CHANGEOVER IN A TRANSFER LINE: NUMERICAL MODELING AND EXPERIMENTAL VALIDATION

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Abstract

In industry, a broad range of polyolefin products are often processed in the same equipment with multiple changeovers daily. Changing the resins in processing equipment such as extruders, transfer lines and dies exerts cost in terms of material waste and production down time. Minimizing these losses by running the products in an optimized sequence and by designing a flow path to reduce this transition time can be a great benefit. We studied the changeover from a single or twin-screw extruder previously [1,2]. Changeover times from transfer lines and dies can be different and even longer than extruder changeover times. These downstream flow channels can have significant impacts on transient operations in the polymer processing industry.

In this study, a series of numerical simulations were conducted to determine the changeover time from a transfer line connecting an extruder to a die. The impact of the polyolefin resin properties and resin sequence on the changeover time was also studied. Congruently, the changeover time was measured experimentally using online and offline optical techniques. These numerical and experimental results provided increased understanding of the influences that resin rheology (viscosity, melt flow and shear thinning index) and resin sequencing have on changeover time. Additionally, this work supports a theoretical framework for the design of flow channels to minimize the changeover delay due to the residence time of the resin in polymer processing equipment downstream of the extruder.

Introduction

For many polymer compounding and fabrication businesses, a broad range of products are often processed in the same set of equipment with multiple changeovers daily. Resin properties and processing characteristics of the different products can vary over a broad range. Transitioning between products requires purging the previous material out from the free volume of the extruder, transfer line and die, resulting in lost production time and an increased production cost. The time needed to achieve and adequate switch out of the materials in the polymer processing equipment can vary significantly depending on the flow rate, viscosity ratio between the resins, and flow channel design. Understanding the fundamental influence of these factors on the changeover operation is of significant practical significance and can be used to minimize the time and cost involved.

We previously studied the changeover from twin- and single-screw extruders [1,2], and identified a few important factors that can impact the extruder changeover time. A polymer discharged from the extruder will flow through the downstream flow channels such as transfer lines and dies, further increasing the changeover time. Unlike the extruder, mixing is very limited in these channels where the materials flow sequentially in a plug flow pattern. Material properties such as melt viscosity, shear thinning and viscoelasticity can be important predictors for the changeover time. The design of the flow channel is another crucial factor in the changeover operation as non-streamlined pathlines and dead volume can significantly increase the changeover time.

In this study, we developed a numerical method and an experimental protocol to determine the resin changeover time from a transfer line. A simple transfer line geometry was modeled to numerically determine a changeover time between two resins with differing rheological properties (shear viscosity and/or shear thinning index) based on a transient flow model. A die was constructed with the same transfer line flow channel to determine the changeover time experimentally. Changeover time from the transfer line was measured by online monitoring of the resin composition change before and after the transfer line using optical methods.

Governing Equations

Simulation of the flow of fluid in a transfer line involves the numerical solution of the equations governing viscous fluid flow on the specified computational domain, subject to the stated boundary conditions. Steady state and transient continuity and momentum equations as well as the transient 2-phase "volume-of-fluid" (VOF) equations [3] can be solved for the flow in a transfer line. For example steady, laminar flow of an isothermal, incompressible, non-Newtonian fluid can be described by the following forms of the equations of continuity and motion:

$$\nabla \cdot v = 0 \quad (1)$$

$$-\nabla p + \nabla \cdot T = \rho a \quad (2)$$

where ρ, v, p, T, and a are the density, velocity vector, pressure, extra stress tensor, and acceleration, respectively.

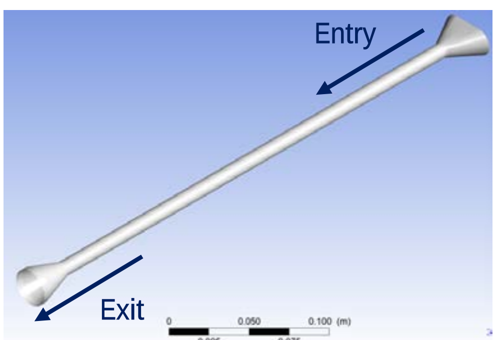
Simulation

Geometry

Two transfer line geometries used for the flow simulations are shown in Figure 1. Geometry A, shown in Figure 1a, has a 38 mm wide, 19 mm high elliptical flow inlet. It transitions to a 10 mm diameter circular channel. This 330 mm long circular channel ends with a 10 mm-to-25 mm diameter conical expansion channel.

