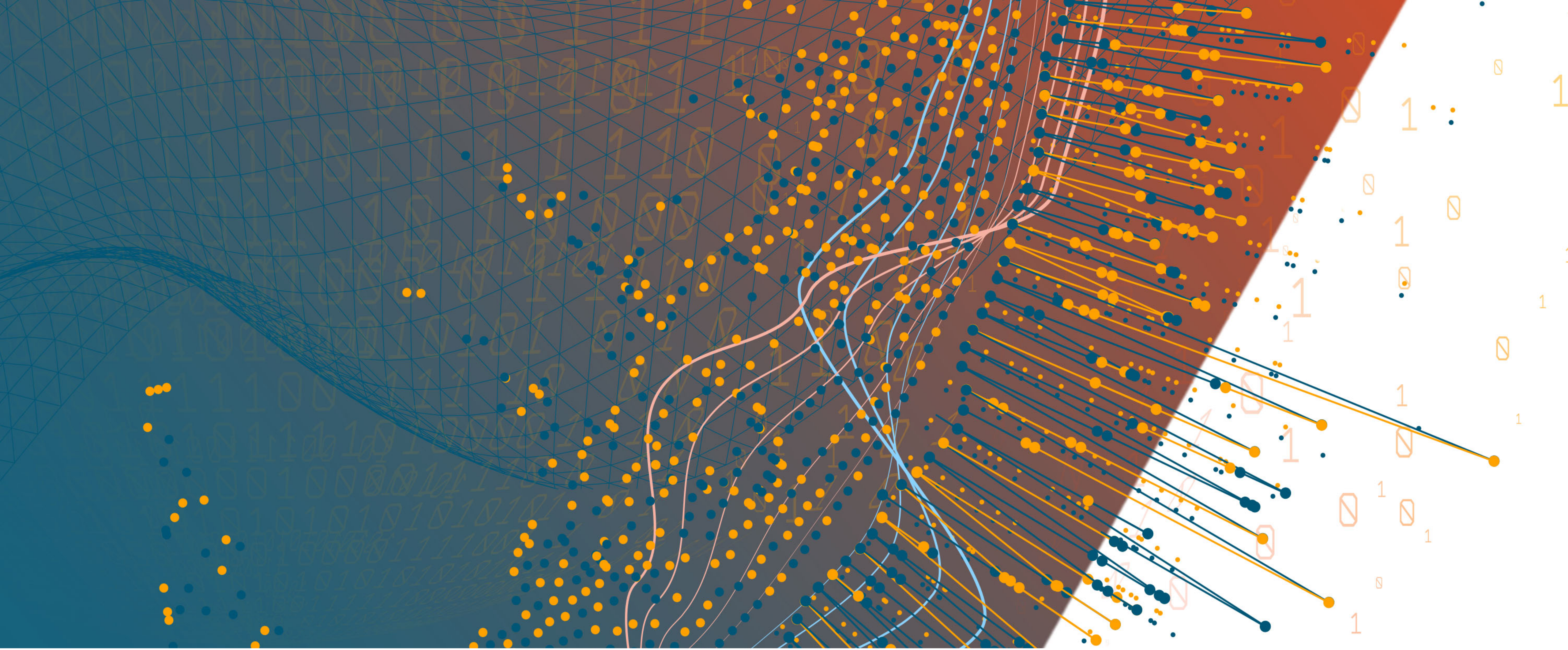

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REFERENCE FOR CREATING NEW MATERIALS WITH ALTAIR POLYMOLD

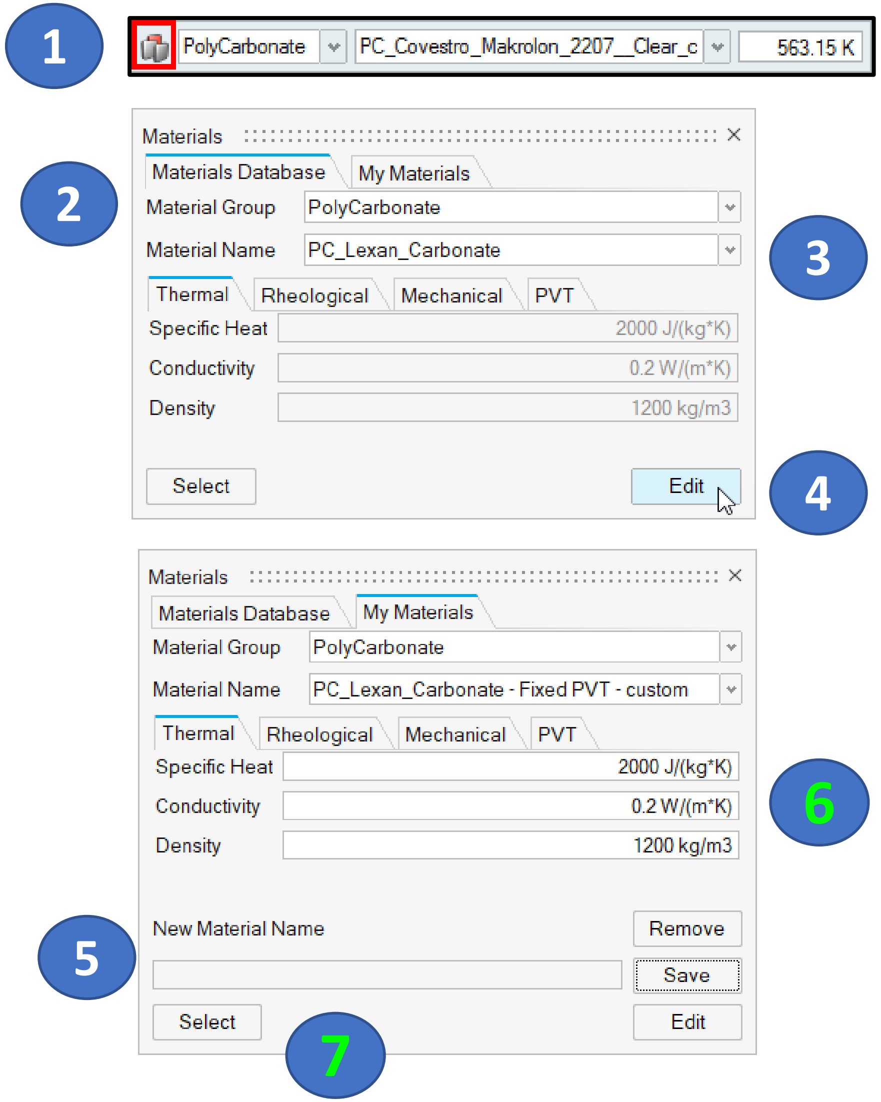
Overview: Creating a New Material

Process Overview: To create a new material in Altair Mold, you select an existing material in the Materials Database, edit the material according to your requirements, and save it as a new material.

Prerequisite: Designate the part cavity in your model geometry. 
The microdialog that appears after you designate a part provides access to the Materials Viewer.

1. Select the **Materials Viewer** icon on the microdialog.
2. From the Materials Database tab, select a Material Group for your new material, for example **PolyCarbonate**.
3. Select a material from which to base your new material, for example **PC_Lexan_Carbonate – Fixed PVT**.
