From Skeletons to Supercontinents: How Fluid Dynamics Can Model It All

PSS Talk

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October 27, 2022

Overview

- Many materials we encounter have viscoelastic properties.
  - Viscosity: measure of resistance to flow.
  - Elasticity: ability of a material to return to its original state after removal of deforming forces.
- Characterised by a *relaxation time* — quantifies 'memory' of deformation history.

Gibson, A., 1972.

Arnold, J., 1955

Disney, 1929.

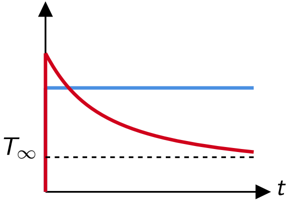
Polymeric Fluids

- Polymer — long chain molecule formed of repeating units/monomers.
- Polymer melt — a thermoplastic heated to a temperature above its melting point.
- (Dilute) polymer solution — polymer molecules suspended in a solvent.

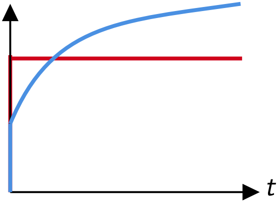
El, A., 2022.

Properties of Polymeric Fluids

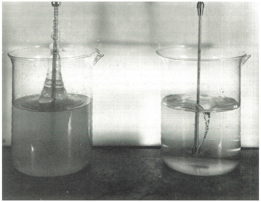
Stress Relaxation:



Creep:

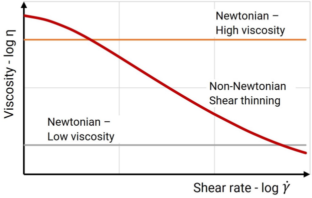


Normal Stress Effects:



Tanner, R. I., 2000

'Variable' Viscosity:

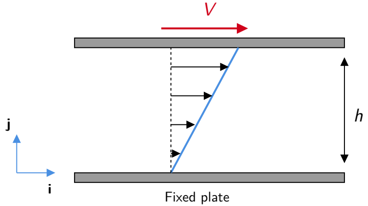


Østergård, A. L., 2020.

Variable Viscosity

- Shear thinning — shear viscosity η_s should drop with shear rate $\dot{\gamma}$.

$$\mathbf{u} = (\dot{\gamma} y, 0, 0)^T, \ \dot{\gamma} = \frac{V}{h}$$



- Strain hardening — elongational viscosity η_e should increase with elongation rate $\dot{\epsilon}$.

$$\mathbf{u} = (\dot{\epsilon} x, -\tfrac{1}{2}\dot{\epsilon} y, -\tfrac{1}{2}\dot{\epsilon} z)^T$$

Viscoelastic Modelling

Overview

Q. How can we model these materials?

A. Use conservation laws.

1. Mass:

$$\nabla \cdot \mathbf{u} = 0.$$

2. Momentum:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) = -\nabla p + \nabla \cdot \boldsymbol{T}, \quad \boldsymbol{T}^T = \boldsymbol{T}.$$

With this notation, we also have

$$\eta_s = \frac{T_{12}}{\dot{\gamma}}, \quad \eta_e = \frac{T_{11} - T_{22}}{\dot{\epsilon}}.$$

Viscoelastic Modelling

Specifying $\boldsymbol{T}$

We still need to specify $\boldsymbol{T}$!

$$\rho\left(\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right)=-\nabla p+\nabla\cdot\boldsymbol{T}.$$

- $\boldsymbol{T}=\mathbf{0}\longrightarrow$ *inviscid fluids*.
- $\boldsymbol{T}=\eta\left[\nabla\mathbf{u}+\nabla\mathbf{u}^{T}\right]:=2\eta\boldsymbol{D}\longrightarrow$ *Newtonian fluids*.
- $\boldsymbol{T}=2\eta(\dot{\gamma})\boldsymbol{D}\longrightarrow$ *generalised Newtonian fluids*.

