Conservation equations – true all materials

Conservation of momentum (Cauchy):

$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \sigma + \rho \mathbf{g}$$

- Often inertia (LHS) is negligible.
- Usually incompressible (plus conservation of mass):

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

  so add pressure to stress, often omitted below.
- Need Constitutive (material dependent) Relation between stress σ and flow $\mathbf{u}$.

Chapter 3

Constitutive equations

- Phenomenology
  - ‘Simple’ materials
  - Perfectly elastic material
  - Time derivatives
- Exact approximations
  - Linear viscoelasticity
  - Second-order fluid
- Semi-empirical models
  - Generalised Newtonian
  - Oldroyd-B
  - K-BKZ

‘Simple’ materials

Lagrangian description

$$\mathbf{X} \to \mathbf{x}(\mathbf{X}, t)$$

Deformation of line element (for micro-lengths $\ll$ macro-lengths)

$$\delta\mathbf{X} \to \delta\mathbf{x} = A \cdot \delta\mathbf{X}, \qquad A_{iJ} = \frac{\partial x_i}{\partial X_J}$$

A has rotation and stretch, see later.
Local and casual dependency

$$\sigma(t) = \sigma\left\{A(\tau)\right\}_{\tau \le t}$$

This functional dependence not useful, except for fast elastic limit and slow viscous limits (each with single parameter)

Material Frame Indifference

‘Tensorial correct’ or result independent of observer, so same stresses if add translation and rotation

$$\mathbf{x}' = \mathbf{a}(t) + Q(t)\mathbf{x}$$

so in new frame

$$\sigma' = \sigma\left\{Q(\tau)A(\tau)Q^T(0)\right\}_{\tau \le t} \equiv Q(t)\sigma\left\{A(\tau)\right\}_{\tau \le t} Q^T(t).$$

Require $\sigma\left\{A\right\}$ to obey this identity for all $Q(t)$.

Perfectly elastic material

Instantaneous, no history.
Decompose deformation A into first a stretch U followed by a rotation R,

$$A = RU, \qquad \text{with} \quad R^T R = I, \qquad \text{by finding } A\text{:} \quad U^2 = A^T A.$$

The set $Q = R^T$ in Material Frame Indifference

$$\sigma\{A\} = R(t) f(U(t)) R^T$$

In incompressible material with isotropic in rest state,

$$f(U^2) = U^2 f_1 + U^{-2} f_2, \quad f_i \text{ scalar functions of invariants of } U,$$

so

$$\sigma = AA^T f_1 + A^{-1\,T} A^{-1} f_2$$

Perfectly elastic material 2

Alternatively for incompressible with isotropic in rest state, use an elastic potential energy w, a function of eigenvalues λ_i of U in invariant combinations

$$\alpha = \tfrac{1}{2}\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2\right), \beta = \tfrac{1}{2}\left(\lambda_1^{-2} + \lambda_2^{-2} + \lambda_3^{-2}\right), \gamma = \lambda_1 \lambda_2 \lambda_3 \equiv 1$$

Virtual work and σ co-diagonal with U gives

$$\sigma_1 = \frac{1}{\lambda_2 \lambda_3}\left(\frac{\partial w}{\partial \lambda_1} = \lambda_1 \frac{\partial w}{\partial \alpha} - \lambda_1^{-3} \frac{\partial w}{\partial \beta}\right),$$

so

$$\sigma = \frac{1}{\gamma}\frac{\partial w}{\partial \alpha} AA^T - \frac{1}{\gamma}\frac{\partial w}{\partial \beta} A^{-1\,T} A^{-1}.$$

Better for data fitting – Ogden model: $w(\lambda_1^n + \lambda_2^n + \lambda_3^n)$

Time derivatives

To express history dependence will use time derivatives and integrals.
But problem : In new frame

$$\sigma' = Q \sigma Q^T$$

so its time derivative

$$\dot{\sigma}' = Q \dot{\sigma} Q^T + \dot{Q} \sigma Q^T + Q \sigma \dot{Q}^T$$

is different in different frames.

Now flow transforms

$$u' = Qu + \dot{Q}x + \dot{a}$$

so velocity gradients transform

$$\frac{\partial u'}{\partial x'} = Q \frac{\partial u}{\partial x} Q^T + \dot{Q} Q^T \qquad \left(\text{watch indices, } \equiv \nabla u^T\right)$$

so

strain-rate $E' = QEQ^T$, vorticity (tensor) $\Omega' = Q \Omega Q^T - \dot{Q} Q^T$

Co-rotational (Jaumann) time derivative

Hence co-rotational (Jaumann) time derivative

$$\overset{\circ}{\sigma} \equiv \frac{D\sigma}{Dt} - \Omega^T \cdot \sigma - \sigma \cdot \Omega$$

has transformation

$$\overset{\circ}{\sigma}{}' = Q \overset{\circ}{\sigma} Q^T$$

Student Exercise

This is the rate of change of σ seen by an observer rotating with the vorticity, and so is universal.

