Microstructural studies for rheology

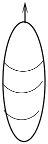
- Micro & macro views
- Einstein viscosity
- Rotations
- Deformations
- Interactions
- Polymers
- Others

Rotations

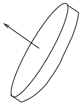
- Rotation of particles
- Macro stress
- Uni-axial straining
  - Extensional viscosity rods
  - Extensional viscosity disks
- Simple shear
  - Shear viscosity
- Anisotropy
- Brownian rotations
  - Macro stress
  - Viscosities
  - Closures

Rotation of particles – rigid and dilute

Spheroid: axes a, b, b, aspect ratio $r = \frac{a}{b}$.



rod $r > 1$



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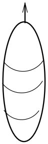

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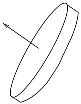

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Direction of axis $\mathbf{p}(t)$, unit vector.

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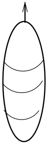

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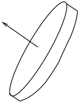

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Direction of axis $\mathbf{p}(t)$, unit vector.

Stokes flow by Oberbeck (1876). See Lamb. Uses ellipsoidal harmonic function in place of spherical harmonic $1/r$

$$\int_{s(\mathbf{x})}^{\infty} \frac{ds'}{\Pi_{i=1}^{3}(a_i^2 + s')^{1/2}}, \qquad \text{where} \quad \sum_{i=1}^{3} \frac{x_i^2}{a_i^2 + s(\mathbf{x})} = 1.$$

Rotation of particles

Microstructural evolution equation

$$\frac{D\mathbf{p}}{Dt} = \Omega \times \mathbf{p} + \tfrac{r^2-1}{r^2+1}\left[\mathbf{E}\cdot\mathbf{p} - \mathbf{p}(\mathbf{p}\cdot\mathbf{E}\cdot\mathbf{p})\right]$$

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Flat disks $\frac{r^2-1}{r^2+1} \to -1$ i.e. Lower Convective Derivative $\overset{\triangle}{A}$

Rotation of particles

Student Exercise

Show that

$$\mathbf{p}(t) = \frac{\mathbf{q}(t)}{|\mathbf{q}(t)|} \quad \text{with} \quad \dot{\mathbf{q}} = \Omega \times \mathbf{q} + \tfrac{r^2-1}{r^2+1}\mathbf{E} \cdot \mathbf{q}$$

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Hence find $\mathbf{p}(t)$ for axisymmetric extensional flow and for simple shear, starting from an arbitrary initial $\mathbf{p}(0)$.

Micro→macro link: stress

$$\overline{\sigma} = -\overline{p}\boldsymbol{I} + 2\mu\mathbf{E} + 2\mu\phi\left[A(\mathbf{p}\cdot\mathbf{E}\cdot\mathbf{p})\mathbf{pp} + B(\mathbf{pp}\cdot\mathbf{E} + \mathbf{E}\cdot\mathbf{pp}) + C\mathbf{E}\right]$$

with A, B, C material constants depending on shape but not size

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	A	B	C
$r \to \infty$	$\frac{r^2}{2(\ln 2r - \frac{3}{2})}$	$\frac{6\ln 2r - 11}{r^2}$	2
$r \to 0$	$\frac{10}{3\pi r}$	$-\frac{8}{3\pi r}$	$\frac{8}{3\pi r}$

Rotation in uni-axial straining

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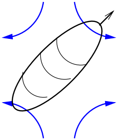

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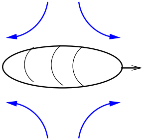

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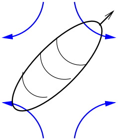

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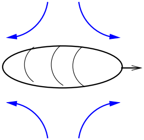

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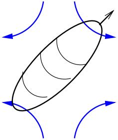

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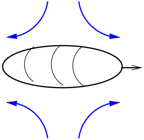

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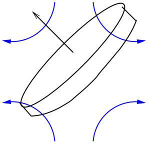

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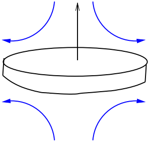

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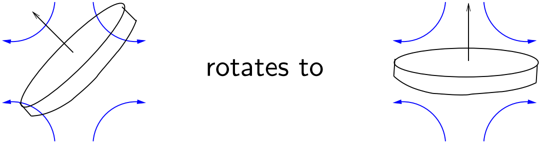

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Effective extensional viscosity for rods

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Dilute requires $na^3 \ll 1$, but extension by Batchelor to semi-dilute $\phi \ll 1 \ll \phi r^2$

$$\mu^*_{\text{ext}} = \mu\left(1 + \frac{4\pi na^3}{9\ln \phi^{-1/2}}\right)$$

Effective extensional viscosity for disks

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No semi-dilute theory, yet.