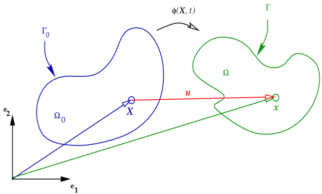
None of these really help us... but we can do better!

Viscoelastic Modelling

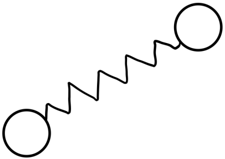
Constitutive Equations

Models fall into four categories:

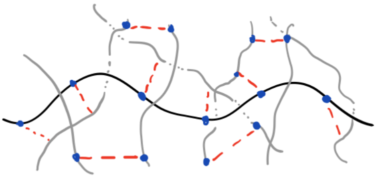
Continuum:



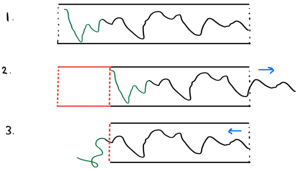
Dumbbell:



Network:



Reptation:



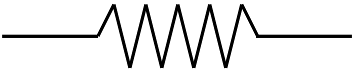
Hutson, M., 2016.

Maxwell Model

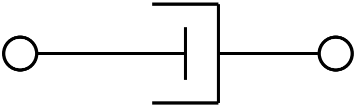
Spring-Dashpot Schematics

- Need to capture effects of elasticity and viscosity.
- Initially work in 1D.
- Represent materials schematically.

Hookean springs
E



Newtonian dashpots
η_0

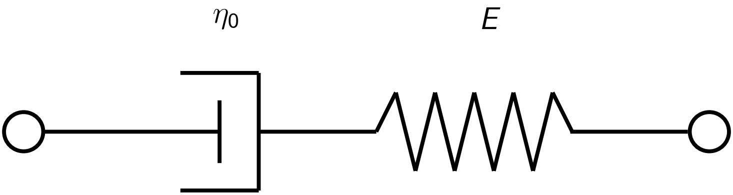


- Build models by combining these elements!

Maxwell Model

Maxwell Material

The simplest construction we can make is

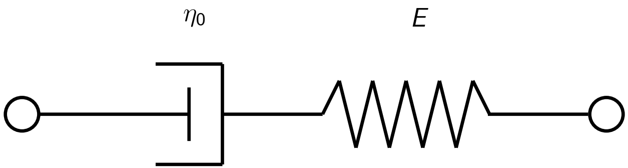


We need to relate the stress T to the strain ϵ.

$$\epsilon = \frac{\text{change in length}}{\text{original length}}.$$

Maxwell Model

Maxwell Equation



Components

Spring: $T_S = E\epsilon_S$ (Hooke's Law)

Dashpot: $T_D = \eta_0 \frac{\partial \epsilon_D}{\partial t}$ (Newton's Law of Viscosity)

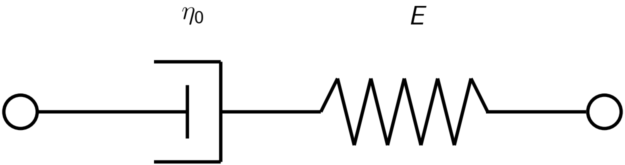
Total

Stress: $T = T_S = T_D$.

Strain: $\epsilon = \epsilon_S + \epsilon_D$.

Maxwell Model

Maxwell Equation



Differentiating total strain yields:

$$T + \lambda \frac{\partial T}{\partial t} = \eta_0 \frac{\partial \epsilon}{\partial t},$$

with relaxation time $\lambda = \frac{\eta_0}{E}$.

This is the Maxwell equation!

Maxwell, J. C. 1867.

Maxwell Model

Is this any good?

