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
Vinckier et al., J. Rheol., 40, 613, 1996.

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

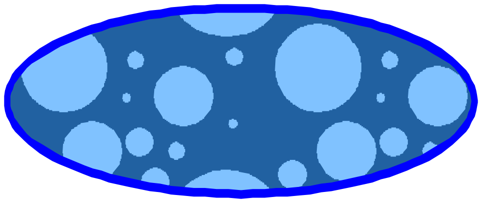
Acknowledgement: Stefano Guido

Outline

- Basics
  - Blends, Morphology, Rheology
- The single drop problem
- The model
  - Viscoelastic Liquids
- Steady flows
- Breakup
- Startup of shear
- Relaxations
- Conclusions

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

- 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**.

Rallison, Ann. Rev. Fluid Mech., 1984;
Kennedy, et al., Computers Fluids, 1994.
Stone, Ann. Rev. Fluid Mech., 1994.
Maffettone & Minale, JNNFM, 1998

The model

- The drop is assumed to be **always** an ellipsoid:

$$\mathbf{Q}(t) : \mathbf{rr} = r_0^2$$

  - r_0 is the radius of the drop at equilibrium (spherical).
  - $\mathbf{r}$ is the generic position vector of a point on the actual drop surface.

- $\mathbf{Q}(t)$ 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

$$\lambda = \frac{\eta_D}{\eta} \qquad Ca = \frac{\eta\, r_0 \left|\nabla \mathbf{v}\right|}{\sigma}$$

$$N = \frac{\Psi_1\, r_0 \left|\nabla \mathbf{v}\right|^2}{\sigma} = p\, Ca^2 \qquad \Psi = -\Psi_2 / \Psi_1$$

$$N_D = \frac{\Psi_{1D}\, r_0 \left|\nabla \mathbf{v}\right|^2}{\sigma} = p_D\, Ca^2 \qquad \Psi_D = -\Psi_{2D} / \Psi_{1D}$$

- N: ratio between the elastic stresses and the interfacial stress.
- p: ratio of a constitutive relaxation time and the interfacial relaxation time.

Greco, JNNFM, 2002

The model

- The evolutive equation for the tensor $\mathbf{Q}(t)$ is

$$\frac{d\mathbf{Q}}{dt}-\left(\boldsymbol{\Omega}\cdot\mathbf{Q}-\mathbf{Q}\cdot\boldsymbol{\Omega}\right)+a\left(\mathbf{D}\cdot\mathbf{Q}+\mathbf{Q}\cdot\mathbf{D}\right)+b\mathbf{D}:\mathbf{QI}+c\mathbf{D}\mathrm{Tr}\left(\mathbf{Q}\right)=f_1\left(\mathbf{Q}-g\,\mathbf{I}\right)$$

- $\mathbf{D}$**:** the deformation rate tensor; $\boldsymbol{\Omega}$**:** vorticity tensor; **at infinity**.
- LHS expresses the most general symmetry preserving time derivative of tensor $\mathbf{Q}$.
- a, b, c are arbitrary numbers.
- A generalization of the analogous equation proposed for the Newtonian case.

Astarita & Marrucci, *Principles of non-Newtonian Fluid Mechanics*, 1974
Maffettone and Minale, JNNFM, 1998.

The model

- Dimensionless model:

$$\frac{d\mathbf{Q}}{dt} + \mathrm{Ca}\left[-(\mathbf{\Omega}\cdot\mathbf{Q} - \mathbf{Q}\cdot\mathbf{\Omega}) + a(\mathbf{D}\cdot\mathbf{Q} + \mathbf{Q}\cdot\mathbf{D}) + c\mathbf{D}\mathrm{Tr}(\mathbf{Q})\right] = f_1(\mathbf{Q} - g\mathbf{I})$$

- Volume preservation ($\det\mathbf{Q}=\mathrm{cost}$) $\Rightarrow$ $b=0$ and:

$$g = \frac{3 - \mathrm{Ca}\dfrac{c}{f_1} I_{\mathbf{Q}} \mathbf{D} : \mathbf{Q}^{-1}}{II_{\mathbf{Q}}}$$

- The coefficients a, c, f_1 are assumed to depend on λ, Ψ, Ψ_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):

$$f_1 = -\frac{40(\lambda+1)}{(2\lambda+3)(19\lambda+16)}, \qquad 2a+3c = \frac{10}{(2\lambda+3)}$$