Geometry B (Figure 1b) was used to aid in comparing the changeover times from numerical modeling and experimental measurements. A die (mimicking a transfer line) having an internal flow channel of Geometry B was designed and used for the changeover time experiments. This geometry is very similar to Geometry A in Figure 1a. This has an extended entry to transition from the twin screw tips to a 10 mm diameter circular channel. This 10 mm diameter channel is 175 mm long and ends with a 3 mm diameter orifice.

(a)



(b)

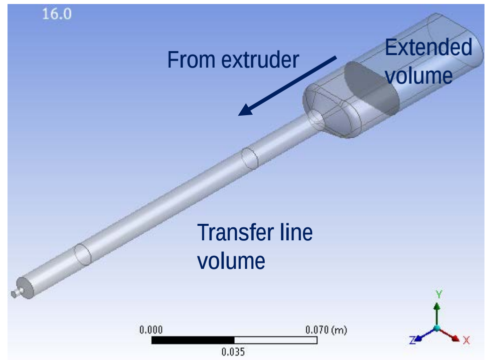


Figure 1. Two transfer line geometries, (a) Geometry A and (b) Geometry B, used for numerical modeling and changeover time experiments.

For the actual flow simulation, the inlet of these two geometries were extended to generate a fully developed inlet flow profile and to simulate the changeover time distribution from the extruder. This extended flow channel volume for Geometry B is shown in Figure 1b.

Computational Grid

The transfer line geometries were meshed using the ANSYS CFD Mesher. In order to reduce the computational time, only one quadrant of the geometry was meshed and modeled after splitting the geometry along two symmetry planes in the flow direction. An all hexahedral mesh was generated and the total mesh counts were around 120,000 elements (Geometry A) and 90,000 elements (Geometry B).

Flow Simulation

The steady or transient laminar, incompressible, isothermal flow of the non-Newtonian polymer was simulated by solving the mass and momentum equations via a finite element formulation using ANSYS Fluent. The following were the flow boundary conditions:

- Flow rate at inlet = 0.5 to 5 kg/h
- No slip boundary conditions on all transfer line walls
- Symmetry boundary conditions along symmetry planes.
- Outflow (i.e., fully developed flow condition) at transfer line exit

In order to simulate the resin changeover, a transient flow model incorporating a two-fluid "volume of fluid" (VOF) method was used to track the evolving shape of the interface between the two resins. VOF is a free-surface modelling technique to track and locate the fluid-fluid interface by solving a scalar advection equation for the volume fraction of one of the fluid phases. The overall fluid physical properties (e.g., density and viscosity) associated with each computational cell are then determined by volume fraction based mixing rules.

The changeover simulations were initiated with a steady state model to develop an initial flow profile of the starting resin at a constant flow rate. This was followed by a transient model incorporating the VOF method, but continuing to add only the Phase 1 fluid at the inlet with the initial flow rate. Finally, the new phase (Phase 2) was introduced to the inlet of the transfer line and the transient solution was computed at every time step, typically using 0.1 to 1 s time intervals.

Changeover times were determined by setting up two solution monitors to record the area average and mass flow rate weighted average of the volume fraction of Phase 2 at the outlet at every time step. These averages are determined by surface integrals (i.e., summations) over all of the computational cell faces (or facets), i, at the outlet;

$$\text{Area average} = \frac{\sum_i \alpha_{i,2} A_i}{\sum_i A_i} \quad (3)$$

$$\text{Mass flow rate weighted average} = \frac{\sum_i \alpha_{i,2} \rho_i v_i A_i}{\sum_i \rho_i v_i A_i} \quad (4)$$

where A_i is the area of the computation facet; $\alpha_{i,2}$ and ρ_i are the volume fraction of Phase 2 and the overall fluid density respectively that are associated with the facet; and v_i is the cell velocity normal to the facet face. The area average is representative of the composition of a frozen slice of extrudate taken at the transfer line exit. In contrast, the flow rate weighted average is representative of a "mixing cup" composition measurement for the fluid extrudate collected at the exit. The VOF simulation was continued until there was no change in the Phase 2 composition at the outlet of the transfer line. CPU times to reach this new steady state were 5-10 h across 20 processors.