In three dimensions:

$$\boldsymbol{T} + \lambda \frac{\partial \boldsymbol{T}}{\partial t} = 2\eta_0 \boldsymbol{D}.$$

Predictions:

- Viscous and elastic limits!
- Stress relaxation — for a step strain $(2\boldsymbol{D} = \boldsymbol{\epsilon_0}\delta(t))$,

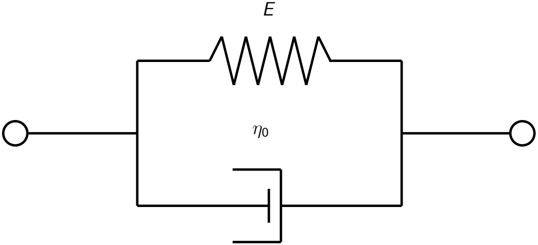
$$\boldsymbol{T} = \boldsymbol{\epsilon}_0 \frac{\eta_0}{\lambda} \mathrm{e}^{-t/\lambda} H(t).$$

- Creep — response to step stress is linear.
- Shear — no shear thinning $(\eta_s = \eta_0)$.
- Elongation — no strain hardening $(\eta_e = 3\eta_0)$.

Further Spring and Dashpot Models

How else can we relate strain (ϵ) and stress (T)?

1. Kelvin-Voigt



$$T = E\epsilon + \eta_0 \frac{\partial \epsilon}{\partial t}.$$

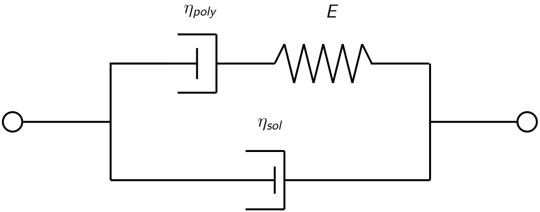
Captures creep behaviour better at expense of stress relaxation.

Thompson, W. 1878.

Further Spring and Dashpot Models

How else can we relate strain (ϵ) and stress (T)?

2. Jeffreys'



$$T + \lambda \frac{\partial T}{\partial t} = \eta_0 \left(\frac{\partial \epsilon}{\partial t} + \lambda_r \frac{\partial^2 \epsilon}{\partial t^2} \right).$$

- Relaxation time: $\lambda = \frac{\eta_{poly}}{E}$
- Zero-shear viscosity: $\eta_0 = \eta_{poly} + \eta_{sol}$
- Retardation time: $\lambda_r = \frac{\eta_{sol}\eta_{poly}}{E\eta_0}$

Jeffreys, H., 1929.

A Major Problem!

- None of these models hold for large deformations!
- Why? They are not *frame invariant*.
  - Relation between stress and strain needs to be independent of the frame of reference.
- Fix: replace $\frac{\partial}{\partial t}$ with a new time derivative!
- Choose an *upper convected derivative*:

$$\overset{\nabla}{\boldsymbol{S}} := \frac{\partial \boldsymbol{S}}{\partial t} + (\mathbf{u} \cdot \nabla)\boldsymbol{S} - (\nabla \mathbf{u})\boldsymbol{S} - \boldsymbol{S}(\nabla \mathbf{u})^T.$$

A Major Solution!

New equations!

- Maxwell $\longrightarrow$ Upper Convected Maxwell (UCM)

$$\boldsymbol{T} + \lambda \overset{\nabla}{\boldsymbol{T}} = 2\eta_0 \boldsymbol{D}.$$

- Jeffreys' $\longrightarrow$ Oldroyd-B

$$\boldsymbol{T} + \lambda \overset{\nabla}{\boldsymbol{T}} = 2\eta_0 (\boldsymbol{D} + \lambda_r \overset{\nabla}{\boldsymbol{D}}).$$

Note that setting $\lambda_r = 0$ gives UCM; setting $\lambda_r = \lambda$ gives the Newtonian stress tensor.

Oldroyd, J. G., 1950.

