Introduction to Rheology of complex fluids
Brief Lecture Notes

Generalized Newtonian Fluids

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- Material functions & Rheological Characterization
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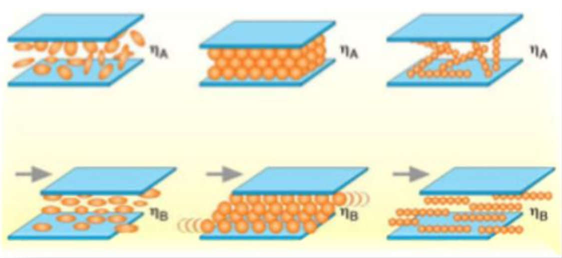

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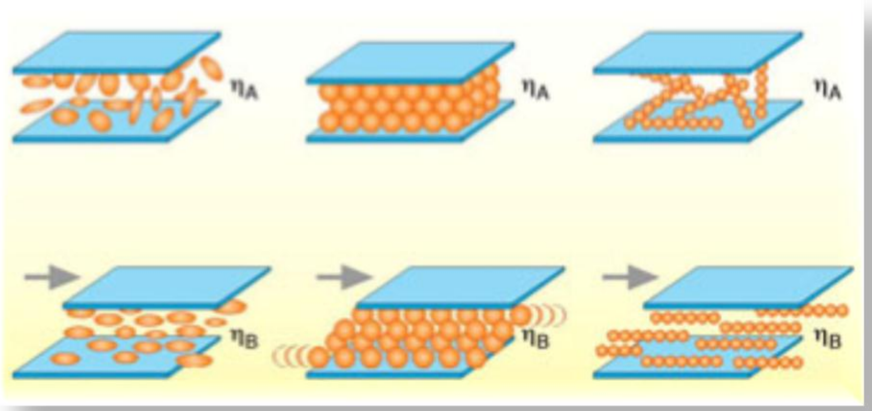

Experimental Observations

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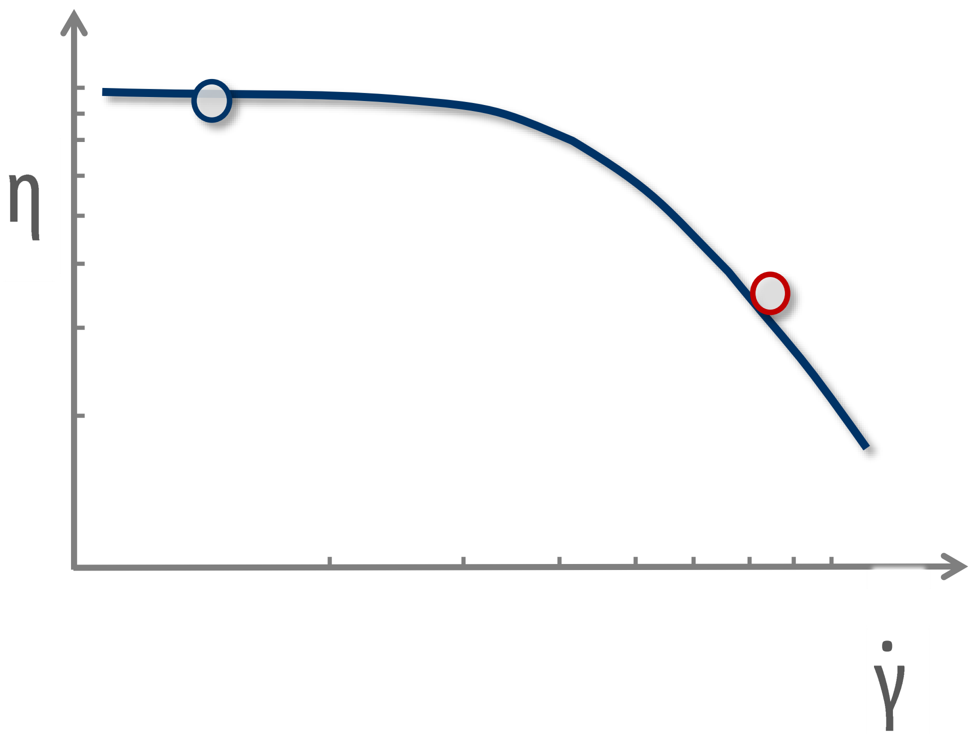
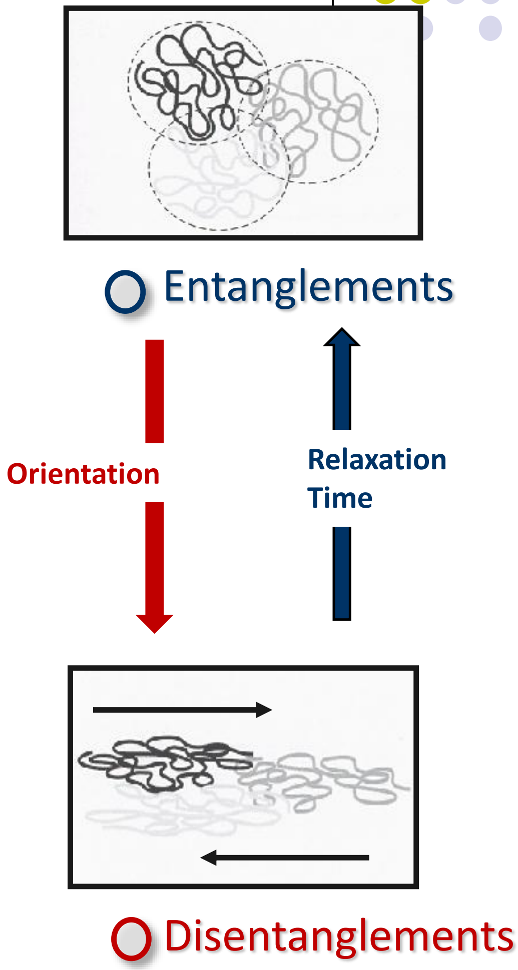
Decrease of shear viscosity

