Low Shear Melt Barrier Screw
Design Target
Poly Lactic Acid

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Introduction

Poly Lactic Acid (PLA) is currently one of the most available and versatile bio-based polymers used by packaging extrusion processors. It is finding wide acceptance in a number of packaging applications; sheet, film, and extrusion coating. Recently we were requested to design an optimized screw to evaluate in comparison to an existing design and an alternate new design. We were tasked to parallel the already on-going development and offer our best design to meet the objectives. Both new screw designs were to be built and evaluated against the design objective for consideration to fulfill their needs in future production applications. This paper reviews the design procedure used to develop the target design and compares the results.

Objectives

Our customer owns a 3 ½” diameter 30:1 L/D extruder. They use this for in-house product development, testing, and scale up. Due to the requirement of their larger production systems they established the target requirement for the 3 ½” extruder, which upon scale up, would meet the requirements of their production extruder.

Following is the design target provided:

Primary Material: PLA, 1.5 to 3.0 MI
Target Rate: 1000 PPH
Target Melt Temp: < 475°F
Pressure Stability: < ± 1.5%
Temp Uniformity: < ± 5°F

Procedure

Our approach to all extrusion systems design problems is consistent:
1. Gather all pertinent system data
2. Gather physical, thermal and rheological material data
3. Gather relevant existing process data
4. Determine any unstated customer expectations
5. Use system, material, and existing process data to develop a simulation model
6. Calibrate the simulation to fit the existing data
7. Develop optimized design geometry and build a simulation model
8. Run simulation experiments considering the “what if” effects of different processing conditions
9. Tweak the design geometry and repeat (steps 7, 8, & 9) until an acceptable design is achieved
10. Manufacture & evaluate

The 3 ½” extruder to be used for testing had the following critical features:

Barrel Diameter  3.5”
Effective Screw Length 28.5 D
Connected Horsepower 200 HP
Screw Speed  200 RPM @ motor base speed
Available torque  5,250 ft-lbs
Heat/Cool Zones  Five (5)

The physical and thermal data for the customer’s PLA resin was obtained. To determine the rheological properties a sample was measured using a capillary rheometer. Shear rates ranged from 1.5 to 2500 (1/sec) at temperatures of 210°C, 230°C, and 250°C. Prior to testing the sample was dried in a vacuum for 12 hours at 80°C. The raw data was adjusted for capillary entrance effects and the corrected shear rate and viscosity values were calculated. The tabulated shear rate and viscosity data were entered into the Compuplast Virtual Extrusion Laboratory (VEL™) simulation suite of programs and fitted to a Carreau model.

<table>
<thead>
<tr>
<th>Shear viscosity – Carreau model</th>
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<tr>
<td>Constant 1</td>
</tr>
<tr>
<td>Constant 2</td>
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<tr>
<td>Constant 3</td>
</tr>
<tr>
<td>Yield stress (τ_y)</td>
</tr>
</tbody>
</table>

\[
\eta(\gamma, T) = \frac{A f(T)}{1 + ([\gamma f(T)]^{1/3})^3} \quad \eta_{\text{total}} = \eta_{\text{model}} + \tau_{\text{yield}}
\]

Fig 1 - Carreau Viscosity Model Parameters of PLA Material
Fig 2 - PLA Rheology Data as modeled

Our customer provided run data from his 3 ½” diameter extruder using the existing screw design. This screw geometry was modeled in the simulation software. We used our best experience to estimate design data that was not specifically provided for the existing design. When the screw geometry was entered in the simulation software the development extruder operating conditions (screw speed, barrel heater set temperatures, head pressure, etc.) were input and a simulation was run. Below is a sample result from the simulation of the existing development extruder screw design.

Fig 3 – Simulation Results for Existing Screw
Since the simulation software incorporates several factors (e.g. coefficient of friction between the pellets and the barrel wall) that are not readily or accurately available the simulation of a known design and a known result are used to “calibrate” these settings in the software set up to obtain a consistent and correlated result. These factors will be used for this application when screw design changes are evaluated.

Although this customer emphasized the need for a screw design dedicated to the optimum performance running PLA they would still have a need to run existing LDPE products. Although their desire was to not change between these products on the extruder line set up for PLA production we still considered the performance on their traditional LDPE resin as an additional design target.

