Material Models in Simulation- Part 3 - New viscosity models

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Evaluation Parameters

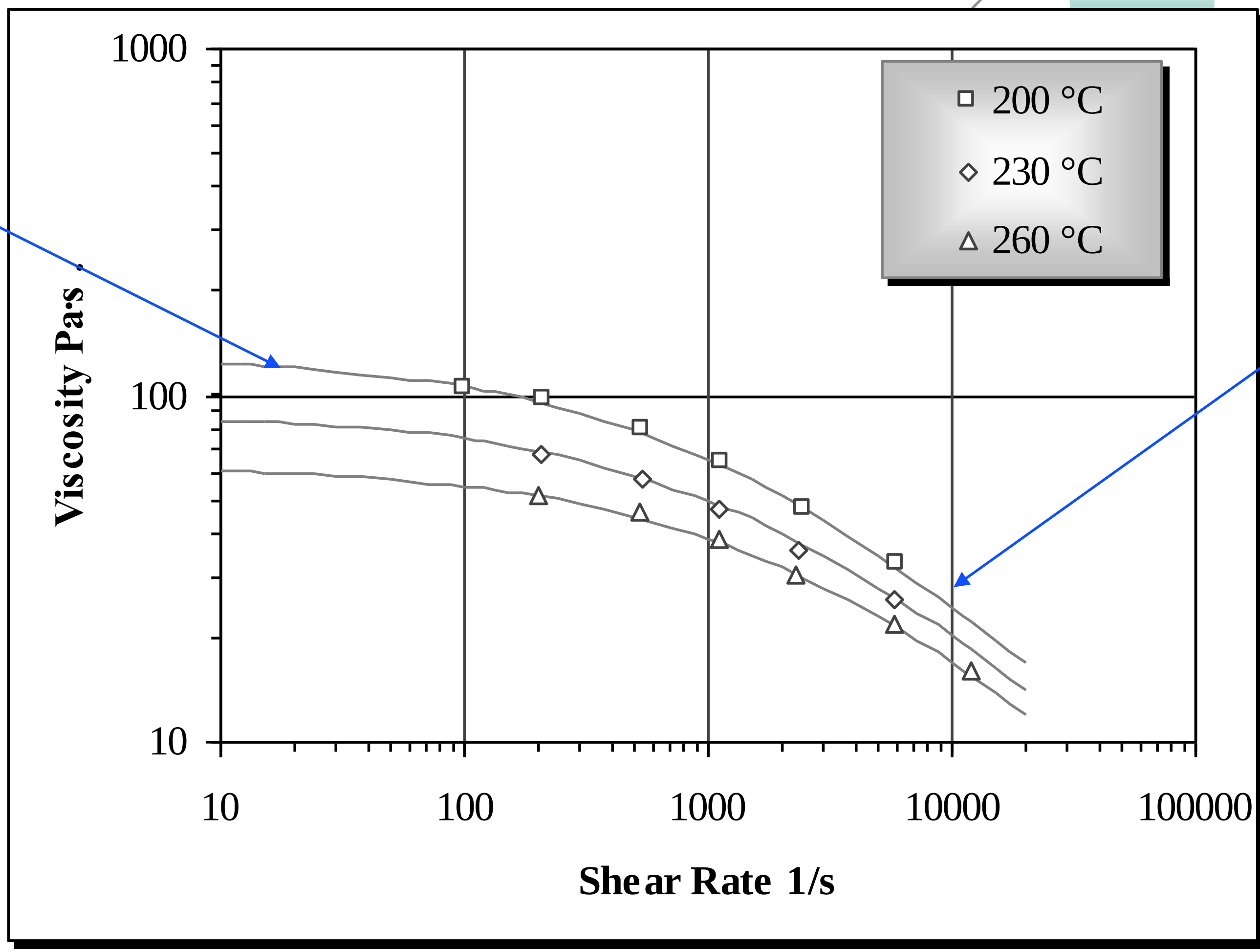
- material property based parameters
- evaluate effects seen in the process
- understand and interpret simulation results
- compare materials
- develop criteria for selection based on desired processability