Recall rotation frames

$$\overset{\circ}{\mathbf{x}} = \dot{\mathbf{x}} + \Omega \mathbf{x}$$

Co-deformational time derivative

Can add multiple of $E\sigma + \sigma E$ to co-rotational derivative.
Hence (upper) co-deformational (Oldroyd-B) derivative

$$\overset{\triangledown}{\sigma} \equiv \frac{D\sigma}{Dt} - \nabla u^T \cdot \sigma - \sigma \cdot \nabla u$$

has transformation

$$\overset{\triangledown'}{\sigma'} = Q\overset{\triangledown}{\sigma}Q^T$$

Student Exercise

Recall stretching material line element

$$\dot{\delta\ell} = \delta\ell \cdot \nabla u$$

so for second-order tensor

$$\dot{\delta\ell\delta\ell} = \nabla u^T \cdot \delta\ell\delta\ell + \delta\ell\delta\ell \cdot \nabla u$$

Linear viscoelasticity

The most general linear response for all materials isotropic in rest state.

Linearise in low stretch: $A^T A \approx I$

$$\sigma(t) = R(t) \int_0^\infty G(s)\dot{\overline{A^T A}}(t-s)\, ds\, R^T(t)$$

The $R(t) \dots R^T(t)$ is a co-rotational integral, but usually dropped in linearisation.

Memory kernel $G(s)$ is the Fourier transform of $G^*(\omega)$ of oscillating shear flow.

For a Newtonian viscous fluid $G(s) = \delta(s)$ and for an elastic solid $G(s) = 1$.

Linear viscoelasticity 2

Student Exercise: If $G(t)$ has a single exponential decay,

$$G(t) = G_0 e^{-t/\tau}$$

show that a polar plot of $Re(G^*)$ versus $Im(G^*)$ as (real) ω varies is part of a circle.

Linear viscoelasticity 3

Scalar form for simple shear flow

$$\sigma(t) = \int_0^\infty G(s)\dot{\gamma}(t-s)\, ds$$

Hence steady shear viscosity (plug in $\dot{\gamma} = \text{const}$)

$$\mu(0) = \int_0^\infty G(s)\, ds$$

Hence recoil after stop steady shear flow $\dot{\gamma}_0$

$$-\dot{\gamma}_0 \frac{\int_0^\infty sG(s)\, ds}{\int_0^\infty G(s)\, ds}$$

Student Exercise

Second-order fluid

For weak and slowly varying flows, the first nonlinear correction

$$\sigma = -pI + 2\mu E - 2\alpha \overset{\triangledown}{E} + \beta E \cdot E$$

where

$$\mu = \int_0^\infty G(s)\, ds, \quad \alpha = \int_0^\infty sG(s)\, ds$$

from 'retarded motion' expansion.

Hence Cox-Mertz is correct in the limit $\dot{\gamma} \to 0$, $\omega \to 0$.

Good for dithering Stokes flow, where accumulation of small effects over a long time can produce a significant change.

Dangerous in stability analyses and numerical studies, where bad behaviour can occur outside limitation of weak and slowly varying.

Second-order fluid 2

Student Exercises

In simple shear

- constant viscosity μ
- Normal stress difference $N_1 = 2\alpha\dot{\gamma}^2$, $N_2 = -\frac{1}{4}\beta\dot{\gamma}^2$

In (axisymmetric pure) extensional flow

- $\mu_{\text{ext}} = \mu + \left(\alpha + \frac{1}{4}\beta\right)\dot{\epsilon}$
- but must keep last term small

Generalised Newtonian

Newtonian viscous fluid, except viscosity depends on shear-rate $\dot{\gamma}$,

$$\sigma = -pI + 2\mu(\dot{\gamma})E \qquad \text{where } \dot{\gamma} = \sqrt{2E : E}.$$

Depends on instantaneous flow, i.e. no elastic part and no history.
'Ad hoc' models to fit experimental data

- Power-law
  $$\mu = k\dot{\gamma}^{n-1}, \quad \text{i.e. stress } \sigma \propto \dot{\gamma}^n$$
- Carreau, Yasuda & Cross
  $$\mu = \mu_\infty + (\mu_0 - \mu_\infty)\left(1 + (\tau\dot{\gamma})^a\right)^{(n-1)/a}$$

  with plateaus at high and low $\dot{\gamma}$.

Generalised Newtonian

More 'ad hoc' models.
Yield fluids which only flow if σ exceeds a yield value σ_Y.

