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A Short Review of Flow Simulation Techniques for Extrusion Die Design

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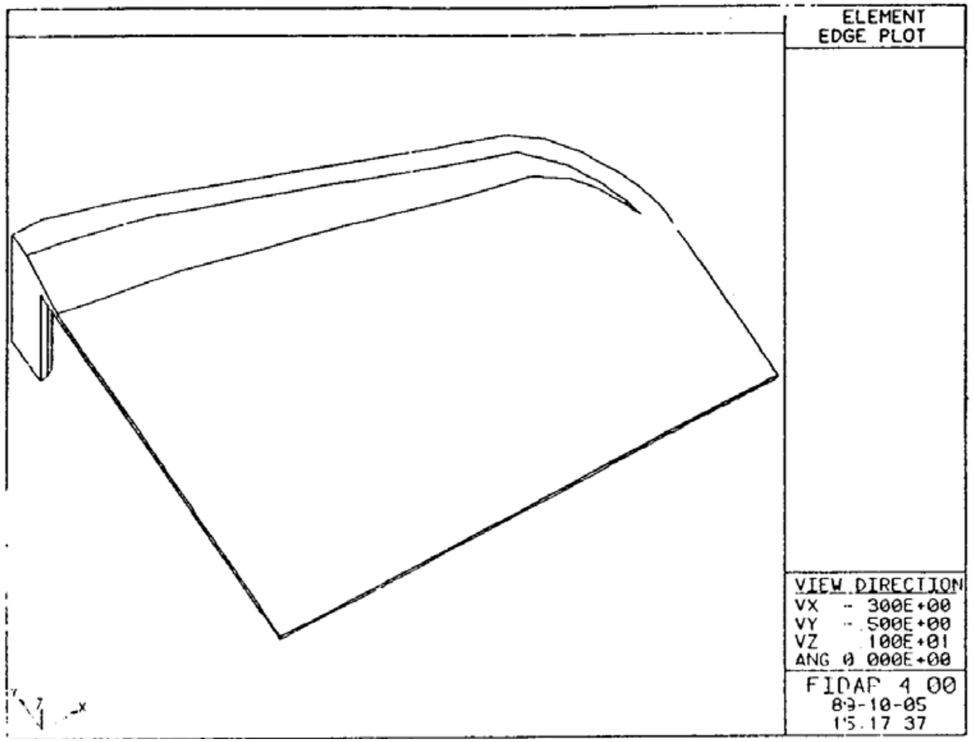
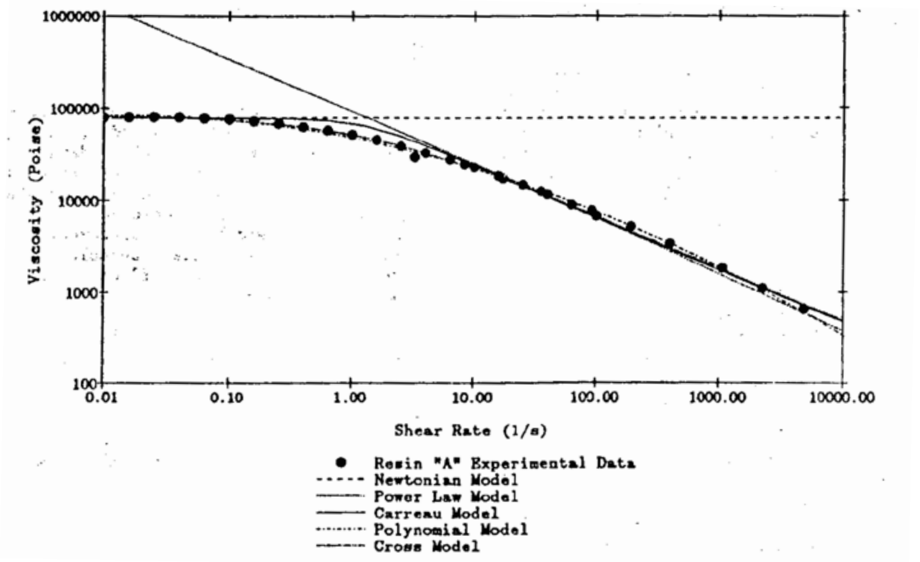
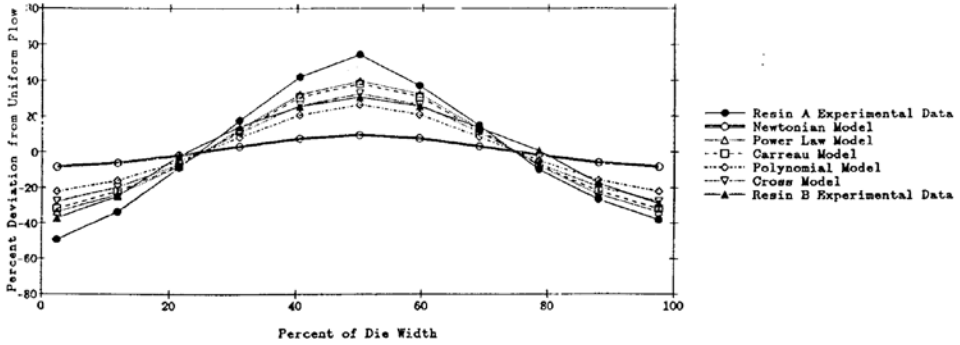
Background

- 3D Flow simulation for complex extrusion die geometries have been commercially available since 1990's
- Today, routine simulation work is possible for complex flow geometries, non-Newtonian and non-isothermal flows with overnight computations
- Automatic routines for geometry optimization / flow balancing
- More complex cases including viscoelastic modeling or multi-layer coextrusion capability are also available

3D flow simulations in the 1990's







J. Dooley, "Simulating the Flow in a Film Die Using Finite Element Analysis", SPE ANTEC Tech Paper 168-171 (1990)

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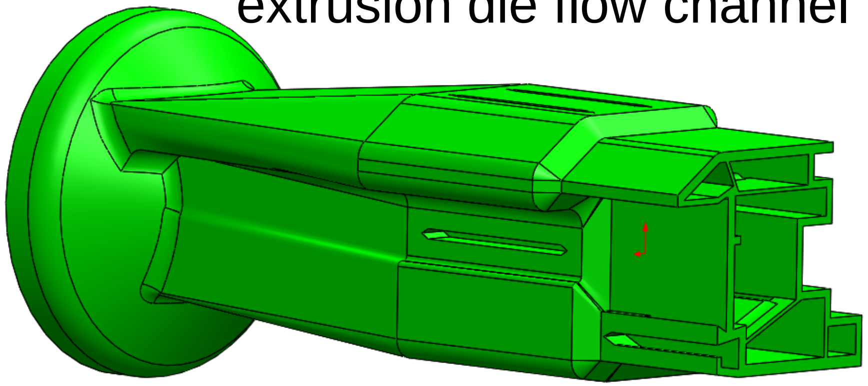
Today: Routine 3D FEA for the industry

- Solving for non-Newtonian, non-isothermal flow using commercial 3D FEA solver for complex geometries

Example of window profile extrusion die

Example of window profile extrusion die flow channel



O. Catherine, "**Advances in Shear Rheology and Flow Simulation for High Performance Extrusion Die Design**", SPE International Polyolefins Conference (2015)

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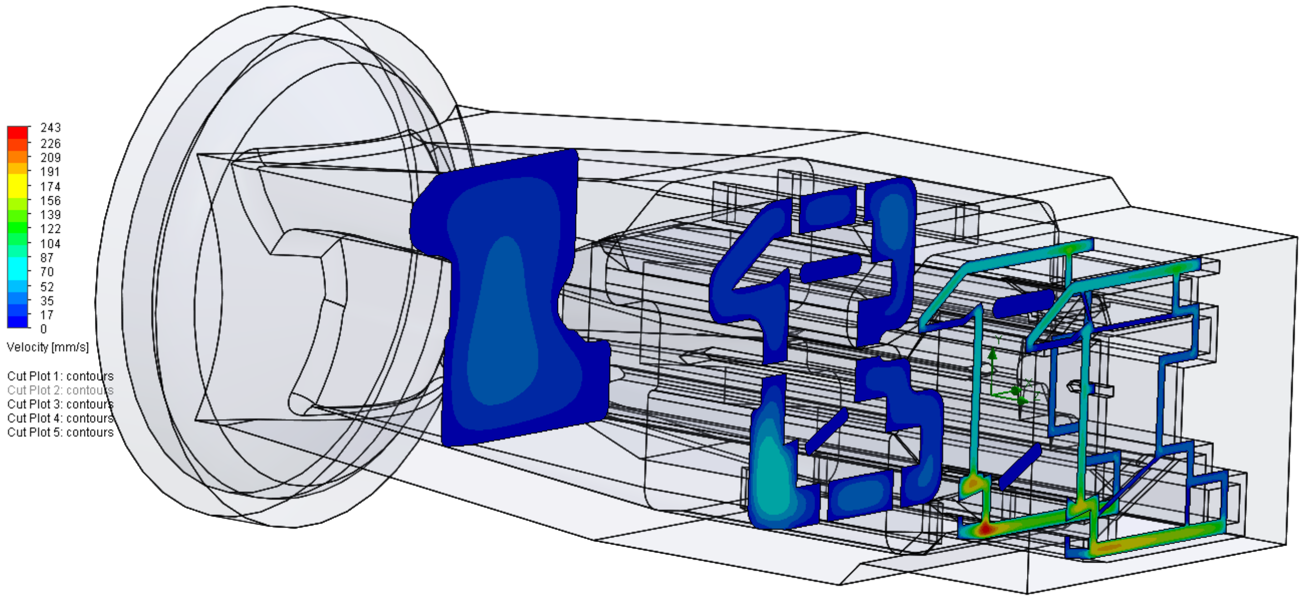