Properties of Evaluation Parameters

- easily available
- measures or estimates of actual effects
- must be considered along with other relevant parameters

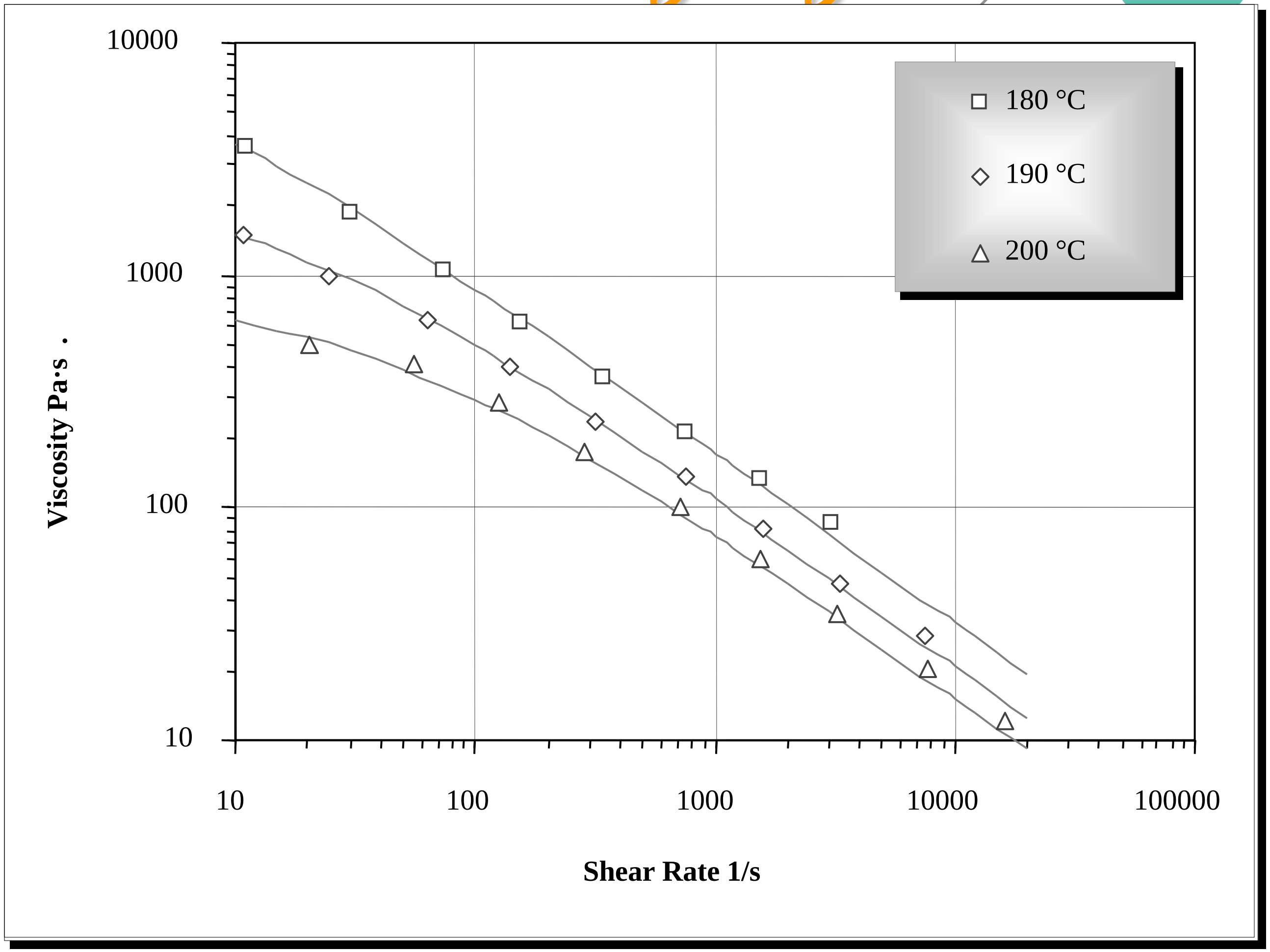
Shear sensitivity of viscosity

Newtonian

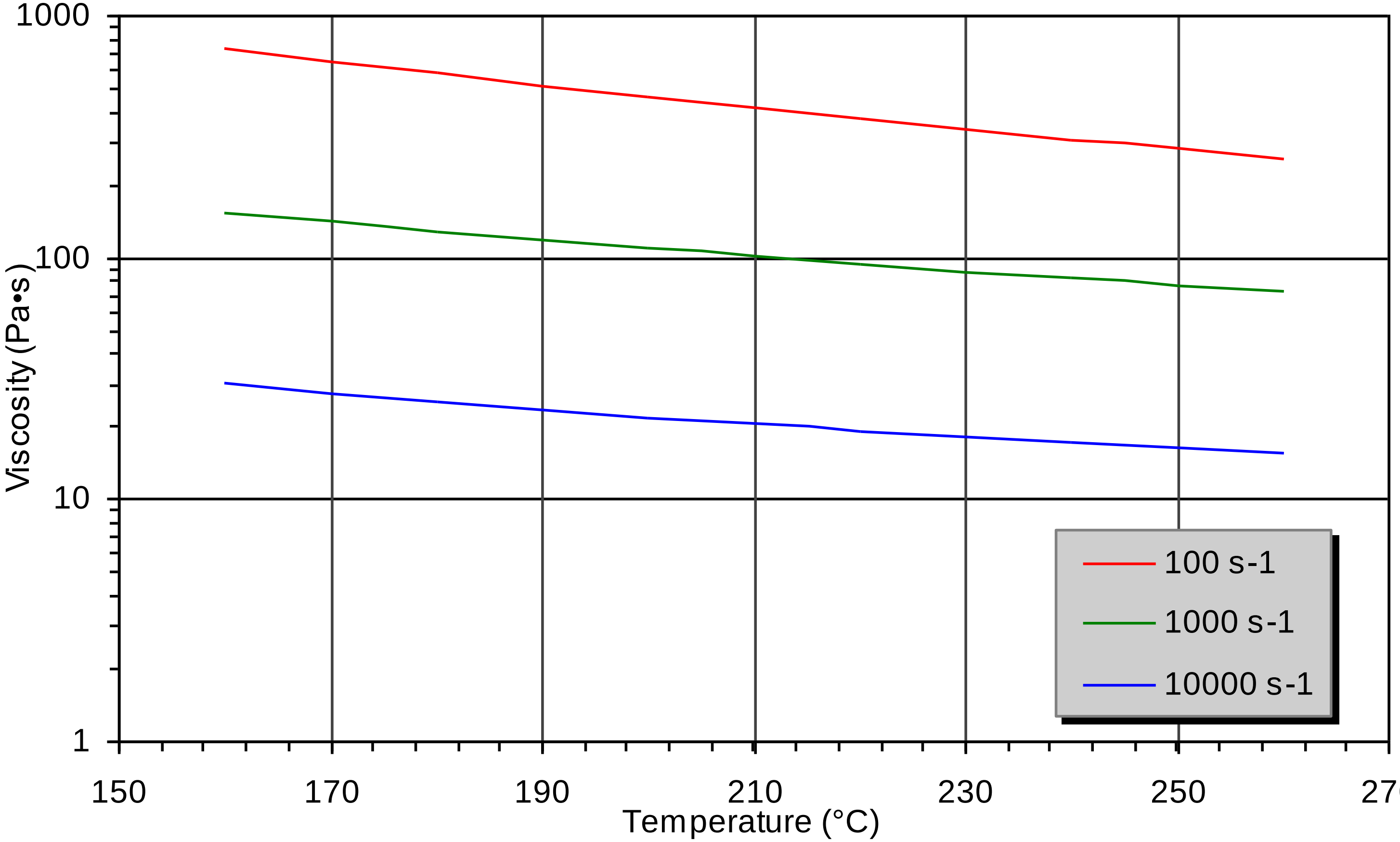


Shear-thinning

Plastics may have large shear thinning regions



Temperature sensitivity of viscosity



Evaluation Parameters - 2nd Order

- nature of the 2nd order matrix
  - temperatures
    - » Tmelt
    - » Tmelt+20
    - » Tmelt-20
  - shear rates
    - » 100
    - » 1000
    - » 10000

