


**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**.

The image displays a series of seven numbered steps illustrating the process of creating a new material in Altair Mold:

- 1:** A toolbar at the top of the interface with the Materials Viewer icon highlighted in a red box.
- 2:** The Materials Database dialog box is open, showing the 'Materials Database' tab. The 'Material Group' is set to 'PolyCarbonate'.
- 3:** The 'Material Name' dropdown is set to 'PC_Lexan_Carbonate'.
- 4:** The 'Edit' button at the bottom right of the dialog is being clicked.
- 5:** The 'New Material Name' field is filled with 'PC_Lexan_Carbonate - Fixed PVT - custom'.
- 6:** The 'Save' button is being clicked.
- 7:** The 'Select' button is being clicked.

Reference for Defining Material Properties

Viscosity Data

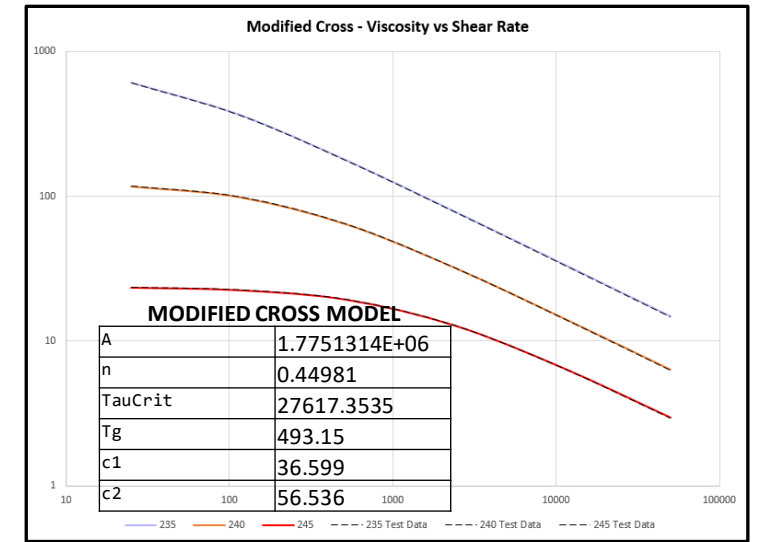
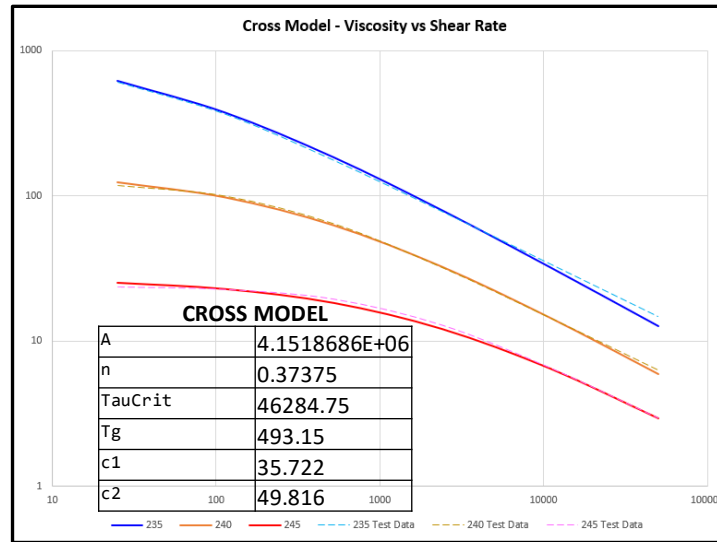
Choose a Constitutive Model:

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

Temperature Dependence

Choose:

- Exponential – $\text{Exp}(-\text{Beta}(T-T_{\text{ref}}))$
- Arrhenius – $\text{Exp}(Q/RT)$
- Williams-Landel-Ferry (WLF)



PVT Data

Select: **2-Domain Tait**

Thermal Quantities

Define:

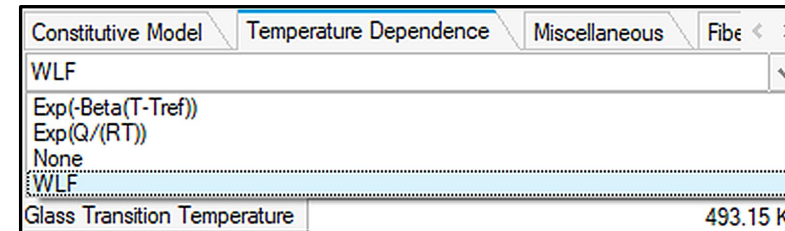
- Thermal Conductivity (k)
- Specific Heat (Cp)
- Melt Density