UCM/Oldroyd-B

$$\boldsymbol{T} + \lambda \overset{\nabla}{\boldsymbol{T}} = 2\eta_0(\boldsymbol{D} + \lambda_r \overset{\nabla}{\boldsymbol{D}})$$

Predictions:

- Stress relaxation/creep inherited from Maxwell model.
- Shear:

$$\eta_s = \eta_0, \quad T_{11} - T_{22} = 2\eta_0(\lambda - \lambda_r)\dot{\gamma}^2, \quad T_{22} - T_{33} = 0.$$

- Extension:

$$\eta_e = \eta_0 \left[\frac{2(1 - \lambda_r \dot{\epsilon})}{1 - 2\lambda\dot{\epsilon}} + \frac{1 + \lambda_r \dot{\epsilon}}{1 + \lambda\dot{\epsilon}} \right]$$

We obtain strain hardening (with a vengeance!)

Going Further

We can improve on this... but the equations become unwieldly!

- White-Metzner:
  Viscosity and relaxation time shear rate dependent.
- Extended White-Metzner:
  Viscosity and relaxation time dependent on trace of stress tensor.
- Corotational UCM:
  Swap $\overset{\triangledown}{\boldsymbol{T}}$ with a *Jaumann* time derivative.

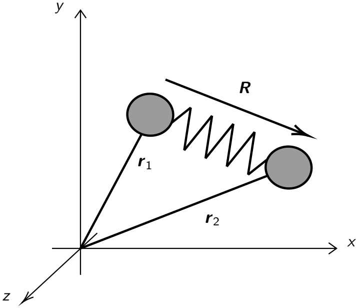
What if we considered molecular arguments instead?

White, J. L. and Metzner, A. B., 1960/Souvaliotis, A. and Beris, A. N. 1992/Jaumann, G., 1911

Dumbbell Modelling

- Consider two beads connected via a Hookean spring, immersed in a Newtonian solvent.
- Acting forces: inertia, spring, friction and Brownian.
- Neglect inertia; friction given by Stokes drag

$$6\pi\eta_{sol}a(\dot{\mathbf{r}}_i - \mathbf{u})$$



$a =$ radius of bead,
$\zeta := 6\pi\eta_{sol}a$,
$\boldsymbol{R} =$ end-to-end vector.

Kuhn, W., 1934/Renardy, M., 2000

Dumbbell Modelling

Stochastic Equation

- Force balance:

$$-\zeta\left(\dot{\mathbf{r}_1} - \mathbf{u}(\mathbf{r}_1, t)\right) + H\mathbf{R} + \mathbf{S}_1 = \mathbf{0},$$
$$-\zeta\left(\dot{\mathbf{r}_2} - \mathbf{u}(\mathbf{r}_2, t)\right) - H\mathbf{R} + \mathbf{S}_2 = \mathbf{0}.$$

- Approximation: since molecules are small,

$$\mathbf{u}(\mathbf{r}_2, t) = \mathbf{u}(\mathbf{r}_1, t) + (\nabla\mathbf{u})(\mathbf{r}_1, t)(\mathbf{r}_2 - \mathbf{r}_1).$$

- Setting $\mathbf{R} = \mathbf{r}_2 - \mathbf{r}_1$:

$$\dot{\mathbf{R}} = \nabla\mathbf{u}\cdot\mathbf{R} - \frac{2H}{\zeta}\mathbf{R} + \frac{1}{\zeta}(\mathbf{S}_2 - \mathbf{S}_1).$$

Dumbbell Modelling

Fokker-Planck Equation

- Assumption:
  Large number of polymer molecules — distribution of end-to-end vectors $\mathbf{R}$ given by $\psi(\mathbf{R}, \mathbf{x}, t)$.
- Center of mass $\mathbf{x} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$.
- Result — Fokker-Planck equation!

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_{\mathbf{x}})\psi = \frac{2}{\beta\zeta}\Delta_{\mathbf{R}}\psi + \nabla_{\mathbf{R}} \cdot \left[-\nabla_{\mathbf{x}}\mathbf{u} \cdot \mathbf{R}\psi + \frac{2H}{\zeta}\mathbf{R}\psi \right].$$

- We can solve this... but we don't need to!