T	γ	η
Tmelt-20	1000	η1
Tmelt	100	η2
Tmelt	1000	η3
Tmelt	10000	η4
Tmelt+20	100	η5
Tmelt+20	1000	η6

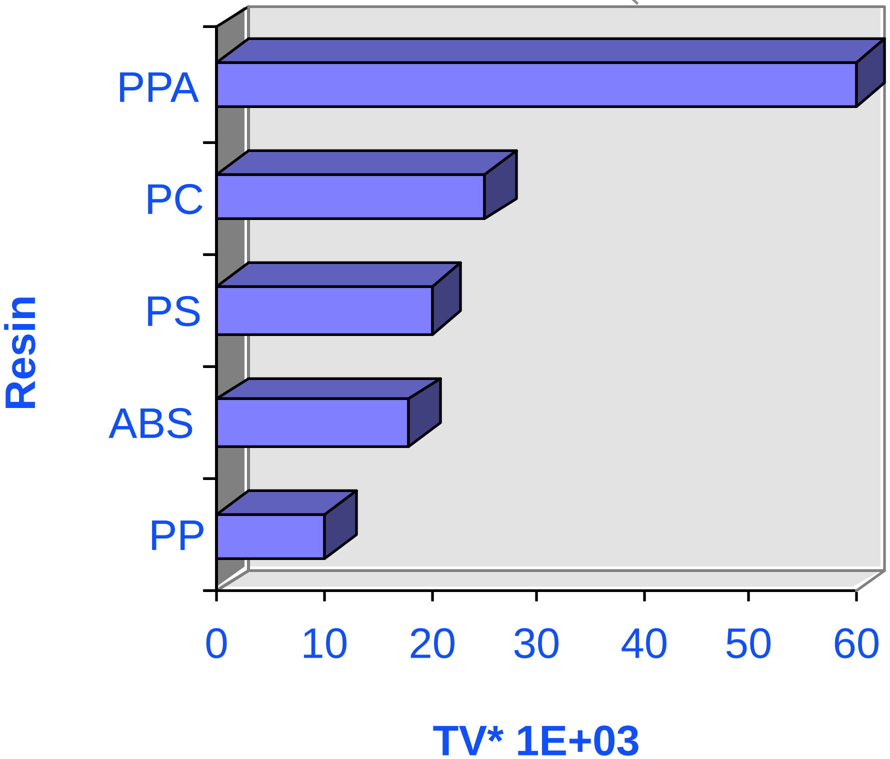
Evaluation Parameters - 2nd Order

- temperature sensitivity of viscosity
  - TVL= (ln $\eta 1$ - ln $\eta 3$) / 20
  - TVH = (ln $\eta 3$ - ln $\eta 6$) / 20

T	γ	η
Tmelt-20	1000	$\eta 1$
Tmelt	100	$\eta 2$
Tmelt	1000	$\eta 3$
Tmelt	10000	$\eta 4$
Tmelt+20	100	$\eta 5$
Tmelt+20	1000	$\eta 6$

Evaluation Parameters - 2nd Order

- rules
  - if TV is large, material is highly sensitive
  - TVL > TVH
  - semi-crystalline
    - » TVL == TVH
  - amorphous
    - » TVL >> TVH



