5 The Oldroyd-B fluid

Last time we started from a microscopic dumbbell with a linear entropic spring, and derived the Oldroyd-B equations:

$$\underline{\nabla} \cdot \underline{u} = 0 \tag{1}$$

$$\rho \left(\frac{\partial \underline{u}}{\partial t} + \underline{u} \cdot \underline{\nabla u} \right) = \underline{\nabla} \cdot \underline{\underline{\sigma}} \tag{2}$$

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + \eta \left(\underline{\nabla u} + (\underline{\nabla u})^\top \right) + G\underline{\underline{A}} \tag{3}$$

$$\frac{\partial \underline{\underline{A}}}{\partial t} + (\underline{u} \cdot \underline{\nabla})\underline{\underline{A}} - \underline{\underline{A}} \cdot \underline{\nabla u} - (\underline{\nabla u})^\top \cdot \underline{\underline{A}} = -\frac{1}{\tau} \left(\underline{\underline{A}} - \underline{\underline{I}} \right) \tag{4}$$

Note that since $\underline{\underline{A}} = \mathbb{E}[\underline{r}\,\underline{r}]$, it must be symmetric.

5.1 Shear flow

Suppose we make our fluid carry out an unsteady shear flow:

$$\underline{u} = (\dot{\gamma}(t)y, 0, 0).$$

If the forcing all depends on y and t only, we expect all the physical variables only to depend on y and t. The mass conservation equation (1) is satisfied. The momentum equation (2) becomes

$$\rho \frac{\partial \underline{u}}{\partial t} = \underline{\nabla} \cdot \underline{\underline{\sigma}}.$$

Now the tensor $\underline{\nabla u}$ is

$$\underline{\nabla u} = \begin{pmatrix} 0 & 0 \\ \dot{\gamma}(t) & 0 \end{pmatrix}$$

so (3) gives

$$\underline{\underline{\sigma}} = \begin{pmatrix} -p & \eta\dot{\gamma}(t) \\ \eta\dot{\gamma}(t) & -p \end{pmatrix} + G\underline{\underline{A}}$$

and (4) becomes

$$\frac{\partial}{\partial t} \begin{pmatrix} A_{xx} & A_{xy} \\ A_{xy} & A_{yy} \end{pmatrix} - \begin{pmatrix} \dot{\gamma}A_{xy} & 0 \\ \dot{\gamma}A_{yy} & 0 \end{pmatrix} - \begin{pmatrix} \dot{\gamma}A_{xy} & \dot{\gamma}A_{yy} \\ 0 & 0 \end{pmatrix} = -\frac{1}{\tau} \begin{pmatrix} A_{xx} - 1 & A_{xy} \\ A_{xy} & A_{yy} - 1 \end{pmatrix}$$

5.1.1 Steady shear flow

Now set $\dot{\gamma}$ as a constant. This means that all the variables should be independent of t:

$$\underline{\nabla} \cdot \underline{\underline{\sigma}} = \underline{0}.$$

$$\underline{\underline{\sigma}} = \begin{pmatrix} -p & \eta\dot{\gamma} \\ \eta\dot{\gamma} & -p \end{pmatrix} + G\underline{\underline{A}}$$

$$-\begin{pmatrix} \dot\gamma A_{xy} & 0 \\ \dot\gamma A_{yy} & 0 \end{pmatrix} - \begin{pmatrix} \dot\gamma A_{xy} & \dot\gamma A_{yy} \\ 0 & 0 \end{pmatrix} = -\frac{1}{\tau}\begin{pmatrix} A_{xx}-1 & A_{xy} \\ A_{xy} & A_{yy}-1 \end{pmatrix}$$

Let's look at the last equation, for the components of $\underline{\underline{A}}$. It gives three scalar equations:

$$\begin{aligned} -\dot\gamma A_{xy} - \dot\gamma A_{xy} &= -\frac{1}{\tau}(A_{xx}-1) \\ -\dot\gamma A_{yy} &= -\frac{1}{\tau}A_{xy} \\ 0 &= A_{yy}-1. \end{aligned}$$