4. Click **Edit** at the bottom of the dialog.
5. Enter a name for your new material that is different from the source material, then click **Save**.
6. Edit the data in each of the tabs as required for your new material: **Thermal**, **Rheological**, **Mechanical** and **PVT**, then click **Save.**
7. Click the **Select** button to apply your new material to your model.

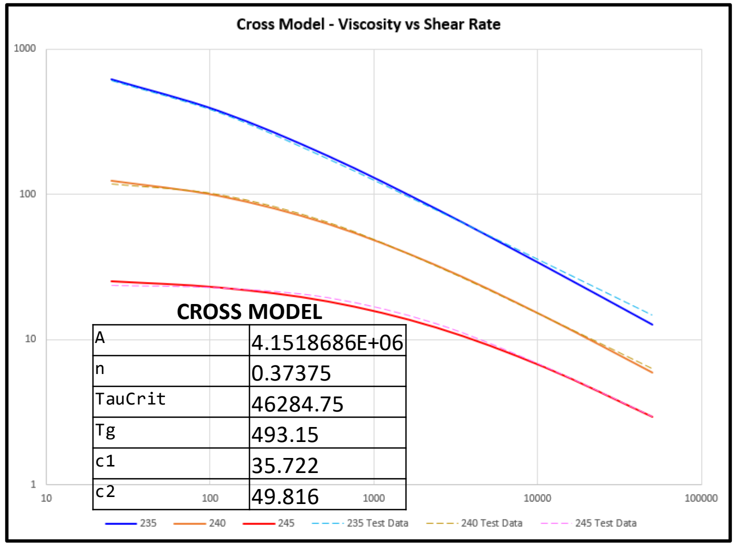
   Note: You can access your new material in the future through the **My Materials** tab on the **Materials Viewer**.

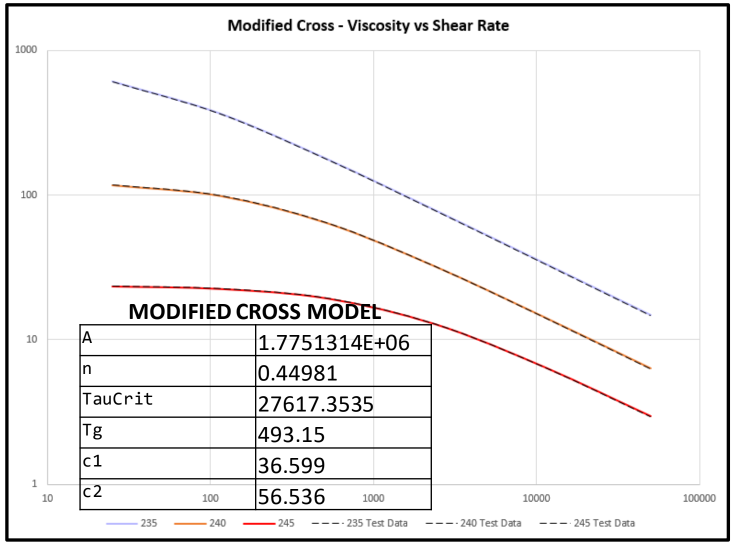


Reference for Defining Material Properties

Viscosity Data
Choose a Constitutive Model:

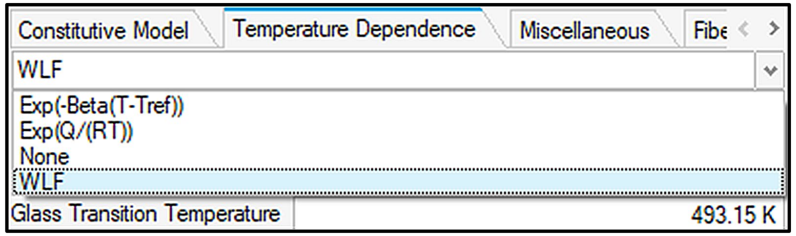
- Cross
- Modified Cross
- Carreau-Yasuda
- Herschel-Buckley
- Power Law





Temperature Dependence
Choose:

- Exponential – Exp(-Beta(T-Tref))
- Arrhenius – Exp(Q/RT)
- Williams-Landel-Ferry (WLF)