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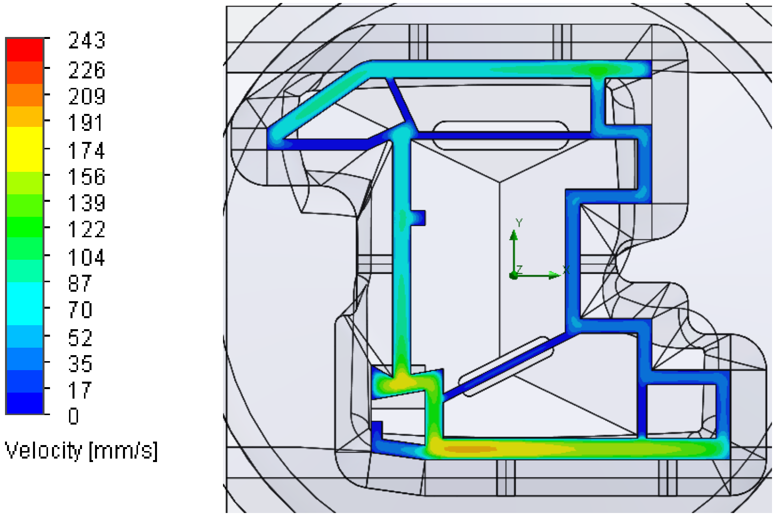
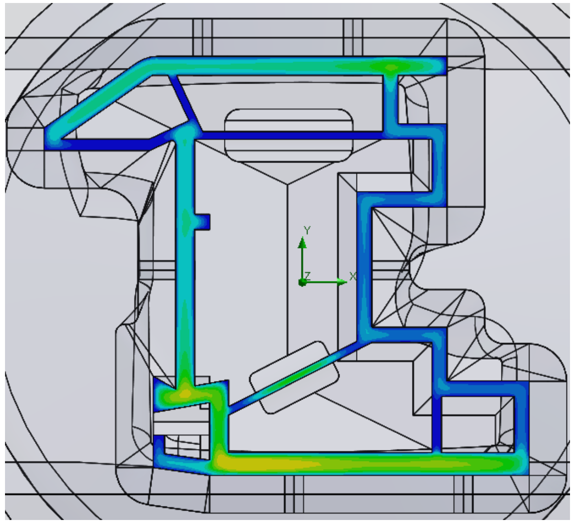


Target of 4 $m.min^{-1}$ => $67 mm.s^{-1}$



1st Revision

More iterations

O. Catherine, "**Advances in Shear Rheology and Flow Simulation for High Performance Extrusion Die Design**", SPE International Polyolefins Conference (2015)

Viscosity model

- Polymer viscosity Shear rate and temperature dependent model

Carreau-Yasuda model

$$\eta(\dot{\gamma}, T) = \eta_0 \times a_T[1 + (\lambda\dot{\gamma} \times a_T)^a]^{\frac{n-1}{a}}$$

η_0 is the zero-shear viscosity in Pa.s
λ is the characteristic time
n is the pseudoplastic index
a is the Yasuda parameter "transition smoothness"

Arrhenius model

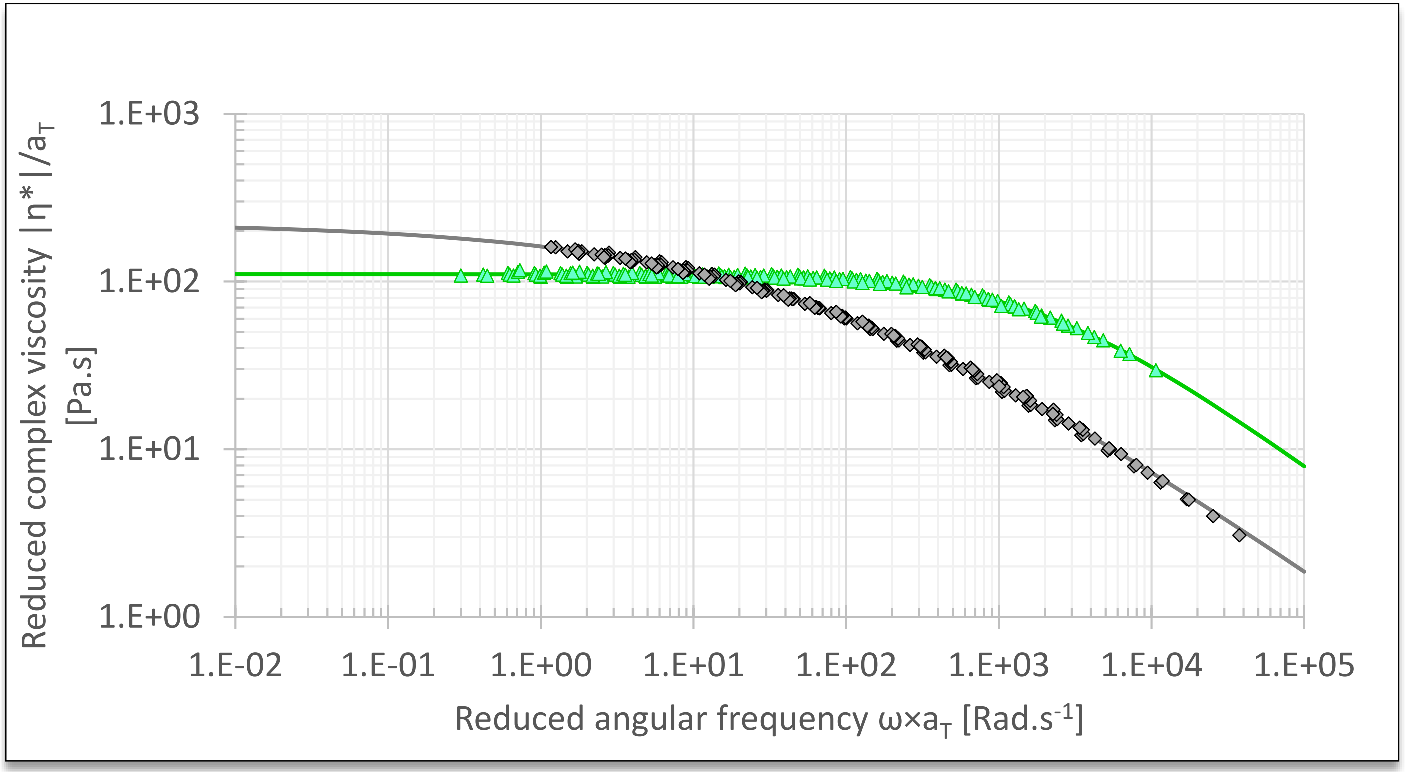
$$a_T = exp\left(\frac{E_a}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$$

Arrhenius empirical model - typically better for $T > T_g + 100°C$.
E_a: Activation Energy ($J.mol^{-1}$)
R: Ideal gas constant =8.3144621 $J.mol^{-1}.K^{-1}$
T_0: Reference temperature (K)

O. Catherine, "**Learning from Shear and Extensional Rheology of a few Extrusion Coating Polyethylenes**", TAPPI PLACE Conference, Fort Worth – TX (2016)

Viscosity model

The Carreau-Yasuda model



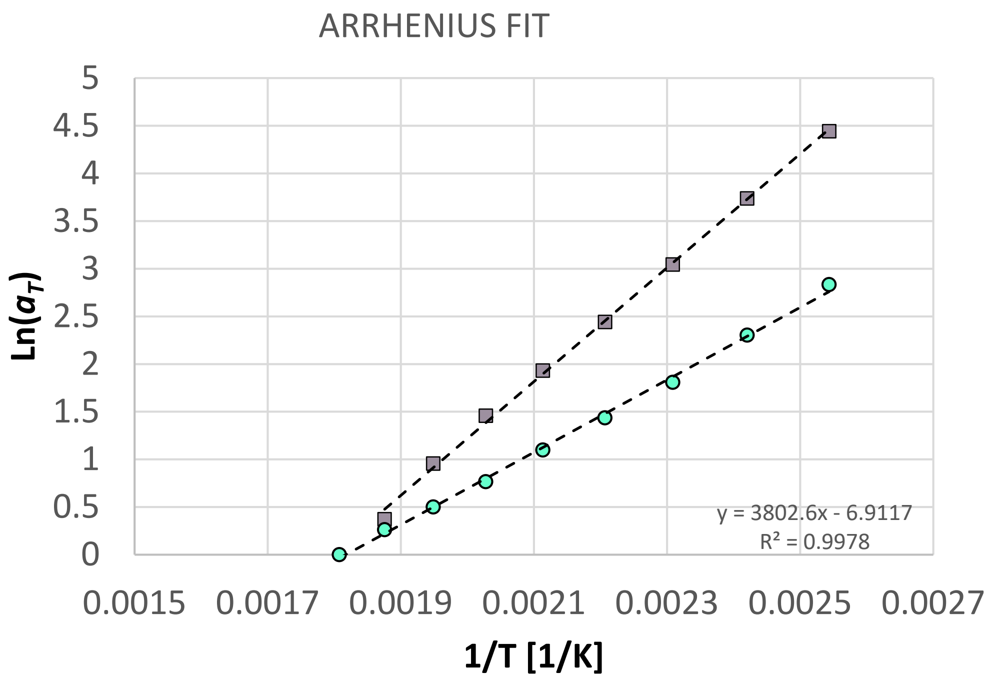
mPE		
Carreau -Yasuda Param.	Value	Unit
η_0	110.50	Pa.s
λ	5.2 x 10^{-4}	s
a	0.818	no unit
n	0.3404	no unit
T_{ref}	280	°C
T_{ref}	553.15	K
E_a	31,599.61	J.mol^{-1}

LDPE2		
Carreau-Yasuda param.	Value	Unit
η_0	223.34	Pa.s
λ	1.14 x 10^{-2}	s
a	0.365	no unit
n	0.3389	no unit
T_{ref}	280	°C
T_{ref}	553.15	K
E_a	44913.06	J.mol^{-1}

O. Catherine, “**Learning from Shear and Extensional Rheology of a few Extrusion Coating Polyethylenes**”, TAPPI PLACE Conference, Fort Worth – TX (2016)