Secondary Material: LDPE, 8.0 to 12.0 MI
Target Rate: 700 PPH
Target Melt Temp: > 580°F
Pressure Stability: < ± 1.5%
Temp Uniformity: < ± 10°F

Using this guiding information from the customer and our existing design data base a preliminary design is developed. The preliminary design geometry is loaded into the simulation software and using the “calibration” settings for the empirically developed variables a series of simulations are run to compare to the existing data, and “calibration” simulations, and our design objectives. Below is a sample simulation for our preliminary design.

Fig 4 – Simulation Results for Preliminary Screw Design

For both the existing design and the preliminary new design a series of simulations were run for outputs from about 1/3 of the target to slightly greater
than the desired 1000 PPH. The following table summarizes the results from these simulations. Note that the preliminary new design yields a higher output per rpm compared to the existing design. The simulations for this higher output screw are run at a lower screw speed.

<table>
<thead>
<tr>
<th>Screw Speed (RPM)</th>
<th>Output (PPH)</th>
<th>Pressure (PSI)</th>
<th>Avg T (F)</th>
<th>Max T (F)</th>
<th>Power (HP)</th>
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<tbody>
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<td>1739 1515</td>
<td>480 488</td>
<td>480 502</td>
<td>147.8 1595</td>
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<td>250</td>
<td>1198 1644</td>
<td>495 495</td>
<td>510 510</td>
<td>180.8</td>
<td></td>
</tr>
</tbody>
</table>

**Table of Simulation Results for Old “Calibration” and New “Preliminary” Designs**

A couple interesting observations are made from these simulation results. The melt temperature of the new (preliminary) design is significantly lower than the old (calibration) screw, 471°F vs. 488°F. This colder temperature results in a higher pressure by 80 psi (~ 5%) due to the viscosity shift at the lower temperature. Also the new screw simulation indicates a very uniform temperature where the average temperature is essentially equal to the maximum. For the old design there is a 14°F difference between the average and maximum temperature. This big difference in melt temperature is also reflected in the specific rate (PPH/HP) for each screw. At 6.68 PPH/HP the existing design has 32% higher mechanical energy input the viscous shear than the new design at 8.83 PPH/HP. This indicates a significant energy efficiency improvement to be expected from the new design.

These results were reviewed with the customer and although the new design simulations indicate a temperature higher than the 475°F target a screw was manufactured to this basic design. Based on the existing screw performance data and “calibration” results we felt the simulations were over predicting the actual melt temperature.

**Test Results**

The new screw was manufactured for evaluation. Our customer tested our new
design and compared the performance to the alternate screw design developed on a parallel path. Each screw was tested at a minimum of three screw speeds and three different extruder barrel profiles. The performance data was collected and analyzed. The plot below shows the operating window for the our screw. The vertical axis shows the maximum barrel heater zone temperature (barrel zone temperatures were ramped from a low temperature at the feed zone to a maximum at the head of the extruder). The horizontal axis is screw speed in rpm. The resulting output and melt temperatures are seen in the contour lines. The white section represents the acceptable operating window. The maximum target output could be achieved at a screw speed of 138 rpm with a barrel temperature profile ending at 444°F in the last barrel heating zone. Lower melt temperatures were achievable at lower settings and a broad window was available at lower screw speeds and outputs.

Fig 5 – Our PLA Screw Operating Window

**Alternate**

The alternate design was also tested. The same test procedure was used with three run speeds and three barrel temperature profiles. This data of the alternate screw was analyzed and the resulting operating window is presented below.

The same vertical and horizontal scales are used in this plot. You can see from
this contour plot that the target output of 1000 PPH was achieved at a screw speed of 110 RPM and a barrel temperature profile ending at 438°F. This is a little bit of a surprising result since we would expect a significantly lower viscous energy input from this deeper screw design. It is suspected the barrier and mixer clearances in this design are significantly tighter than in our design. The alternate design results in a substantially smaller operating window and a greater sensitivity between outputs and melt temperatures. Note that this result is actually an indicator of pressure sensitivity since the lower temperature melt corresponds to a higher operating pressure with a fixed downstream forming system. This would be an anticipated result with a deeper screw design.