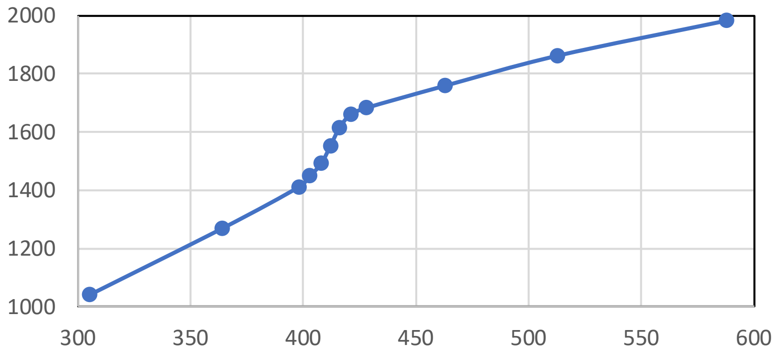


PVT Data
Select: **2-Domain Tait**

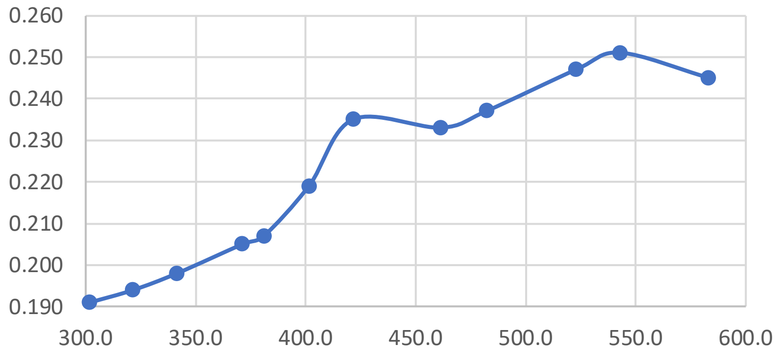
Thermal Quantities
Define:

- Thermal Conductivity (k)
- Specific Heat (Cp)
- Melt Density

Specific Heat (Cp) versus Temp



Thermal Conductivity vs Temp



Mechanical Properties
Keep the Default Values for these properties:

- Young's Modulus
- Poisson's Ratio
- Yield Stress
- CLTE

Note: SI (m-kg-sec) units

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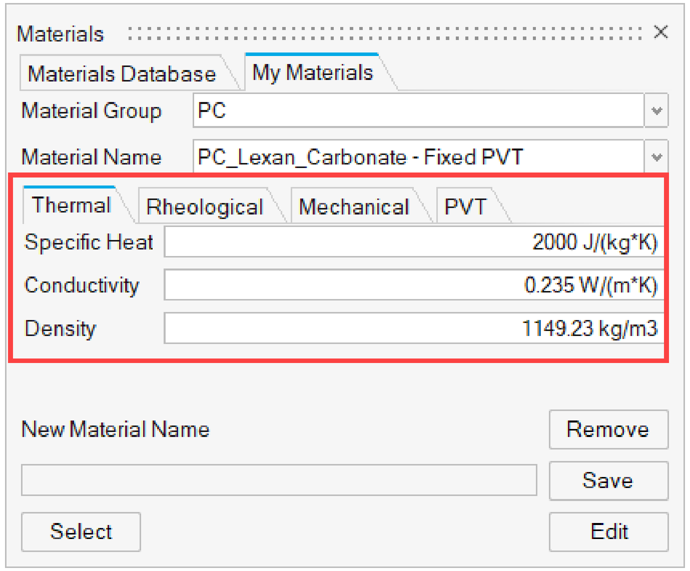
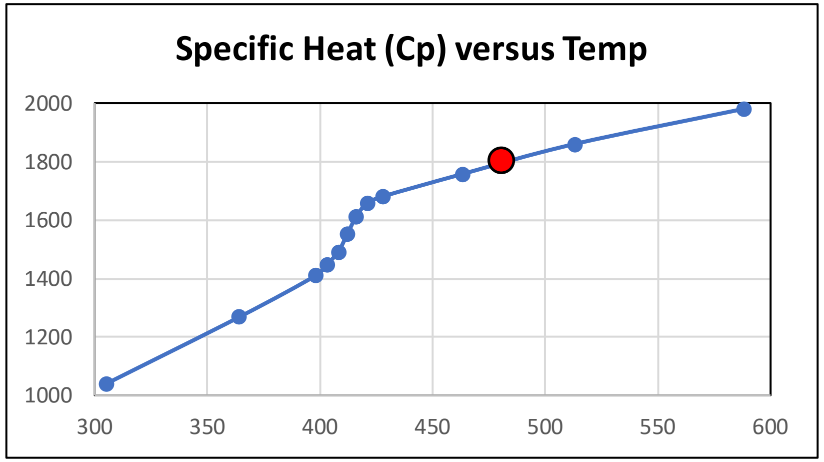
Material Reference for Defining Thermal Properties

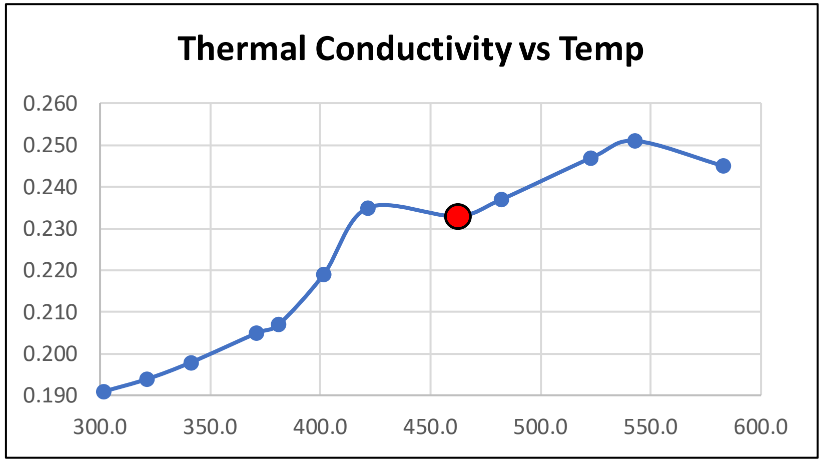


From the Thermal tab, review and enter the Specific Heat, Conductivity and Density values for your material.