Experimental

Materials and Rheology

Experimental shear viscosity data for three polyethylene resins (PE) and one polystyrene (PS) resin were used for numerical modeling. Resin A is a 1.0 dg/min melt index (190 °C/2.16 kg), 0.92 g/cm^3 density linear low density polyethylene (LLDPE) resin. Resin B is a 2.3 dg/min melt index, 0.917 g/cm^3 density LLDPE resin. Resin C is a 1.9 dg/min melt index, 0.919 g/cm^3 density low density polyethylene (LDPE) resin. Resin D is a 1.5 dg/min melt index (200 °C/5 kg) PS resin. The rheologies of the three PE resins used for changeover simulation (Resin A, B and C) at 280 °C are compared in Figure 2a. The rheology of Resin A at 243 °C and Resin D at 233 °C used for changeover experiments are compared in Figure 2b. Temperatures were the actual melt temperatures of the polymers measured during the changeover experiments.

The rheological behaviors of the polymers were described for numerical modeling based on the Cross model:

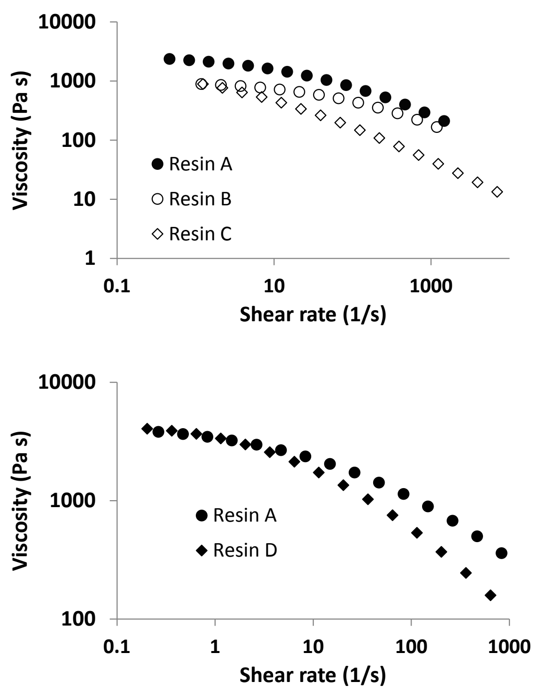
$$\eta = \frac{\eta_\circ}{1+\left(\dfrac{\eta_\circ \gamma'}{\tau^*}\right)^{1-n}} \quad (5)$$

where:

η = viscosity, Pa.s
$\eta_\circ$ = zero shear viscosity, Pa.s
τ^* = stress constant, Pa.s
γ' = shear rate, 1/s
n = exponent

It should be noted that the trend for the PE resins based on viscosity is A > B > C; and the trend based on the extent of shear thinning is C > A > B.

(a)



(b)

Figure 2. Resin rheology (a) for Resin A, B and C at 280 °C and (b) for Resin A at 243 °C and Resin D at 233 °C.

Changeover Experiments

Geometry B (Figure 2b) was used for the changeover experiments. The experimental set-up is illustrated in Figure 3. The transfer line (die) was connected to an 18 mm twin-screw extruder. Two optical probes were installed near the inlet and outlet of the transfer line to monitor the resin changeover based on a Raman signal. More details about the optical measurements to monitor resin changeover can be found elsewhere [1,2].

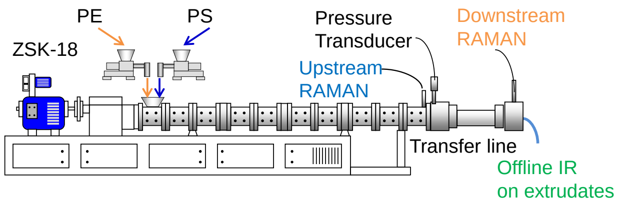


Figure 3. Experimental set-up to determine the changeover time from a transfer line.

PE (Resin A) and PS (Resin D) were selected for the changeover experiments due to their distinctive Raman response. For a typical experiment, the line was run for at least 15 minutes to ensure that steady-state conditions of either PE or PS (Phase 1) had been reached at a constant flowrate before introducing the Phase 2 material. Once steady state was reached, the feeding of Phase 1 was stopped and feeding of the new resin (Phase 2) started simultaneously at the same feed rate. Changeover from the upstream and downstream locations shown Figure 3 were monitored until > 99% changeover was obtained. During the experiment, extrudate samples were also collected from the transfer line discharge every 30 s, and the resin composition was determined off-line from Infrared (IR) measurements.