Dumbbell Modelling

Closure Approximations

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_{\mathbf{x}})\psi = \frac{2}{\beta\zeta}\Delta_{\mathbf{R}}\psi + \nabla_{\mathbf{R}} \cdot \left[-\nabla_{\mathbf{x}}\mathbf{u} \cdot \mathbf{R}\psi + \frac{2H}{\zeta}\mathbf{R}\psi \right] \quad (*)$$

- We can show that the polymer contribution to the stress is

$$\boldsymbol{T}_p = \int_{\mathbb{R}^3} nH\mathbf{R}\mathbf{R}^T \psi \, d\mathbf{R}.$$

- Multiplying Fokker-Planck (*) by $nH\mathbf{R}\mathbf{R}^T$ and integrating gives

$$\overset{\nabla}{\boldsymbol{T}}_p + \frac{4H}{\zeta}\boldsymbol{T}_p = \frac{4nH}{\beta\zeta}\boldsymbol{I}.$$

Have we seen this before?

Dumbbell Modelling
Déjà Vu?

$$\overset{\nabla}{\boldsymbol{T}}_p + \frac{4H}{\zeta}\boldsymbol{T}_p = \frac{4nH}{\beta\zeta}\boldsymbol{I}.$$

- Setting $\boldsymbol{T}_p = \frac{n}{\beta}\boldsymbol{I} + \tilde{\boldsymbol{T}}_p$, $\lambda = \frac{\zeta}{4H}$ and $\eta_p = \frac{n\zeta}{4\beta H}$, we get

$$\lambda \overset{\nabla}{\tilde{\boldsymbol{T}}}_p + \tilde{\boldsymbol{T}}_p = 2\eta_p \boldsymbol{D}.$$

  This is the UCM model again!
- Total extra stress is

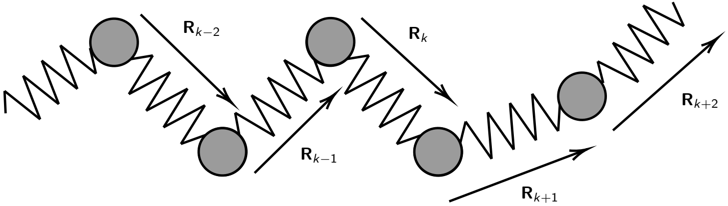
$$\boldsymbol{T} = \tilde{\boldsymbol{T}}_p + 2\eta_{sol}\boldsymbol{D},$$

  which gives us Oldroyd-B!

Dumbbell Modelling

What do we learn from this?

1. UCM/Oldroyd-B aren't stupid choices!
2. Can easily obtain an extension $\longrightarrow$ Rouse model.
   - Each 'spring' satisfies its own UCM equation.
   - Applicable to polydisperse solutions.



Rouse, P. E., 1953.

An Advanced Dumbbell Model

- Based on the idea of *direction dependent drag*.
- In absence of solvent ($\eta_{sol} = 0$, $\eta_p = \eta_0$), modify UCM equation as

$$\lambda \overset{\nabla}{\boldsymbol{T}} + \boldsymbol{M}\boldsymbol{T} = 2\eta_0 \boldsymbol{D}.$$

- Choosing $\boldsymbol{M} = \boldsymbol{I} + \frac{\alpha\lambda}{\eta_0}\boldsymbol{T}$ gives the *Giesekus* model:

$$\lambda \overset{\nabla}{\boldsymbol{T}} + \boldsymbol{T} + \frac{\alpha\lambda}{\eta_0}\boldsymbol{T}^2 = 2\eta_0 \boldsymbol{D}, \quad \alpha \in (0, 1).$$

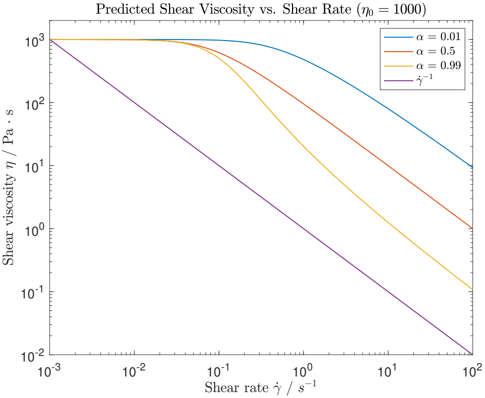
- This is no longer linear in stress!

