Complex Fluids

CFD Spring 2013, A. Dower

Simple fluid → internal microstructure of molecules and atoms is independent of the transport processes occurring.

Complex fluid → Complex microstructure that responds and affects the flow. Examples: polymeric fluids, polymeric suspensions, colloidal suspensions, gels, blood, nano-fluids, etc.
The simplest type of complex fluid, or non-Newtonian fluid, is a linearly visco-elastic fluid:

\[ \gamma \times \mathbf{y} = \eta \dot{\gamma} \]

\[ \dot{\gamma} (t) = \eta \mathbf{y} \]

\[ \gamma \times \mathbf{y} \rightarrow \text{Viscous or shear stress} \]

\[ \text{Viscosity} = \text{constant} \]

Based on a book by H.C. Ottinger
Non-Newtonian

\[ \sigma_{xy} = - \int_{-\infty}^{t} G(t-t') \dot{\gamma}(t') \, dt' \]

Shear relaxation modulus

Assume

\[ \dot{\gamma}(t) = \begin{cases} \dot{\gamma} & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases} \]

Start-up shear flow

\[ \Rightarrow \sigma_{xy}(t) = -\dot{\gamma} \int_{0}^{t} G(t') \, dt' \]

\[ \Rightarrow \eta = \int_{0}^{\infty} G(t') \, dt' \]
Generalized constitutive law relating stress with strain rate:

$$\sigma(t) = -\int_{-\infty}^{t} G(t-t') \left[ \dot{\vec{v}} + \left( \dot{\vec{v}} \right)^T \right] dt'$$

A common simple model is the multi-relaxation model:

$$G(t) = \eta_{\infty} \delta(t) + \sum_{j} \frac{\eta_j}{\tau_j} e^{-t/\tau_j} + G_0$$

Sum over internal relaxation processes
\( \eta_0 = 0 \) for a true liquid

\[
\eta = \eta_\infty + \frac{e_j}{j}
\]

Example: Maxwell Model of a visco-elastic fluid

\[
\frac{\partial \varepsilon_{\text{el}}}{\partial t} = -6\varepsilon_{\text{el}} + \eta_1 \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right)
\]

\[
6 = \eta_\infty \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) + 6\varepsilon_{\text{el}}
\]

\[\varepsilon + \nabla \mathbf{p} = -\nabla \cdot \mathbf{\varepsilon}, \quad \nabla \cdot \mathbf{u} = 0\]
To go beyond such simple phenomenological models, we must add internal variables (fields) that describe the microstructure of the complex fields. Here we will focus on a polymeric fluid in the dilute limit:
Let's assume for now (to be justified later) that the local microstructure of the dumbbell "polymeric" molecules can be described via two fields:

A scalar number density of polymers field $N(r,t)$ and a tensor conformation tensor field $\mathbf{C}(r,t) = \langle \mathbf{Q} \mathbf{Q}^T \rangle$.

Local average over many polymers.
Then, in addition to the Navier-Stokes equations, one can "derive" (i.e., justify, see book by Ottinger) evolution laws for $n(r,t)$ and $\vec{e}(r,t)$.

$$\frac{\partial \vec{e}}{\partial t} = - \nabla \cdot (\vec{v} \vec{e}) + \nabla \cdot (\vec{v} \vec{e}) + \vec{e} \cdot \nabla \vec{v}$$

- Relaxation:
  $$\frac{1}{2} (\vec{e} - n \vec{I})$$
  - Advection
  - Identity tensor

- Diffusion tensor:
  $$\nabla \cdot (\vec{D} \nabla \vec{e})$$
  - $\vec{D} \geq 0$
and the usual advection:

\[ \frac{\partial n}{\partial t} = -\nabla \cdot (\Omega n) + \nabla \cdot (D \nabla n) \]

Here $D$ is the diffusion tensor of the polymer molecules (in the dilute limit, equal to the self-diffusion coeff.).

