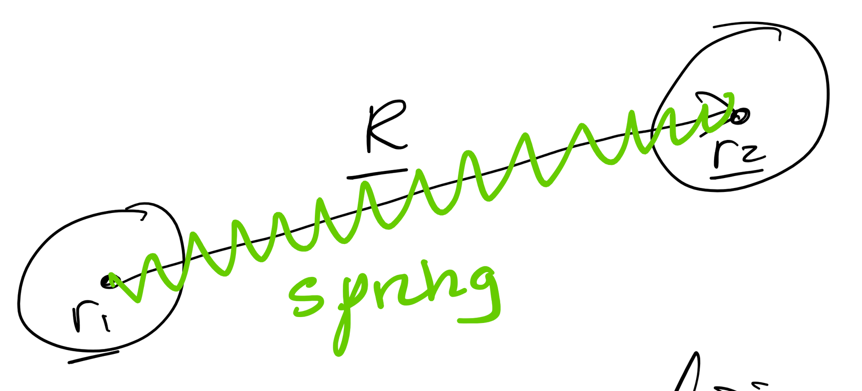
Advanced Fluid Dynamics lecture 4

Monday, 25 January 2021 00:01

Spheres with springs: the upper convected Maxwell viscoelastic fluid



Consider two spheres, radii a, with centres $\mathbf{r}_1(t)$ and $\mathbf{r}_2(t)$, separation $\mathbf{R} = \mathbf{r}_2 - \mathbf{r}_1$, joined by a linear spring that exerts a force $-\mathbf{R}H$ on sphere 2.

Suppose further that this device is embedded in a linear flow

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}(0,t) + \mathbf{x}\cdot\nabla\mathbf{u}$$

[Beware of other conventions that write $(\nabla\mathbf{u})\mathbf{x}$ instead but mean the same thing.]

and that $|\mathbf{R}| \gg a$ so the separation is much larger than the spheres' radii.

Sufficiently small spheres will experience stochastic Brownian forces $\mathbf{S}_1$ and $\mathbf{S}_2$ from collisions with molecules of the surrounding fluid.

The centres $\mathbf{r}_1$ and $\mathbf{r}_2$ move according to 2 Langevin equations:

$$m\,\ddot{\mathbf{r}}_1 = -\zeta(\dot{\mathbf{r}}_1 - \mathbf{u}(\mathbf{r}_1, t)) + H\mathbf{R} + \mathbf{S}_1$$

$$m\,\ddot{\mathbf{r}}_2 = -\zeta(\dot{\mathbf{r}}_2 - \mathbf{u}(\mathbf{r}_2, t)) - H\mathbf{R} + \mathbf{S}_2,$$

where m is the mass of a sphere and $\zeta = 6\pi\mu a$ is the Stokes drag coefficient.

Neglect inertia for the particles, consistent with Stokes flow, so the net forces balance instantaneously.

Consider a suspension of many widely-separated bead-spring pairs with a distribution function $\Psi(\mathbf{r}_1, \mathbf{r}_2, t)$. No dependence on $\dot{\mathbf{r}}_1$ and $\dot{\mathbf{r}}_2$ in Stokes flow.

Following Chandrasekhar (1943) we can find an evolution equation for Ψ by putting

$$\mathbf{S}_i = -k_B T\,\nabla_{\mathbf{r}_i}\log\Psi,$$

where k_B is Boltzmann's constant and T is temperature.

This will make sense later in a Liouville equation for Ψ.

Easier to change variables to $\mathbf{R} = \mathbf{r}_2 - \mathbf{r}_1$ and

$$\mathbf{x} = \tfrac{1}{2}(\mathbf{r}_2 + \mathbf{r}_1), \text{ mean position,}$$

and write

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = n\psi(\mathbf{R}, \mathbf{x}, t)$$

where n is the number density of bead-spring pairs, and for each $\mathbf{x}$ & t, ψ is normalized by

$$\int \psi(\mathbf{R}, \mathbf{x}, t)\,d\mathbf{R} = 1.$$

In these coordinates, the Brownian forces become

$$\nabla_{\mathbf{r}_1}\log\Psi = \left(\tfrac{1}{2}\nabla_{\mathbf{x}} - \nabla_{\mathbf{R}}\right)\log\psi,$$

$$\nabla_{\mathbf{r}_2}\log\Psi = \left(\tfrac{1}{2}\nabla_{\mathbf{x}} + \nabla_{\mathbf{R}}\right)\log\psi.$$