Viscosity model

- **The Arrhenius model**



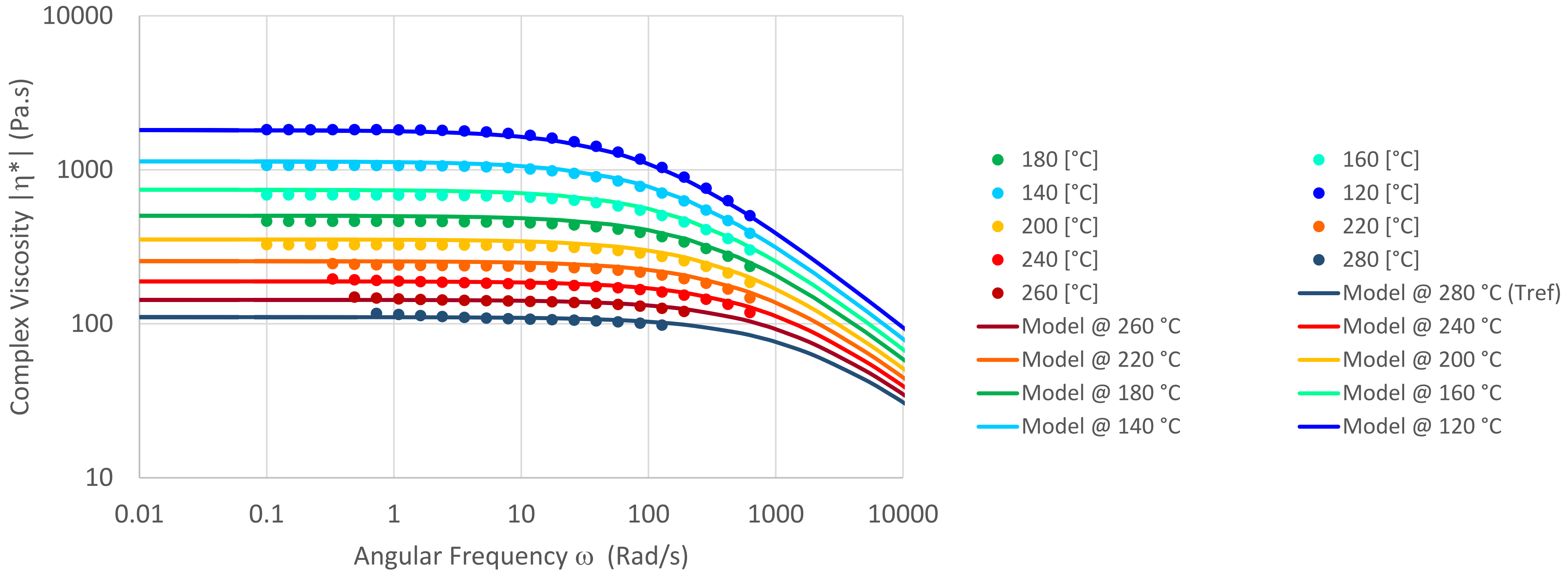
T [℃]	*1/T [1/K]*	a_T	*Ln (a_T)*
120	0.002544	17	2.833213
140	0.00242	10	2.302585
160	0.002309	6.1	1.808289
180	0.002207	4.2	1.435085
200	0.002113	3	1.098612
220	0.002028	2.15	0.765468
240	0.001949	1.65	0.500775
260	0.001876	1.3	0.262364
280	0.001808	1	0

O. Catherine, “**Learning from Shear and Extensional Rheology of a few Extrusion Coating Polyethylenes**”, TAPPI PLACE Conference, Fort Worth – TX (2016)

Viscosity model

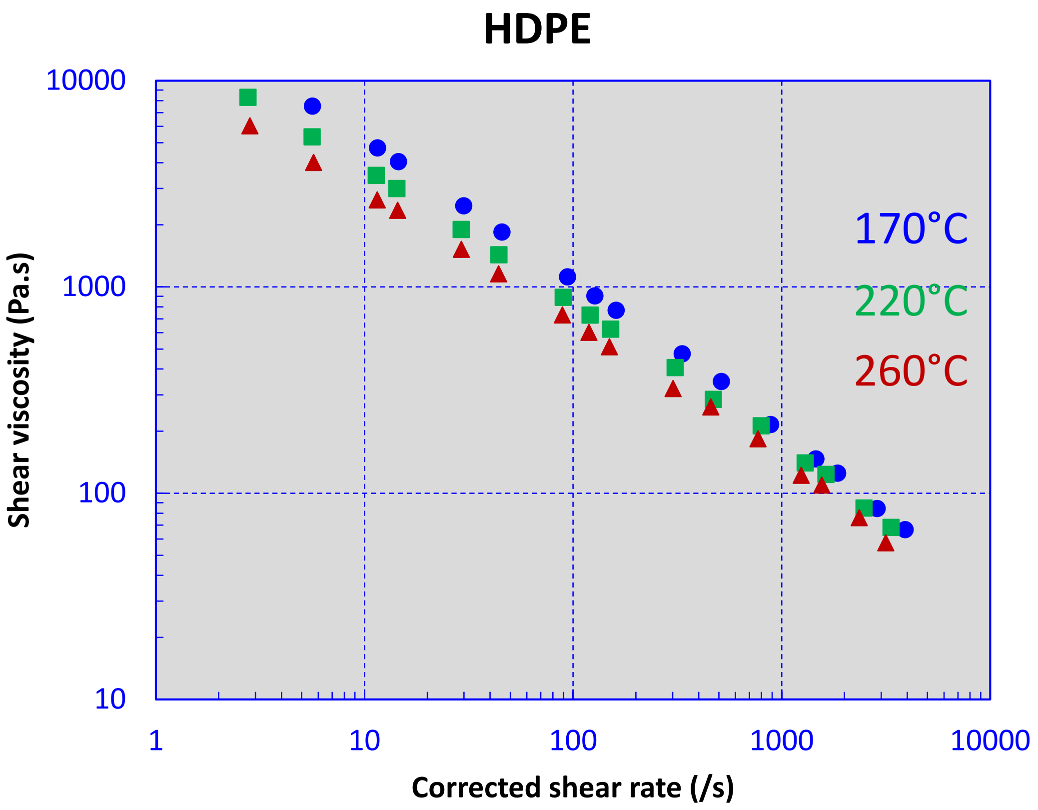
Full shear rate and temperature dependent model

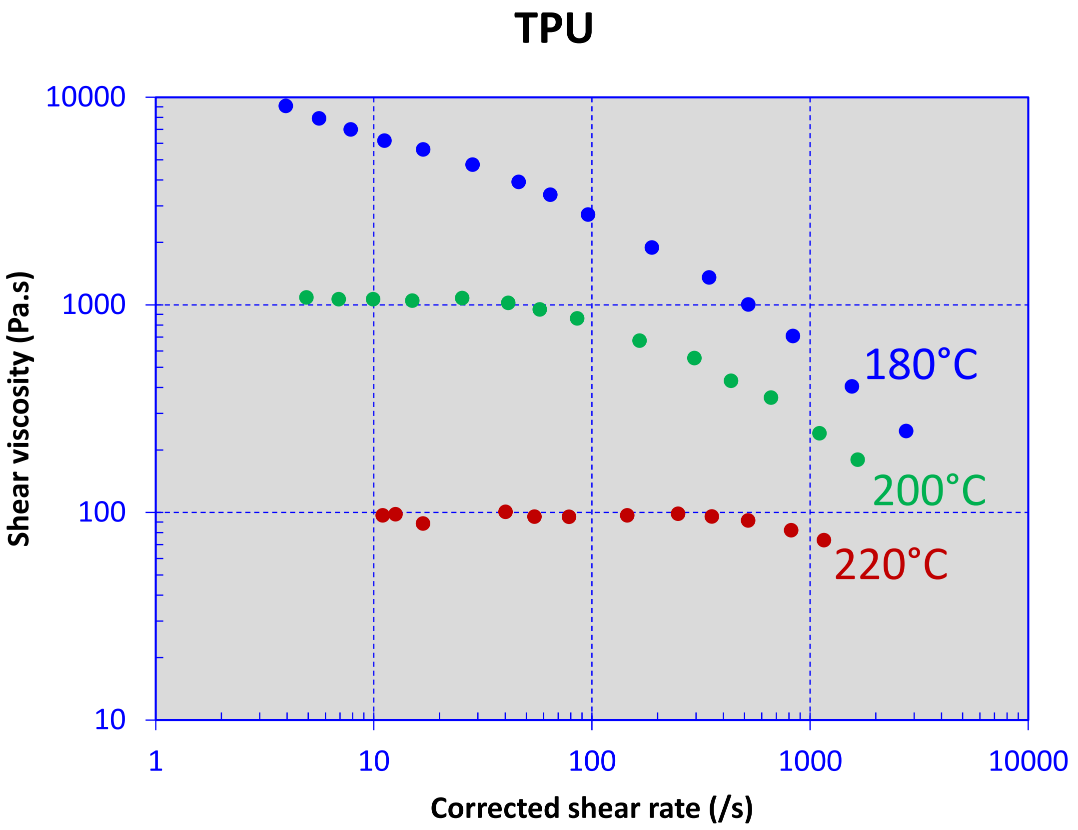
- Model vs. measured data



The importance of thermal aspect of the flow

- Polymer viscosity can be very temperature sensitive





The importance of thermal aspect of the flow

- Thermal / mechanical coupling within the flow:

Steady State Energy balance: $\rho C(\mathbf{V} \cdot \nabla T) = k\Delta T + \boldsymbol{\tau} : \dot{\boldsymbol{\varepsilon}}$

- $\rho C(\mathbf{V} \cdot \nabla T)$ → Convection
- $k\Delta T$ → Conduction
- $\boldsymbol{\tau} : \dot{\boldsymbol{\varepsilon}}$ → Mechanically generated = flow / thermal coupling

With:

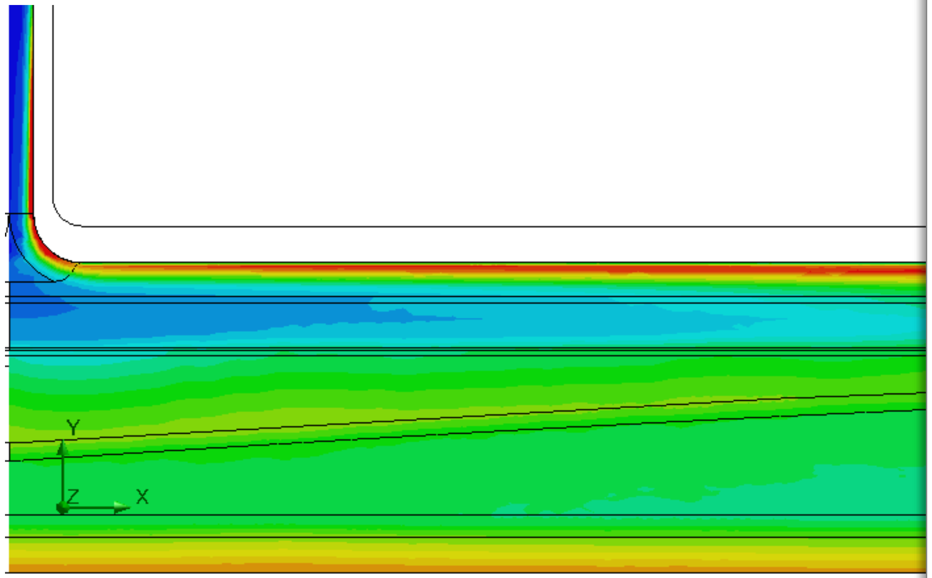
$\boldsymbol{\tau} = 2\eta\dot{\boldsymbol{\varepsilon}}$ "Viscous" Stress tensor

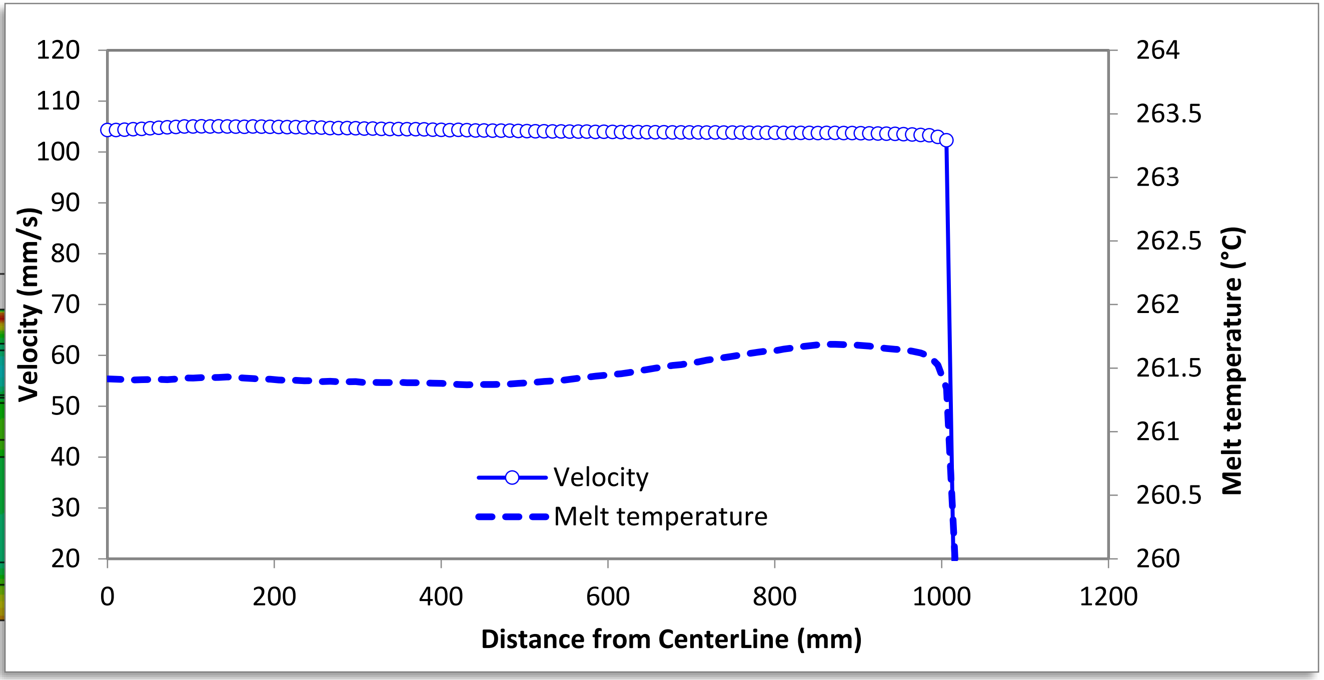
$\dot{\boldsymbol{\varepsilon}} = \frac{1}{2}\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^{\mathrm{T}}\right)$ Rate of deformation tensor

For simple shear flow, the mechanically generated energy is $= \eta\dot{\gamma}^2$

The importance of thermal aspect of the flow

- Generally, viscous dissipation in die flow channel is small

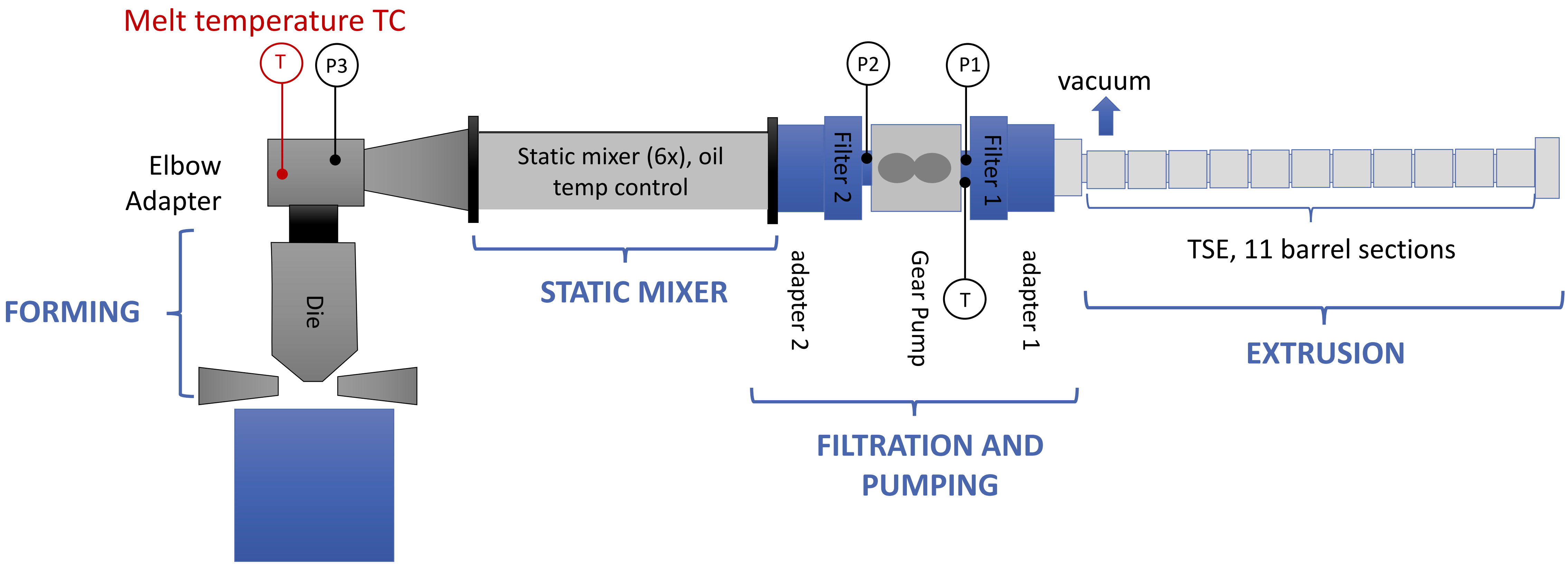




O. Catherine, "**Effect of Typical Melt Temperature non-Uniformity on Flow Distribution in Flat Dies**", SPE ANTEC Conference (2012)

The importance of thermal aspect of the flow

- Actual example of excessive viscous dissipation: PVB extrusion



O. Catherine, "**A Practical Example of Film Extrusion Process Troubleshooting and Fine Tuning**", SPE ANTEC Conference, Orlando FL (2015)

The importance of thermal aspect of the flow

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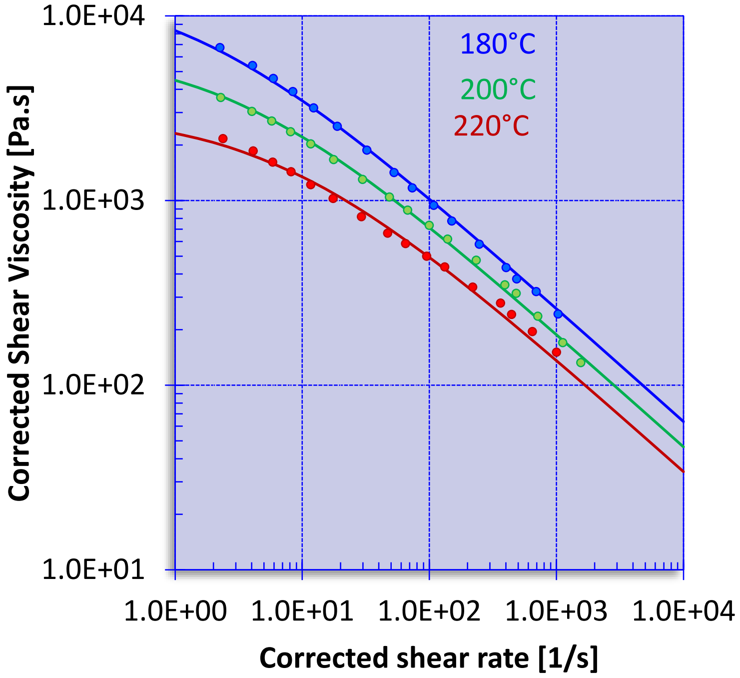
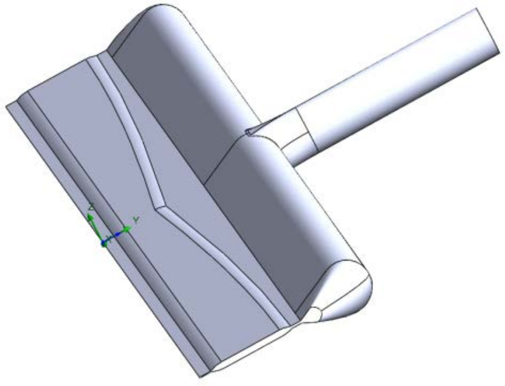