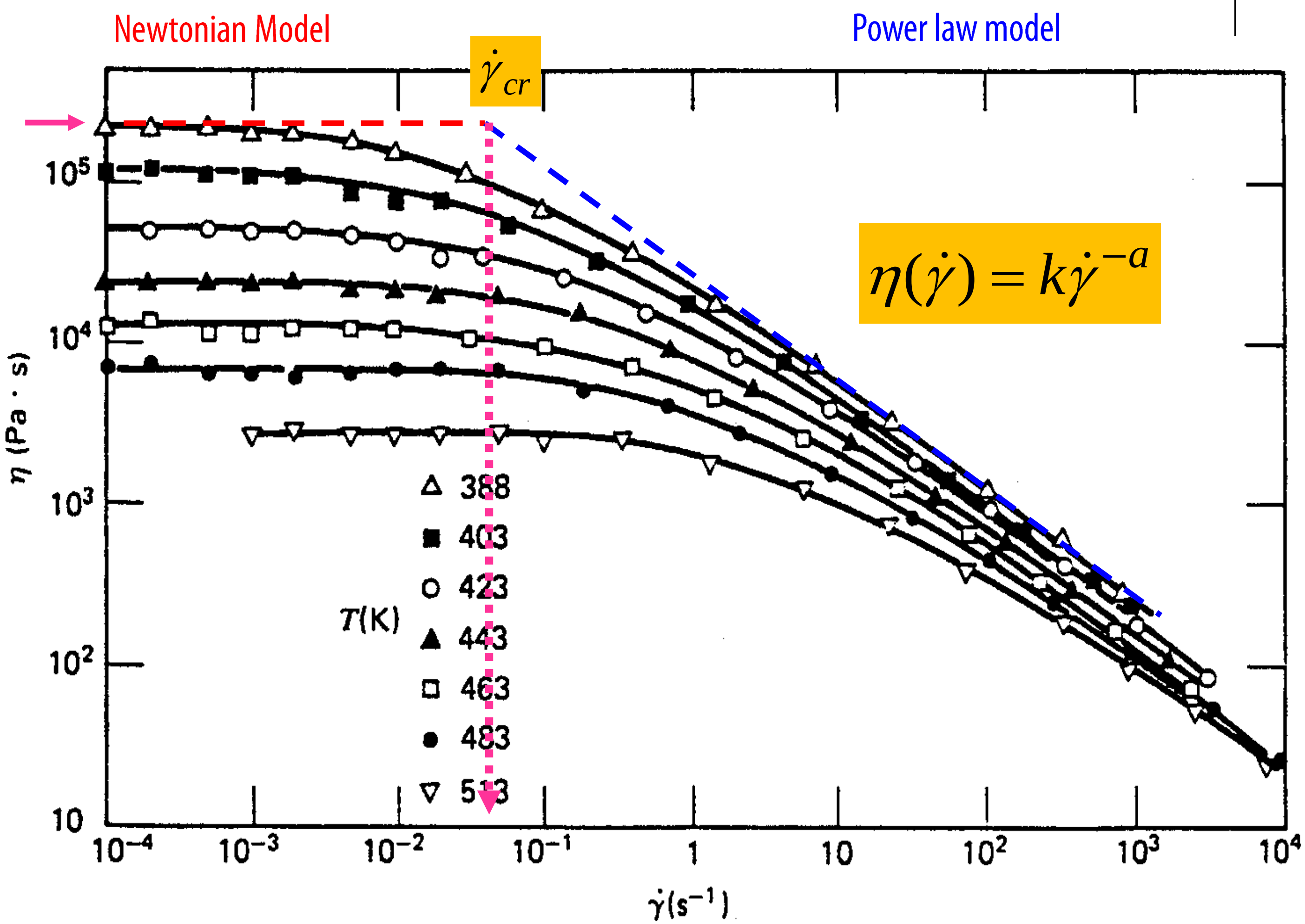
- Shear viscosity decreases due to the rearrangement of the macromolecules with increasing shear rate.
- This effect is observed in polymer melts and solutions of high polymeric concentration.





Reduction of shear viscosity

Zero-shear viscosity η_0



Relaxation time???

$\lambda = 1/\dot{\gamma}_{cr}$

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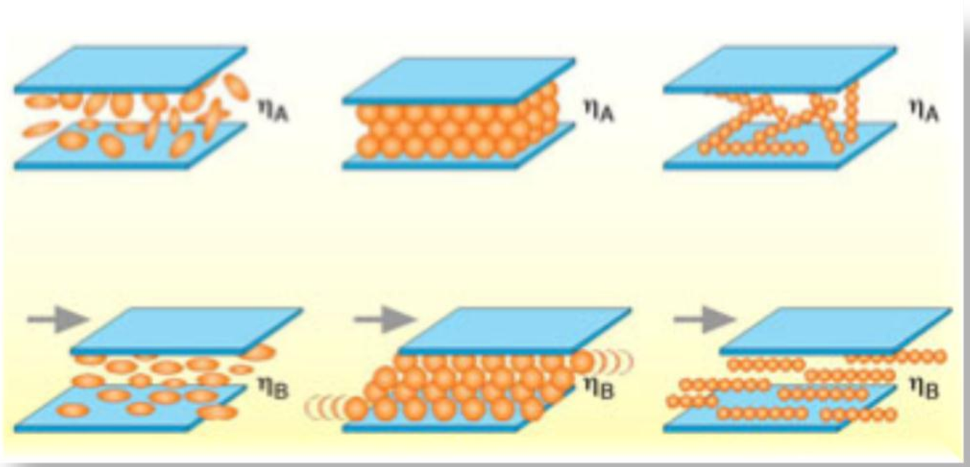

General principles for constitutive modeling

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Basic ideas for the Generalized Newtonian Fluid

Total Stress tensor

$$\underline{\underline{\sigma}} = \underline{\underline{f}}(\underline{\underline{\dot{\gamma}}})$$

Polynomial Approximation

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + a_1\underline{\underline{\dot{\gamma}}} + a_2\underline{\underline{\dot{\gamma}}}\cdot\underline{\underline{\dot{\gamma}}} + a_3\underline{\underline{\dot{\gamma}}}\cdot\underline{\underline{\dot{\gamma}}}\cdot\underline{\underline{\dot{\gamma}}} + \cdot$$

From the Cayley-Hamilton Theorem

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + f_1\underline{\underline{\dot{\gamma}}} + f_2\underline{\underline{\dot{\gamma}}}\cdot\underline{\underline{\dot{\gamma}}}$$

Reiner-Rivlin Constitutive Model

$$f_1 = f_1(I_{\underline{\underline{\dot{\gamma}}}}, II_{\underline{\underline{\dot{\gamma}}}}, III_{\underline{\underline{\dot{\gamma}}}})$$
$$f_2 = f_2(I_{\underline{\underline{\dot{\gamma}}}}, II_{\underline{\underline{\dot{\gamma}}}}, III_{\underline{\underline{\dot{\gamma}}}})$$

Basic ideas for the Generalized Newtonian Fluid

Q: Do we need all the invariants of the Rate of deformation Tensor?