Tip:

- The specific heat and thermal conductivity are entered as single values. You may find it advantageous to set these to the value near the expected melt temperature.
- The Density value required here refers to the melt density.





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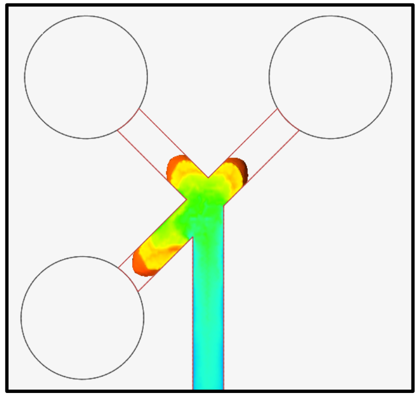
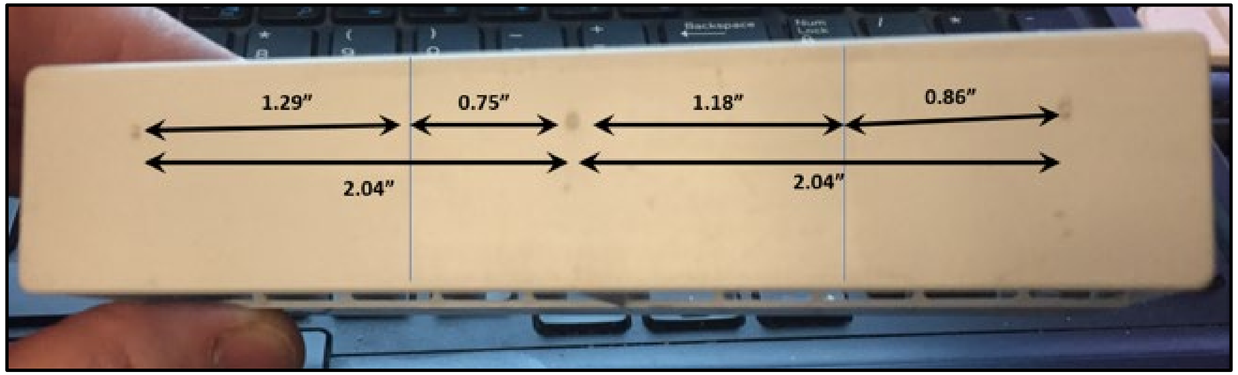
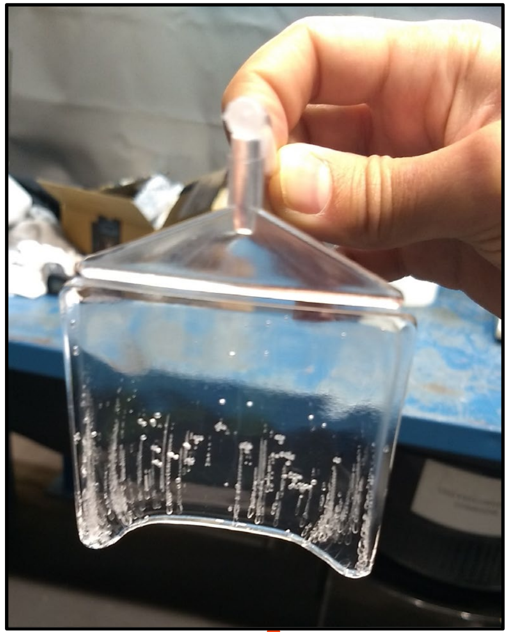
Reference for Rheological Properties: Viscosity Models

Model	Parameters	Literal	Simplified	Viscosity at Critical Shear Rate
Cross Model	A: Consistency n: Power law index τ^*: Reference Shear Stress	$\eta(T,\dot{\gamma}) = \frac{A\alpha}{1+\left[\frac{A\alpha\cdot\dot{\gamma}}{\tau^*}\right]^{(1-n)}}$	$\eta(T,\dot{\gamma}) = \frac{\eta_0(T)}{1+\left[\frac{\dot{\gamma}}{\dot{\gamma}_{Crit}}\right]^{(1-n)}}$	$\eta(T,\dot{\gamma}_{Crit}) = \frac{\eta_0(T)}{2}$
Modified Cross Model	A: Consistency n: Power law index τ^*: Reference Shear Stress	$\eta(T,\dot{\gamma}) = \frac{A\alpha}{\left[1+\frac{A\alpha\cdot\dot{\gamma}}{\tau^*}\right]^{(1-n)}}$	$\eta(T,\dot{\gamma}) = \frac{\eta_0(T)}{\left[1+\frac{\dot{\gamma}}{\dot{\gamma}_{Crit}}\right]^{(1-n)}}$	$\eta(T,\dot{\gamma}_{Crit}) = \frac{\eta_0(T)}{[2]^{(1-n)}}$
Carreau-Yasuda Model	A: Consistency n: Power law index λ: Time Constant a: Width of transition region η_∞: Infinite Shear Rate Viscosity	$\eta(T,\dot{\gamma}) = \eta_\infty + \frac{A\alpha-\eta_\infty}{[1+(\lambda\dot{\gamma})^a]^{\frac{1-n}{a}}}$	$\eta(T,\dot{\gamma}) = \eta_\infty + \frac{\eta_0-\eta_\infty}{[1+(\lambda\dot{\gamma})^a]^{\frac{1-n}{a}}}$	$\eta(T,\dot{\gamma}_{Crit}) = \frac{\eta_0(T)}{[2]^{\frac{1-n}{a}}}$
Herschel-Bulkley Model (Thermosets)	A: Consistency n: Power law index τ_0: Shear Stress Threshold m: Smoothing Parameter	$\eta(T,\dot{\gamma}) = \frac{A\alpha_T}{\dot{\gamma}^{(1-n)}} + \frac{\tau_0\left(1-e^{-m\dot{\gamma}}\right)}{\dot{\gamma}}$	$\eta(T,\dot{\gamma}) = \frac{\eta_0(T)}{\dot{\gamma}^{(1-n)}} + \frac{\tau_0\left(1-e^{-m\dot{\gamma}}\right)}{\dot{\gamma}}$	





