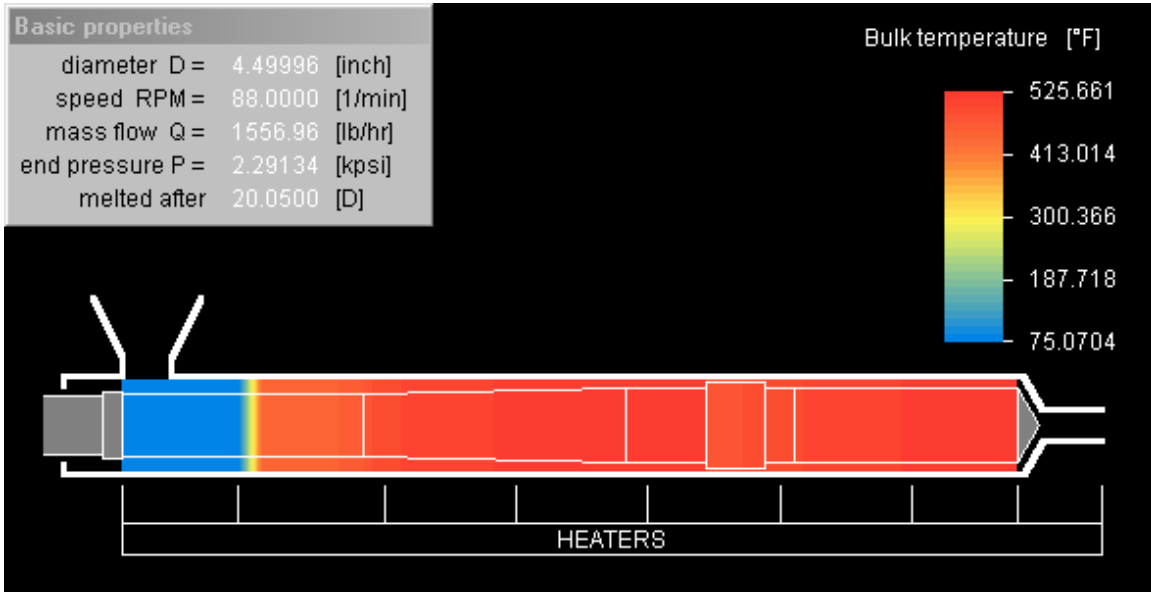


FIGURE 9

Figure 10 shows the cross channel temperature differential of the material as it leaves the screw. As a general rule, the temperature differential should be no more than +/- 5.6C (10F).

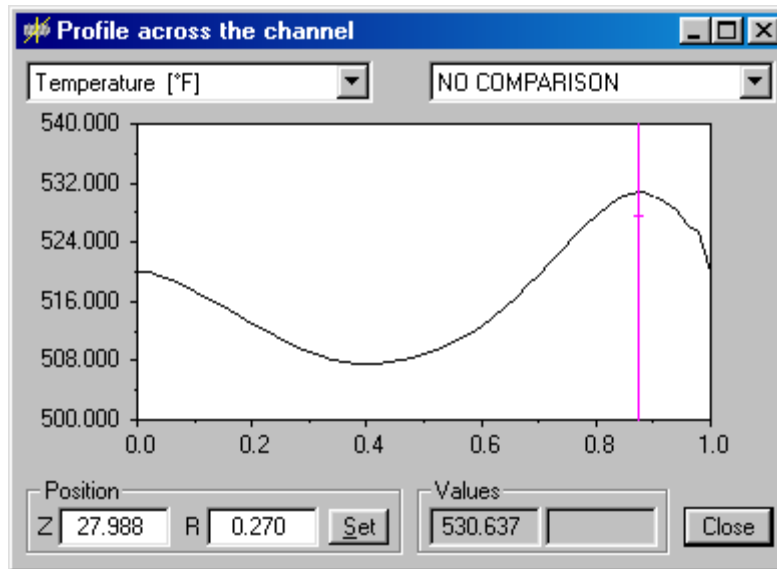


FIGURE 10

The cross channel differential is at about the maximum acceptable differential. The results from all three simulations showed that the last design would produce the best results. In most cases, only the one tip would be manufactured and used. We were fortunate in this case that all three designs were made and tested.

The first tip tested was the one with no mixer (Tip #1). The simulation gave the result of unmelted material. The trial was set up with this tip first. Upon running the material through the system, bubbles were seen in the melt curtain. These bubbles were thought to be moisture but upon closer examination, small unmelted particles could be seen at the start of the bubbles. The material was moisture tested and found to be 0.1% moisture. The target temperature should be less than 273C (523F). This was done to confirm that there were no inherent moisture problems. The material was run at slow screw speed due to the appearance of the melt curtain. Temperature and pressure were not too high but the screw speed was slow. As an experiment, the head pressure was increased from 1400 psi to 4000 psi. This cleared up the curtain, confirming the unmelts.