<table>
<thead>
<tr>
<th>HorizVert Factor</th>
<th>Current X</th>
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<tbody>
<tr>
<td>Screw Mfr</td>
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<tr>
<td>Barrel Temp, F</td>
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<tr>
<td>Screw Speed, rpm</td>
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</table>

<table>
<thead>
<tr>
<th>Response</th>
<th>Contour</th>
<th>Current Y</th>
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<th>Hi Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Avg Melt Temp, F</td>
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<td>440</td>
<td>460</td>
</tr>
<tr>
<td>Output, lb/hr</td>
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<td>0</td>
<td>1000</td>
</tr>
<tr>
<td>Barrel Pressure, psi</td>
<td>4000</td>
<td>2867.8952</td>
<td>0</td>
<td>4000</td>
</tr>
</tbody>
</table>

Fig 6 - Alternate Screw PLA Operating Window

Summary

This paper has described a design procedure using a combination of experimental data, experiential data, and simulation data to evaluate an existing screw design and develop a new and optimized design for a specific target application. The design procedure is a robust method that depends on a calibration of the simulation to real world processing data before evaluating alternative designs. In addition to field process data to correlate to the simulation reliable physical data and rheological data must be obtained in the range of
shear rates and temperatures to be simulated. With this fundamental data new screw design geometry can be simulated and evaluated with a strong correlative confidence. The results of this design procedure provided a screw design for the target application with a wide operating window satisfying the design target supplied by the customer.

Reference:

Foederer, Beth M., “Equipment and Processing Considerations for Extruding Bio-Resins”, TAPPI-PLACE

Christie, Andrew W., “Equipment Design Considerations for Processing with Metallocene Resins”, Polyolefins

Perdikoulias, John, Personal Communication (2010)

Compuplast, Virtual Extrusion Laboratory™, Version 6.3, Compuplast International Inc. 2009
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Original Publication
SPE FlexPackCon 2010
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Outline

• Introduction
• Design Objective
• Design Procedure
• Simulation Calibration
• New Design & Fit
• Test Data
• Summary
Introduction

• Bio-based materials for sustainability
  – Poly Lactic Acid (PLA)
  – Bio-based polyesters
  – Starch modified
  – PolyHydroxy Butyrate (PHB)

• Material properties / process requirements

• Design process
  – Existing data
  – Simulation calibration
  – Design evaluation
  – Build & test
Bio-based materials

- Commercial bio-polymers ≠ LDPE
  - Hydroscopic – Dry to < 50 ppm
  - Shear sensitivity
  - Temperature limited
  - Rheological space
Design Objective

• Design Optimized for PLA
  – Primary Material: PLA, 1.5 to 3.0 MI
  – Target Rate: 1000 PPH
  – Target Melt Temp: < 475°F
  – Pressure Stability: < ± 1.5%
  – Temp Uniformity: < ± 5°F

• Secondary Consideration – LDPE
  – Secondary Material: LDPE, 8.0 to 12.0 MI
  – Target Rate: 700 PPH
  – Target Melt Temp: > 580°F
  – Pressure Stability: < ± 1.5%
  – Temp Uniformity: < ± 10°F
Design Procedure

• Gather all pertinent system data
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• Gather relevant existing process data
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• Calibrate the simulation to fit the existing data
• Develop optimized design geometry and build a simulation model
• Run simulation experiments considering the “what if” effects of different processing conditions
• Tweak the design geometry and repeat (steps 7, 8, & 9) until an acceptable design is achieved
• Manufacture & evaluate
Customer Test Extruder

- Barrel Diameter: 3.5”
- Effective Screw Length: 28.5 D
- Connected Horsepower: 200 HP
- Screw Speed: 200 RPM @ motor base speed
- Available torque: 5,250 ft-lbs
- Heat/Cool Zones: Five (5)
Melt Index / Rheology

- **Melt Index**
  - Simple test
  - One temperature
  - One shear rate
  - Relative indicator

- **Capillary Rheology**
  - Multiple temperatures
  - Multiple shear rates
  - Bracket operating range
Carreau Model
Capillary Rheology
Extrusion Coating Comparison
Existing Screw Design

- Single Flight Design
  - Constant Depth Feed
  - Tapered Transition
  - Long Meter
  - Maddocks (UCC) Mixer
  - Short 2nd Meter
Simulation Model Existing Design