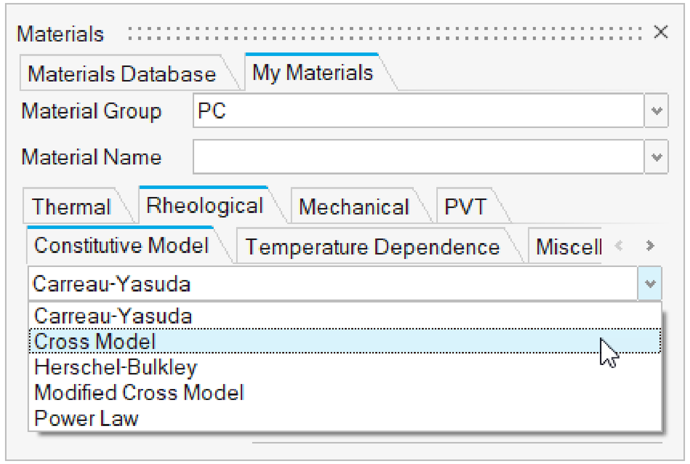


Reference for Defining Rheological Properties
Part I: Cross Model

$$\alpha = e^{\frac{-C_1\,(T-T_g)}{C_2+(T-T_g)}}$$

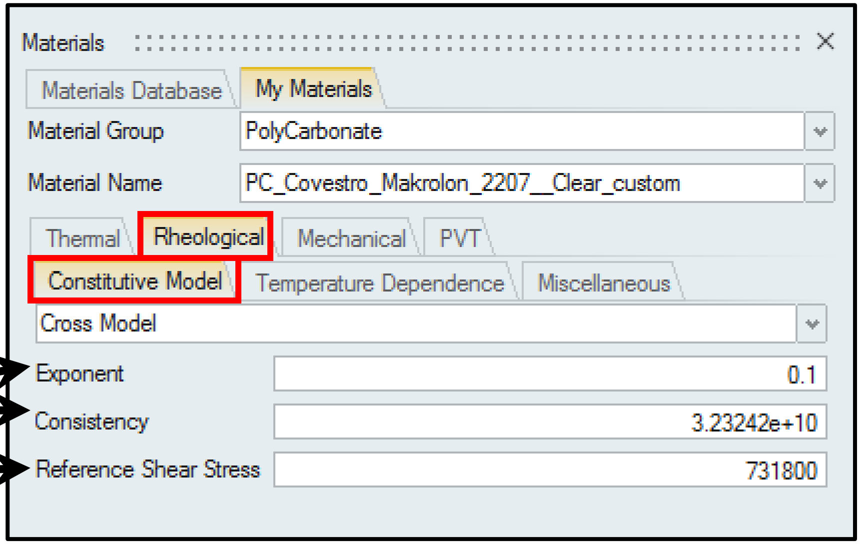
$$A = \eta^*$$

$$\eta_0(T) = A\alpha$$



Modified Cross - WLF

Eta*	3.23242E+10
n	0.1
Tau*	7.318E+05
Tg	411.15K
D3	3.72E-07
C1	25.708
C2	51.6



$$\eta(T,\dot{\gamma}) = \frac{A\alpha}{1+\left[\frac{A\alpha\cdot\dot{\gamma}}{\tau^*}\right]^{(1-n)}}$$

$$\eta(T,\dot{\gamma}) = \frac{\eta_0(T)}{1+\left[\frac{\eta_0(T)\cdot\dot{\gamma}}{\tau^*}\right]^{(1-n)}}$$

Note: The Cross Model and Modified Cross Model in the pull-down list are DIFFERENT as shown in the previous slide.

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Reference for Defining Rheological Properties
Part II: Williams-Landel-Ferry (WLF)

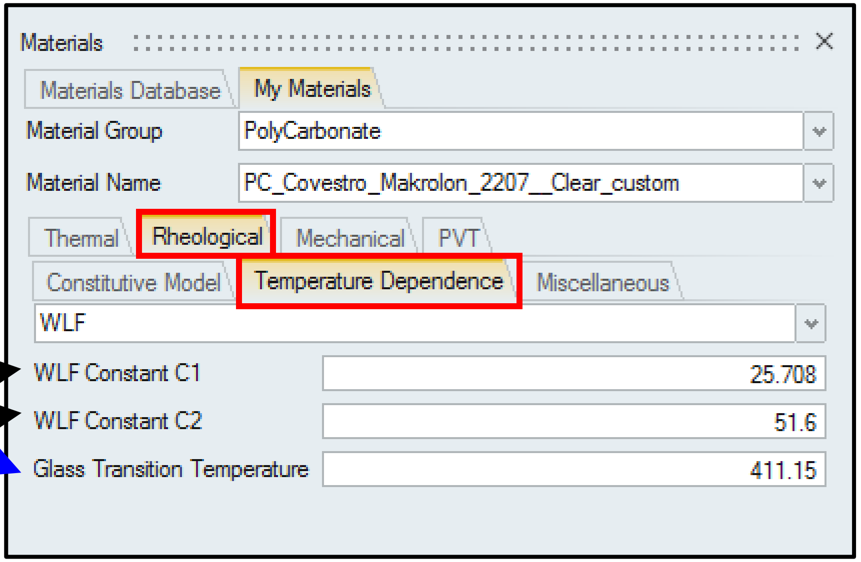
$$\alpha = e^{\frac{-C_1\,(T-T_g)}{C_2+(T-T_g)}}$$