- Bingham
  $$\sigma = \begin{cases} \infty, \text{ so } E = 0 & \text{if } \sigma < \sigma_Y \\ \mu_0 + \sigma_Y/\dot{\gamma} & \text{if } \sigma > \sigma_Y \end{cases}$$
- Herchel-Buckley
  $$\sigma = \begin{cases} \infty, \text{ so } E = 0 & \text{if } \sigma < \sigma_Y \\ \mu_0\dot{\gamma}^{n-1} + \sigma_Y/\dot{\gamma} & \text{if } \sigma > \sigma_Y \end{cases}$$

Oldroyd-B model fluid

History dependence through time differentials.
Easier for computing than with time integrals

$$\sigma + \lambda_1 \overset{\triangledown}{\sigma} = 2\mu_0 \left(E + \lambda_2 \overset{\triangledown}{E} \right) \quad \text{with } 0 \leq \lambda_2 \leq \lambda_1.$$

Three constants

- a viscosity μ_0,
- a relaxation time λ_1 and
- a retardation time λ_2.

Special cases

- Maxwell UCM $\lambda_2 = 0$
- Newtonian $\lambda_1 = \lambda_2$

Oldroyd-B model fluid 2

Student Exercises

In simple shear

- constant viscosity $\mu = \mu_0$
- Normal stress difference $N_1 = 2\mu_0(\lambda_1 - \lambda_2)\dot{\gamma}^2$, $N_2 = 0$

In (axisymmetric pure) extensional flow

- $$\mu_{\text{ext}} = \mu_0 \frac{1 - \lambda_2\dot{\epsilon} - 2\lambda_1\lambda_2\dot{\epsilon}^2}{(1 - 2\lambda_1\dot{\epsilon})(1 + \lambda_1\epsilon)}$$
- becomes negative just above $\dot{\epsilon} = 1/2\lambda_1$!!!!!

Variants of Oldroyd-B

- White-Metzner to incorporate shear-thinning $\mu(\dot{\gamma})$

$$\sigma + \frac{\mu(\dot{\gamma})}{G} \overset{\triangledown}{\sigma} = 2\mu(\dot{\gamma})E$$

- Giesekus for positive extensional viscosity

$$\sigma + \frac{\alpha\lambda_1}{\mu_0}\sigma^2 + \lambda_1 \overset{\triangledown}{\sigma} = 2\mu_0 E$$

- PTT-exponential Phan-Thien & Tanner

$$\sigma + \left[\exp\left(\frac{\lambda_1}{\mu_0} \text{trace } \sigma \right) - 1 \right] \sigma + \lambda_1 \overset{\triangledown}{\sigma} = 2\mu_0 E$$

- Multi-mode versions of above

Molecular reformulation of Oldroyd-B

also for better numerics

Microstructure A:

$$\overset{\triangledown}{A} + \frac{f}{\tau}(A - I) = 0$$

Stress σ:

$$\sigma = -pI + 2\mu_0 E + Gf(A - I)$$

Oldroyd-B $f = 1$

FENE modification, for nice behaviour in extensional flow

$$f = \frac{L^2}{L^2 - \text{trace } A}$$

K-BKZ model fluid

Kay-Bernstein-Kearsley-Zappa

History dependence through time integrals
Merging of linear viscoelasticity and nonlinear elasticity

$$\sigma = \int_0^\infty \dot{G}(s) \left[\frac{\partial w}{\partial \alpha} \left(\tilde{A}\tilde{A}^T - I \right) - \frac{\partial w}{\partial \beta} \left(\tilde{A}^{-1\,T} \tilde{A}^{-1} - I \right) \right] ds$$

where the relative deformation from s to t is

$$\tilde{A} = A(t) A^{-1}(t-s)$$

$\frac{\partial w}{\partial \alpha}$ and $\frac{\partial w}{\partial \beta}$ are usually replaced by ϕ_1 and ϕ_2 'damping functions,
not derivatives of some w,
functions of combinations α and β eigenvalues of $\tilde{A}$.

K-BKZ model fluid 2

Student Exercises

In simple shear

$$\mu = \int_0^\infty \dot{G}(s) \left(\phi_1 + \phi_2 \right) s \, ds$$

$$N_1 = \int_0^\infty \dot{G}(s) \left(\phi_1 + \phi_2 \right) s^2 \, ds, \qquad N_2 = -\int_0^\infty \dot{G}(s) \phi_2 s^2 \, ds,$$

In extensional flow

$$\mu_{\text{ext}} = \int_0^\infty \dot{G}(s) \left[\phi_1 \left(e^{2\dot{\epsilon}s} - e^{-\dot{\epsilon}s} \right) + \phi_2 \left(e^{\dot{\epsilon}s} - e^{-2\dot{\epsilon}s} \right) \right] s \, ds / \dot{\epsilon}$$

K-BKZ model fluid 3

Wagner model

$$\phi_2 = 0 \quad \text{so } N_2 = 0$$

and

$$\phi_1 = \exp \left(-k \sqrt{\alpha - 3 + \theta(\beta - \alpha)} \right)$$

In shear shear

$$\phi_1 = \exp \left(-k \dot{\gamma} (t-s) \right)$$