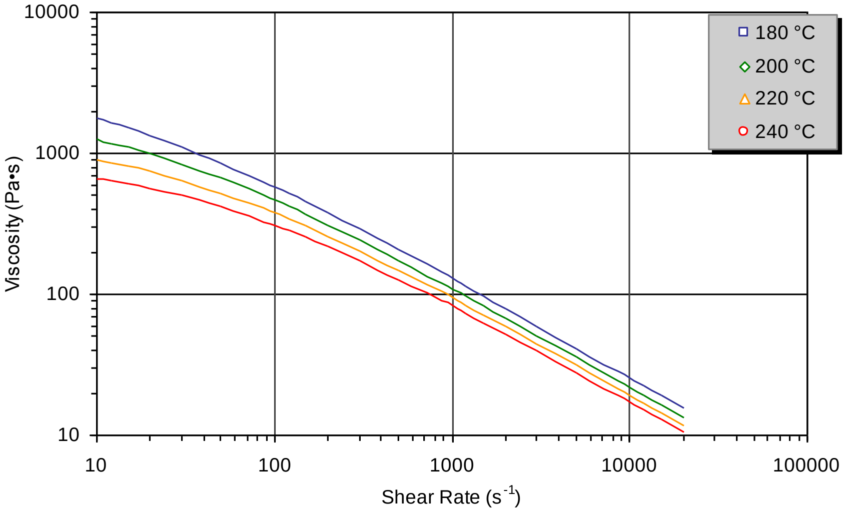
Evaluation Parameters - 2nd Order

- shear sensitivity of viscosity
  - defining a limited power-law index.
    - » SHB= (ln $\eta 3$ - ln $\eta 4$) / 2.303

T	γ	η
Tmelt-20	1000	$\eta 1$
Tmelt	100	$\eta 2$
Tmelt	1000	$\eta 3$
Tmelt	10000	$\eta 4$
Tmelt+20	100	$\eta 5$
Tmelt+20	1000	$\eta 6$

Evaluation Parameters - 2nd Order

- rules
  - 0<SHB < 1
  - large SHB = shear sensitive
  - important exception:
    - » broad newtonian PC)



New models used in Moldflow

- viscosity:
- Cross Model

$$\eta = \frac{\eta_0}{1 + \left(\frac{\eta_0 \dot{\gamma}}{\tau^*}\right)^{(1-N)}}$$

$$\eta_0 = B \exp\left(\frac{T_b}{T}\right) \exp(\beta P)$$

η Viscosity $(Pa.\mathrm{sec})$

$\dot{\gamma}$ Shear Rate (sec^{-1})

T Temperature (C)

P Pressure (Pa)

Unknowns: B, $\mathrm{T_b}$, β, τ^*, N

Evaluation Parameters - Cross Model

- B -no direct relevance
- measures η_o when taken with Tb
- "zero shear viscosity normalized for temperature"

$$\eta_0 = B \exp\left(\frac{T_b}{T}\right)$$

Evaluation Parameters - Cross Model

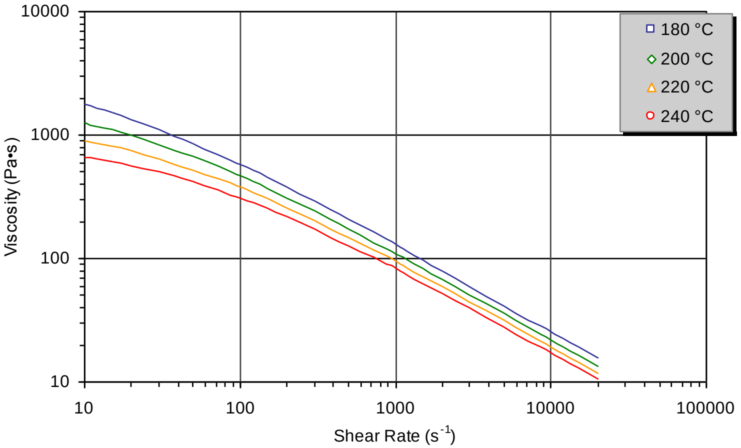
- Tb -measures temperature sensitivity of viscosity
- rules
  - if Tb is large, material is highly sensitive
  - semi-crystalline
    - » Tb is small and relatively constant
  - amorphous
    - » Tb is larger and increases with temperature

Evaluation Parameters - Cross Model

- τ^* -critical transition stress for shear-thinning behavior
- rules
  - if τ^* is large, wide Newtonian region
  - if τ^* is small, narrow Newtonian region
  - τ^* is small for simple linear polymers
    - eg HDPE, LDPE, PP
  - τ^* is large for polymers with large side chains
    - eg. PC

Evaluation Parameters - Cross Model

- N - measures shear thinning behavior
  - inverse of the power-law index
- rules for N
  - 0 < N < 1
  - small N = shear sensitive
  - important exception:
    - » fails if shear thinning region is not defined