Giesekus, H., 1966.

Giesekus Predictions

Shear Viscosity

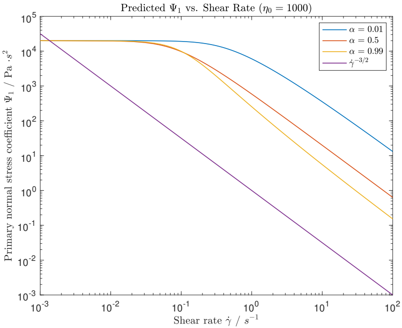
We actually predict shear thinning!

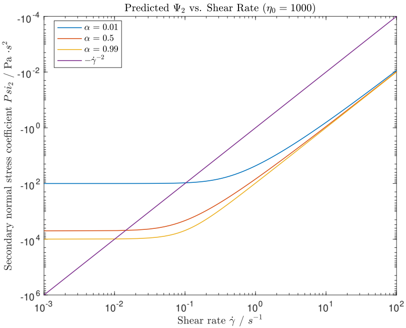


Giesekus Predictions

Shear Normal Stress Coefficients

Positive primary normal stresses; *negative* secondary normal stresses.

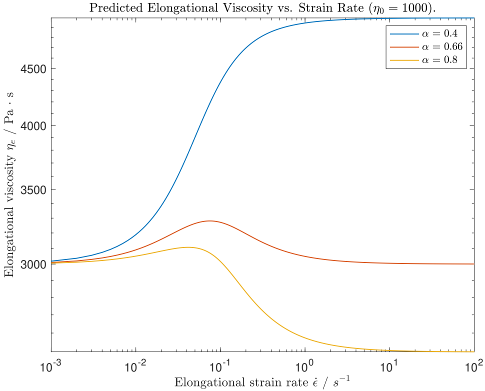




Giesekus Predictions

Elongational Viscosity

Strain *hardening* for $\alpha < 2/3$; strain *softening* for $\alpha \geq 2/3$.



Giesekus Predictions

In fact...

Constitutive model	Small-strain	Steady viscometric η	Steady viscometric N_1	Steady viscometric N_2	Steady elongation	Start/stop in shearing flow	Elongational start/recoil	Single shear step	Double-step shear	Remark
Newtonian, eqn (1.7)	P	M	U	U	M	P	U	U	U	Infinite stresses in step strains.
Generalized Newtonian, e.g. eqns (4.4, 4.11)	P	E	U	U	M	P	U	U	U	Infinite stresses in step strains.
Lodge–Maxwell, (UCM) eqns (4.25, 5.150)	E	M	M	U	P	M	M	M	M	Useful for illustrative purposes.
Giesekus eqn (5.111)	E	E	E	G-E	G	G	G	M	M	

...Giesekus can have fairly good predictions in many situations!

Tanner, R. I., 2000.

Summary

In this presentation, we have

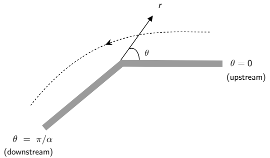
- Discussed the basics of viscoelastic modelling.
- Looked at some mechanical-based continuum models and motivated the UCM model.
- Motivated the UCM model again via molecular theory (so it's certainly not a bad model!)
- Discussed a more complicated model which can make more useful predictions.

Where Do I Fit into This?