Consider Simple Shear flow

$$\underline{\underline{\dot{\gamma}}} = \begin{pmatrix} 0 & \dot{\varsigma} & 0 \\ \dot{\varsigma} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \underline{\underline{\dot{\gamma}}} \cdot \underline{\underline{\dot{\gamma}}} = \begin{pmatrix} \dot{\varsigma}^2 & 0 & 0 \\ 0 & \dot{\varsigma}^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

where

$$I_{\underline{\underline{\dot{\gamma}}}} = tr(\underline{\underline{\dot{\gamma}}}) = 0$$

$$II_{\underline{\underline{\dot{\gamma}}}} = tr(\underline{\underline{\dot{\gamma}}} \cdot \underline{\underline{\dot{\gamma}}})$$

$$III_{\underline{\underline{\dot{\gamma}}}} = det(\underline{\underline{\dot{\gamma}}}) = 0$$

Q: Should the second order term be used in 2D?

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + f_1 \begin{pmatrix} 0 & \dot{\varsigma} & 0 \\ \dot{\varsigma} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + f_2 \begin{pmatrix} \dot{\varsigma}^2 & 0 & 0 \\ 0 & \dot{\varsigma}^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

thus →

$$\sigma_{xx} - \sigma_{yy} = 0$$

$$\sigma_{yy} - \sigma_{zz} = f_2 \dot{\varsigma}^2$$

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Conclusions for the Generalized Newtonian Fluid

1st Conclusion

$$I_{\underline{\underline{\dot{\gamma}}}} = tr(\underline{\underline{\dot{\gamma}}}) = 0$$

$$II_{\underline{\underline{\dot{\gamma}}}} = tr(\underline{\underline{\dot{\gamma}}} \cdot \underline{\underline{\dot{\gamma}}})$$

$$III_{\underline{\underline{\dot{\gamma}}}} = det(\underline{\underline{\dot{\gamma}}}) = 0$$

In Simple Shear flow, two of the three Invariants are identically zero, hence they are not needed.

2nd Conclusion

$$\sigma_{xx} - \sigma_{yy} = 0$$

$$\sigma_{yy} - \sigma_{zz} = f_2 \dot{\varsigma}^2$$

The second order term results in normal stresses with no physically observed values:
$N_1=0$ and $N_2>0$

Hence:

$$f_1 \to \eta(\mathrm{II}_{\dot{\gamma}})$$

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + \eta(II_{\underline{\underline{\dot{\gamma}}}})\underline{\underline{\dot{\gamma}}}$$

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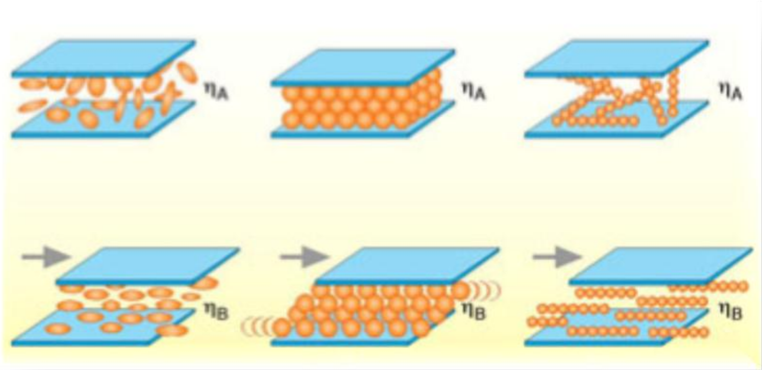
Pros and cons of the Generalized Newtonian Fluid

- Generalized Newtonian models are useful in many industrial applications, due to their simplicity.
- They describe with accuracy the reduction of the shear viscosity with increasing rate of deformation.
- Generalized Newtonian models cannot predict normal stresses or transient phenomena.



Generalized Newtonian Fluid models for polymeric fluids

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Power-Law Model

- The constitutive relation for stresses is given by: $\underline{\underline{\tau}} = \eta(\dot{\gamma})\underline{\underline{\dot{\gamma}}}$

Power Law

- Power-law model: $\eta(\dot{\gamma}) = K\dot{\gamma}^{n-1}$ $\quad \dot{\gamma} = |\underline{\underline{\dot{\gamma}}}|$
  - $K = \eta_o$ $\quad n = 1$ $\quad$ Newtonian Fluids
  - K $\quad n > 1$ $\quad$ Shear-Thickening
  - K $\quad 0 < n < 1$ $\quad$ Shear-Thinning
  - K: consistency index
- The slope of log(η) vs. log(γ) is constant.
- Advantages: simple, can predict the volumetric flow rate Q =Q(ΔP)
- Disadvantages: cannot predict the Newtonian Plateau for small values of rate of strain.

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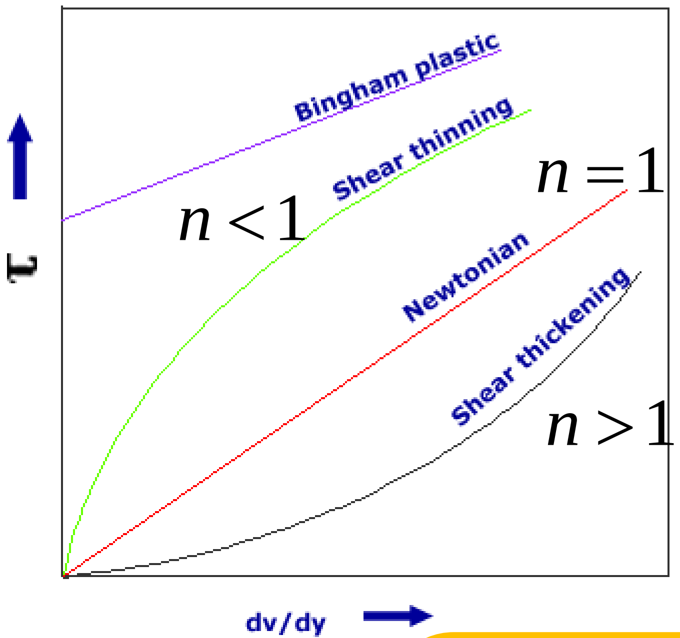
Power-law Model



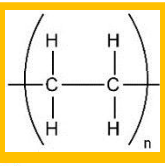
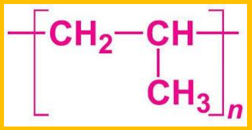
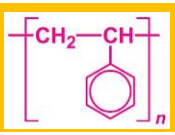
Typical values of the index n