Rallison, Ann. Rev. Fluid Mech., 1984

The model

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

$$r = 1 + \mathrm{Ca}T\mathbf{D}:\mathbf{uu} + \mathrm{Ca}^2\left[s_1\mathbf{DD}::\mathbf{uuuu} + s_2\mathbf{D}\cdot\mathbf{D}:\mathbf{uu} + s_3\mathbf{D}:\mathbf{D} + s_4\left(\boldsymbol{\Omega}\cdot\mathbf{D} - \mathbf{D}\cdot\boldsymbol{\Omega}\right):\mathbf{uu}\right]$$

  - Ellipsoidal

$$r = 1 + \mathrm{Ca}\alpha\mathbf{D}:\mathbf{uu} + \mathrm{Ca}^2\left[\frac{3}{2}\alpha^2\mathbf{DD}::\mathbf{uuuu} + \frac{2\alpha}{f_1}a\mathbf{D}\cdot\mathbf{D}:\mathbf{uu} - \frac{\alpha}{9}\left(\alpha + \frac{4a-3c}{f_1}\right)\mathbf{D}:\mathbf{D} - \frac{\alpha}{f_1}\left(\boldsymbol{\Omega}\cdot\mathbf{D} - \mathbf{D}\cdot\boldsymbol{\Omega}\right):\mathbf{uu}\right]$$

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

Greco, JNNFM, 2002

The model

1) $2Tf_1 + 2a + 3c = 0$ ← Steady state behaviour at order Ca

2) $s_4 f_1 = -T$ ← Newtonian ($p=p_D=0$) dynamics at order Ca

3) $s_2 f_1 - 2Ta = 0$

4) $\left(9s_3 + T^2\right) f_1 + 4Ta - 3Tc = 0$

- 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

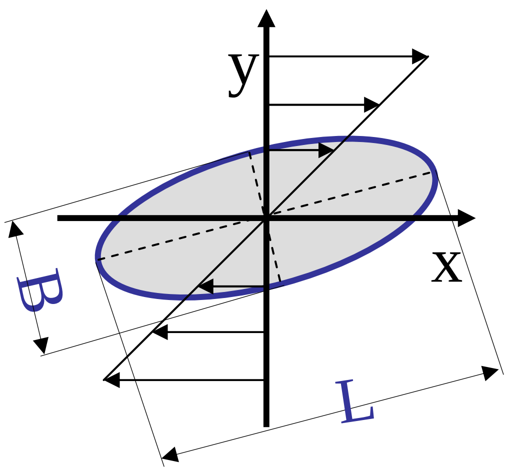
Steady state — shear flow

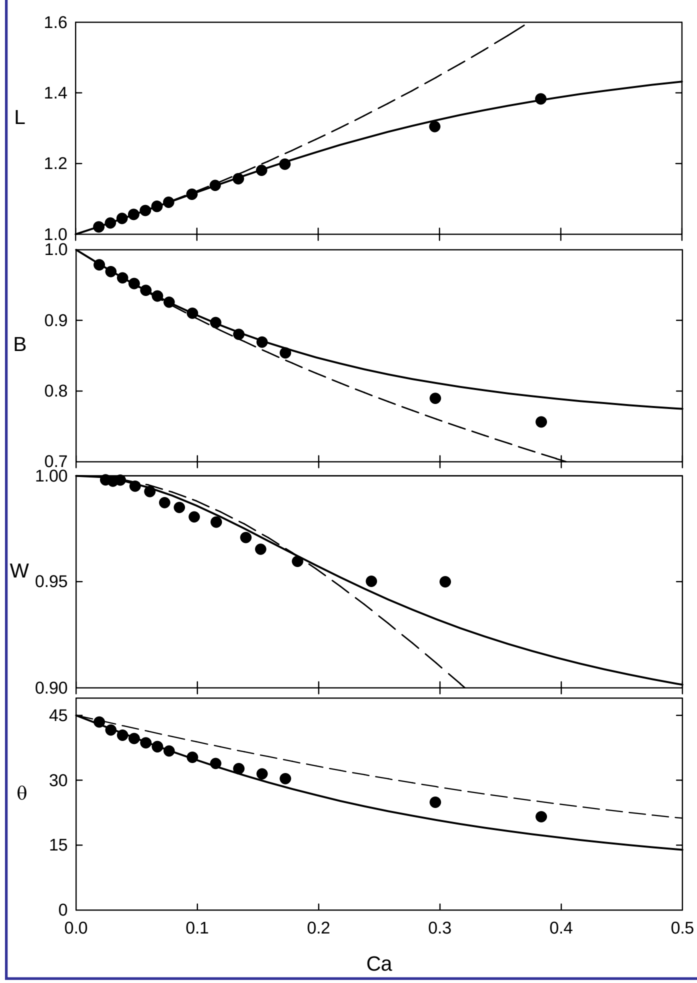
$\lambda=1$, $p=1.8$, $\Psi=-.2$, $p_D=0$

- Experiments

—— Non-Newtonian model

— —Newtonian model.