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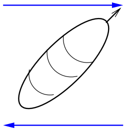

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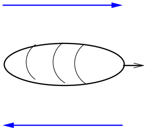

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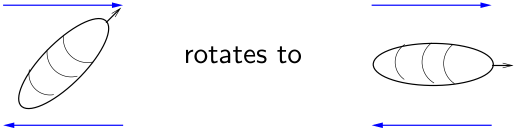

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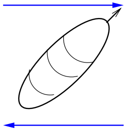

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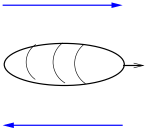

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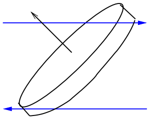

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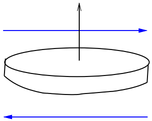

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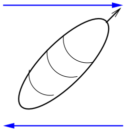

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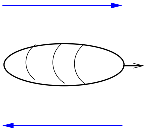

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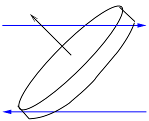

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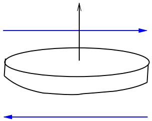

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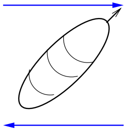

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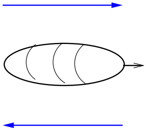

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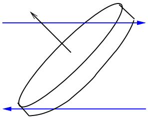

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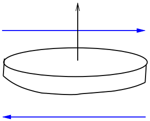

Rotates to lie in flow $\rightarrow$ minimum dissipation

Both Tumble: flip in $1/\gamma$, then align for r/γ $\quad (\delta\theta = 1/r$ with $\dot{\theta} = \gamma/r^2)$

Effective shear viscosity

Jeffery orbits (1922)

$$\begin{aligned}
\dot{\phi} &= \frac{\gamma}{r^2+1}\left(r^2 \cos^2\phi + \sin^2\phi\right) \\
\dot{\theta} &= \frac{\gamma(r^2-1)}{4(r^2+1)} \sin 2\theta \sin 2\phi
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Solution with orbit constant C.

$$\tan\phi = r\tan\omega t, \quad \omega = \frac{\gamma r}{r^2+1}, \quad \tan\theta = Cr(r^2\cos^2\phi + \sin^2\phi)^{-1/2}$$

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Effective shear viscosity   Leal & H (1971)

$$\mu^*_{\mathrm{shear}} = \mu \left(1 + \phi \begin{cases} 0.32r/\ln r & \text{rods} \\ 3.1 & \text{disks} \end{cases} \right)$$

numerical coefficients depend on distribution across orbits, C.

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Important to Turbulent Drag Reduction

Three measures of concentration of rods

$$\begin{cases} \phi r^2 \doteq na^3 & \text{for} \quad \mu^*_{\text{ext}} \\ \phi r \doteq na^2 b & \text{for} \quad \mu^*_{\text{shear}} \\ \phi \doteq nab^2 & \text{for permeability} \end{cases}$$

Brownian rotations – for stress relaxation

Rotary diffusivity: for spheres,

$$D_{\mathrm{rot}} = kT \Big/ 8\pi\mu a^3,$$

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After flow is switched off, particles randomise orientation in time $1/6D \quad \sim 1$ second for $1\mu m$ in water.

State of alignment: probability density $P(\mathbf{p}, t)$ in orientation space $=$ unit sphere $|\mathbf{p}| = 1$.

Brownian rotations – for stress relaxation

Rotary diffusivity: for spheres, rods and disks

$$D_{\mathrm{rot}} = kT \Big/ 8\pi\mu a^3, \quad kT \Big/ \frac{8\pi\mu a^2}{3(\ln 2r - 1.5)}, \quad kT \Big/ \tfrac{8}{3}\mu b^3$$

NB largest dimension, again

After flow is switched off, particles randomise orientation in time $1/6D \quad \sim 1$ second for $1\mu m$ in water.

State of alignment: probability density $P(\mathbf{p}, t)$ in orientation space $=$ unit sphere $|\mathbf{p}| = 1$.

Fokker-Plank equation

$$\frac{\partial P}{\partial t} + \nabla\cdot(\dot{\mathbf{p}}P) = D_{\mathrm{rot}}\nabla^2 P$$

$\dot{\mathbf{p}}(\mathbf{p})$ earlier deterministic.