The second tip with the mixer at the end (Tip #2) was placed in the extruder. Initial testing indicated that the screw was completely melting the material. Temperatures were not as high as the simulation predicted but output was higher so this was understandable. As the material was run for a longer period of time at high screw speeds, poly skips started to appear. These poly skips looked like elongated holes in the product. This material was being coextruded with two other materials. Each layer was run separately to determine if the skips were due to the Nylon material. This was indeed the case. The poly skips had no evidence of unmelted polymer. It was felt that the holes were due to the higher local polymer temperature and the saturated moisture content at that temperature.

The final tip was placed on the end of the screw (Tip #3). The screw was run at 70 rpm for 15 minutes to stabilize the process. The melt curtain was clear. The cross channel melt temperature was checked and ran between 289-293C (553-560F). Figure 11 shows the summary for all three predicted conditions versus the actual for each tip. This chart shows that the simulation was not exact for temperature and output, it was relative. More importantly, the simulation tool provided an excellent means of detecting problems before the tips were even run. This is an extremely beneficial tool to have when designing for unknown materials. In this case, if only one design could have been used based on customer input, there would have been problems as were seen with the tip #1 design. It may have taken several tries without this tool to find the right screw design. Keep in mind that this was a material with a very narrow processing range.

Condition	Simulation	Actual
Tip #1		
Screw RPM	55 rpm	55 rpm
Melt Temperature	275C (527F)	272C (521F)
Head Pressure	1400 psi	1400 psi
Output	287kg/hr (632pph)	249kg/hr (548pph)
Problems	unmelts	unmelts
Tip #2		
Screw RPM	103 rpm	103 rpm
Melt Temperature	296C (565F)	293C (560F)
Head Pressure	2400 psi	2400 psi
Output	527kg/hr (1160pph)	505kg/hr (1110pph)
Problems	high temp	temp/moisture
Tip #3		
Screw RPM	75 rpm	75 rpm
Melt Temperature	281C (537F)	289C (553F)
Head Pressure	3600 psi	3600 psi
Output	405kg/hr (892pph)	368kg/hr (810pph)
Problems	none	none

FIGURE 11 – CASE 1 SUMMARY

DISCUSSION – CASE STUDY 2

BACKGROUND

The second case study involved newly developed Biodegradable Polyester. This resin was going to be tested in our extrusion lab. The manufacturer of this resin was DuPont.

MATERIAL SPECS & PROCESSING

This resin was DuPont Biomax 4026. It is a hydro/biodegradable polyester resin with an intrinsic viscosity of 0.7. It has a melting point of 195C (383F) and an amorphous density of 1.35.

Very little was known about processing this resin, including what feed screw would be the best. The supplier recommended that the material be run at low temperatures (desired melt temperature 238C (460F)) and residence time needed to be kept to a minimum. This material is a type of PET and that was deemed a good place to start in looking at screw designs. There were two different designs that were examined for this trial. The first was a single screw with two twisted mixers and the second was a barrier screw with one twisted mixer. The first was chosen because of its low residence time and the second because it would keep the temperature lower.