Processing parameters

Process parameter	Value
Die wall temperature	210°C
Initial melt temperature	210°C
Extrusion output	800 kg/h

Viscosity model

Parameter	Value
η_0 (Pa.s)	6.67 ×10^3
τ_*(Pa)	2.14.10^4
m	0.38335
T_{ref} (K)	473.15 (200°C)
C_1	104.26
C_2 (K)	2591.3



PVB Flow Channel was designed and optimized

O. Catherine, "**A Practical Example of Film Extrusion Process Troubleshooting and Fine Tuning**", SPE ANTEC Conference, Orlando FL (2015)

The importance of thermal aspect of the flow

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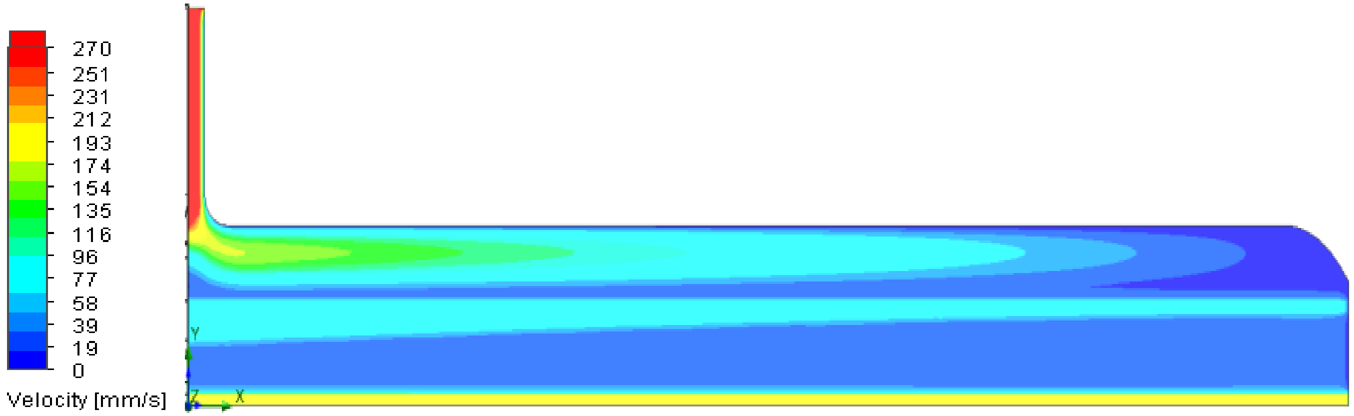

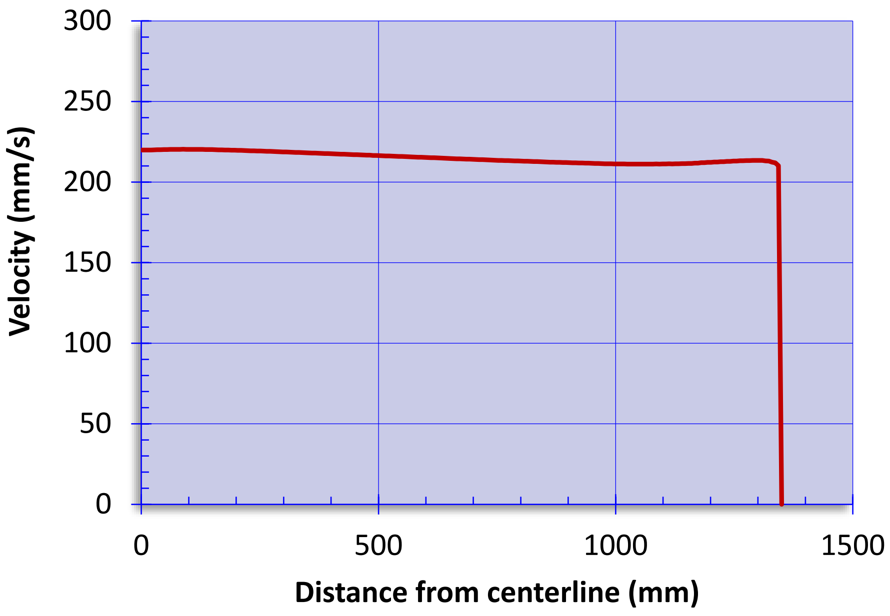

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The importance of thermal aspect of the flow

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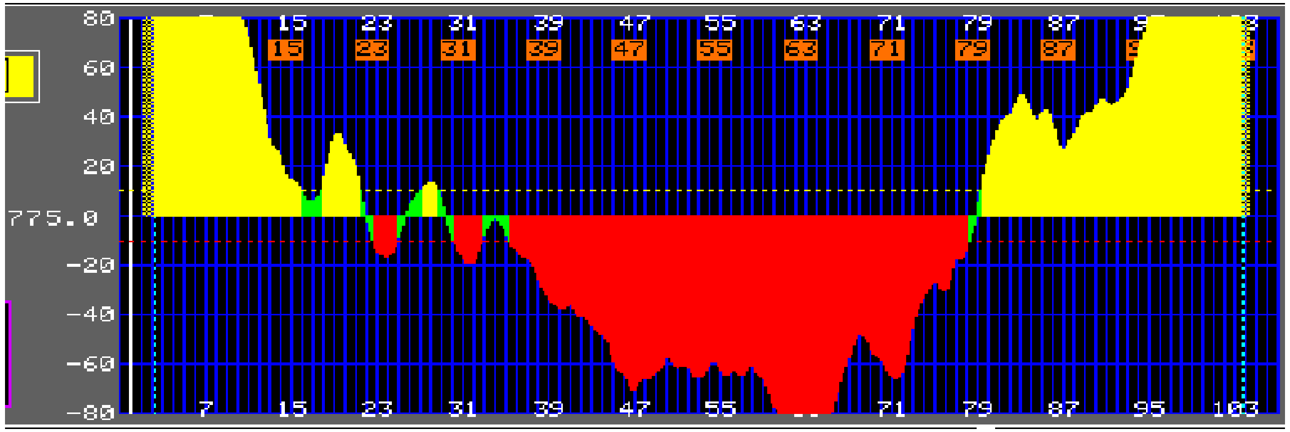

Unfortunately at start-up, without lip adjustment, a very non-uniform flow was coming out of the die (non-uniform film thickness measured by online gauge system):

- 2σ variation of 131.28 µm for an average thickness of 780 µm
  - 16.8% variation

<u>Process troubleshooting concluded to:</u>

1) The processed material was a different formulation
2) The melt temperature was too high due to viscous dissipation in the extruder.
   - Adapters were run colder
   - Output was lowered
3) Flow model with adjusted parameters was run for confirmation

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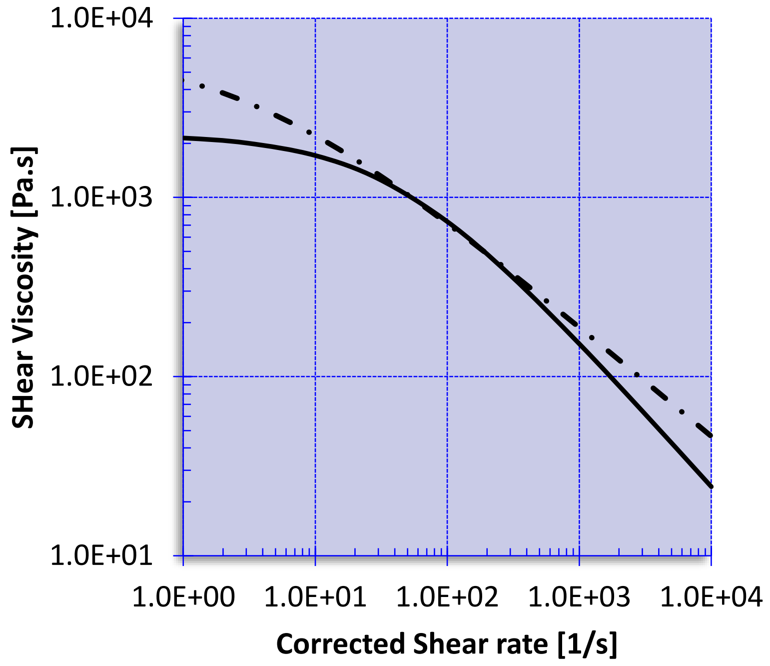
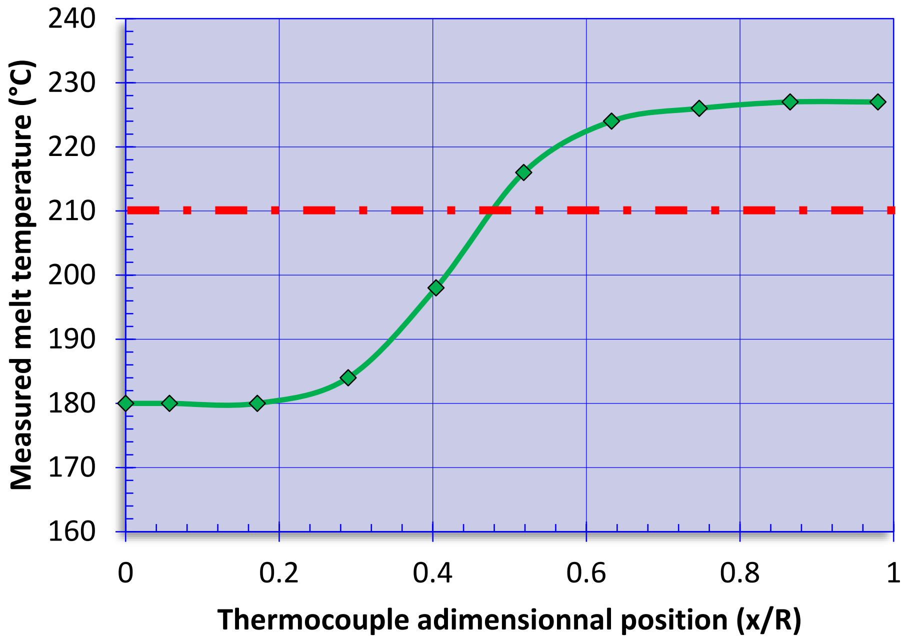


