An ellipsoidal drop model for single drop dynamics with non-Newtonian fluids

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Motivation

• Systems consisting of two immiscible substances are important in different fields:
  - Polymer blends
  - Food
  - Biomedics
  - Cosmetics.

• Processing implies interactions between morphology and rheology

• The properties of the final product depend on the properties of the constituents and on the morphology of the system.

Utracki, Polymer Alloys and Blends, 1989
Motivation

• Motivation: Description of the shape of the dispersed phase, and its evolution under the action of a well-controlled flow field.

• **FOCUS**: the effects of *viscoelasticity* of the fluid components on the shape dynamics of isolated droplets

Acknowledgement: Stefano Guido
Basics

- Hypothesis: **dilute** systems, consisting of drops dispersed in a matrix.

- Globular morphology

- In dilute conditions the deformation of the drops and the stress response are only slightly affected by the hydrodynamic interactions between droplets.

- A good description of the deformation of a single drop immersed in a matrix subjected to flow is of value.
The single drop problem

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- The deformation of a buoyancy-free, Newtonian drop immersed in a Newtonian fluid undergoing viscous flow:
  - Perturbation analysis of the Navier-Stokes equations
  - Simulation of the Navier-Stokes equations

- The case of **viscoelastic** components has received less attention for the much more complex constitutive equations.

- Our model is based on the assumption that the drop shape is always **ellipsoidal**.

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Maffettone & Minale, JNNFM, 1998
The model

- The drop is assumed to be **always** an ellipsoid:
  \[ Q(t) : rr = r_0^2 \]
  - \( r_0 \) is the radius of the drop at equilibrium (spherical).
  - \( r \) is the generic position vector of a point on the actual drop surface.

- \( Q(t) \) is a second rank **symmetric** and **positive definite**, and time dependent tensor that describes the ellipsoidal surface.

- The drop dynamics is dictated by relaxation effects and deformation induced by flow.

Maffettone & Greco, J. Rheol, 2004
The model

- From dimensional analysis of the non-Newtonian case: six nondimensional parameters

\[
\begin{align*}
\lambda &= \frac{\eta_D}{\eta} \\
N &= \frac{\Psi_1 r_0 |\nabla \mathbf{v}|^2}{\sigma} = p C a^2 \\
N_D &= \frac{\Psi_{1D} r_0 |\nabla \mathbf{v}|^2}{\sigma} = p_D C a^2
\end{align*}
\]

- \( \lambda \): ratio between the elastic stresses and the interfacial stress.
- \( p \): ratio of a constitutive relaxation time and the interfacial relaxation time.

\[
\begin{align*}
\text{Ca} &= \frac{\eta r_0 |\nabla \mathbf{v}|}{\sigma} \\
\Psi &= -\frac{\Psi_2}{\Psi_1} \\
\Psi_D &= -\frac{\Psi_{2D}}{\Psi_{1D}}
\end{align*}
\]
The model

- The evolutive equation for the tensor $Q(t)$ is

$$\frac{dQ}{dt} - (\Omega \cdot Q - Q \cdot \Omega) + a(D \cdot Q + Q \cdot D) + b D : QI + c D \text{Tr}(Q) = f_1(Q - gI)$$

- $D$: the deformation rate tensor; $\Omega$: vorticity tensor; at infinity.

- LHS expresses the most general symmetry preserving time derivative of tensor $Q$.

- $a, b, c$ are arbitrary numbers.

- A generalization of the analogous equation proposed for the Newtonian case.

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The model

- Dimensionless model:
  \[
  \frac{dQ}{dt} + Ca \left[ - (Q \cdot Q - Q \cdot Q) + a (D \cdot Q + Q \cdot D) + c D \text{Tr}(Q) \right] = f_1 (Q - g I)
  \]

- Volume preservation (det\(Q=\text{cost}\)) \(\Rightarrow b=0\) and:
  \[
  g = \frac{3 - Ca \left\{ \frac{c}{f_1} I_Q D : Q^{-1} \right\}}{II_Q}
  \]

- The coefficients \(a, c, f_1\) are assumed to depend on \(\lambda, \Psi, \Psi_D, p\) and \(p_D\).

- The mathematics of the model is now completely specified

- The model is nonlinear.
The model

- The non-Newtonian model is so built as to recover the steady state in the small deformation limit.

- The phenomenological parameters of the model are determined in the small deformation limit only.