Results and Discussions

Effects of Resin Rheology on Changeover

A series of transient flow simulation based on the VOF method described above was carried out to determine the changeover times within a transfer line. Figure 4a and Figure 4b show the simulated flow profiles when Resin B (red) is changed over to Resin A (blue) and when Resin A is changed over to Resin B in transfer line Geometry A (Figure 1a) flowing at 5 kg/h. Note that the inlet of the transfer line was extended to create a fully developed velocity profile before reaching the original inlet plane. Time, t = 0 was defined when a fully developed profile of Phase 2 first reached the original inlet. Comparing Figure 4a and 4b suggests that the resin viscosity and resin sequencing can significantly affect the evolution of the interface for this two-phase flow system. The flow front of Phase 2 reaches the transfer line exit around t = 10 s for both cases. Then the Phase 2 resin continues to replace the original Phase 1 resin within the transfer line at an increasing proportion. For the changeover from Resin B to Resin A (Figure 4a), Resin B is completely replaced by Resin A at 74 s. However, for the changeover from Resin A to Resin B (Figure 4b), changeover was never completed within a simulated time frame of 117 s. The final changeover state is a Phase 2 core stream encapsulated by a Phase 1 skin near the wall.

Figure 5 shows that resin changeover monitored at the transfer line exit based on the flow rate weighted and area average of the volume fraction of Phase 2 during the transient flow modeling. Changeover profiles can be affected by the resin sequence used for the changeover of resins with differing shear viscosities. For both cases shown in Figure 5, the flow rate weighted average increased very rapidly as soon as the Phase 2 resin reached the transfer line exit. Due to the parabolic nature of the velocity profile, Phase 2 resin in the core flows out faster at the exit plane than the Phase 1 resin near the wall. This has a strong effect on the "mixing cup" average.

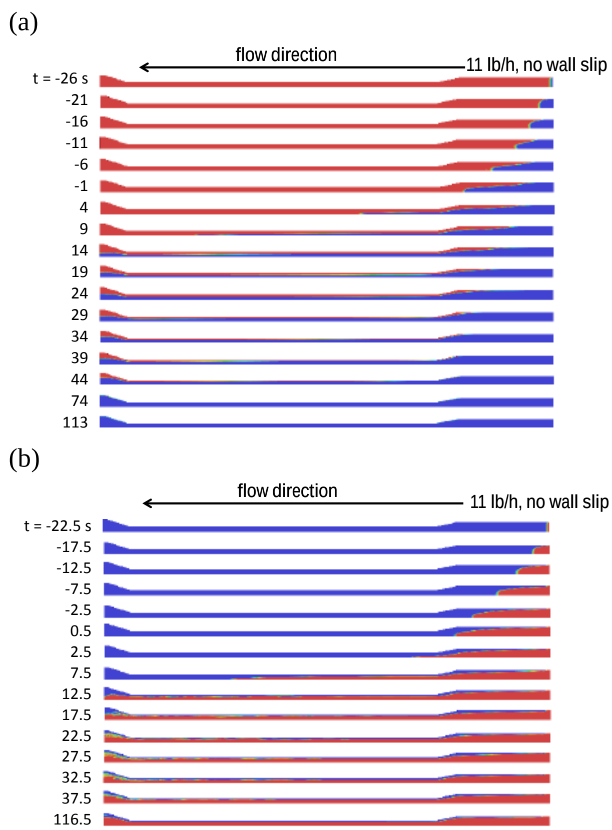


Figure 4. Changeover simulation results in a transfer line Geometry A (a) from Resin B to Resin A, and (b) from Resin A to Resin B flowing at 5 kg/h.

The trends seen for the area weighted average data were different from the flow rate weighted average data, and varied depending on the resin sequence. In this case, the monitored average composition is not affected by the velocity profile. When a lower viscosity Resin B was switched over to a higher viscosity Resin A (Figure 5a), the area average of the volume fraction of Phase 2 increased gradually until complete changeover was achieved. However, when Resin A was changed over to Resin B (Figure 5b), the area average reached a new steady state at slightly less than 60% of complete changeover, never reaching a full changeover state even at the final simulation time of 120 s.