Mechanical Properties

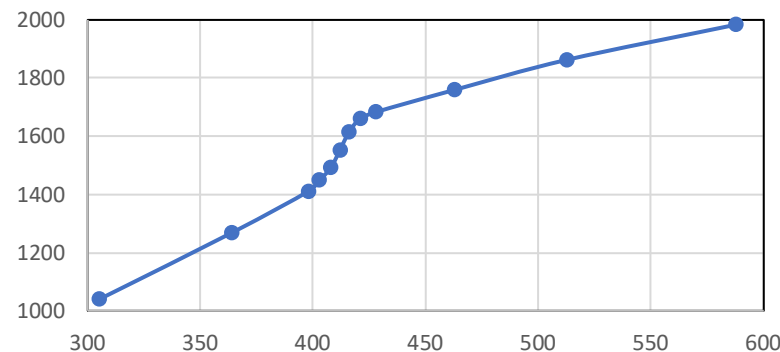
Keep the Default Values for these properties:

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

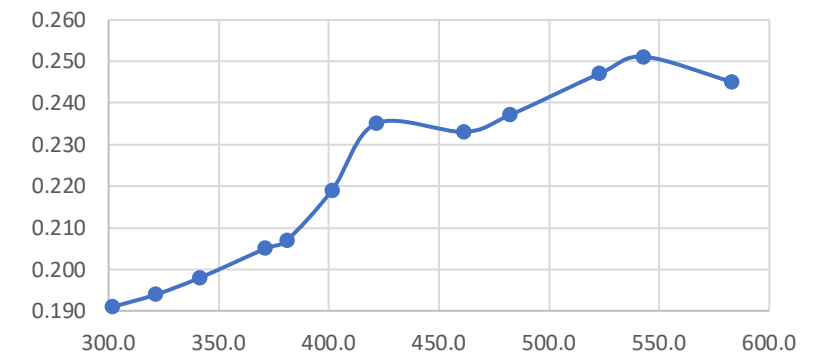
Note: SI (m-kg-sec) units



Specific Heat (Cp) versus Temp



Thermal Conductivity vs Temp



Material Reference for Defining Thermal Properties

Materials Database | My Materials

Material Group: PC

Material Name: PC_Lexan_Carbonate - Fixed PVT

Thermal | Rheological | Mechanical | PVT

Specific Heat: 2000 J/(kg*K)

Conductivity: 0.235 W/(m*K)

Density: 1149.23 kg/m³

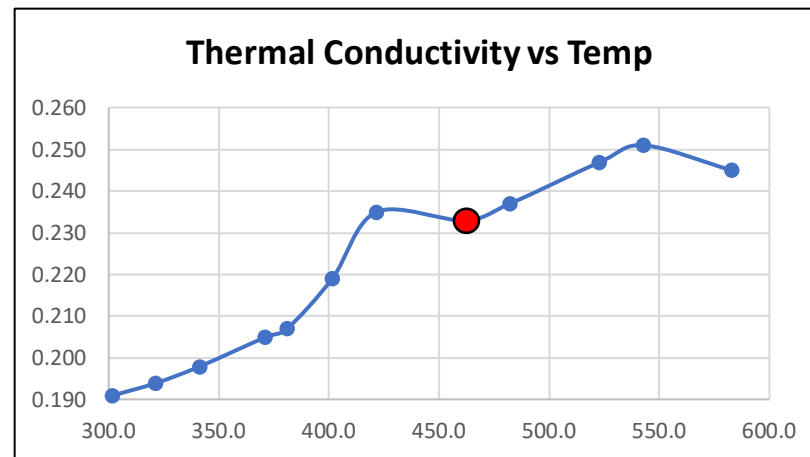
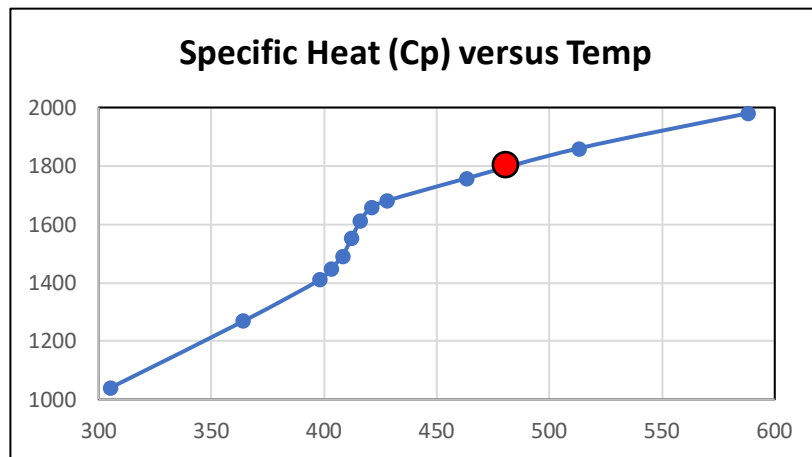
New Material Name:

Remove Save Select Edit

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.



Reference for Rheological Properties: Viscosity Models

Cross Model

A: Consistency
 n: Power law index
 τ^* : Reference Shear Stress

Literal

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

Simplified

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

Viscosity at Critical Shear Rate

$$\eta(T, \dot{\gamma}_{Crit}) = \frac{\eta_0(T)}{2}$$

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

$$\eta(T, \dot{\gamma}) = \eta_\infty + \frac{A\alpha - \eta_\infty}{[1 + (\lambda\dot{\gamma})^a]^{\frac{1-n}{a}}}$$

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

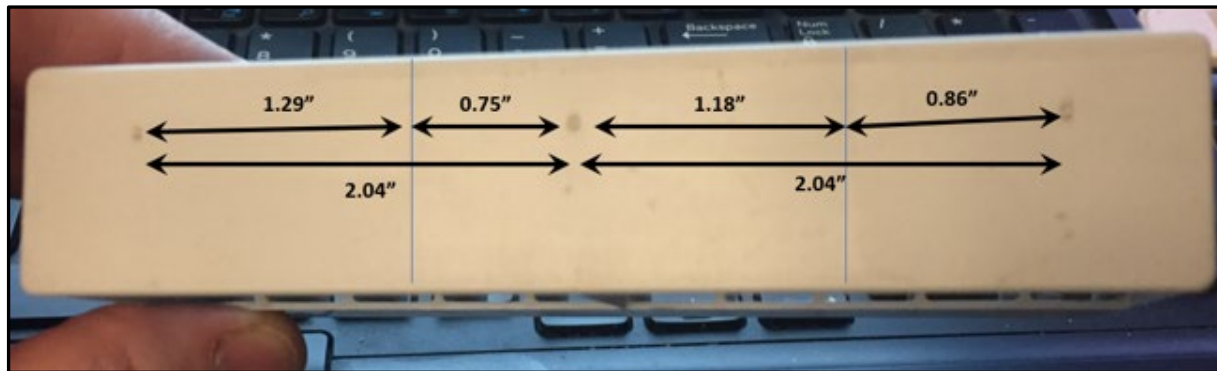
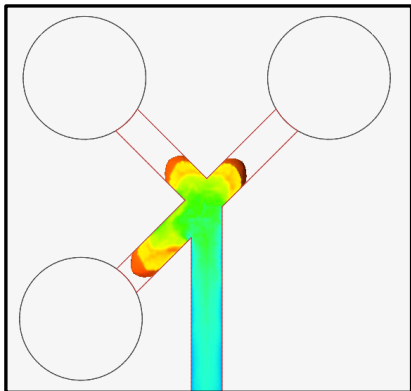
$$\eta(T, \dot{\gamma}_{Crit}) = \frac{\eta_0(T)}{[2]^{\frac{1-n}{a}}}$$

Herschel-Bulkley Model (Thermosets)

A: Consistency
 n: Power law index
 τ_0 : Shear Stress Threshold
 m: Smoothing Parameter

$$\eta(T, \dot{\gamma}) = \frac{A\alpha\tau}{\dot{\gamma}^{(1-n)}} + \frac{\tau_0(1 - e^{-m\dot{\gamma}})}{\dot{\gamma}}$$

$$\eta(T, \dot{\gamma}) = \frac{\eta_0(T)}{\dot{\gamma}^{(1-n)}} + \frac{\tau_0(1 - e^{-m\dot{\gamma}})}{\dot{\gamma}}$$