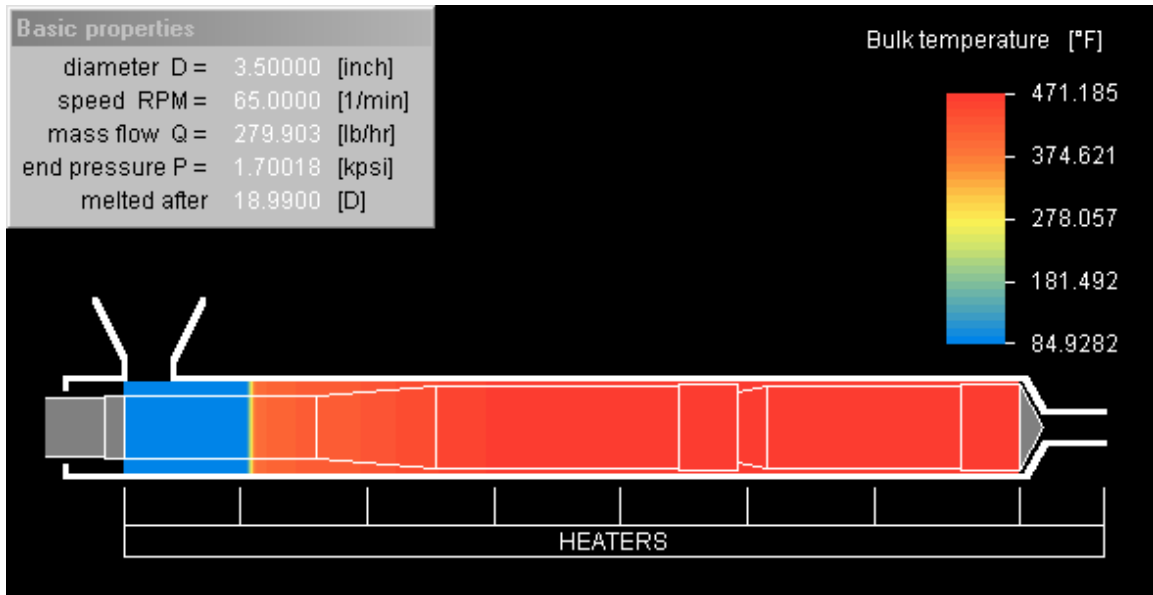


FIGURE 12

SIMULATIONS

The first screw was run with a goal of getting about 127-132 kg/hr (280-290 pph) at about 1700 psi head pressure. Figure 12 shows the melt temperature through the screw. As can be seen from the simulation, the bulk temperature is about 244C (471F). This is with the barrel zones set to achieve about 238C (460F). This means that the simulation is predicting that this resin will overheat in this screw. It was not known if this temperature would be too high for processing this resin. Figure 13 shows the amount of residence time in this screw. As can be seen, the mean residence time is about 133 seconds. This can be compared to a melt separation barrier design screw.

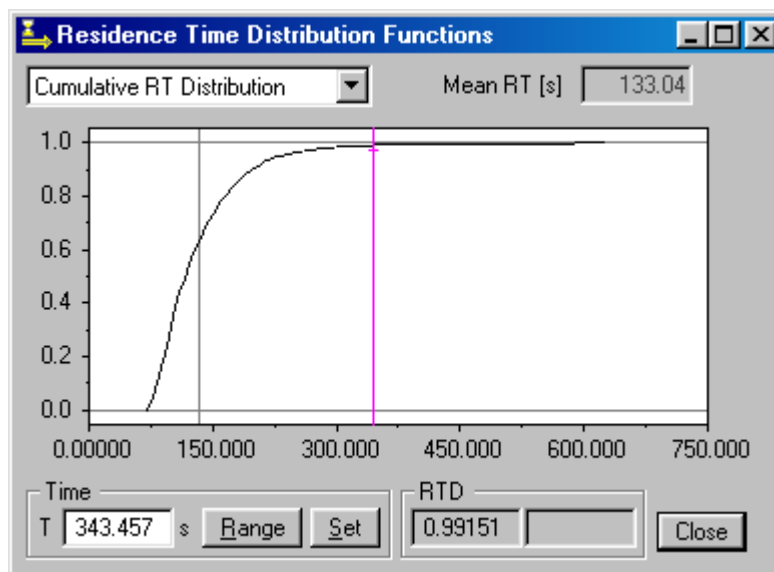


FIGURE 13

A proprietary barrier design (Black Clawson patents 5599097 and 5599098) was examined. Using the same set up conditions and adjusting screw speed to match the output of the previous simulation.