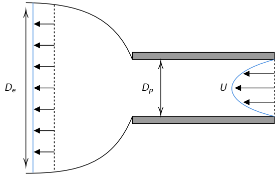
PhD aim: *Apply asymptotic techniques to study White-Metzner fluids.*

$$\overset{\nabla}{\boldsymbol{T}} + \lambda_0 \dot{\gamma}^{q-1} \boldsymbol{T} = 2\eta_0 \dot{\gamma}^{n-1} \boldsymbol{D}, \quad \dot{\gamma} = \sqrt{2\mathrm{tr}(\boldsymbol{D}^2)}.$$

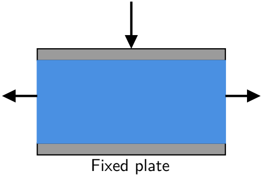
Re-entrant corners



Die swell



Squeeze flow



Thank you for listening!

Happy Halloween!

Ericksen Blog, n.d.

References

Dracula:
Dracula A.D. 1972 (1972), Directed by Alan Gibson [Film], London, Hammer Film Productions Ltd.
Spider:
Tarantula! (1955), Directed by Jack Arnold [Film], Universal Pictures
Skeletons:
The Skeleton Dance, 1929, Directed by Walt Disney [Film], Walt Disney Productions
Lego:
El, A., 2022 '*Halloween Lego Minifigures*' [Online]. Germany Detail Zero. Available from: https://germany.detailzero.com/technology/79249/New-Halloween-minifigures-in-the-LEGO-Build-a-Minifigure-Tower.html
Shear diagram:
Østergård., A. L., 2020. '*Why Shear Rate Matters in Process Control*' [Online]. Fluidan. Available from: https://fluidan.com/why-shear-rate-matters-in-process-control/ [Accessed 04-10-22].
Weissenberg Effect/Viscoelastic Table:
R. I. Tanner. Engineering Rheology. 2nd ed. New York, N.Y.: Oxford University Press, 2000.

References

ZZ Top:
Hutson, M. 2016. '*Billy Gibbons, Frank Beard and Dusty Hill of ZZ Top pose for a group portrait backstage at Glastonbury Festival, United Kingdom, 24th June 2016.*'. Redferns.
Maxwell:
Maxwell. J. C. "IV. On the dynamical theory of gases". In: Philos. Trans. Royal Soc. 157 (1867), pp. 49–88.
Kelvin Voigt:
Thompson, W. (Lord Kelvin), "Elasticity" in Encyclopaedia Britannica, 9th ed., Vol. VII, Charles Screibner's, New York, (1878) p. 803d,
Jeffreys:
Jeffreys, H., "The Earth: Its Origin, History and Physical Constitution". Cambridge: Cambridge University Press, (1929), p. 265.
Oldroyd:
Oldroyd, J. G., "On the formulation of rheological equations of state". In: Proc. Royal Soc. A. 200.1063 (1950), pp. 523–541.
White-Metzner:
White, J. L. and Metzner, A. B., "Development of constitutive equations for polymeric melts and solutions". In: J. Appl. Polym. Sci. 7 (1963), pp. 1867– 1889.

References

Extended White-Metzner:
A. Souvaliotis and A. N. Beris. "An extended White–Metzner viscoelastic fluid model based on an internal structural parameter". In: Journal of Rheology 36.2 (1992), pp. 241–271.
Jaumann Derivative:
Jaumann, G., Grundlagen der Bewegungslehre. Springer, Leipzig, (1905).
Kuhn:
Kuhn, W., "Shape of fibre-forming molecules in solutions". In: Kolloid Zeitschrift 68 (1934), pp. 2–15.
Renardy:
Renardy, M., Mathematical Analysis of Viscoelastic Flows. Society for Industrial and Applied Mathematics, 2000
Rouse:
Rouse, P.E., "A Theory of the Linear Viscoelastic Properties of Dilute Solutions of Coiling Polymers". In: J. Chem. Phys. 21.7 (1953), pp. 1272–1280.
Giesekus:
Giesekus, H., "Die Elastizität von Fl üssigkeiten". In: Rheol. Acta 5.1 (1966), pp. 29–35.
Pumpkin:
Ericksen Blog, '*Rick Astley carved into a pumpkin*', Available from:
https://www.reddit.com/r/rickroll/comments/qetfd6/rickroll_pumpkin/ [Accessed: 25-10-22]