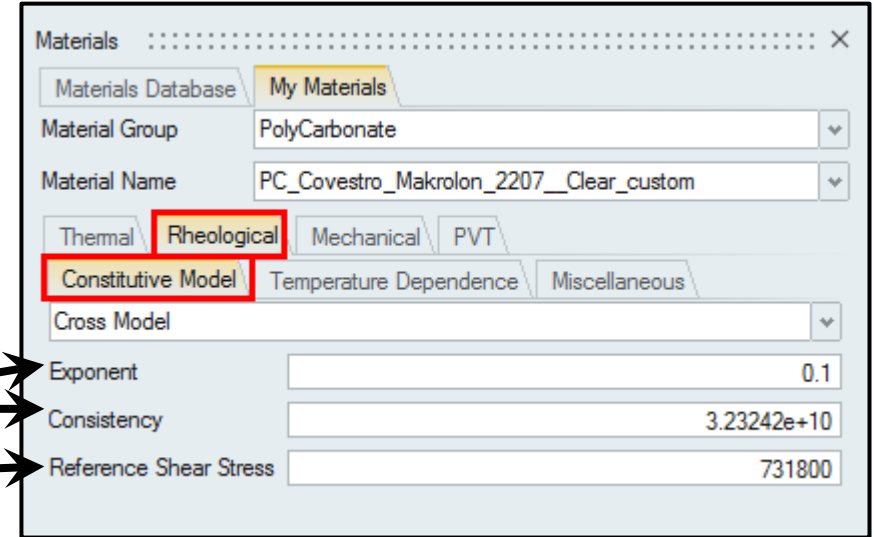
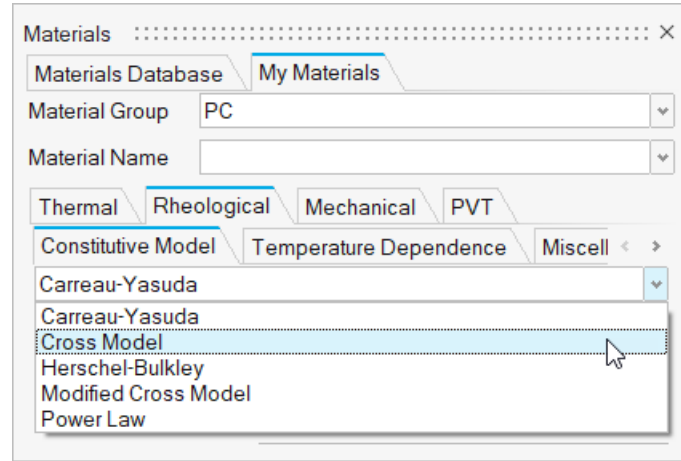
Reference for Defining Rheological Properties

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

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

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

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

Materials

Materials Database: My Materials

Material Group: PolyCarbonate

Material Name: PC_Covestro_Makrolon_2207_Clear_custom

Thermal | **Rheological** | Mechanical | PVT

Constitutive Model: **Temperature Dependence** | Miscellaneous

WLF

WLF Constant C1: 25.708

WLF Constant C2: 51.6

Glass Transition Temperature: 411.15

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).

Materials X

Materials Database: My Materials

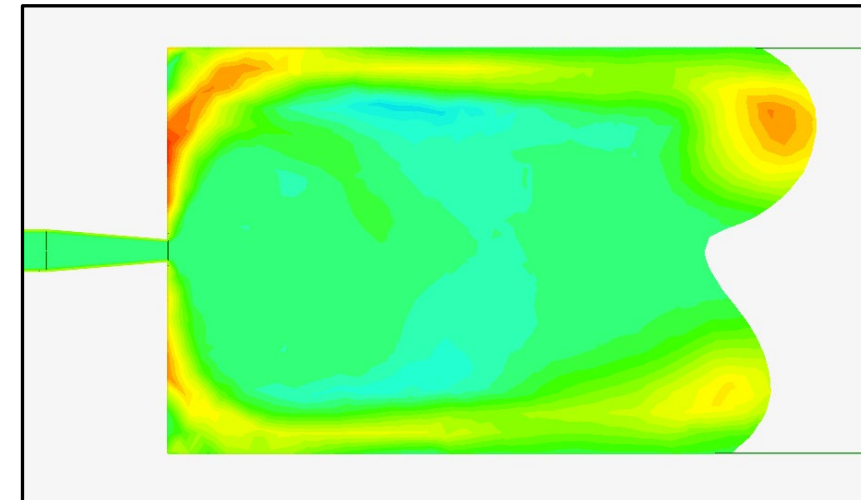
Material Group: PolyCarbonate

Material Name: PC_Lexan_Carbonate - FixedPVT

Thermal | **Rheological** | Mechanical | PVT

Constitutive Model | Temperature Dependence | **Miscellaneous** | Fibre < >

Reference Temperature	310 C
No Flow Temperature	144 C
Minimum Strain Rate Limit	1.0 1/s
Maximum Strain Rate Limit	100000.0 1/s
Air Density	1e-09 kg/mm3