Table 1 summarizes times required for 97% changeover based on flow rate weighted average and area average. Changeover times determined by flow rate weighted average were shorter when a higher viscosity Resin A was switched over to a lower viscosity Resin B than for the low to high viscosity changeover. However, the changeover time based on area average of volume fraction of Phase 2 was significantly longer for the changeover from Resin A to Reins B (where a changeover of 97% was never achieved in the simulated time frame).

(a)

(b)

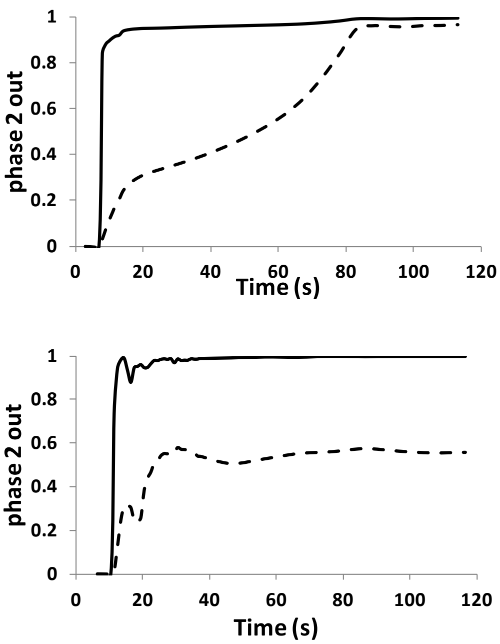


Figure 5. Changeover monitors at the transfer line exit based on flow rate weighted (solid) and area average (dashed) of volume fraction of Phase 2 from transient flow models for (a) Resin B to Resin A and for (b) Resin A to Resin B.

Table 1. Changeover time between Resin A and Resin B for > 97% conversion at transfer line exit

	Flow rate weighted avg	Area average
Resin B to Resin A	67 s	120 s
Resin A to Resin B	23 s	very long time

This difference in changeover responses depending on the resin sequence and monitors used can be explained by the resin and velocity profile of a transient two-phase flow. Figure 6 compares the velocity profiles of a two-phase flow from the exit of the transfer line plotted from the center (Position = 0) to the transfer line wall (Position = 0.0125 m) at t = 20 s. When a low viscosity resin (Resin B) is changed over to a high viscosity resin (Resin A), flow modeling predicted that high viscosity resin would form a core stream with a fairly flat velocity profile encapsulated by a relatively high (as compared to Figure 6b) velocity boundary layer of the low viscosity resin as illustrated in Figure 6a. Thus, a high viscosity plug flow can drag the low viscosity skin layer along, allowing for complete removal within a finite time frame. However, when a higher viscosity resin (Resin A) is changed over to a lower viscosity resin (Resin B), the transient two-phase flow consists of a low viscosity core with a more parabolic velocity flow profile (fast at the center and low near the interface) encapsulated by a very sluggish high viscosity boundary layer (Figure 6b). The low viscosity core flow moves over the almost stationary boundary layer, without removing the higher viscosity skin.

(a)

(b)