$$A = \eta^*$$

$$\eta_0(T) = A\alpha$$

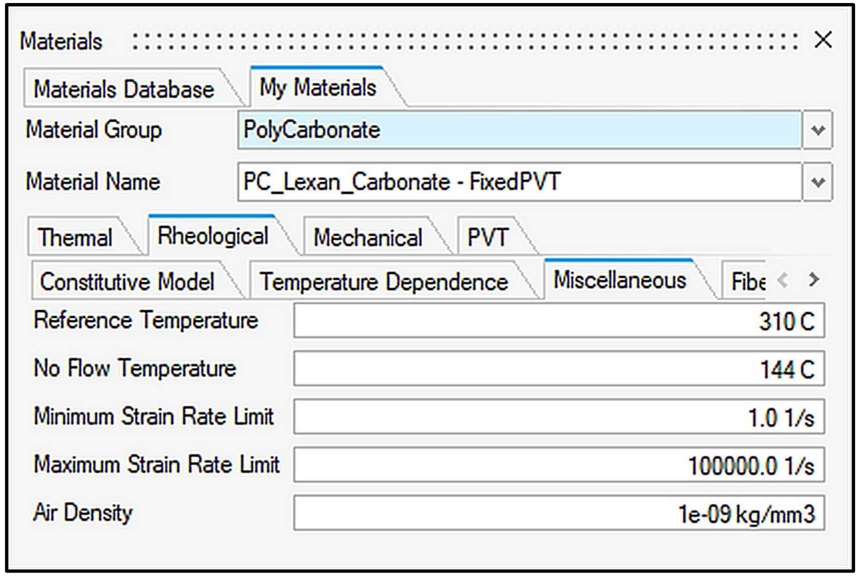
Modified Cross - WLF

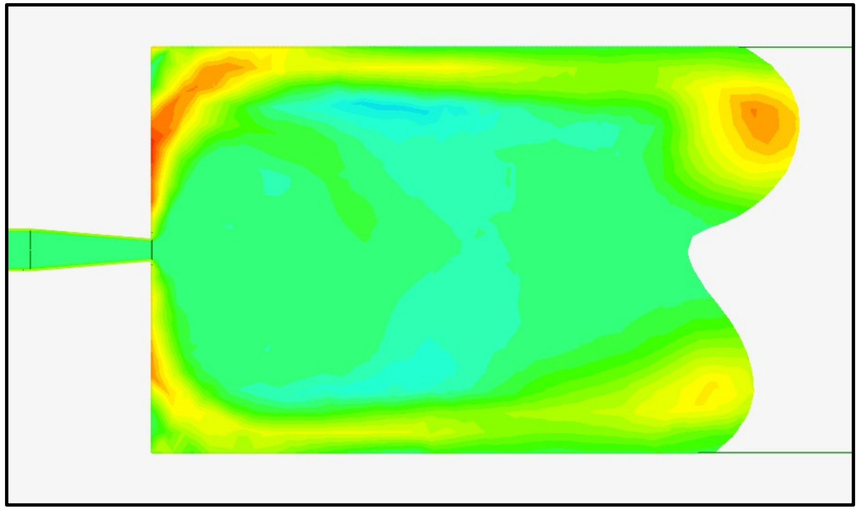
Eta*	3.23242E+10
n	0.1
Tau*	7.318E+05
Tg	411.15K
D3	3.72E-07
C1	25.708
C2	51.6



Reference for Defining Rheological Properties Part III: Miscellaneous Properties

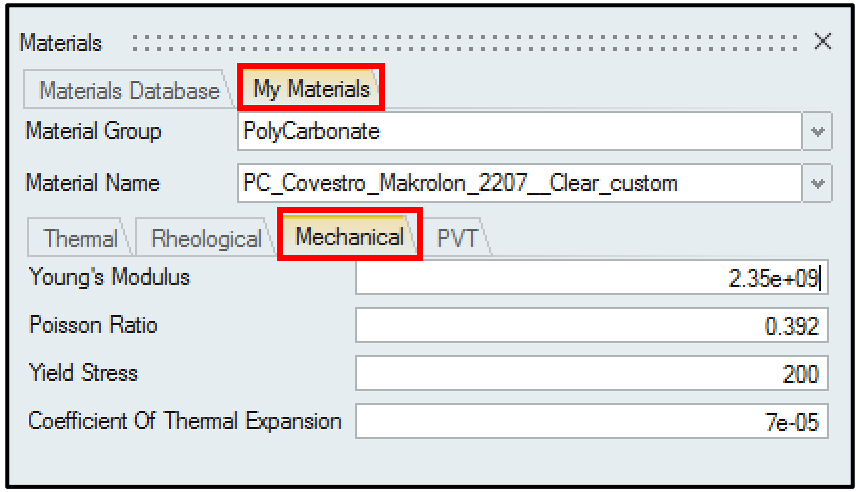
1. **Reference Temperature** (K).
2. **No Flow Temperature**: Temperature at which the material will, for all intents and purposes, stop flowing; generally, this is the Tg (K).
3. **Minimum Strain Rate Limit**: Shear rate below which viscosity is not expected to materially change. This is the “practical” zero-shear rate limit.
4. **Maximum Strain Rate Limit**: Maximum shear rate for which the data is considered valid & useful.
5. **Density**: Assumed melt density. During filling, the polymer is assumed to be incompressible (kg/m³).
6. **Air Density**: Assumed density of the air being displaced in the mold during filling (kg/m³).