- n =1 for fluids with small MW
- n ~ 0.4-0.8 for polymeric melts
- n ~ 0.2 for high MW liquids

The values of K depend on the power-law index n

Example for typical Polymeric Fluids

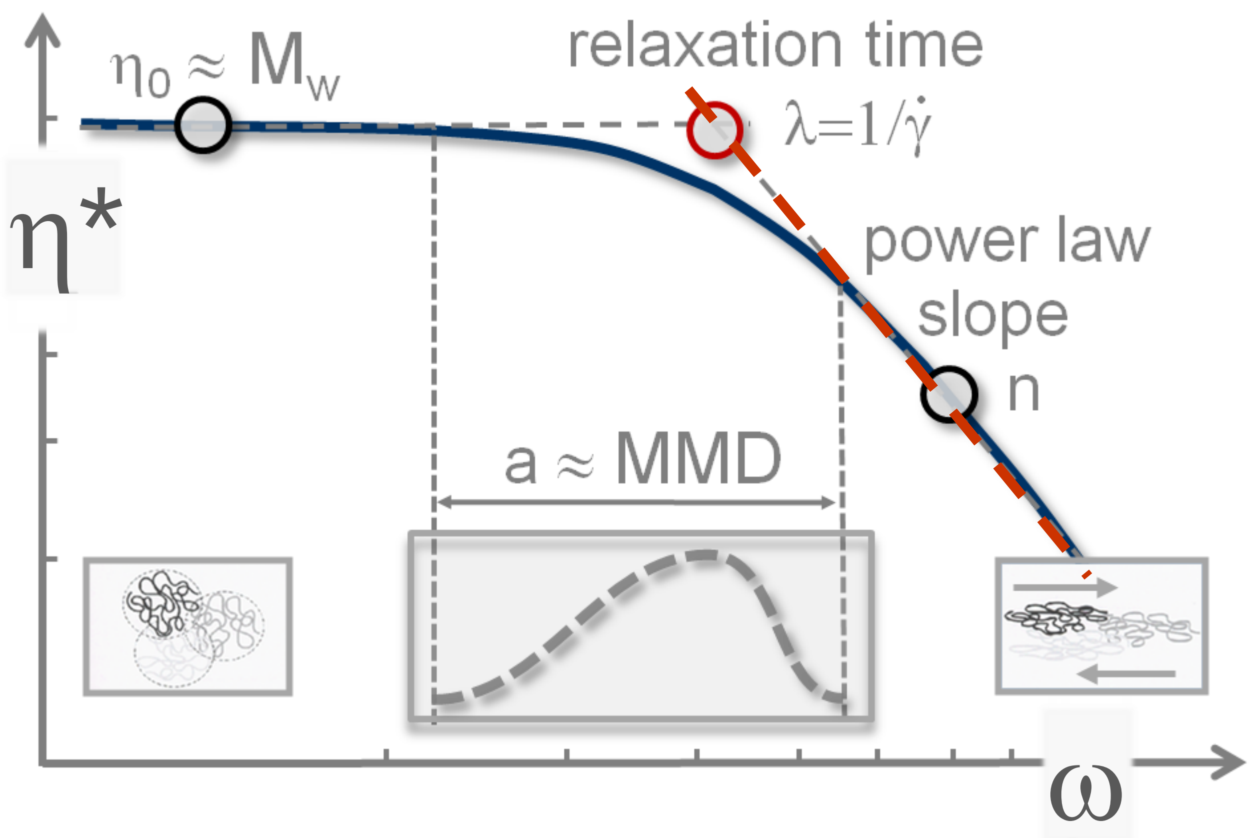
$$K = 1.3x10^3 \; Pa\, s^{-0.52} \quad \text{for} \quad n = 0.52$$

PE		$T_m \sim 135\ {}^oC$	$T_{process} \sim 150-200\ {}^oC$
PP		$T_m \sim 170\ {}^oC$	$T_{process} \sim 180-200\ {}^oC$
PS		$T_m \sim 100\ {}^oC$	

Power-law Model

- η_0 Zero Shear Viscosity ~ Molecular Weigh
- **n** Index = qualitative expression of macromolecular orientation in the direction of shear
- **a** Width of transition = proportional to **MMD** and **PDI** -> Narrow distribution MMD=steep, Wide distribution MMD=flat)
- **λ** Relaxation Time = Mean Recovery Time of the original stress state?

PDI = M_w/M_n



De Deborah number

$$De = \frac{\text{Relaxation Time}}{\text{Processing Time}} = \lambda \cdot \dot{\gamma}$$

Empirical Law for Application:

Deborah number should be small

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Power-law fluid model

$$\eta(\dot{\gamma}) = K\dot{\gamma}^{n-1}$$

+

$$\dot{\gamma} = \left|\frac{dv_x}{dy}\right|$$

In Steady Shear Flow

$$\eta(\dot{\gamma}) = K\left|\frac{dv_x}{dy}\right|^{n-1}$$

Log Form:

$$\log(\eta(\dot{\gamma})) = \log(K) + (n-1)\log\left(\left|\frac{dv_x}{dy}\right|\right)$$

The Optimal values of (b, a) and, hence, that of (K, n) are determined linear Least-Squares

Of the linear form: $y \;=\; b \;+\; a \;\; x$

Carreau-Yasuda Model

- Carreau-Yasuda model

$$\underline{\underline{\tau}} = \eta(\dot{\gamma})\underline{\underline{\dot{\gamma}}} \qquad \dot{\gamma} = |\underline{\underline{\dot{\gamma}}}|$$

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

a – affects the decrease of shear viscosity

λ – time constant which shows when there is a change in the power law

n – describes also the rate of reduction of viscosity

η_0, η_∞ - are the viscosities in the plateau regions

- Advantages:

  Represent the majority of the cases with polymeric fluids

- Disadvantages: has five parameters

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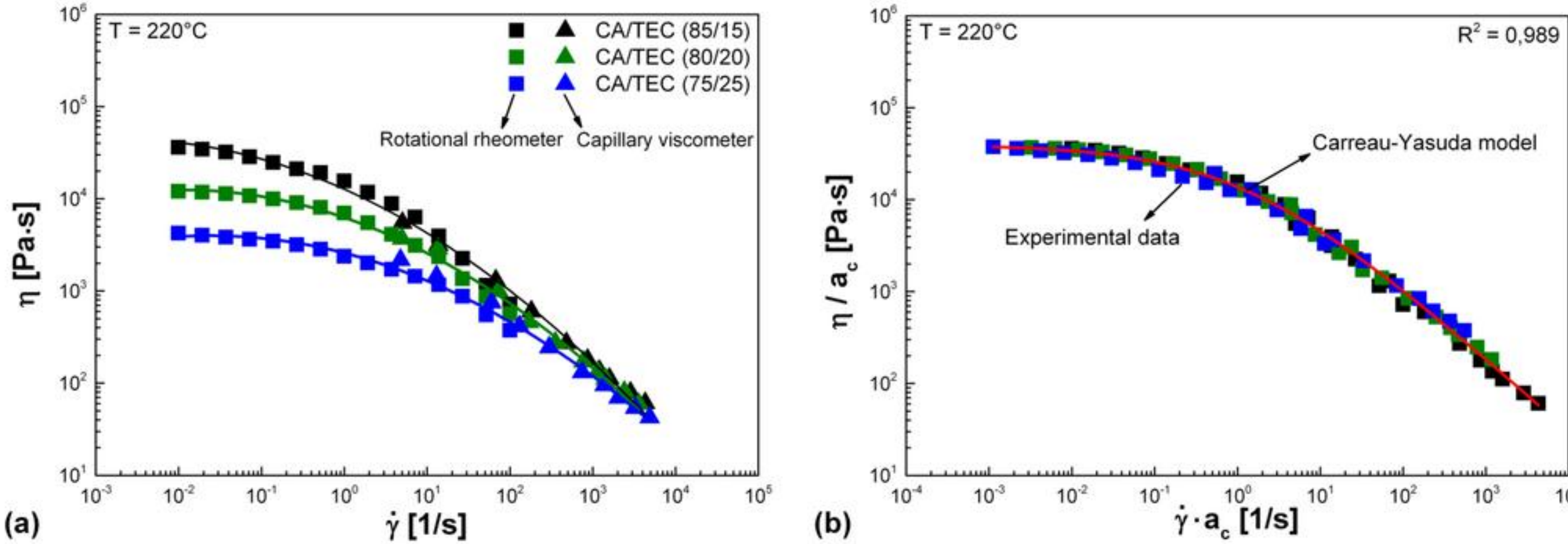
Carreau-Yasuda Model



Generalized models for Newtonian Fluids containing Microstructures

(gels, foams, colloidal pastes, emulsions and granular suspensions)

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Bingham Plastic Model
(Herschel-Bulkley when shear thinning is included)

- It describes the viscosity of viscoplastic materials

- Bingham Model:

$$\underline{\underline{\tau}} = \eta(\dot{\gamma})\underline{\underline{\dot{\gamma}}}$$

$$\dot{\gamma} = |\underline{\underline{\dot{\gamma}}}|$$

$$\eta(\dot{\gamma}) = \begin{cases} \infty & \tau \le \tau_y \\ \eta_0 + \dfrac{\tau_y}{\dot{\gamma}} & \tau \ge \tau_y \end{cases}$$

τ_y = Yield Stress

η_o = Viscosity for large shear rates (plastic viscosity)

Cross Model

- Similar to the Carreau-Yasuda Model

$$\underset{=}{\tau} = \eta(\dot{\gamma})\underset{=}{\dot{\gamma}}$$

$$\dot{\gamma} = |\underset{=}{\dot{\gamma}}|$$

$$\frac{\eta(\dot{\gamma}) - \eta_\infty}{\eta_0 - \eta_\infty} = \left(1 + (\dot{\gamma}\lambda)^n\right)^{-1}$$

λ – time constant which shows when there is a change in the power law

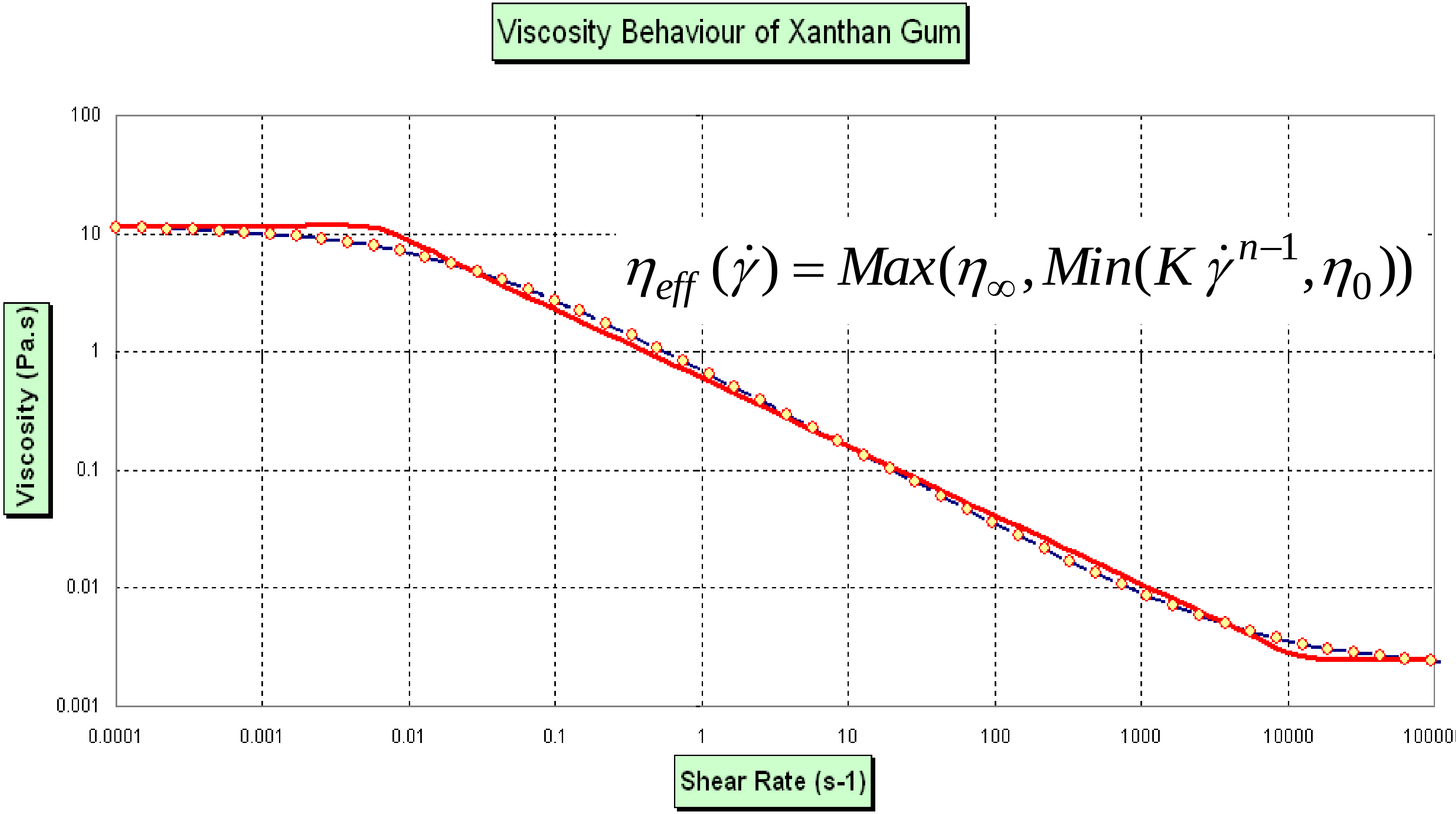
n – describes the viscosity rate of reduction