Solving from the bottom up gives

$$A_{yy} = 1 \qquad A_{xy} = \dot\gamma\tau \qquad A_{xx} = 1 + 2\dot\gamma^2\tau^2.$$

The total stress becomes

$$\underline{\underline{\sigma}} = \begin{pmatrix} -p + G + 2G\dot\gamma^2\tau^2 & (\eta + G\tau)\dot\gamma \\ (\eta + G\tau)\dot\gamma & -p + G \end{pmatrix}.$$

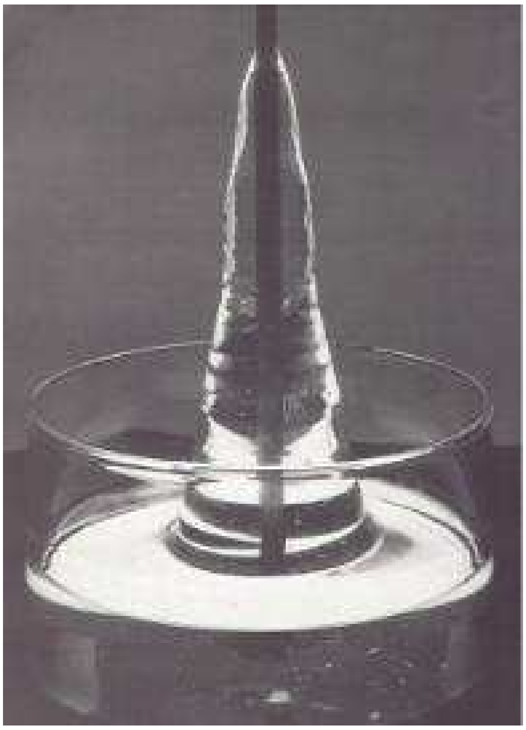
The presence of the polymers has made two changes to the Newtonian stress:

- The viscosity is increased from η to $\eta + G\tau$
- There is a difference between the two diagonal stress components.

This difference is called the **first normal stress difference**

$$N_1 = \sigma_{xx} - \sigma_{yy} = 2G\tau^2\dot\gamma^2.$$

As a stress acting along the flow lines (xx-direction) it has the opposite sign to pressure so it acts like a tension: the streamlines are like stretched rubber bands. It is the driving force behind the rod-climbing experiment:



This picture is from Boger & Walters' book "Rheological Phenomena in Focus". The rod in the middle is rotated, causing a shear flow round the outside. The streamlines are circular, so their tension causes the fluid to move to the middle – and the only place it can go is up the rod.

5.1.2 Linear rheology

Let's return to the time-dependent shear flow:

$$\underline{u} = (\dot{\gamma}(t)y, 0, 0).$$

$$\rho\frac{\partial \underline{u}}{\partial t} = \underline{\nabla} \cdot \underline{\underline{\sigma}}; \qquad \underline{\underline{\sigma}} = \begin{pmatrix} -p & \eta\dot{\gamma}(t) \\ \eta\dot{\gamma}(t) & -p \end{pmatrix} + G\underline{\underline{A}}$$

and

$$\frac{\partial}{\partial t}\begin{pmatrix} A_{xx} & A_{xy} \\ A_{xy} & A_{yy} \end{pmatrix} - \begin{pmatrix} \dot{\gamma}A_{xy} & 0 \\ \dot{\gamma}A_{yy} & 0 \end{pmatrix} - \begin{pmatrix} \dot{\gamma}A_{xy} & \dot{\gamma}A_{yy} \\ 0 & 0 \end{pmatrix} = -\frac{1}{\tau}\begin{pmatrix} A_{xx}-1 & A_{xy} \\ A_{xy} & A_{yy}-1 \end{pmatrix}$$

For the standard linear rheology experiment, we set

$$\dot{\gamma}(t) = \alpha\omega\cos(\omega t).$$

We'll assume the motion starts at $t = 0$. Before that there is no flow so the fluid was relaxed and $\underline{\underline{A}} = \underline{\underline{I}}$.