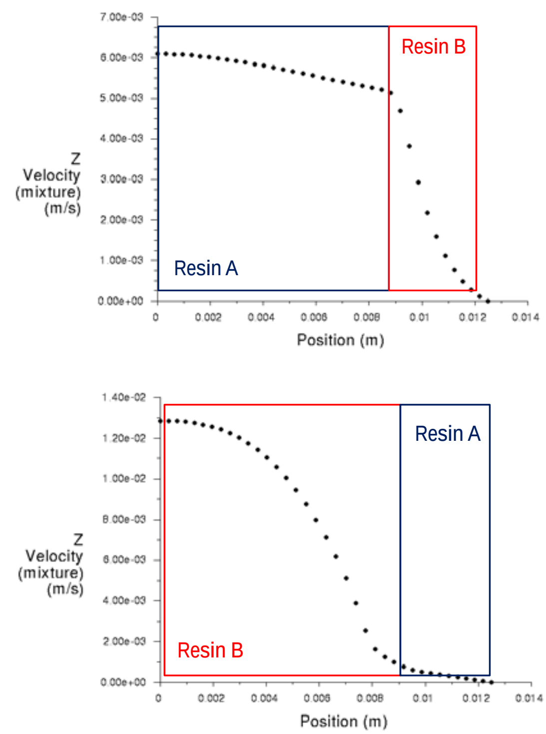


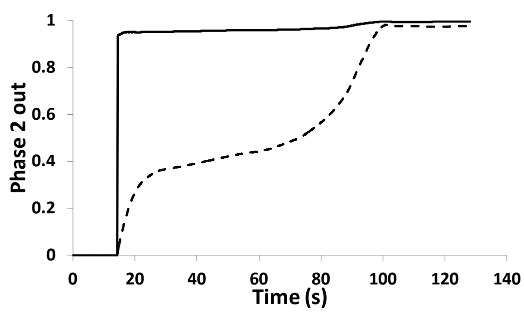
Figure 6. Two-phase velocity profiles at t = 20 s from the VOF transient flow modeling for (a) Resin B to Resin A and for (b) Resin A to Resin B at 5 kg/h.

A transient flow modeling was also conducted for Resin B and Resin C. As shown in Figure 2a, Resin B and Resin C have the same zero shear viscosity, but their shear thinning behaviors are distinguished in that as the

LDPE resin (Resin C) shear thins more pronouncedly compared to the LLDPE resin (Resin B). Figure 7 compares the changeover from Phase 1 to Phase 2 monitored at the transfer line exit for Resin B to Resin C (Figure 7a) and for Resin C to Resin B (Figure 7b). Depending on the extent of shear thinning and resin sequence, they exhibited dissimilar changeover profiles. For both cases, flow rate weighted average showed a sharp increase when the Phase 2 resin first reached the transfer line exit. For Resin B (LLDPE) to Resin C (LDPE), the area average of Phase 2 volume fraction gradually increased and eventually reached complete changeover. For Resin C (LDPE) to Resin B (LLDPE), the area average reached a steady state at less than 50% conversion and a complete changeover state was never achieved at the final simulation time of 130 s.

Table 2 compares the changeover results from the transient flow modeling for Resin B to Resin C and for Resin C to Resin B. These results indicate that the changeover time varies significantly depending on the resin sequence for polymers with different degree of shear thinning. The simulations predicted that it would take a longer time to change over from less shear thinning (resulting in higher viscosity) Resin B to Resin C if a flow rate weighted average of volume fraction of Phase 2 is used. However, if an area average is used, the transient model predicted a finite changeover time for Resin B to Resin C but an infinitely long time for Resin C to Resin B. This is contrary to what would be expected from the relative resin viscosities based on Table 1 trends discussed above, and suggests that the extent of shear thinning could have a stronger influence on the changeover time than the resin viscosity. It also suggests that it is the rheological nature of the skin layer (Phase 1) that dominates.

(a)



(b)

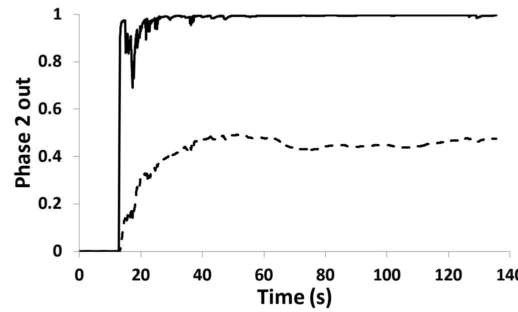


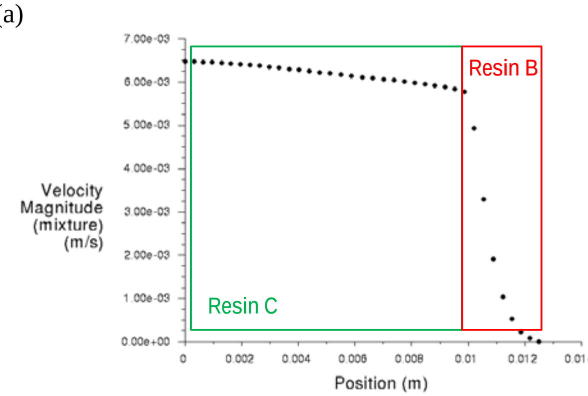
Figure 7. Changeover monitors at the transfer line exit based on flow rate weighted (solid) and area (dashed) average of volume fraction of Phase 2 from transient flow models for (a) Resin B to Resin C and for (b) Resin C to Resin B.