New Material rheology (solid line)



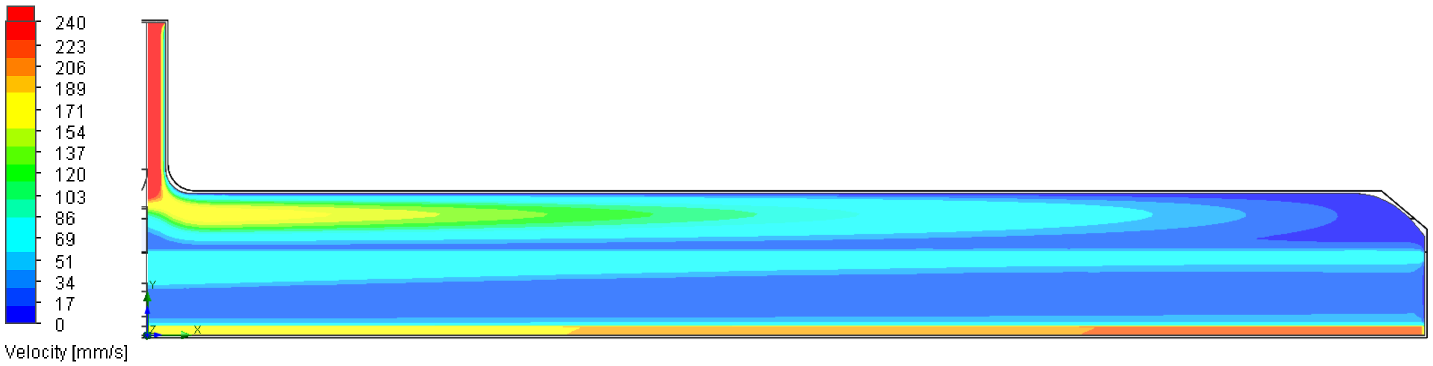
Non-Uniform melt temperature at die inlet

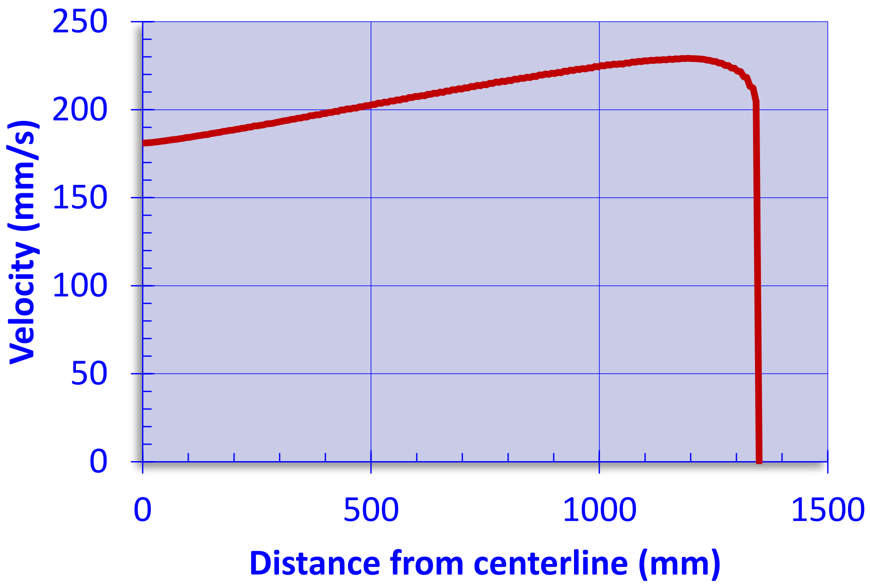
O. Catherine, “**A Practical Example of Film Extrusion Process Troubleshooting and Fine Tuning**”, SPE ANTEC Conference, Orlando FL (2015)

The importance of thermal aspect of the flow

- Actual example of excessive viscous dissipation: PVB extrusion

  - Model predict the issue well
  - Model validates the origins of the extrusion problem



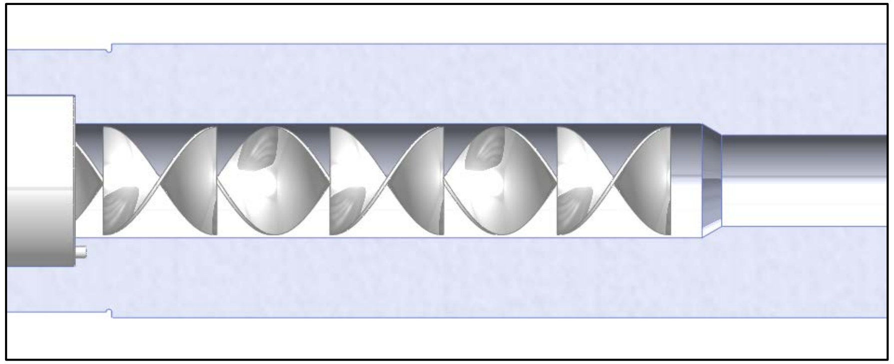


$$\frac{2\sigma}{ave} = 14.8\%$$

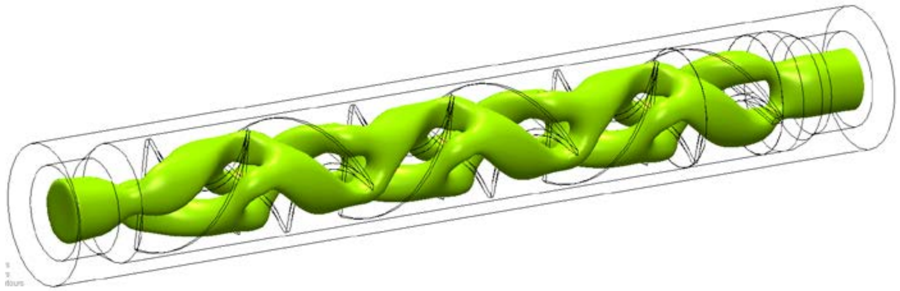
O. Catherine, "**A Practical Example of Film Extrusion Process Troubleshooting and Fine Tuning**", SPE ANTEC Conference, Orlando FL (2015)

The importance of thermal aspect of the flow

- Can a static mixer help?



- Mixer with six “bow-tie” mixing elements
- Commonly used in sheet, film and extrusion coating applications
- 3D flow simulations run to evaluate the



- Complex flow – only 3D FEA can capture

O. Catherine, “**Evaluation of the Flow Performance of a Static Mixer for non-Uniform Incoming Melt Temperature with Computational Fluid Dynamics (CFD)**”, SPE Eurotec, Lyon France (2013)

The importance of thermal aspect of the flow

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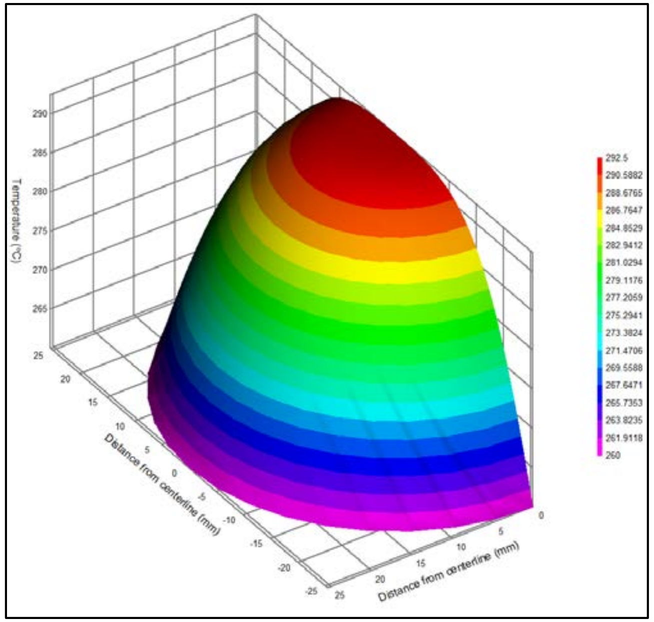