Predictions – Shear flow

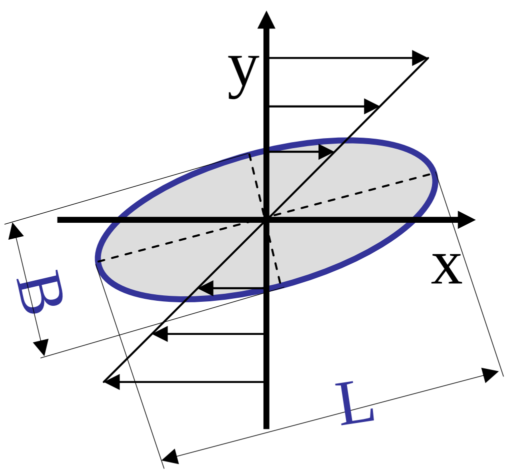
Steady state — shear flow

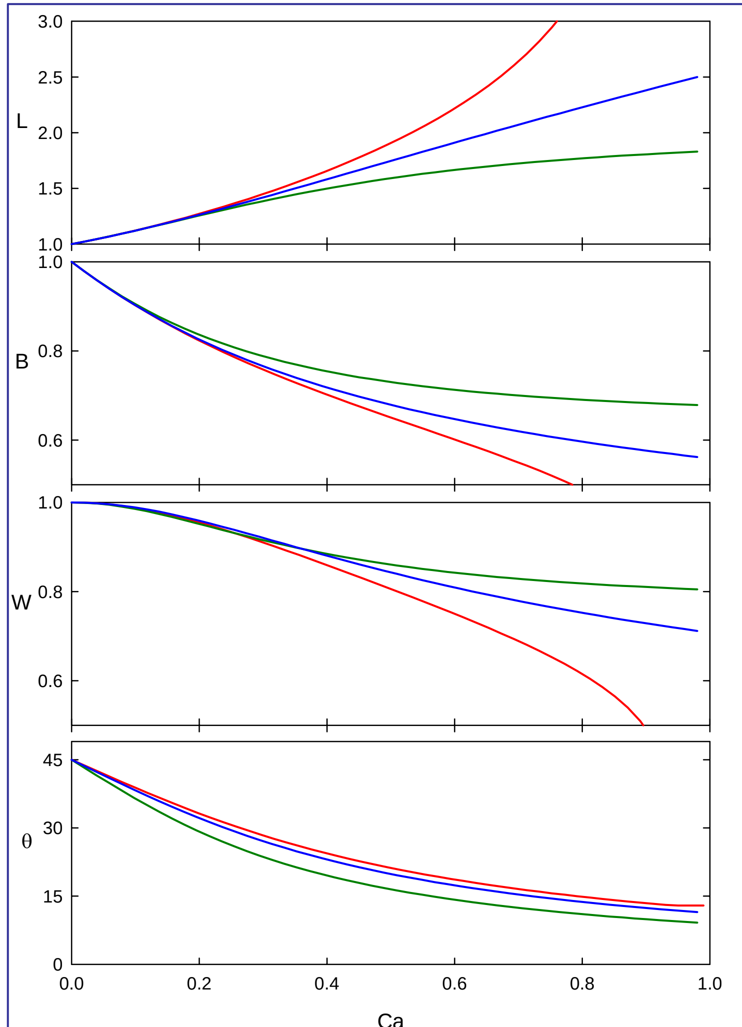
$\lambda=1$,

Newtonian

VE Matrix $p=1$

VE Drop $p_D=1$

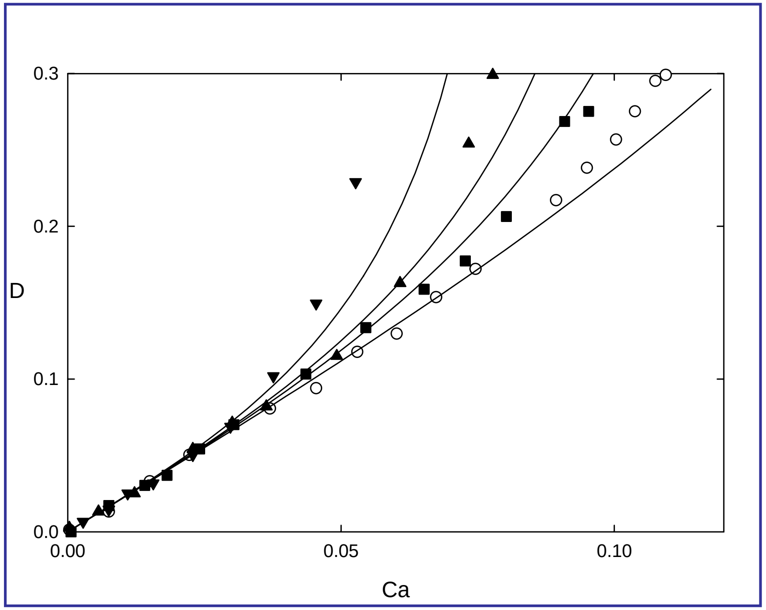




Predictions – Elongational flow

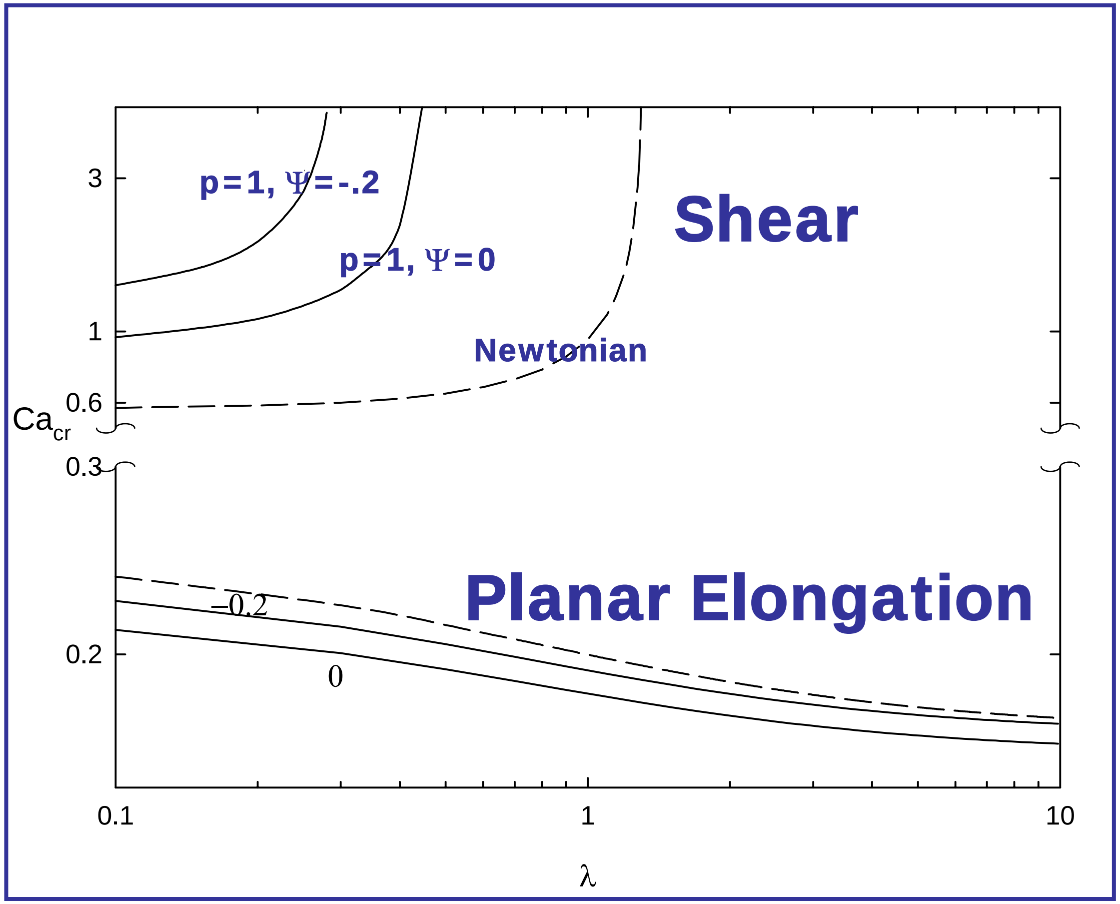
- **Steady state under planar elongation**
  - Experiments λ=1.08: ○ fully Newtonian; ■ p=2.95, Ψ=0, p_D=0; ▲ p=4.38, Ψ=0, p_D=0; ▼ p=7.16, Ψ=0, p_D=0
  - Solid line: Non-Newtonian model

$$D = \frac{L-B}{L+B}$$



Tretheway and Leal, JNNFM, 2001

Predictions – Break-up



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.