Table 2. Resin changeover time between Resin B and Resin C for > 97% conversion at transfer line exit

	Flow rate weighted avg	Area average
Resin B to Resin C	85 s	99 s
Resin C to Resin B	26 s	very long time

Figure 8 shows velocity profiles simulated for a two-phase transient flow for the changeover from Resin B to Rein C and from Resin C to Resin B across the transfer line exit at 5 kg/h. When compared to Figure 6b, using the same Phase 2 (core) material, we see that the velocity profile of the Phase 1 material near the wall in Figure 8b is significantly flatter for the more shear thinning (and in this case less viscous) Resin C, which in turn increases the height of the parabolic profile for the core material. Flushing out this near zero velocity skin layer will take an infinitely long time as reflected in the area average changeover time, while the flow rate weighted average will indicate that only Phase 1 is being collected (in a mixing cup) at relatively short times.

(a)



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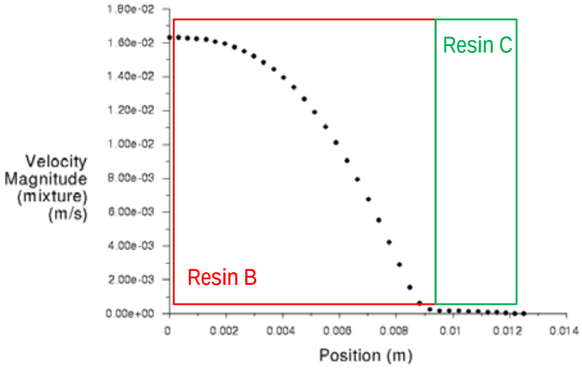


Figure 8. Two-phase velocity profile at t = 20 s from VOF transient flow modeling for (a) Resin B to Rein C and (b) Resin C to Resin B at 5 kg/h.

If we reconsider the results in Table 1 from a shear thinning effect standpoint, we see the same trends as seen in Table 2 in that Resin A is more shear thinning than Resin B, and the higher shear thinning skin layer tends to have a flatter velocity profile. However, the differences in the degree of shear thinning are less when comparing Resins A and B so that the viscosity effects will be more dominant.

Changeover Time Experiments

In order to validate the changeover time results from the transient flow simulation, changeover extrusion trials were conducted on a setup described in Figure 3 to determine the changeover time experimentally. The changeover between PE and PS was quantified by attaching transfer line (die) Geometry B to a twin-screw extruder and using on-line optical measurements. The changeover time from the same flow channel geometry (Figure 1b) was also estimated via flow simulation using the resin rheology data in Figure 2b. For the changeover simulations, the flow rate weighted average of volume fraction of Phase 2 was monitored at both the entry and exit of the transfer line (upstream and downstream locations in Figure 9) to quantify the changeover from the transfer line. Figure 10 compares the changeover between Resin A and Resin D determined via numerical modeling (dashed lines) and a changeover experimental trial (solid lines). For the changeover measurements from the upstream location of the transfer line, online Raman measurements were utilized. Downstream changeover was measured using offline IR measurements on extrudate samples from the die.

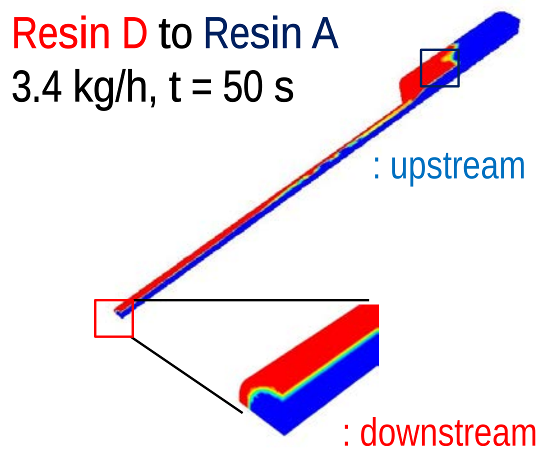
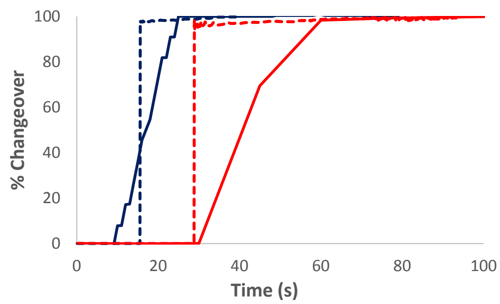


Figure 9. Transient VOF flow modeling on Geometry B for changeover from Resin D to Resin A flowing at 3.4 kg/h and upstream and downstream locations where the changeover based on flow rate weighted average of volume fraction of Phase 2 was monitored.