These equations are nothing but advection-diffusion equations (generalized to tensor fields) and can be solved as usual. They do, however, couple back to the fluid flow via the stress tensor $\sigma(c, n, \nabla)$.
where $\vec{f} = \nabla$
For example, 

$$\sigma_c = + \beta (k_B T) (n_c - c)$$

extra pressure due to polymers

$$+ k \left[ \left( \frac{\partial c}{\partial t} - \nabla \cdot \mathbf{C} \right) - c \cdot \nabla \mathbf{C} \right]$$

material constant

where \( \dot{\mathbf{J}} = \nabla \mathbf{U} + \nabla ^T \mathbf{U} \) is the rate of deformation.
The previous way of modeling complex fluids relies on closure approximations to give a simple closed-form constitutive law for the stress-strain relations. A more detailed and general description is the kinetic theory level of description. Here, we describe the state of the polymers with a probability density function

\[ f(\theta, r) = \text{prob. to find conf. } \theta \text{ around position } r \]
Note that \( f(r, \theta) \) is a very high-dimensional object: at every point in space we have a whole distribution to describe.

\[
\begin{align*}
N &= \int f(r, \theta) \, d\theta - \text{first moment} \\
C &= \text{const.}, \quad \int f(r, \theta) \, \mathbf{\hat{r}} \mathbf{\hat{r}}^T \, d\theta - \text{second moment}
\end{align*}
\]

If we assume \( f(r, \theta) \) is Gaussian, then \( N \) and \( C \) are sufficient to describe \( f \) → reduced model.
The contribution to the stress tensor coming from the polymers (dumbbells) is given in terms of moments of $f$, e.g.

\[ \sigma = \int f(x) \left[ 2k_BT \cdot I - \frac{\partial^2 \Phi}{\partial x^2} \right] dx \]

where $\Phi(x)$ is the entropy of the coiled polymer spring as a function of its end-to-end distance (vector).
For example, for linear entropic springs,

$$y(\theta) = \frac{H \theta^2}{2} \Rightarrow \frac{\partial y}{\partial \theta} = H \theta$$

Spring constant

Kramers' expression

$$\sigma_r = 2k_B T \cdot \mathcal{N} - HC$$

$$= 2k_B T \left( n - \frac{H}{2k_B T} \right)$$

To close the equations we need an evolution equation for \( f(r, \theta) \).

This is the Fokker-Planck equation of kinetic theory.
\[
\dot{f} = -4 \cdot (vf) - \frac{2}{2a} \left[ \nu \cdot \frac{\partial}{\partial x} \right] f \\
+ \nu_0 \left( \frac{k_B T}{2a} \right) f + \frac{3}{3a} \left( \frac{2 k_B T}{3} \right) \frac{\partial f}{\partial x}
\]

**Side note:** This corresponds to a Langevin equation of motion for the dumbbells.

\[
\frac{dQ}{dt} = \mathbf{u}(Q) + \nabla \cdot \mathbf{Q} - \frac{2}{3} \frac{\partial}{\partial x} + \sqrt{4 k_B T \left\langle f_0 \right\rangle} \frac{dW}{dt}
\]

(Brownian dynamics or Monte Carlo approach to expectation values of \( f \))
From the equation for \( \tilde{f} \) one can derive

\[
\tilde{f} = k_{\beta T} N + \frac{\varepsilon}{4} \left[ \frac{\partial c}{\partial t} - \nu \cdot \nabla c - c \cdot \nabla \nu \right]
\]

which is very similar to the previous phenomenological model for \( \tilde{c} \).

The difference here is that there is no approximate closure equation for \( \tilde{c} \), rather, \( \tilde{c} = \langle \tilde{c} \tilde{c}^T \rangle \) is obtained from \( \tilde{f} \) as an expectation value (local in space)
A final and most detailed description is one in which the dynamics of each polymer chain is described explicitly (stochastic ODE or Langevin equation) and coupled bidirectionally with the surrounding fluid flow. This is very expensive but can be done using an Immersed Boundary-like approach (see my own research) and Coarse-Graining Course next Fall.