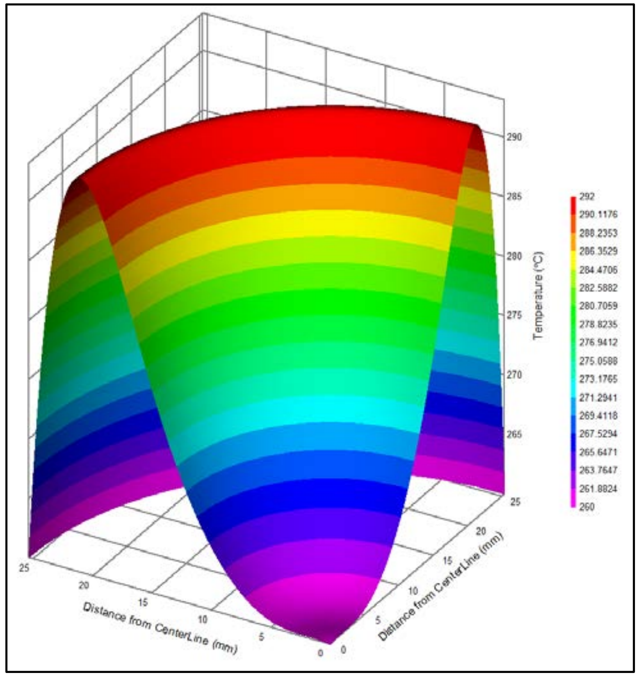

(1) Input entrance temperature profile
Maximum at center of flow channel

(2) Input entrance temperature profile
Maximum near the wall of the flow channel

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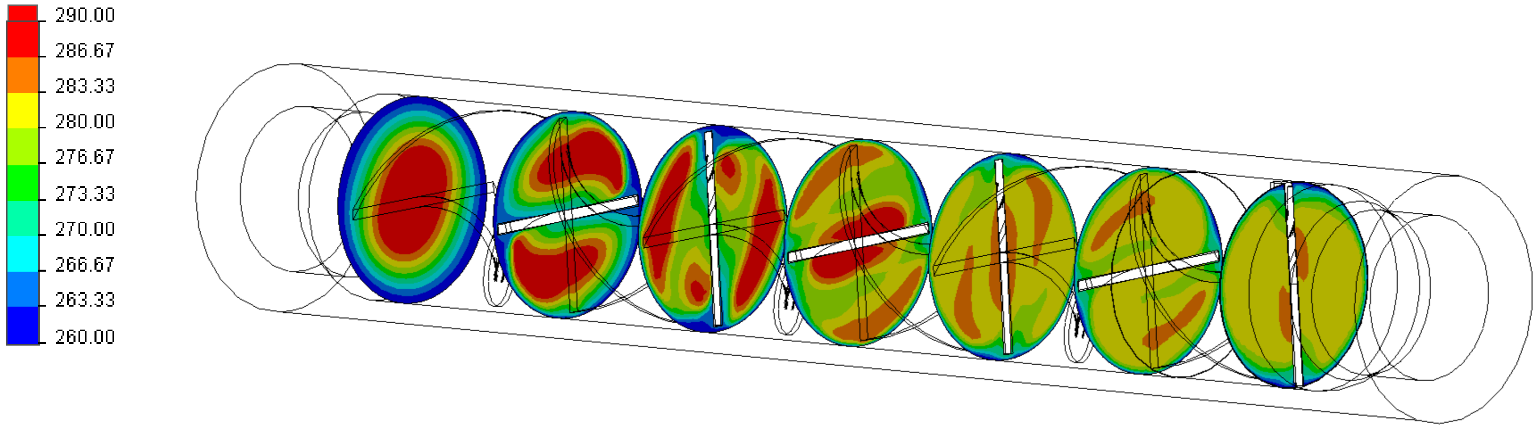
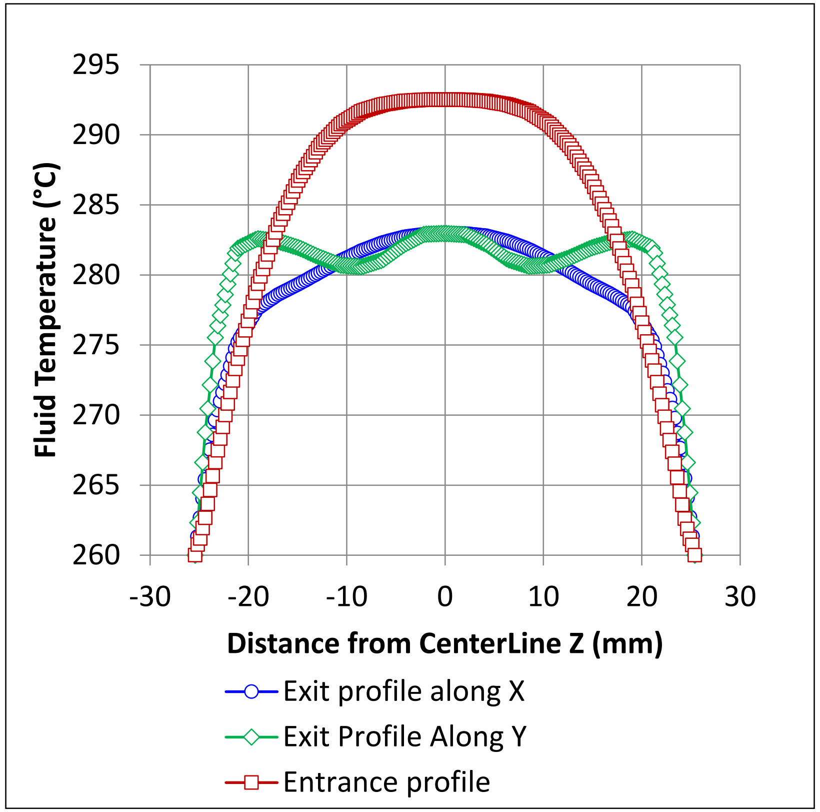


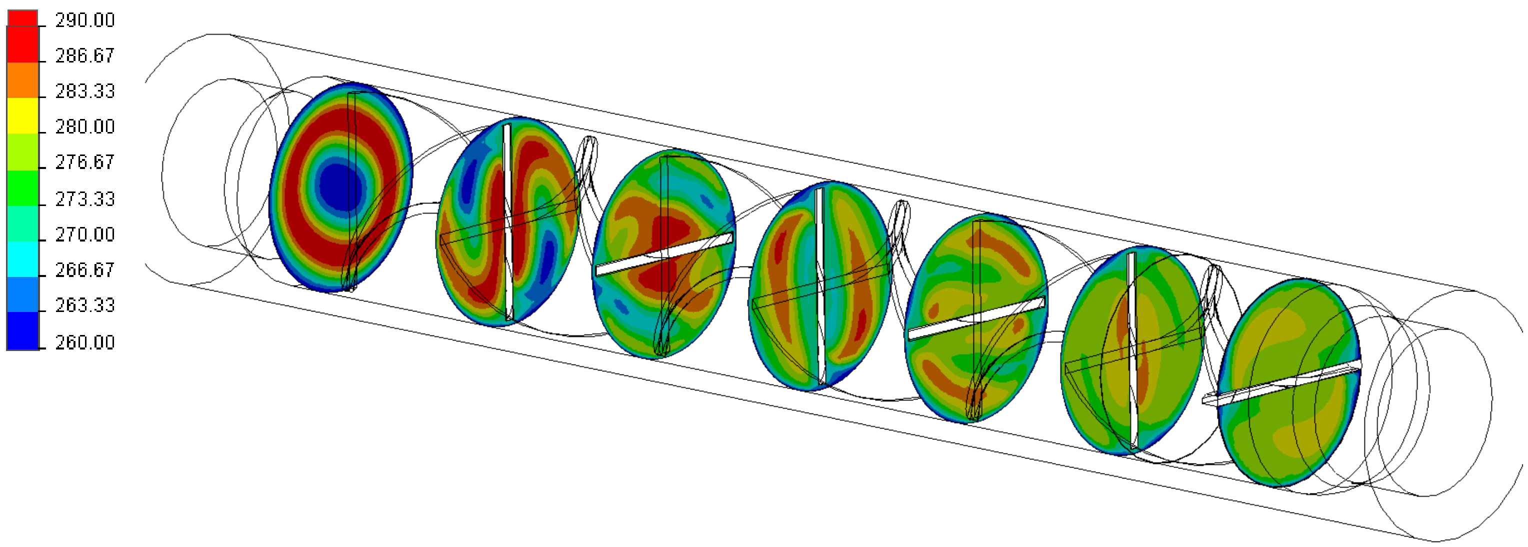


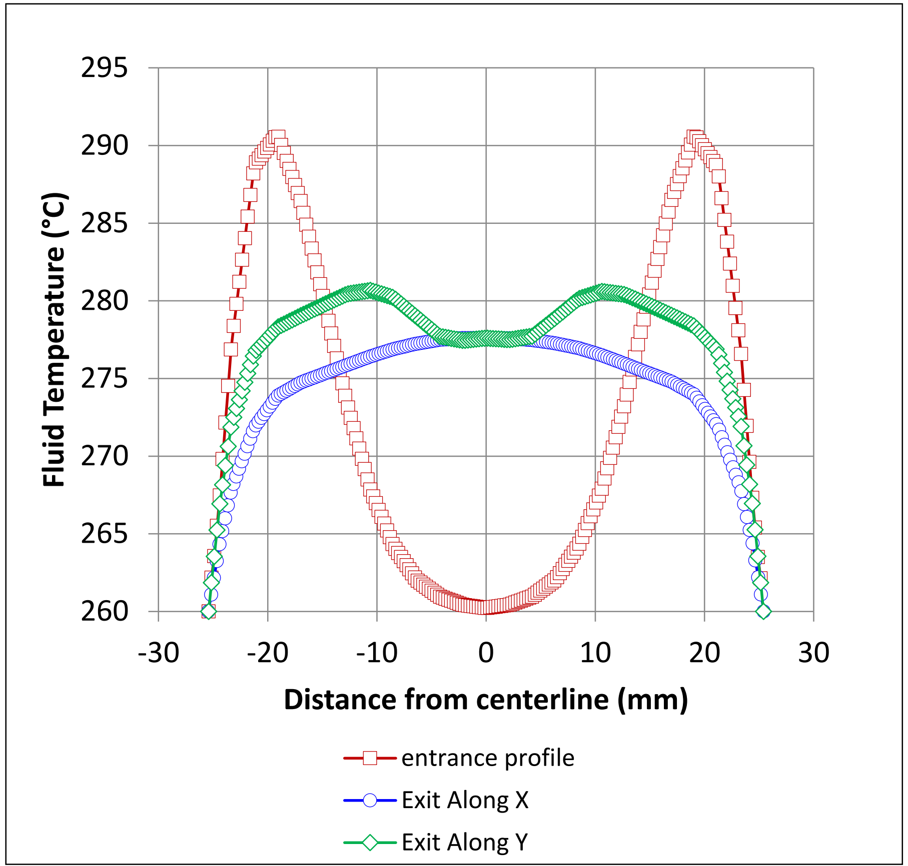
O. Catherine, "**Evaluation of the Flow Performance of a Static Mixer for non-Uniform Incoming Melt Temperature with Computational Fluid Dynamics (CFD)**", SPE Eurotec, Lyon France (2013)

The importance of thermal aspect of the flow

- Can a static mixer help?