Figure 10 shows the % changeover versus time at two different locations, inlet (blue) and outlet of the transfer line (red); time zero represents the moment when the extruder feed stream resin switch is made. Clearly, there is a reasonable agreement between the changeover determined through numerical modeling and experimental measurement. In particular, the numerical modeling was able to predict the onset of the changeover from both upstream and downstream locations reasonably well. The main discrepancy between numerical modeling and experimental result is on the slope of the lines. Experimental results showed a more gradual change in % changeover over time while the numerical simulation based on flow rate weighted averages predicted a sudden jump from 0 to 100% changeover. This mismatch can be due to the significant phase mixing inside the extruder that leads to a broad distribution in the resin composition feeding the transfer line. Whereas, the simulations were conducted based on an assumption of an instantaneous 100% feed change between two resins that will flow sequentially from a pure Phase 1 to Phase 2 transition in a plug flow.

(a)



(b)

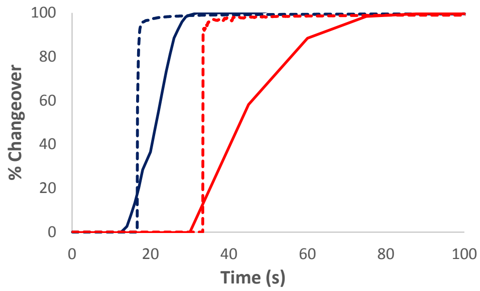


Figure 10. Changeover at 1.7 kg/h rate (a) from Resin D to Resin A and (b) from Resin A to Resin D monitored from inlet (blue) and outlet (red) of Geometry B determined from flow simulation (dashed line) and experimental measurements (solid line).

Table 3 lists experimentally and numerically determined changeover times for > 99% changeover between Resin A and Resin D from the transfer line. Changeover times were recorded from the upstream and downstream locations in Figure 9 and the differences between the upstream and downstream values are reported in Table 3. There are reasonable agreements in the changeover times determined through flow simulation and changeover experiments. Both experiments and simulation predicted faster changeover at a higher flow rate, 3.4 kg/h versus 1.7 kg/h as expected. Experiments and simulation both predicted a longer changeover for Resin A (PE) to Resin D (PS) at 3.4 kg/h, (where the shear thinning characteristics would be stronger, with Resin A being less shear thinning), and a longer changeover for Resin D to Resin A at 1.7 kg/h (where the shear thinning characteristics are weaker, with Resin D having lower viscosity).

Table 3. Time for > 99% changeover between Resin A and Resin D from a transfer line.

Changeover time (s)	**Experimental**		**Simulation**	
Flowrate (kg/h)	1.7	3.4	1.7	3.4
Resin D to Resin A	> 115	50	161	36
Resin A to Resin D	> 56	60	83	65

Conclusions

This study has shown how the resin changeover from a transfer line can be significantly affected by the resin rheology and resin sequencing. The numerical definition of changeover time; i.e., based on flow-rate average versus area average; can affect the trends observed and needs to be taken into account when interpreting the results. When changeover time is based on flow rate weighted average (i.e., “mixing cup” composition in an extrudate), the flow simulation predicted that at similar flow conditions, switching the resins from high to low viscosity (with similar shear thinning characteristics) takes place faster than the opposite order. The reverse trend is predicted using area averages, which reflects the development of an almost stationary high viscosity skin layer that is very hard to remove from the system. When resins with different degrees of shear thinning are involved, area-average based changeover is predicted to be faster inside a transfer line when a less shear thinning (LLDPE) resin is purged out by a more shear thinning (LDPE) resin. These results suggest that higher viscosity and more shear thinning (LDPE) resins make a good purge material for lower viscosity and less shear thinning (LLDPE) resins.

Changeover time from a transfer line was also determined via experiments. However, once again the nature of the changeover time being measured needs to be understood in order to correctly interpret the results. Changeover times based on mixing cup sampling may be very different from those based on point probe measurements or frozen resin analysis. In this work, changeover times between PE and PS resins measured using an optical technique appeared to correlate well with what were estimated from numerical modeling, using flow-rate-average based predictions. Both experiments and modeling predict a longer changeover time at a lower flow rate. The results emphasize the importance of understanding the rheology and resin sequencing of polymer resins for the changeover from a transfer line. Optimizing these factors will help minimize the changeover time for the polymer processing equipment for reduced production time and cost.

References

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