Let's look at the evolution of $\underline{\underline{A}}$. To get the rheology, we will only need A_{xy}, so we'll only use the A_{xy} and A_{yy} equations.

$$\begin{aligned} \frac{\partial A_{xy}}{\partial t} - \dot{\gamma}A_{yy} &= -\frac{1}{\tau}A_{xy} \\ \frac{\partial A_{yy}}{\partial t} &= -\frac{1}{\tau}(A_{yy}-1). \end{aligned}$$

The second of these is satsfied by $A_{yy} = 1$, so the first gives

$$\begin{aligned} \frac{\partial A_{xy}}{\partial t} - \alpha\omega\cos(\omega t) &= -\frac{1}{\tau}A_{xy} \\ \frac{\partial A_{xy}}{\partial t} + \frac{1}{\tau}A_{xy} &= \alpha\omega\cos(\omega t) \\ \frac{\partial}{\partial t}\left[A_{xy}e^{(t/\tau)}\right] &= \alpha\omega\cos(\omega t)e^{(t/\tau)} \end{aligned}$$

This is one of those tricky integrals that works iteratively by parts:

$$\begin{aligned} I &= \int_0^t \alpha\omega\cos(\omega t')e^{(t'/\tau)}\ \mathrm{d}t' \\ &= [\alpha\omega\tau\cos(\omega t')e^{(t'/\tau)}]_0^t + \int_0^t \alpha\omega^2\tau\sin(\omega t')e^{(t'/\tau)}\ \mathrm{d}t' \\ &= [\alpha\omega\tau\cos(\omega t')e^{(t'/\tau)}]_0^t + [\alpha\omega^2\tau^2\sin(\omega t')e^{(t'/\tau)}]_0^t - \int_0^t \alpha\omega^3\tau^2\cos(\omega t')e^{(t'/\tau)}\ \mathrm{d}t' \\ &= \alpha\omega\tau\cos(\omega t)e^{(t/\tau)} + \alpha\omega^2\tau^2\sin(\omega t)e^{(t/\tau)} - \alpha\omega\tau - \omega^2\tau^2 I \end{aligned}$$

Finally the expression for A_{xy} is

$$A_{xy} = \frac{1}{1+\omega^2\tau^2}\left(\alpha\omega\tau\cos(\omega t) + \alpha\omega^2\tau^2\sin(\omega t) - \alpha\omega\tau e^{-(t/\tau)}\right)$$

For long times, the $e^{-(t/\tau)}$ term becomes very small so we will neglect it. The total shear stress σ_{xy} then becomes

$$\sigma_{xy} = \left[\eta + \frac{G\tau}{1+\omega^2\tau^2}\right]\dot{\gamma}(t) + \frac{G\omega^2\tau^2}{1+\omega^2\tau^2}\gamma(t)$$

Thus the linear rheology functions for the Oldroyd-B fluid are

$$G' = \frac{G\omega^2\tau^2}{1+\omega^2\tau^2} \qquad G'' = \eta\omega + \frac{G\omega\tau}{1+\omega^2\tau^2}.$$

This is just like the single exponential relaxation fluid if we set $\eta = 0$; that would give the **Upper Convected Maxwell** model. With a nonzero viscosity, although the relaxation time is still τ, the storage and loss modulus no longer cross at $\omega = \tau^{-1}$.