2 Input entrance temperature profile
Maximum near the wall of the flow channel





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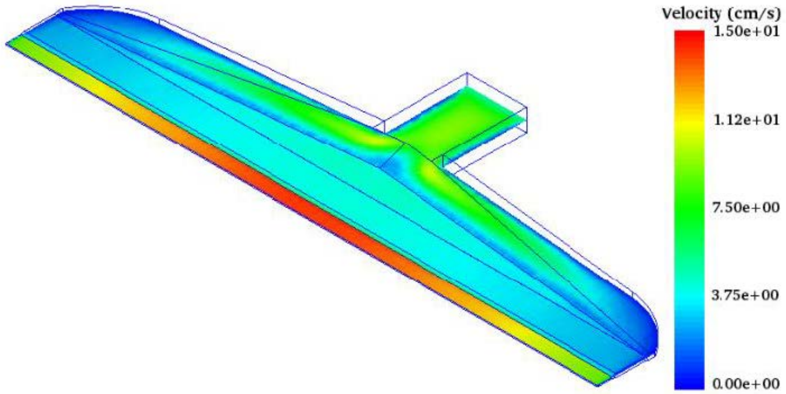
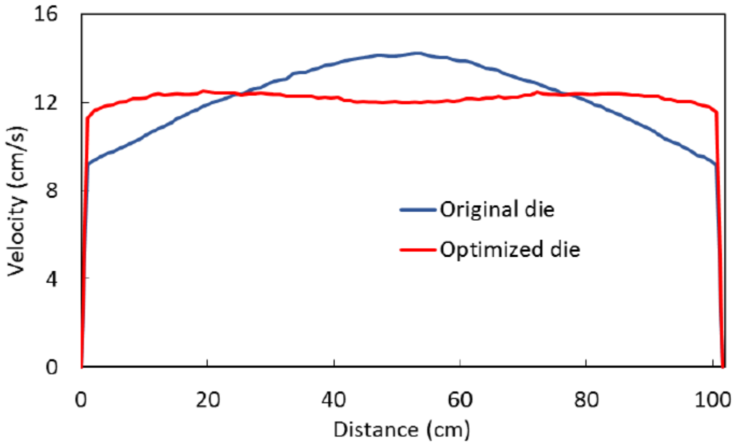
Automatic Optimization

- Several studies - complex optimization procedure and constraints definition





Optimization with PolyXtrue commercial software

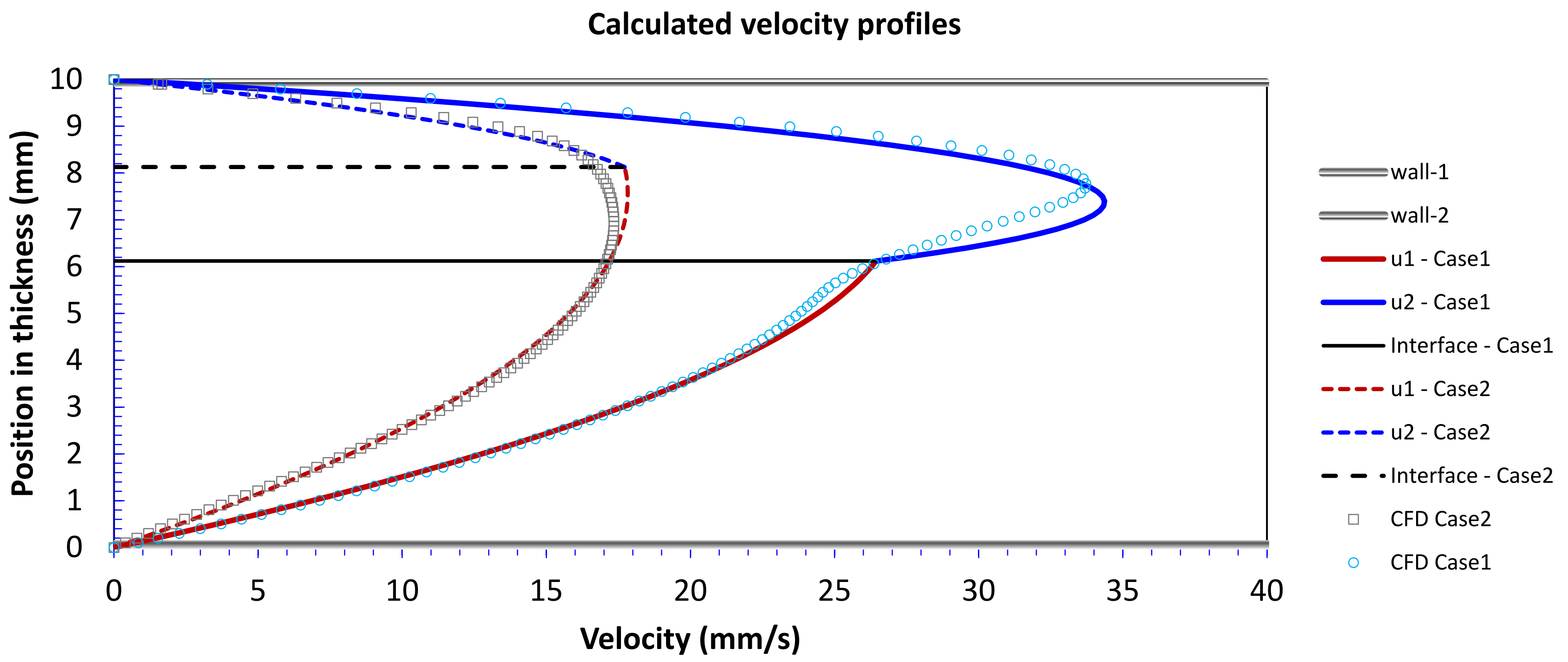
M. Gupta: “Automatic Optimization of Extrusion Dies”, SPE ANTEC Conference, Indianapolis, IN (2016)

Coextrusion

- Analytical models for Newtonian flows can provide some valuable information
- Non-Newtonian analytical models are more involved
- Some 2D and 3D software based on finite element analysis can model multi-layer flows
  - Advantages: complex geometry can be modeled, non-Newtonian and in some cases non-isothermal models can be run
  - Limitations: lack of precision at the interface, no physics for viscous encapsulation

Coextrusion

- Example I: comparison of analytical solution with 3D FEA



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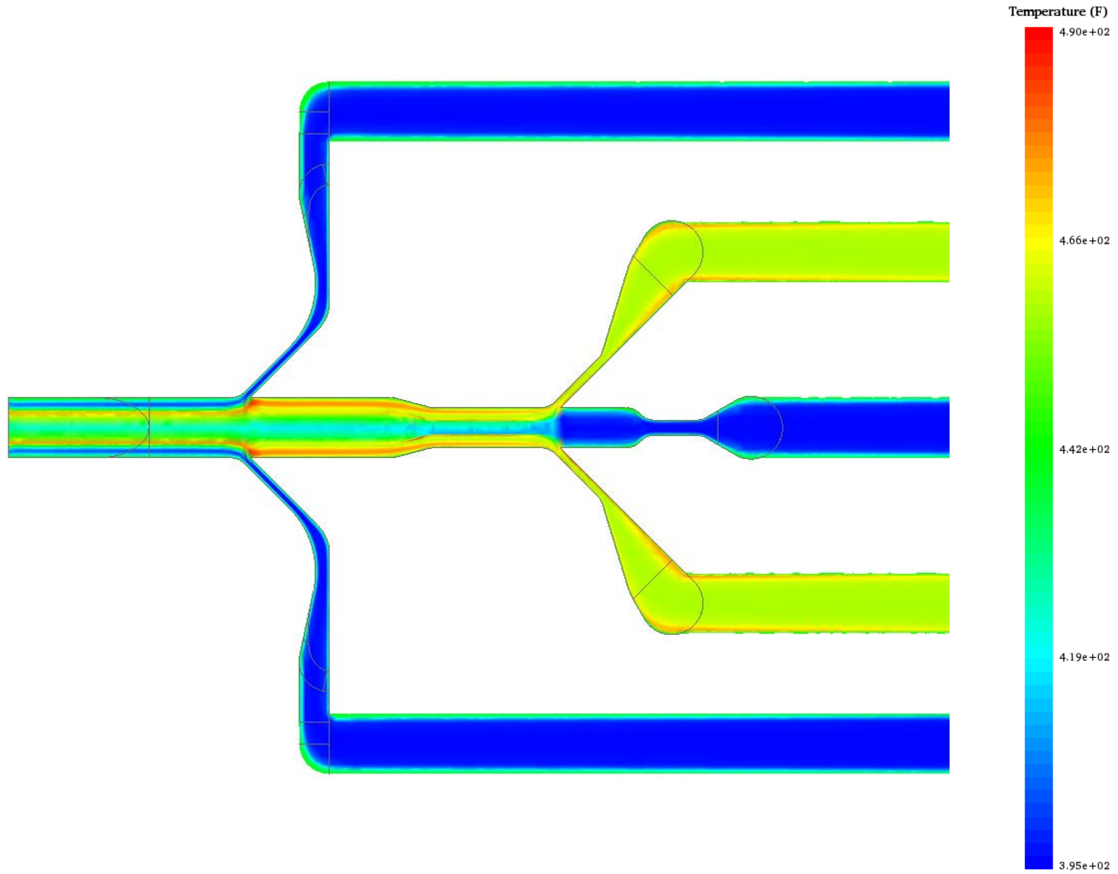
Coextrusion

- Example II: 3D FEA non-isothermal non-Newtonian Flow (PolyXtrue)



Conclusion

- Since the 1990's with the first 3D modeling work, significant progress has been made that makes flow simulation technology very valuable for die design and optimization
- Routine 3D non-isothermal non-Newtonian models are run with complex flow geometry
- On the practical level, the thermal aspect of the flow is at the origin of a significant number of extrusion problems
- Residence time evaluation is also an important parameter (not discussed today)
- More advanced modeling such as automated optimization, coextrusion and viscoelastic flows is making also substantial progress