η_0, η_∞ - are the viscosities in the plateau regions

- Advantages:

  Represent the majority of the cases of colloids & emulsions
- Disadvantages: has four parameters

Cross Model



$$\eta_{eff}(\dot{\gamma}) = Max(\eta_{\infty}, Min(K\,\dot{\gamma}^{n-1}, \eta_0))$$

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Model Comparison

Power-law Model

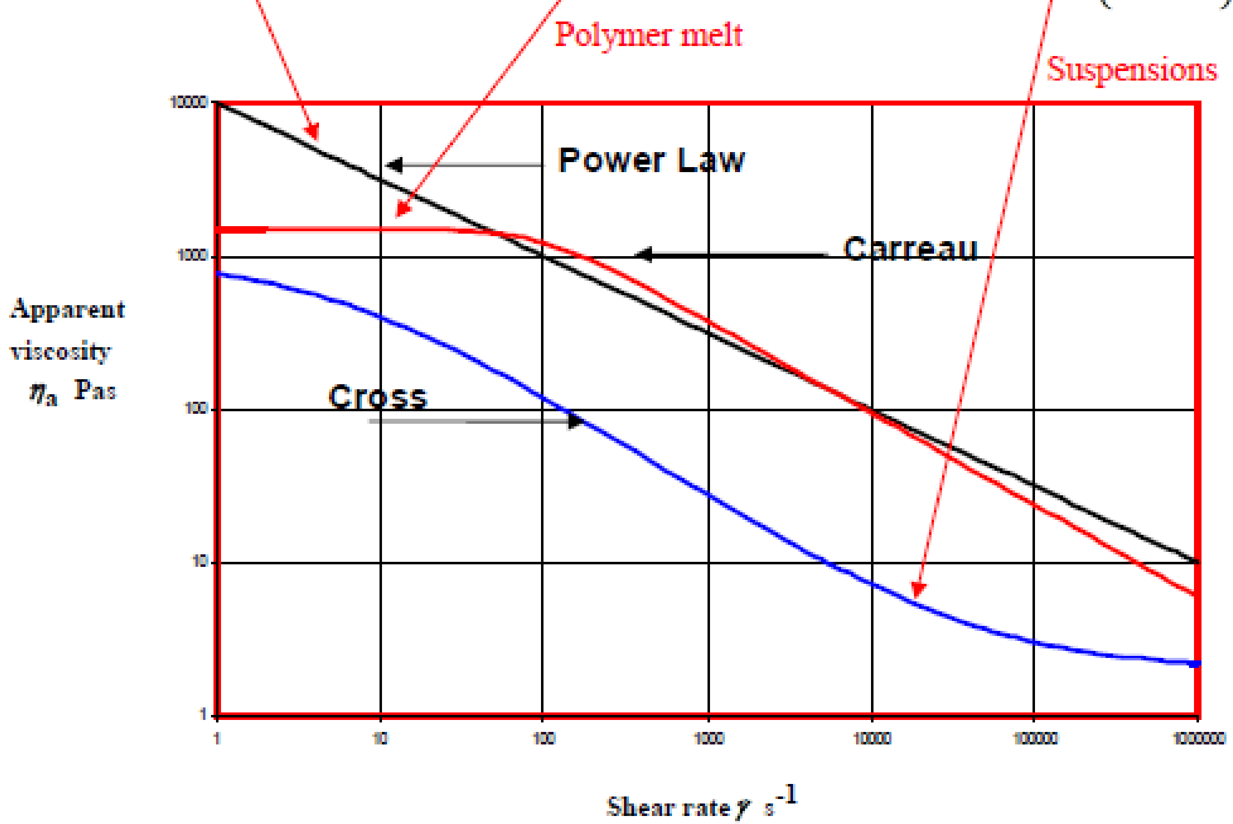
$$\eta(\dot{\gamma}) = K\dot{\gamma}^{n-1}$$