- Existing Geometry “Calibrated” to Data
## Calibration Simulation Summary

<table>
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<th>Screw Speed (RPM)</th>
<th>Output (PPH)</th>
<th>Pressure (Psi)</th>
<th>Avg T (F)</th>
<th>Max T (F)</th>
<th>Power (HP)</th>
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<td>1198</td>
<td>1644</td>
<td>495</td>
<td>510</td>
<td>180.8</td>
</tr>
</tbody>
</table>
What did we learn – 200 rpm

- Over heating due to high shear input
- Aggressive feeding
  - Pre-heated pellets
  - Higher density
New Screw Design

• Lower compression ratio
• Long melt barrier design
  – Less aggressive transition
• Low shear input
  – Liberal barrier clearance
  – Liberal mixer clearance
• No stagnation points
  – Twisted helical mixer with tapered root
  – Modified “Gregory” patent
Melt Separation Barrier
Barrier Efficiencies

The Maillefer barrier, patented in 1967, was the first melt-separation device. It retains solids in the primary channel, eliminating the break-up of the solids bed and improving melting capacity and melt quality.

The Schippers/Barr primary melting channel gets shallower as the auxiliary channel deepens. A straight primary flight increases melting area in contact with the barrel wall, relative to Maillefer's design.

Wheeler's DSB-1 barrier for Davis-Standard borrows from Maillefer, Schippers/Barr, and Dray. It uses three different lead widths, which reduces the melting area.

The width of Dray's primary channel carrying the solids stays the same even after it joins the auxiliary channel, allowing a larger melting area than other barrier designs.
Maddock’s (UCC) Mixer

- Dispersion – high shear over barrier
- Distribution – splits & recombines flow
- Depends on pressure for flow
- Dead ended channels
- Wiping flight
Modified Gregory Mixer

- Dispersive – high shear over barrier
- Distribution – splits & recombines flow
- Helical channels pump at all speeds
- Tapered channel ends
- No wiping flight
New Design Simulation

[Image: Simulation software interface showing various graphs and data points related to extruder results for PLA, including temperature profiles, pressure data, and material flow rates.]

Details:
- Diameter: 8.66 mm
- Speed: 100 RPM
- Mass flow: 0.0819 kg/s
- Screw pressure: 9.989 MPa
- End pressure: 0.990 MPa
- Melt temperature: 238.0°C
- Viscosity: 1 Pa·s
- Temperature profile across the channel
- Pressure profile along the screw
- Extruder results for PLA
- PLA module
- Screw RPM: 100
- Mass flow rate: 20.41 kg/h
- Solids transport angle: 15°
- Maximum solids conveying mass flow rate: 265.5 kg/h
- Energy consumption: 39.44 kW
- Screw torque: 5208.7 N·m
- Screw back force on the tip: 6200 N

[Additional graphs and data points shown, including temperature and pressure variations along the channel and screw.]
## New Design Simulation Summary

<table>
<thead>
<tr>
<th>Screw Speed (RPM)</th>
<th>Output (PPH)</th>
<th>Pressure (PSI)</th>
<th>Avg T (F)</th>
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## Field Test

### 445 F BARREL SET TEMPS

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<th>Motor LOAD (318 FLA)</th>
<th>LOAD/RPM</th>
<th>% Maximum Load</th>
<th>Output</th>
<th>Output/RPM</th>
<th>Barrel Pressure</th>
<th>Adaptor Pressure</th>
<th>Average Melt Temperature</th>
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<td>lb/hr</td>
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<td>psi</td>
<td>psi</td>
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New Design Operating Window

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<th>Contour</th>
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<th>Lo Limit</th>
<th>Hi Limit</th>
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<tbody>
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Alternate Design Operating Window

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<tr>
<td>Barrel Temp, F</td>
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<td>Screw Speed, rpm</td>
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<td>Barrel Pressure, psi</td>
<td>4000</td>
<td>2867.8952</td>
<td>0</td>
<td>4000</td>
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Graph showing the relationship between Screw Speed, rpm, Barrel Temp, F, and Output, lb/hr.
Summary

• Screw design objectives need to be clearly defined
• Material physical & rheological properties in the processing range are required for valid simulations
• Experiential data must be correlated to “calibrate” the simulation model
• New design can be modeled and modified relative to known design operating point
• Good design results are expected based on
  – Reasonable and valid objectives
  – Accurate material data
  – Good experiential data
  – Open discussion of expectations and limitations
  – Fundamental design concepts
  – Precise manufacture to design within tolerances
Thank You

Questions?