Assessment of the Cross Model

- easy model
  - terms have direct physical relevance
  - easy to assess and evaluate
- temperature sensitivity of viscosity is constant
  - cannot model temperature sensitivity for amorphous materials

New models used in Moldflow

- viscosity:
- Cross-WLF

$$\eta = \frac{\eta_0}{1+\left(\frac{\eta_0\dot{\gamma}}{\tau^*}\right)^{(1-N)}}$$

$$\eta_0 = D_1 \exp\left[\frac{-A_1\left(T-T^*\right)}{A_2+\left(T-T^*\right)}\right]$$

$$T^* = D_2 + D_3 P$$

η Viscosity $(Pa.\mathrm{sec})$

$\dot{\gamma}$ Shear Rate (sec^{-1})

T Temperature (C)

P Pressure (Pa)

Unknowns: $D_1\ D_2\ D_3\ A_1\ A_2\ \tau^*\ N$

Evaluation Parameters - Cross-WLF Model

- D1 -no direct relevance
- similar to B
- measures η_o when taken with WLF equation
- "zero shear viscosity normalized for temperature"

$$\eta_0 = D_1 \exp\left[\frac{-A_1\left(T - T^*\right)}{A_2 + \left(T - T^*\right)}\right]$$

Evaluation Parameters - Cross-WLF Model

- D_2 - a reference temperature
- theoretically, the temperature where η goes to ∞
- typically D2=Tg, and $\eta = 10^9$ Pa.s
- D_3 defines the pressure sensitivity of D_2

$$T^* = D_2 + D_3 P$$

Evaluation Parameters - Cross-WLF Model

- A_1 & A_2 - WLF parameters
- A_1 defines the temperature sensitivity of viscosity
- A_2 defines change in temperature sensitivity with temperature
- classical WLF parameters are
  - $A_1 = 40.1$, $A_2 = 51.6$; if D2 = Tg
  - not always so for plastics

New models used in Moldflow

- viscosity:
- Carreau Model

$$\eta = \frac{\eta_0}{\left[1+\left(\frac{\eta_0 \dot{\gamma}}{\tau^*}\right)^2\right]^{\left(\frac{1-N}{2}\right)}}$$

$$\eta_0 = B \exp\left(\frac{T_b}{T}\right) \exp\left(\beta P\right)$$

η Viscosity $(Pa.\mathrm{sec})$

$\dot{\gamma}$ Shear Rate (sec^{-1})

T Temperature (C)

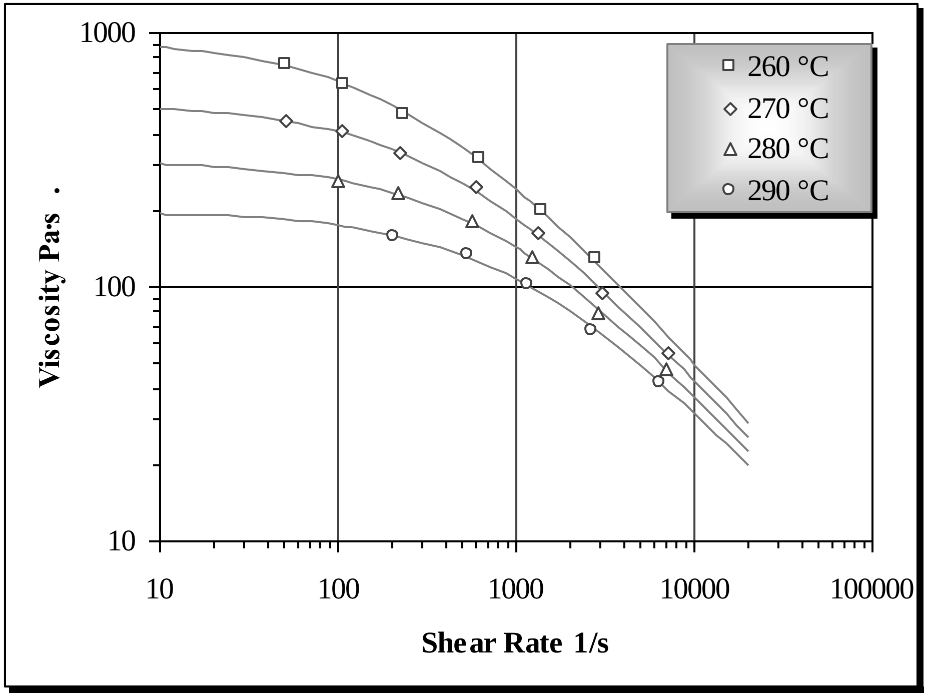
P Pressure (Pa)