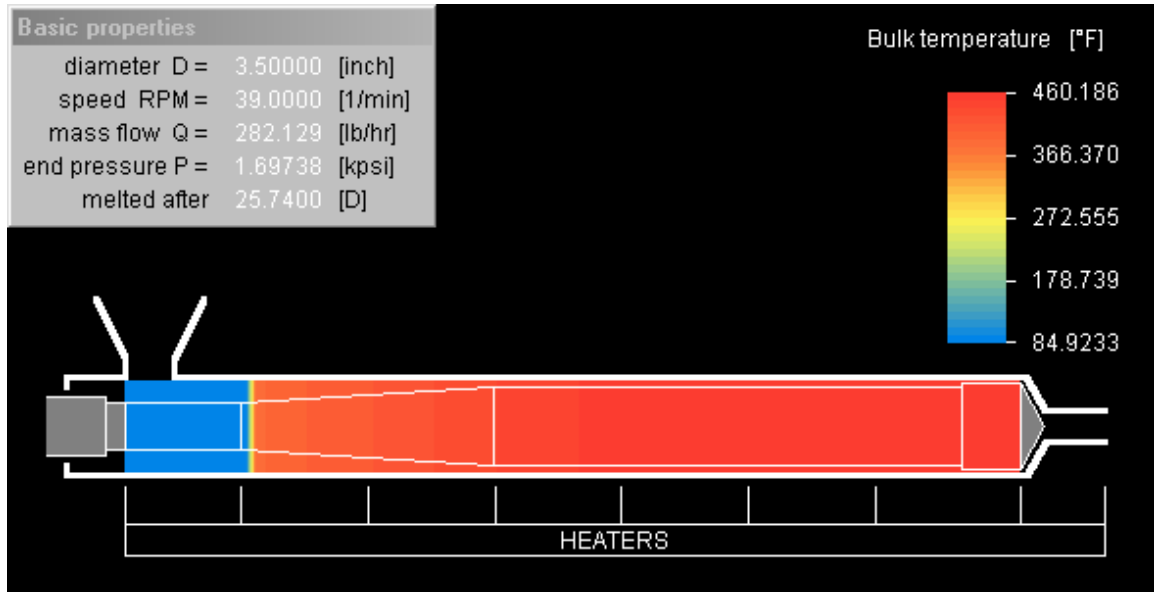


FIGURE 14

As can be seen from Figure 14, this screw keeps the temperature right at 238C (460F). This screw runs at 39 rpm to achieve about the same output as the first screw. The rpm of the first screw was 65 rpm. This screw does have longer residence time due to the increased channel volume.

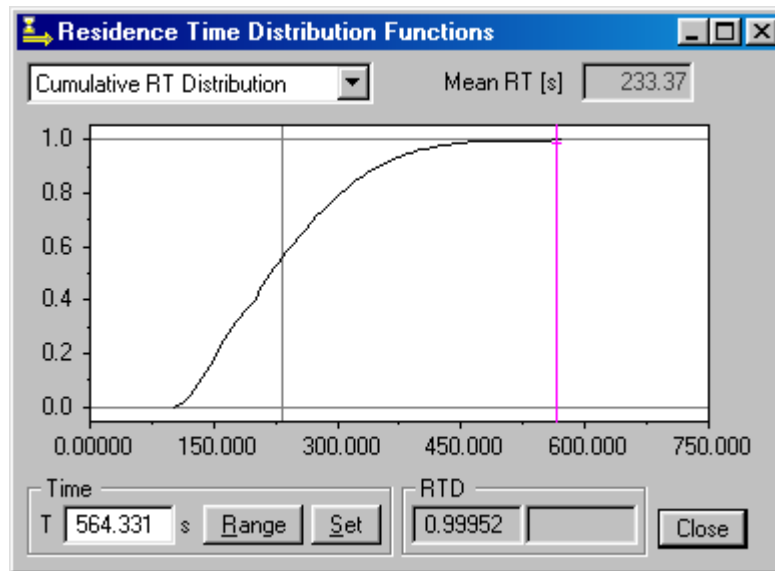


FIGURE 15

In Figure 15, the mean residence time is 233 seconds. This is about 1.67 minutes longer than the time for the first screw. It was decided by both parties involved to stay with the deeper screw to better control the temperature. Several months earlier, the first screw that was had been run in a different lab trial. This afforded us the opportunity to compare the flow simulation software once again to determine if the

simulation was giving us the results that we hoped for. We also ran the screw that we chose for the trial with better results.

Condition	Simulation	Actual
Screw #1		
Screw RPM	65 rpm	65 rpm
Melt Temperature	243C (470F)	247C (477F)
Head Pressure	1700 psi	1633 psi
Output	127kg/hr (280pph)	127kg/hr (280pph)
Problems	High melt temp	High melt temp
Screw #2		
Screw RPM	39 rpm	39 rpm
Melt Temperature	238C (460F)	238C (461F)
Head Pressure	1700 psi	1400 psi
Output	128kg/hr (282pph)	127kg/hr (280pph)
Problems	none	none

FIGURE 16 – RESULTS CASE STUDY 2

The chart in figure 16 shows that the first screw did overheat. It was actually worse than the simulation predicted. The rest of the variables for this screw were actually very accurate. The results for this material were much closer than the previous example. This could be due to many factors that make up each resin. The extrapolation of data from the viscosity curves follows the power law much more closely with this resin most likely being the main reason. The results from screw #2 were just as accurate.

SUMMARY

What can be learned from these two case studies? The use of a simulation tool cannot always be assumed to give 100% accurate results but can help us understand the behavior of the extruder and predict relative performance. The simulation tool can spot and pinpoint potential problems that can save considerable amounts of time and money. Careful interpretation of the data is necessary to achieve good results.

ACKNOWLEDGEMENTS

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