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)

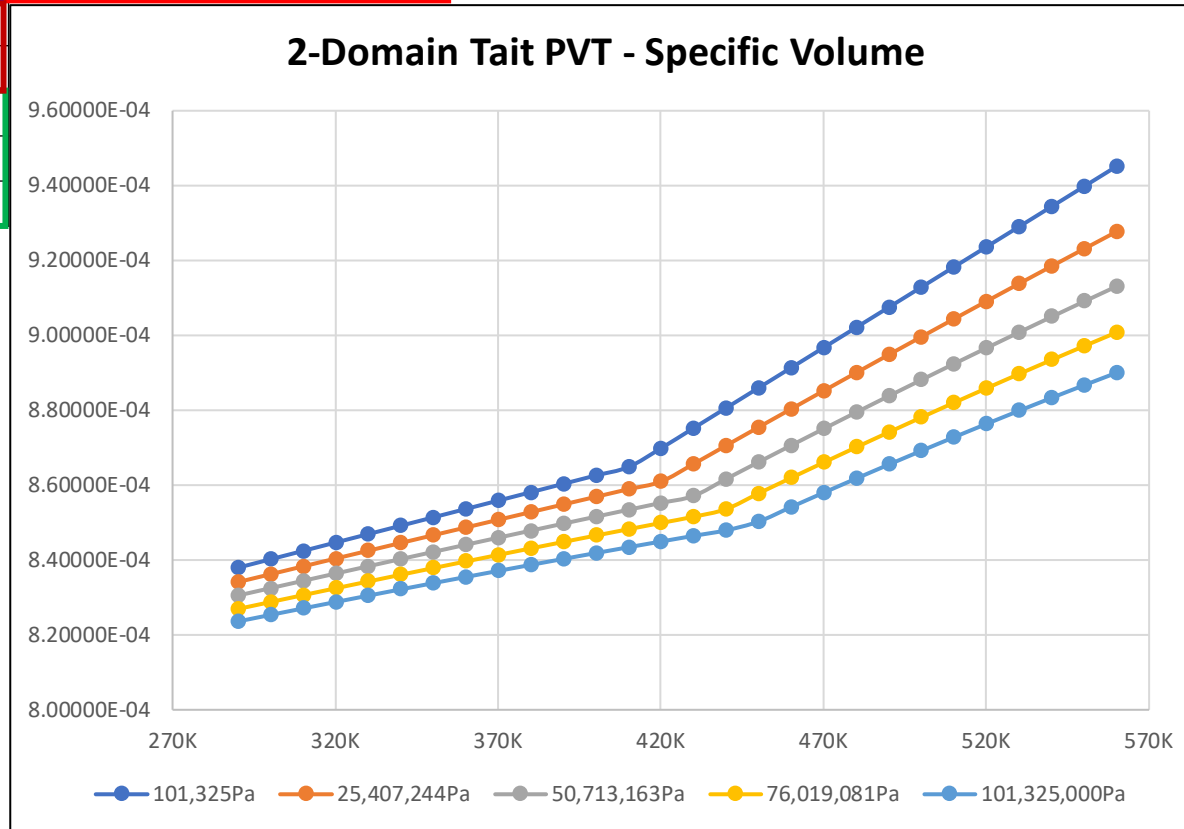
The screenshot shows a software window titled "Materials" with a close button (X). It features a "Materials Database" dropdown menu set to "My Materials". Below this, "Material Group" is set to "PolyCarbonate" and "Material Name" is set to "PC_Covestro_Makrolon_2207_Clear_custom". A tabbed interface at the bottom includes "Thermal", "Rheological", "Mechanical" (which is highlighted with a red box), and "PVT". Under the "Mechanical" tab, four properties are listed with their values in input fields: Young's Modulus (2.35e+09), Poisson Ratio (0.392), Yield Stress (200), and Coefficient Of Thermal Expansion (7e-05).