Reference for Defining Mechanical Properties

1. **Young's Modulus (Pa)**
2. **Poisson's Ratio**
3. **Yield Stress (Pa)**
4. **Coefficient of Linear Thermal Expansion (CLTE)**



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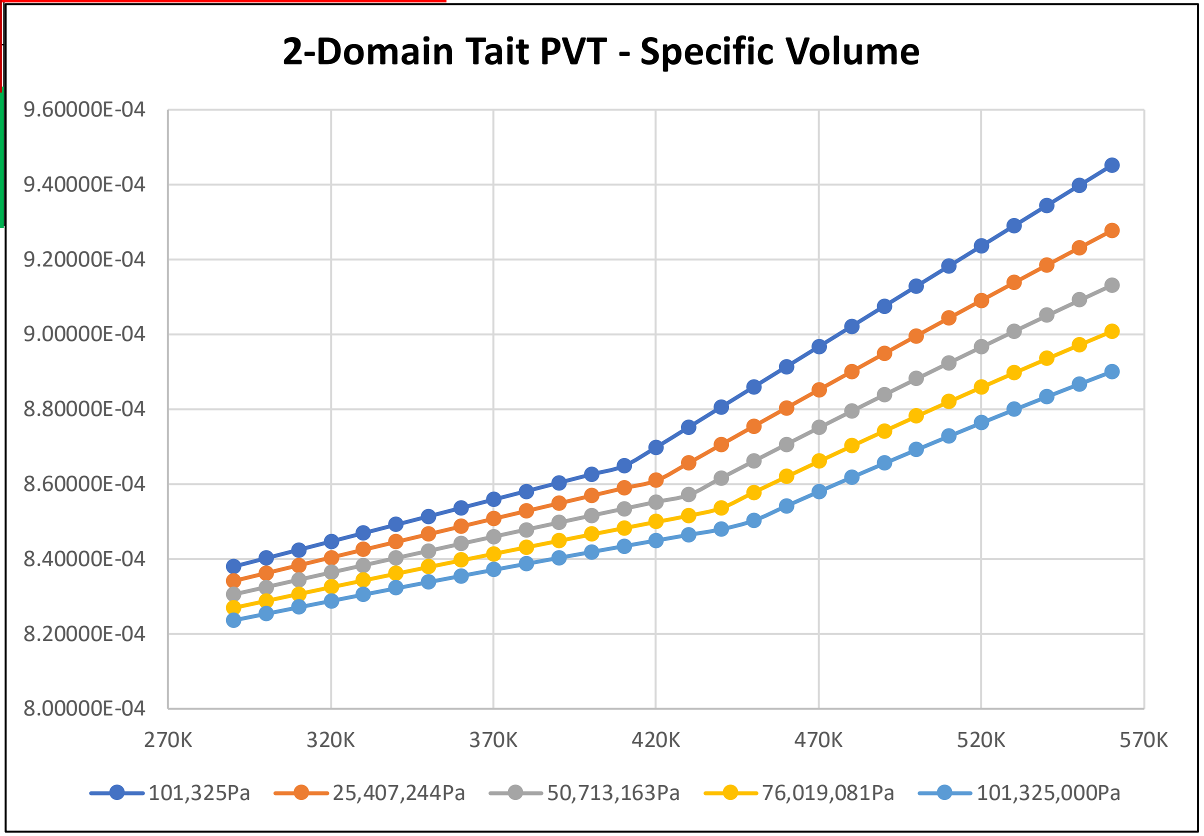
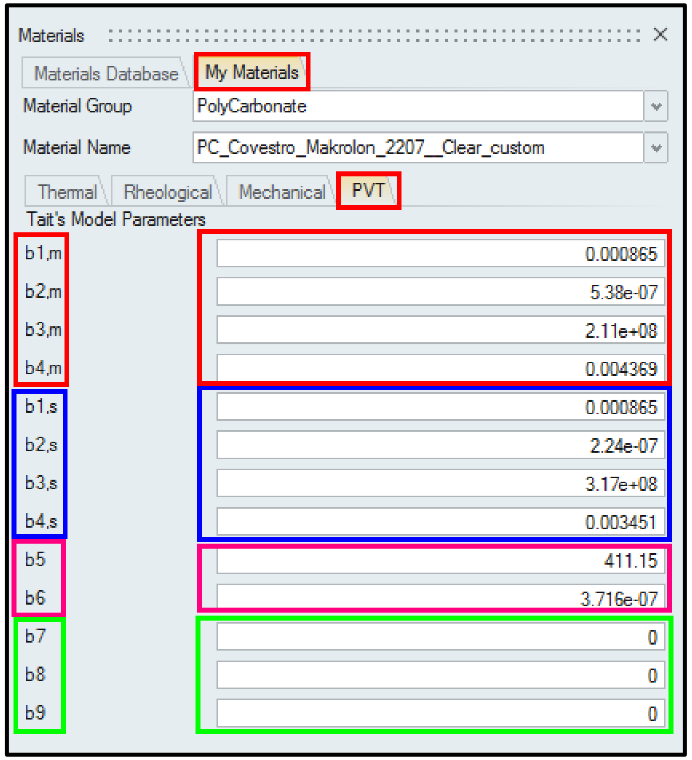
Reference for Defining PVT Parameters
Part I: Equation of State (Tait) – Solid & Liquid Domains

Solid Domain		Molten Domain	
b1s	8.650E-04	b1m	8.650E-04
b2s	2.240E-07	b2m	5.380E-07
b3s	3.170E+08	b3m	2.110E+08
b4s	3.451E-03	b4m	4.369E-03
b5	411.15		
b6	3.716E-07		
b7	0		
b8	0		
b9	0		





$$b_{1m} = b_{1s} + b_7$$

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Reference for Defining PVT Parameters
Part II: Equation of State (Tait) – (pvT) – Solid & Liquid Domains

$$v(T,p) = v_0(T)\left[1 - C\,ln\left(1 + \frac{p}{B(T)}\right)\right] + v_{tr}(T,p)$$