Carreau Model

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

Cross Model

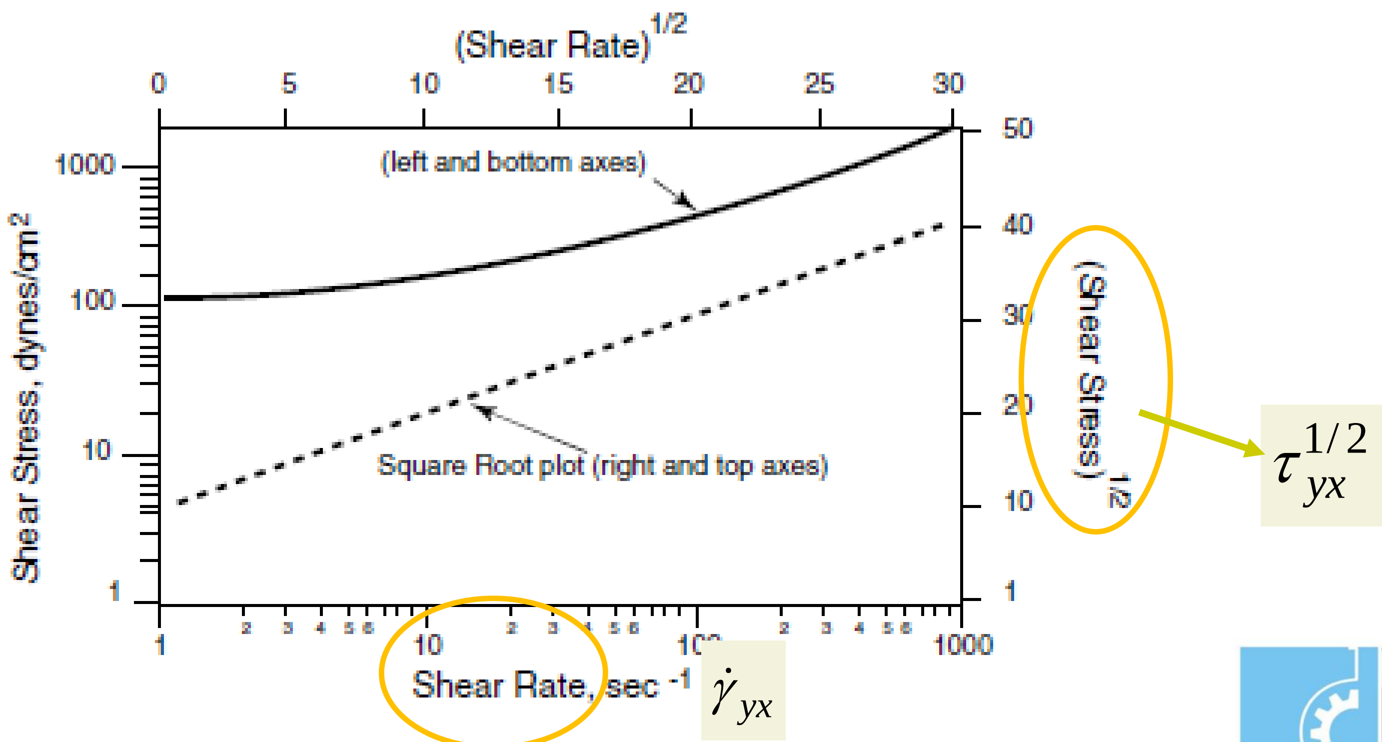
$$\frac{\eta(\dot{\gamma})-\eta_\infty}{\eta_0-\eta_\infty} = \left(1+(\dot{\gamma}\lambda)^n\right)^{-1}$$



Casson Model

- This model is recommended for the rheological description of blood and mud.
- Unfortunately, there is no analytical expression for the shear viscosity.

$$\begin{cases} \underline{\underline{\tau}} = \eta(\dot{\gamma})\underline{\underline{\dot{\gamma}}}: & \left|\underline{\underline{\tau}}\right|^{1/2} - \tau_y^{1/2} = \eta_0^{1/2}\dot{\gamma}^{1/2}, & \left|\underline{\underline{\tau}}\right| > \tau_y \\ & \underline{\underline{\dot{\gamma}}} = \underline{\underline{0}}, & \left|\underline{\underline{\tau}}\right| < \tau_y \end{cases}$$



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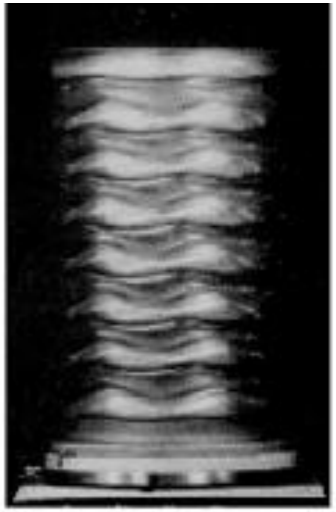

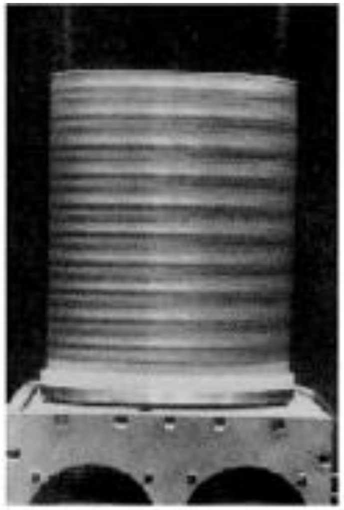

Other predictions of the Generalized Newtonian Models in Rheological Flows

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Stress Tensor

$$\underline{\underline{\tau}} = \eta(\dot{\gamma})\underline{\underline{\dot{\gamma}}} \quad \text{where} \quad \dot{\gamma} = \left|\underline{\underline{\dot{\gamma}}}\right|$$

$$\underline{\underline{\tau}} = \eta(\dot{\gamma})\begin{pmatrix} 2\frac{\partial v_x}{\partial x} & \frac{\partial v_y}{\partial x}+\frac{\partial v_x}{\partial y} & \frac{\partial v_z}{\partial x}+\frac{\partial v_x}{\partial z} \\ \frac{\partial v_x}{\partial y}+\frac{\partial v_y}{\partial x} & 2\frac{\partial v_y}{\partial y} & \frac{\partial v_z}{\partial y}+\frac{\partial v_y}{\partial z} \\ \frac{\partial v_x}{\partial z}+\frac{\partial v_z}{\partial x} & \frac{\partial v_y}{\partial z}+\frac{\partial v_z}{\partial y} & 2\frac{\partial v_z}{\partial z} \end{pmatrix}$$

Stress Tensor in Simple Shear Flow

$$\underline{v} = v_x(y,t)\underline{e}_x \quad \text{και} \quad \dot{\gamma} = \left|\underline{\underline{\dot{\gamma}}}\right| = \left|\frac{\partial v_x}{\partial y}\right|$$

Zero Normal Stresses

$$\underline{\underline{\tau}} = \eta(\dot{\gamma})\begin{pmatrix} 0 & \frac{\partial v_x}{\partial y} & 0 \\ \frac{\partial v_x}{\partial y} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