The Langevin equations become

$$\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}, t) - \frac{k_B T}{\zeta}\nabla_{\mathbf{x}}\log\psi,$$

$$\dot{\mathbf{R}} = \mathbf{R}\cdot\nabla\mathbf{u} - \frac{2H}{\zeta}\mathbf{R} - \frac{2k_B T}{\zeta}\nabla_{\mathbf{R}}\log\psi.$$

To make sense of the Brownian terms, substitute into the Liouville equation for ψ,

$$\frac{\partial\psi}{\partial t} + \nabla_{\mathbf{x}}\cdot(\dot{\mathbf{x}}\psi) + \nabla_{\mathbf{R}}\cdot(\dot{\mathbf{R}}\psi) = 0,$$

to get the Fokker–Planck equation

$$\partial_t\psi + \mathbf{u}\cdot\nabla\psi = \underbrace{\nabla_{\mathbf{x}}\cdot\left(\frac{k_B T}{\zeta}\nabla_{\mathbf{x}}\psi\right)} + \nabla_{\mathbf{R}}\cdot\left(-\psi\mathbf{R}\cdot\nabla\mathbf{u} + \frac{2H}{\zeta}\psi\mathbf{R} + \frac{2k_B T}{\zeta}\nabla_{\mathbf{R}}\psi\right)$$

This term gives Brownian diffusion in physical space $\mathbf{x}$, cf separation or internal space $\mathbf{R}$. If $|\mathbf{R}| \ll |\mathbf{x}|$, so spatial variation is on scales $\gg |\mathbf{R}| \sim$ molecular scale, so the green term is $O\left(\left(\frac{|\mathbf{R}|}{|\mathbf{x}|}\right)^2\right)$ smaller than diffusion in $\mathbf{R}$. Commonly omitted.

Taking the second moment w.r.t. $\underline{R}$ of the Fokker-Planck equation, and assuming $\psi \to 0$ as $|\underline{R}| \to \infty$, shows that conformation tensor

$$\underline{\underline{C}} = \langle \underline{R}\,\underline{R} \rangle = \int \underline{R}\,\underline{R}\,\psi \, d\underline{R}$$

obeys the closed evolution equation

$$\partial_t \underline{\underline{C}} + \underline{u}\cdot\nabla\underline{\underline{C}} - (\nabla\underline{u})^T\cdot\underline{\underline{C}} - \underline{\underline{C}}\cdot(\nabla\underline{u}) = \frac{4k_BT}{\zeta}\underline{\underline{I}} - \frac{4H}{\zeta}\underline{\underline{C}}$$

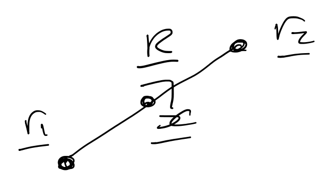
The LHS is called the upper convected derivative $\overset{\triangledown}{\underline{\underline{C}}}$, in components

$$[\overset{\triangledown}{C}]_{ij} = \frac{\partial C_{ij}}{\partial t} + u_k \frac{\partial C_{ij}}{\partial x_k} - \frac{\partial u_i}{\partial x_k} C_{kj} - C_{ik}\frac{\partial u_j}{\partial x_k}.$$

It's a material derivative for rank-2 tensors that respond to local fluid stretching & rotation.

To motivate it, omitting H and S_i gives

$$\dot{\underline{R}} = \underbrace{\frac{\partial \underline{R}}{\partial t} + \underline{u}\cdot\nabla\underline{R}}_{\text{advection}} = \underbrace{\underline{R}\cdot\nabla\underline{u}}_{\text{stretching}}$$



$$\underline{u}(\underline{x} + \tfrac{1}{2}\underline{R}) - \underline{u}(\underline{x} - \tfrac{1}{2}\underline{R}) = \underline{R}\cdot\nabla\underline{u}$$

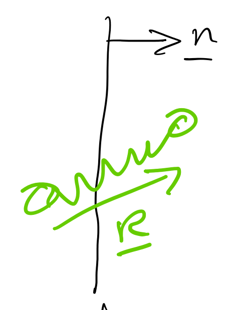
This is the equation for magnetic field $\underline{B}$ in ideal MHD, and for vorticity in ideal fluids.