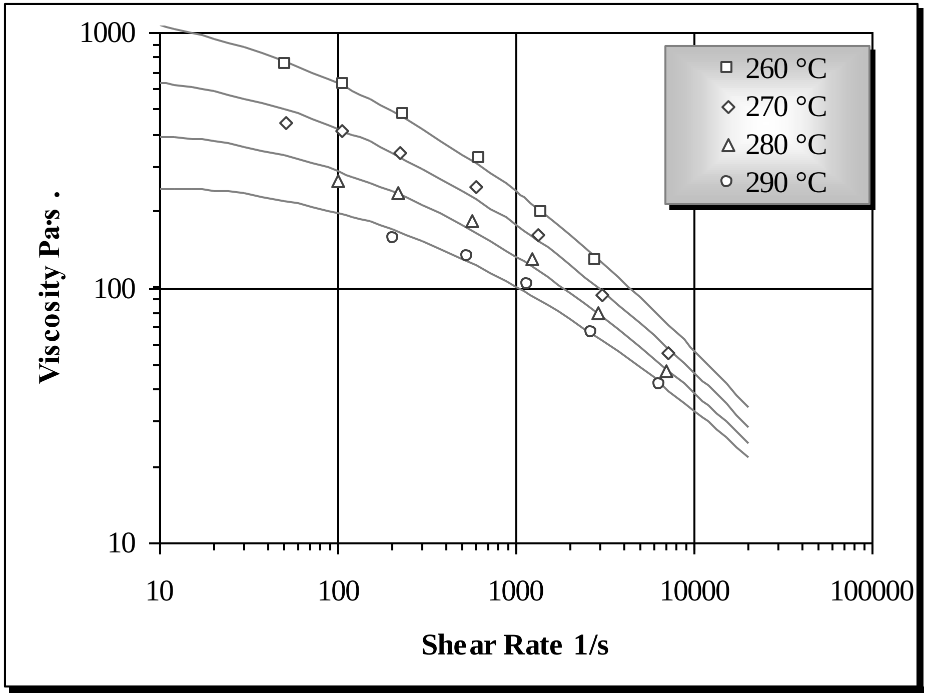
Unknowns: B, T_b, β, τ^*, N

Evaluation Parameters - Carreau Model

- similar to Cross model
- terms have similar relevance
- Carreau Model will give sharper transitions from Newtonian to shear thinning region