Property	Value
Young's Modulus	2.35e+09
Poisson Ratio	0.392
Yield Stress	200
Coefficient Of Thermal Expansion	7e-05

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		



Materials Database: My Materials

Material Group: PolyCarbonate

Material Name: PC_Covestro_Makrolon_2207_Clear_custom

Thermal | Rheological | Mechanical | **PVT**

Tait's Model Parameters

b1,m	0.000865
b2,m	5.38e-07
b3,m	2.11e+08
b4,m	0.004369
b1,s	0.000865
b2,s	2.24e-07
b3,s	3.17e+08
b4,s	0.003451
b5	411.15
b6	3.716e-07
b7	0
b8	0
b9	0

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

Reference for Defining PVT Parameters

Part II: Equation of State (Tait) – (pvT) – Solid & Liquid Domains

SOLID DOMAIN:

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

$C = 0.0894$

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

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

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

Data Fit Coefficients:

$$b_{1s}, b_{2s}, b_{3s}, b_{4s}, b_5, b_6, b_7, b_8, b_9$$

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.

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

$$b_5 = T_{tr}(0)$$

LIQUID DOMAIN:

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

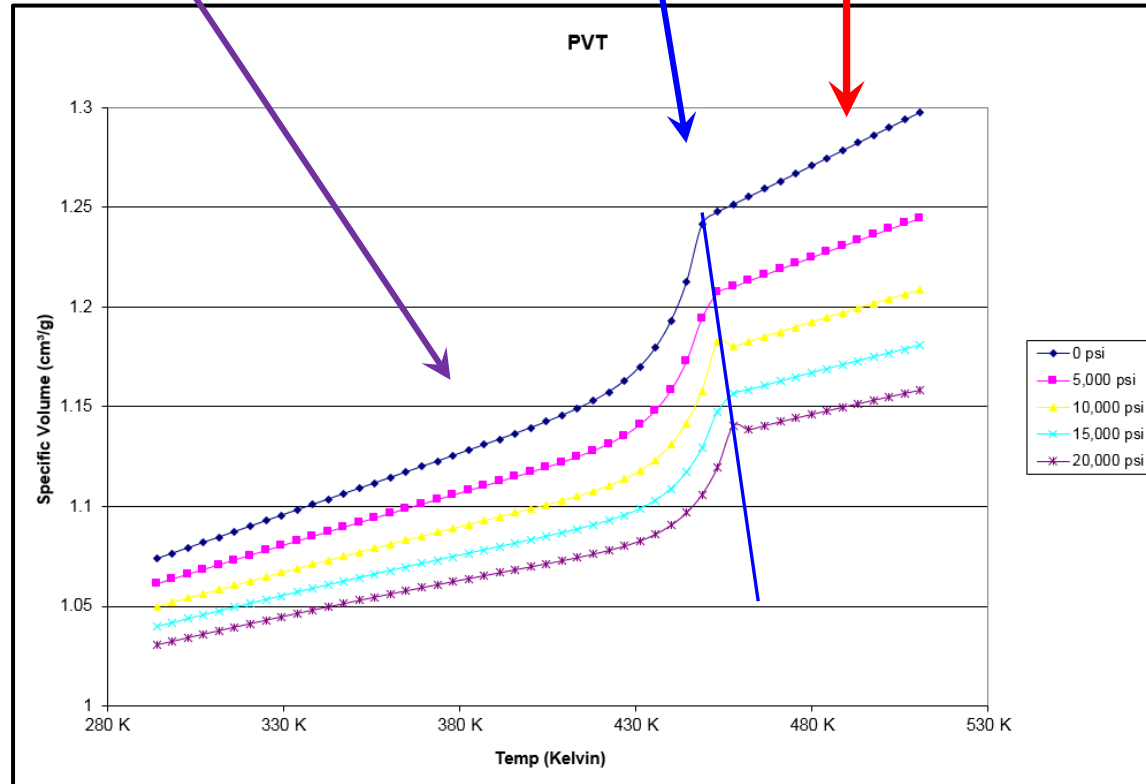
$$B(T) = b_{3l} e^{-b_{4l}(T - b_5)}$$

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

Data Fit Coefficients:

$$b_{1l}, b_{2l}, b_{3l}, b_{4l}, b_5 \text{ \& } b_6$$

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



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 Vydyn 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:
100-180°F
Melt Temperature Range:
530-590°F