$C = 0.0894$

SOLID DOMAIN:

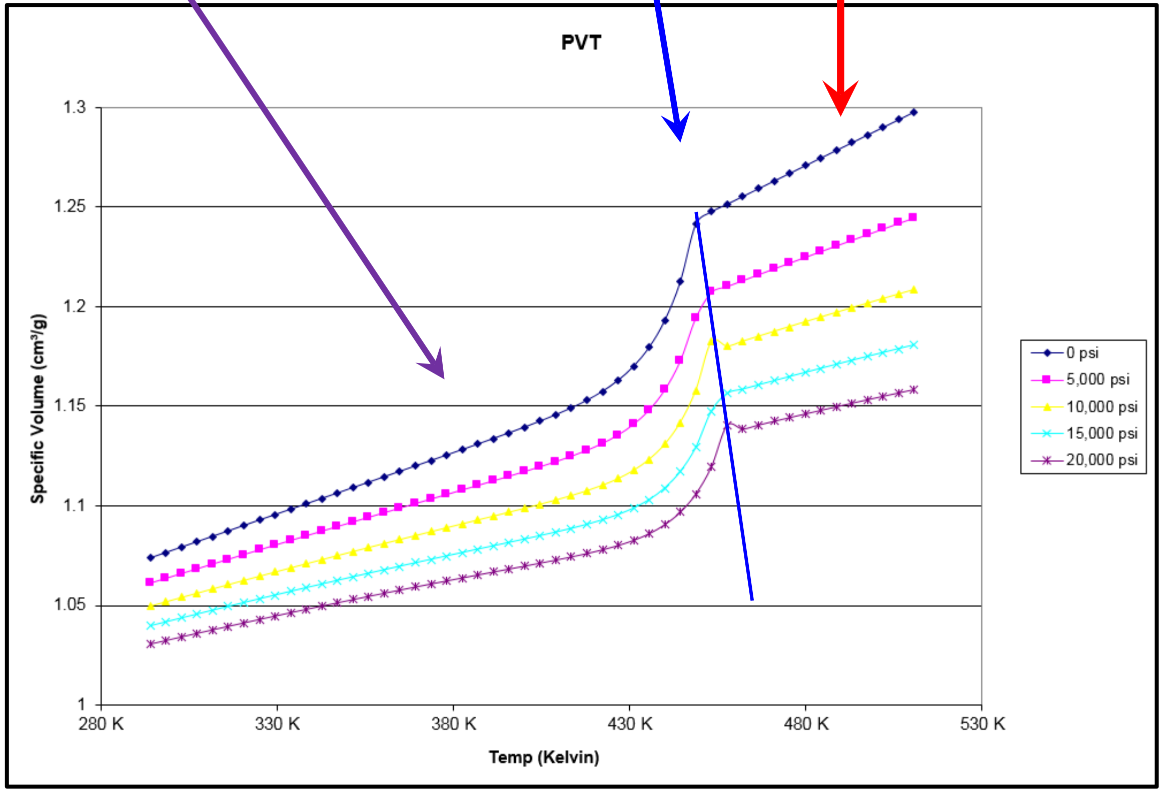
$v_0 = b_{1s} + b_{2s}(T - b_5)$

$B(T) = b_{3s}e^{[-b_{4s}(T-b_5)]}$

$v_{tr}(T,p) = b_7 e^{[(b_8(T-b_5))-(b_9 p)]}$

Data Fit Coefficients:
$b_{1s}, b_{2s}, b_{3s}, b_{4s}, b_5, b_6, b_7, b_8, b_9$

$$T_{tr}(p) = b_5 + b_6 p$$
$$b_5 = T_{tr}(0)$$



LIQUID DOMAIN:

$v_0 = b_{1l} + b_{2l}(T - b_5)$

$B(T) = b_{3l}e^{[-b_{4l}(T-b_5)]}$

$v_{tr}(T,p) = 0$

Data Fit Coefficients:
$b_{1l}, b_{2l}, b_{3l}, b_{4l}, b_5$ & b_6

$$b_{1l} = b_{1s} + b_7$$

Important: Sometimes an error occurs when the solid and liquid domains do not match-up correctly. This discontinuity is not physical; it is due to curve fitting. Check and adjust the b_{1s} value accordingly.

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Material Data Exercise

1. Select an existing material in the Materials Viewer.
2. Modify properties of the material according to the data provided in the tables, which is based on Vydyne R543H BK02 (PA-66, 43% Glass Filled) a popular material made by Ascend Polymers.
3. Save the material with a new name and access it from the Material Viewer on the **My Materials** tab.

Specific Heat	1908
Conductivity	0.330
Density	1305.3
Cross Model	
Exponent	0.33358
Consistency	4.80707E+19
Critical Shear Stress	2.26362E+05
WLF	
C1	47.535
C2	51.60
D3	0.0
Tg	323.15
Reference Temperature	491.15
No Flow Temperature	491.15
Minimum Shear Rate Limit	0.01
Maximum Shear Rate Limit	100,000
Young's Modulus	1.01974e+011
Poisson's Ratio	0.391
Yield Stress	9.00E+06
CLTE	3.525E-05

Tait PVT	Solid	Molten
b1	0.000705	0.000753
b2	2.100E-07	3.918E-07
b3	3.38522E+08	1.71450E+08
b4	0.001937	0.004512
b5	532.15	
b6	8.166E-08	
b7	0.000047	
b8	0.023396	
b9	5.623E-09	

Fiber Percentage	43.00
Average Diameter	8.33E-06
Max Length	4.50E-04
Min Length	1.50E-04

Mold Temperature Range:
100-180ºF
Melt Temperature Range:
530-590ºF

The material properties for this example were created and provided by Ascend Polymers.