5.2 Extensional flow

Finally, we look at a steady 2D extensional flow:

$$\underline{u} = (\dot{\varepsilon}x, -\dot{\varepsilon}y).$$

Again, this satisfies mass conservation. This time we have

$$\underline{\nabla u} = \begin{pmatrix} \dot{\varepsilon} & 0 \\ 0 & -\dot{\varepsilon} \end{pmatrix}.$$

The stress is

$$\underline{\underline{\sigma}} = \begin{pmatrix} -p+2\eta\dot{\varepsilon} & 0 \\ 0 & -p-2\eta\dot{\varepsilon} \end{pmatrix} + G\underline{\underline{A}}$$

and the evolution of $\underline{\underline{A}}$ (independent of time and position) becomes

$$-\begin{pmatrix} \dot{\varepsilon}A_{xx} & -\dot{\varepsilon}A_{xy} \\ \dot{\varepsilon}A_{xy} & -\dot{\varepsilon}A_{yy} \end{pmatrix} - \begin{pmatrix} \dot{\varepsilon}A_{xx} & \dot{\varepsilon}A_{xy} \\ -\dot{\varepsilon}A_{xy} & -\dot{\varepsilon}A_{yy} \end{pmatrix} = -\frac{1}{\tau}\left(\underline{\underline{A}} - \underline{\underline{I}}\right)$$

so

$$A_{xx} = \frac{1}{(1-2\dot{\varepsilon}\tau)} \qquad A_{xy} = 0 \qquad A_{yy} = \frac{1}{(1+2\dot{\varepsilon}\tau)}$$

The total stress is

$$\underline{\underline{\sigma}} = \begin{pmatrix} -p+2\eta\dot{\varepsilon}+G/(1-2\dot{\varepsilon}\tau) & 0 \\ 0 & -p-2\eta\dot{\varepsilon}+G/(1+2\dot{\varepsilon}\tau) \end{pmatrix}.$$

Since in a Newtonian fluid we have

$$\underline{\underline{\sigma}} = \begin{pmatrix} -p+2\eta\dot{\varepsilon} & 0 \\ 0 & -p-2\eta\dot{\varepsilon} \end{pmatrix}$$

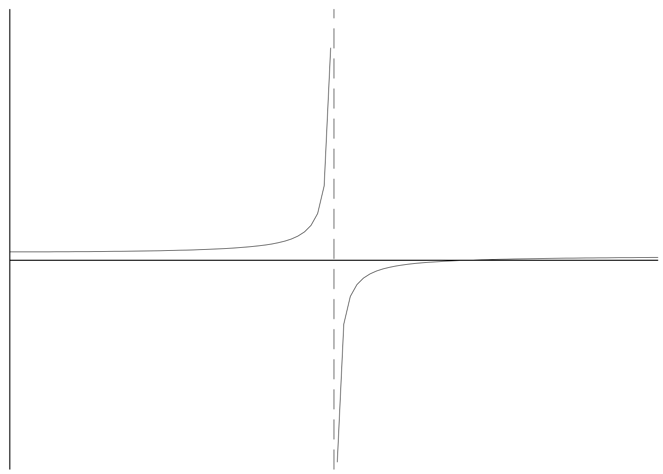
we can define an *extensional viscosity* as

$$\eta_{\text{ext}} = \frac{\sigma_{xx} - \sigma_{yy}}{4\dot{\varepsilon}}.$$

The Oldroyd-B fluid has extensional viscosity

$$\eta_{\text{ext}} = \eta + \frac{G\tau}{(1 - 4\dot{\varepsilon}^2\tau^2)}$$

This strain-hardens (gets thicker with increasing speed) for low strain rates but for higher strain rates disaster strikes:



The viscosity diverges at a strain rate of $\dot{\varepsilon} = 1/2\tau$ and for strain rates slightly larger, the viscosity value is negative!

The moral of this: a linear spring is fine for shear flows, where the stretch is fairly moderate; for stretching flows, a linear spring can stretch indefinitely and give infinite forces. The standard workaround at this point is to use a nonlinear spring law (FENE model, finie extensibility nonlinear elasticity) – which brings with it its own complications.

There is no single right answer to polymer modelling – but hopefully you now have an idea about how to start!