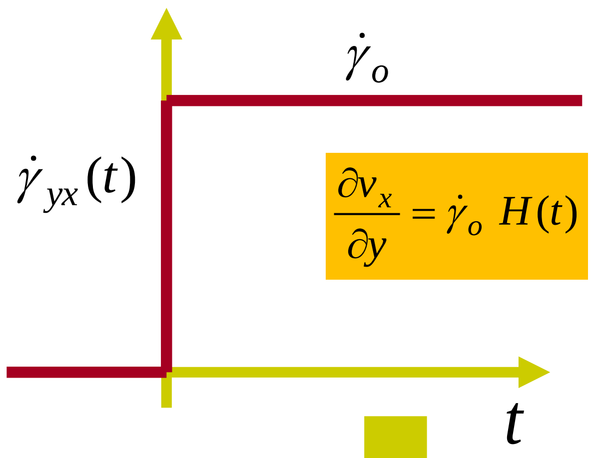
$$\tau_{xx} = 0$$

$$\tau_{yy} = 0$$

$$\tau_{zz} = 0$$

Stress tensor in start-up of steady shear flows

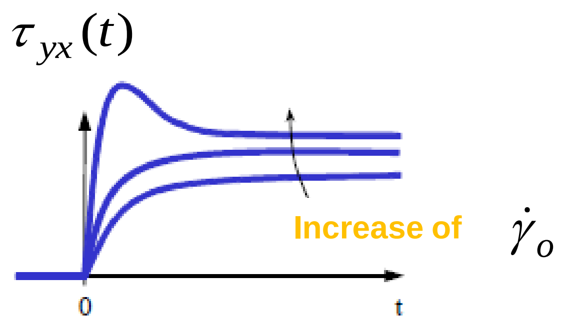
Imposed Rate of Strain



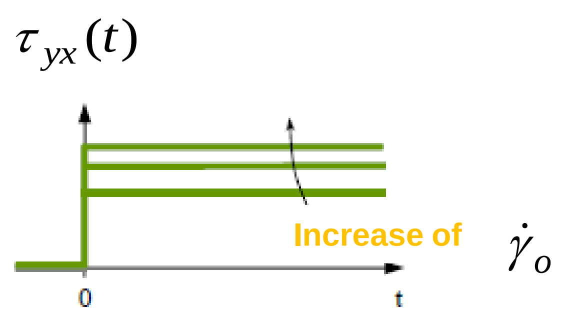
$$\frac{\partial v_x}{\partial y} = \dot{\gamma}_o \; H(t)$$

$$\tau_{yx}(y,t) = \eta(\dot{\gamma}_o)\frac{\partial v_x}{\partial y} = \eta(\dot{\gamma}_o)\,\dot{\gamma}_o \; H(t)$$

Experimental Observations



Model Predictions



Steady Uniaxial Elongational Flow

Flow Kinematics

$$\dot{\varepsilon}(t) = \dot{\varepsilon}_o$$

$$v_x(x,y,z) = -\frac{1}{2}\dot{\varepsilon}_o x$$

$$v_y(x,y,z) = -\frac{1}{2}\dot{\varepsilon}_o y$$

$$v_z(x,y,z) = \dot{\varepsilon}_o z$$

For main flow in the z-direction

Rate of Strain tensor and its magnitude

$$\underline{\underline{\dot{\gamma}}} = \underline{\nabla}\underline{v} + \left(\underline{\nabla}\underline{v}\right)^T = 2\dot{\varepsilon}_o \begin{pmatrix} -1/2 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\dot{\gamma} = \left|\underline{\underline{\dot{\gamma}}}\right| = \sqrt{\frac{1}{2}tr\left(\underline{\underline{\dot{\gamma}}} \cdot \underline{\underline{\dot{\gamma}}}\right)} = \sqrt{\frac{1}{2}tr\left(4\dot{\varepsilon}_o^2 \begin{pmatrix} -1/2 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} -1/2 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right)}$$

$$= \sqrt{\dot{\varepsilon}_o^2 tr\left(\begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 2 \end{pmatrix}\right)} = \sqrt{3\dot{\varepsilon}_o^2} = \sqrt{3}\dot{\varepsilon}_o$$

Stress Tensor in Uniaxial Elongational Flow

The stresses

$$\underline{\underline{\tau}} = \eta(\dot{\gamma})\underline{\underline{\dot{\gamma}}} \quad \text{where} \quad \dot{\gamma} = \left|\underline{\underline{\dot{\gamma}}}\right| = \sqrt{3}\dot{\varepsilon}_o$$

$$\underline{\underline{\tau}} = \eta(\sqrt{3}\dot{\varepsilon}_o)\begin{pmatrix} -\dot{\varepsilon}_o & 0 & 0 \\ 0 & -\dot{\varepsilon}_o & 0 \\ 0 & 0 & 2\dot{\varepsilon}_o \end{pmatrix}$$

Elongational Viscosity

$$\bar{\eta} = \frac{\tau_{zz} - \tau_{xx}}{\dot{\varepsilon}_o} = \frac{\eta(\sqrt{3}\dot{\varepsilon}_o)2\dot{\varepsilon}_o + \eta(\sqrt{3}\dot{\varepsilon}_o)\dot{\varepsilon}_o}{\dot{\varepsilon}_o} = 3\eta(\sqrt{3}\dot{\varepsilon}_o)$$

$$\bar{\eta}_o = \lim_{\dot{\varepsilon}_o \to 0}\left(\bar{\eta}\right) = \lim_{\dot{\varepsilon}_o \to 0}\left(3\eta(\sqrt{3}\dot{\varepsilon}_o)\right) = 3\lim_{\dot{\varepsilon}_o \to 0}\left(\eta(\sqrt{3}\dot{\varepsilon}_o)\right) = 3\eta_o$$

Trouton Ratio $\quad Tr = \frac{\bar{\eta}}{\eta_o} = 3\frac{\eta(\sqrt{3}\dot{\varepsilon}_o)}{\eta_o}$

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Limitations of the Generalized Newtonian Fluid Models

- Cannot approximate always the viscosity curve.
- Cannot predict non-shear flows.
- Cannot predict elastic effects.
- Cannot predict transient phenomena.
- Do not take into account the deformation history.

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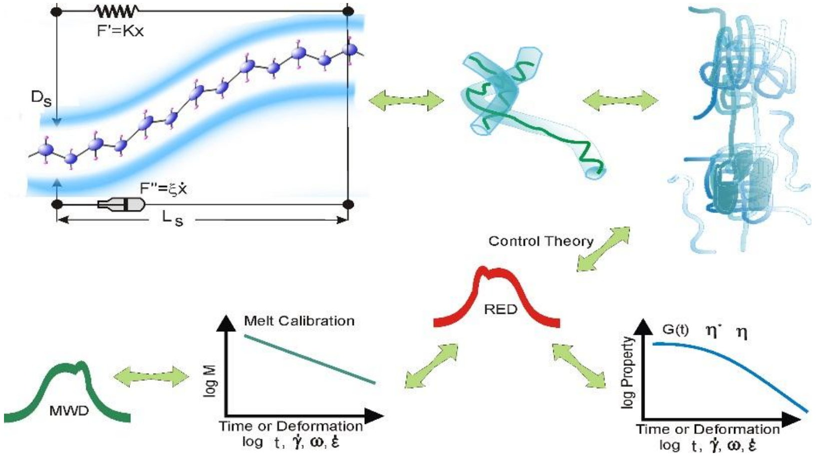

End of lecture