Then the tensor $\underline{R}\,\underline{R}$ evolves according to

$$\overset{\triangledown}{\langle \underline{R}\,\underline{R} \rangle} = 0$$

Effect of the springs on the fluid

The number density of bead-spring pairs crossing a unit area with normal $\underline{n}$ is $\underline{n}\cdot\underline{R}\,\psi$.



surface

The momentum transferred across this area is

$$\int (H\underline{R})\,\underline{n}\cdot\underline{R}\,\psi\, d\underline{R} = \underline{\underline{\sigma}}^{\text{spring}}\cdot\underline{n}.$$

Requiring this to hold for all normals $\underline{n}$ gives

$$\underline{\underline{\sigma}}^{\text{spring}} = nH\langle \underline{R}\,\underline{R}\rangle = nH\underline{\underline{C}}.$$

In steady state with no flow,

$$\underline{\underline{C}} = \frac{k_BT}{H}\underline{\underline{I}} \quad \text{so} \quad \underline{\underline{\sigma}}^{\text{spring}} = nk_BT\underline{\underline{I}}.$$

This is <u>minus</u> the pressure in an ideal gas. There's another contribution $-2nk_BT\underline{\underline{I}}$ from the beads (number density $2n$) crossing the surface. The overall pressure in an incompressible fluid comes from $\nabla\cdot\underline{u} = 0$ anyway.

We can write

$$\underline{\underline{\sigma}}^{\text{spring}} = nH\underline{\underline{C}} = nk_BT\underline{\underline{I}} + \underline{\underline{\sigma}}^{P}$$

where $\underline{\underline{\sigma}}^{P}$ vanishes with no flow.

The upper convected derivative of $\underline{\underline{I}}$ is

$$\overset{\triangledown}{\underline{\underline{I}}} = \partial_t\underline{\underline{I}} + \underline{u}\cdot\nabla\underline{\underline{I}} - (\nabla\underline{u})^T\cdot\underline{\underline{I}} - \underline{\underline{I}}\cdot(\nabla\underline{u})$$
$$= -(\nabla\underline{u})^T - (\nabla\underline{u})$$
$$= -2\underline{\underline{e}}$$

Using this to eliminate $\underline{\underline{\sigma}}^{\text{spring}}$ gives

$$\overset{\triangledown}{\underline{\underline{\sigma}}}{}^{P} + \frac{4H}{\zeta}\underline{\underline{\sigma}}^{P} = 2nk_BT\underline{\underline{e}},$$

the upper convected Maxwell fluid, commonly written as

$$\underline{\underline{\sigma}}^{P} + \tau\overset{\triangledown}{\underline{\underline{\sigma}}}{}^{P} = 2\mu'\underline{\underline{e}},$$

where $\mu' = \frac{nk_BT\zeta}{4H}$ is the steady state viscosity, and $\tau = \frac{\zeta}{4H}$ is the stress relaxation time. Replacing $\overset{\triangledown}{\underline{\underline{\sigma}}}{}^{P}$ by $\partial_t\underline{\underline{\sigma}}^{P}$ gives the linear Maxwell model from kinetic theory of gases.

The upper convected Maxwell model is <u>objective</u>, so the stress behaves consistently under rotations.

A more realistic version adds a Newtonian viscous stress from the solvent:

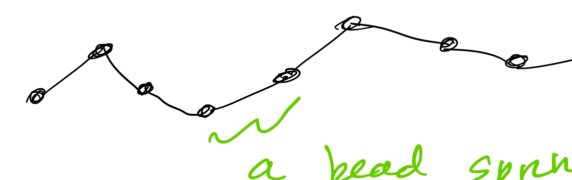
$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + 2\mu\underline{\underline{e}} + \underline{\underline{\sigma}}^{P}$$

This is the Oldroyd-B model for viscoelastic liquids, e.g. Boger fluids.

Bubbles in shampoo:

$\Leftarrow$ cusp due to viscoelasticity

Long chain polymer:



a bead spring pair models one link in the chain. It's not a bad conceptual model for the whole chain.