- Thereafter, the model is used to obtain predictions for whatever deformation of the drop, and both at steady state and in time dependent situations.

- First order Ca (steady state and dynamics):
  \[ f_1 = -\frac{40(\lambda + 1)}{(2\lambda + 3)(19\lambda + 16)}, \quad 2a + 3c = \frac{10}{(2\lambda + 3)} \]

The model

- Second order Ca (only steady state):
  - Perturbative (all is known)

\[
r = 1 + \text{Ca} \mathbf{T} : \mathbf{u} \mathbf{u} + \text{Ca}^2 \left[ \mathbf{s}_1 \mathbf{D} :: \mathbf{u} \mathbf{u} \mathbf{u} + \mathbf{s}_2 \mathbf{D} : \mathbf{u} \mathbf{u} + \mathbf{s}_3 \mathbf{D} : \mathbf{D} + \mathbf{s}_4 \left( \mathbf{\Omega} \cdot \mathbf{D} - \mathbf{D} \cdot \mathbf{\Omega} \right) : \mathbf{u} \mathbf{u} \right]
\]

- Ellipsoidal

\[
r = 1 + \text{Ca} \alpha \mathbf{D} : \mathbf{u} \mathbf{u} + \text{Ca}^2 \left[ \frac{3}{2} \alpha^2 \mathbf{D} :: \mathbf{u} \mathbf{u} \mathbf{u} + \frac{2\alpha}{f_1} \mathbf{a} \mathbf{D} : \mathbf{u} \mathbf{u} - \frac{\alpha}{9} \left( \alpha + \frac{4\alpha - 3c}{f_1} \right) \mathbf{D} : \mathbf{D} - \frac{\alpha}{f_1} \left( \mathbf{\Omega} \cdot \mathbf{D} - \mathbf{D} \cdot \mathbf{\Omega} \right) : \mathbf{u} \mathbf{u} \right]
\]

- with \( T = \frac{19\lambda + 16}{8(\lambda + 1)} \)
  \( \alpha = -\frac{2a + 3c}{2f_1} \)
The model

1) \(2Tf_1 + 2a + 3c = 0\) \(\rightarrow\) Steady state behaviour at order Ca
2) \(s_4 f_1 = -T\) \(\rightarrow\) Newtonian \((p=p_D=0)\) dynamics at order Ca
3) \(s_2 f_1 - 2Ta = 0\)
4) \((9s_3 + T^2)f_1 + 4Ta - 3Tc = 0\)

- The linear system is overdetermined. Thus, we arbitrarily chose:
  - Eq 1 and 2 always fulfilled to recover the Newtonian Ca-limit correctly.
  - Two systems with Eqs. 1,2,3 and with Eqs. 1,2,4 solved, and the two solutions averaged.
Predictions - Shear flow

Steady state — shear flow
\( \lambda = 1, p = 1.8, \Psi = -.2, p_D = 0 \)
- Experiments
  - Non-Newtonian model
  - Newtonian model.
Steady state — shear flow
\( \lambda = 1 \),

- Newtonian
- VE Matrix \( p=1 \)
- VE Drop \( p_D=1 \)
Predictions - Elongational flow

- **Steady state under planar elongation**
  - Experiments $\lambda = 1.08$:  
    - Circles: fully Newtonian; ■ $p = 2.95$, $\Psi = 0$, $p_D = 0$;
    - ▲ $p = 4.38$, $\Psi = 0$, $p_D = 0$; ▼ $p = 7.16$, $\Psi = 0$, $p_D = 0$
  - Solid line: Non-Newtonian model

\[
D = \frac{L - B}{L + B}
\]
Predictions - Break-up

Shear

Planar Elongation

Motivation
Outline
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Single drop
The model
Shear Flow
Elong. Flow
Break-up
Startup Shear
Relaxation
Conclusions

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Conclusions

- The phenomenological model describes drop deformation and orientation under the action of a generic flow field imposed “at infinity” was presented.

- The model applies to blends consisting in Newtonian as well as non-Newtonian components.

- The model parameters are determined once and for all in the small deformation limit, by comparison with existing analytic solutions. Thus, no adjustable parameter appears in the model.

- Model predictions agree with experimental results at steady state.
Conclusions

- Break-up predictions are in qualitative agreement with experimental results.

- In the case of viscoelastic phases, the description of transients is accurate only for "low elasticities".

- The model should be improved to adequately describe the dynamics at "large elasticities". No asymptotic limit, however, is available so far.