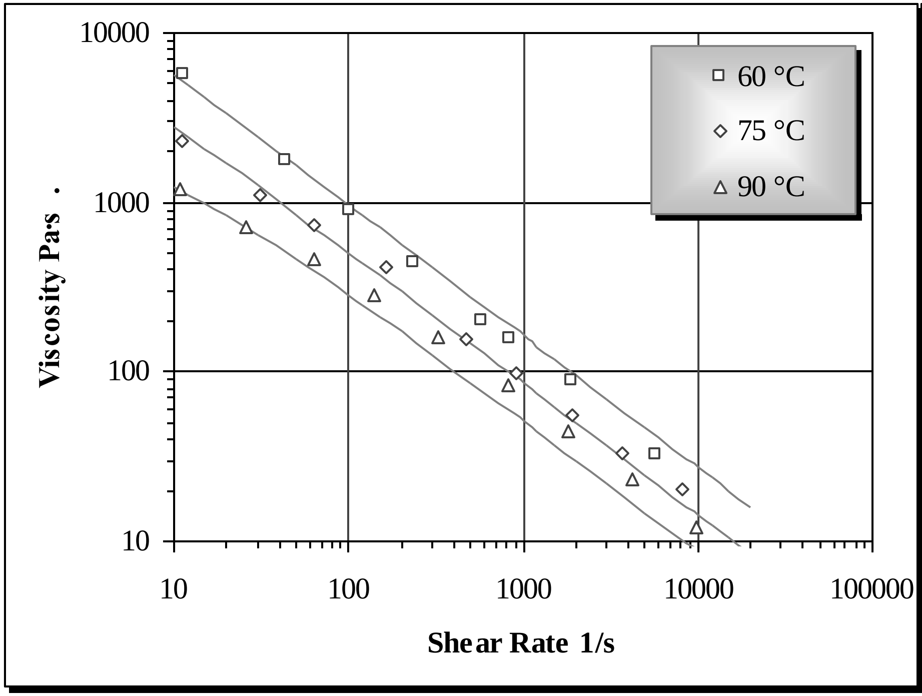
If the data follows the model

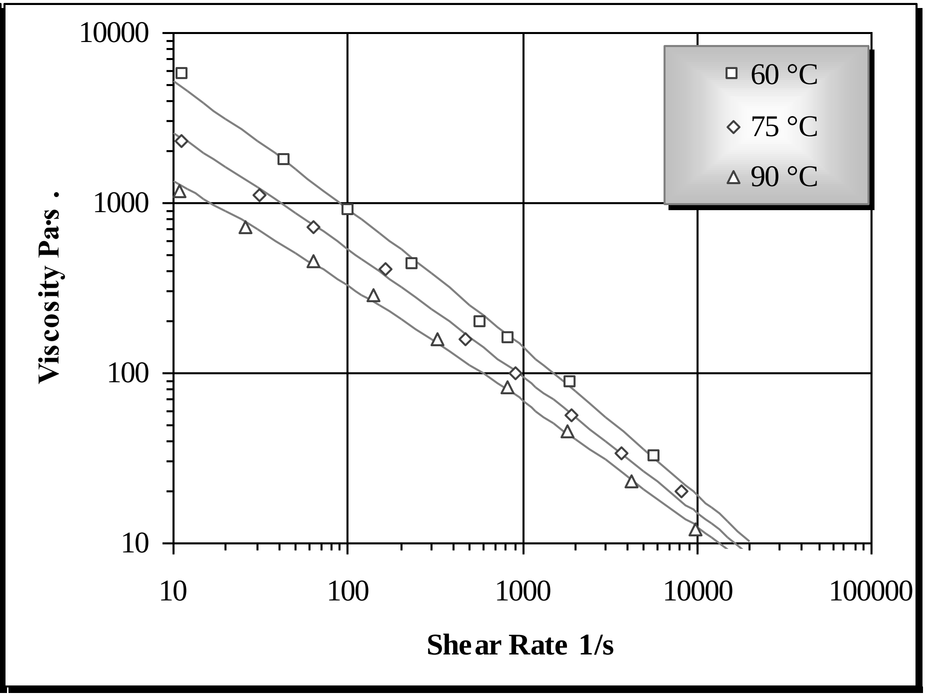




Datapoint Testing Services

If the data does not follow the model





Issues in data fitting

- rheological data may not be complete
- complete data should contain Newtonian & shear thinning regions
- data must show the right temperature sensitivity trends
- if not, model coefficients are indeterminate
- extrapolation will be dangerous

New models are constrained models

- not generalized; designed for polymers
- predict the expected trends for polymers
- incorporate both Newtonian and shear-thinning behavior
- do not work well if polymer does not follow expected trend (rare cases)

Benefits of constrained models

- predict a particular kind of behavior
- prevent inaccuracies in measured data from affecting the model
- safer to use
- model coefficients have useful interpretations
- are adaptable to master-curves

Conclusions

- we have a wider range of models for simulation
- each has its own benefits
- with new Moldflow formats, we can select the best model.
- model coefficients contain vital information
  - if properly understood, they will save you time and money
- see previous presentations (MUG ‘96 & MUG’97) for details on how to use evaluation parameters.