Average stress over distribution P

Averaged stress

$$\sigma = -pI + 2\mu E + 2\mu\phi[AE : \langle \mathbf{pppp} \rangle + B(E\cdot\langle \mathbf{pp} \rangle + \langle \mathbf{pp} \rangle \cdot E) + CE + FD_{\mathrm{rot}}\langle \mathbf{pp} \rangle]$$

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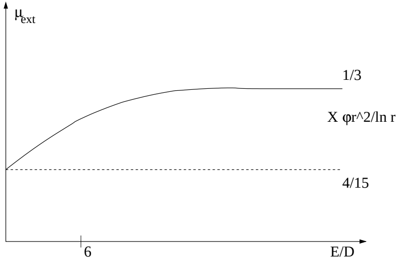
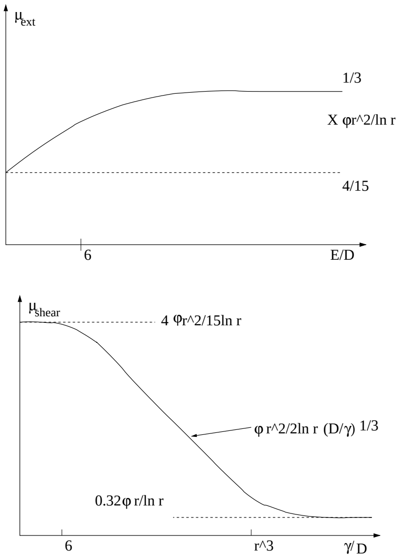
Solve Fokker-Plank: numerical, weak and strong Brownian rotations

Extensional and shear viscosities



Small
strain-hardening

Extensional and shear viscosities



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Large
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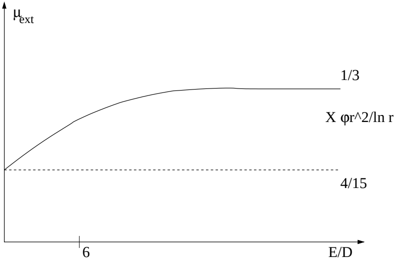

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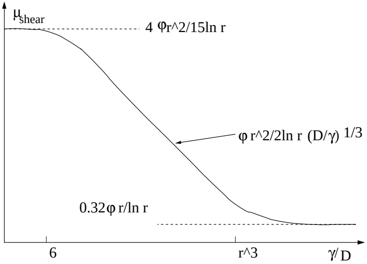

Large shear-thinning

Also $N_1 > 0$,
N_2 small < 0.

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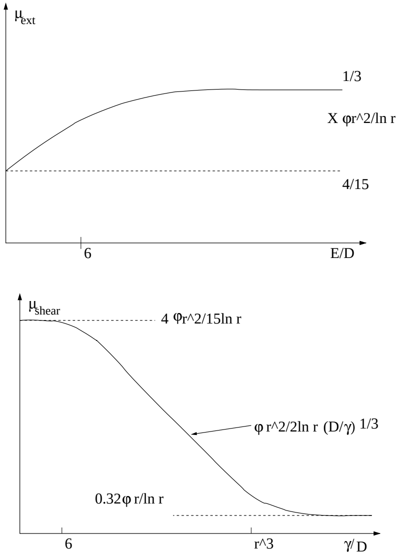

Small
strain-hardening

↕ Orientation effects

Large
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The closure problem

- Second moment of Fokker-Plank equation

$$\frac{D}{Dt}\langle \mathbf{pp}\rangle - \Omega\cdot\langle \mathbf{pp}\rangle\langle \mathbf{pp}\rangle\cdot\Omega$$
$$= \tfrac{r^2-1}{r^2+1}\left[E\cdot\langle \mathbf{pp}\rangle + \langle \mathbf{pp}\rangle\cdot E - 2\langle \mathbf{pppp}\rangle : E\right] - 6D_{\mathrm{rot}}\left[\langle \mathbf{pp}\rangle - \tfrac{1}{3}I\right]$$

Hence this and stress need $\langle \mathbf{pppp}\rangle$, so an infinite hierarchy.

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- New idea Brownian fields: simulate many random walks in orientation space for each point of the complex flow.

Rotations

- Rotation of particles
- Macro stress
- Uni-axial straining
  - Extensional viscosity rods
  - Extensional viscosity disks
- Simple shear
  - Shear viscosity
- Anisotropy
- Brownian rotations
  - Macro stress
  - Viscosities
  - Closures

Microstructural studies for rheology

- Micro & macro views
- Einstein viscosity
- Rotations
- Deformations
- Interactions
- Polymers
- Others

Deformations

- Emulsions
  - Rupture
  - Theories
  - Numerical
- Flexible thread
- Double layer

Emulsions - deformable microstructure

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Reviews: Ann. Rev. Fluid Mech. Rallison (1984), Stone (1994)

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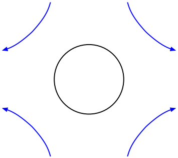

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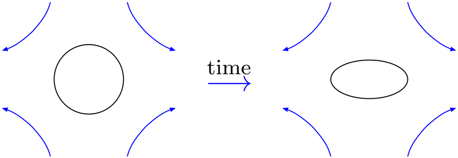

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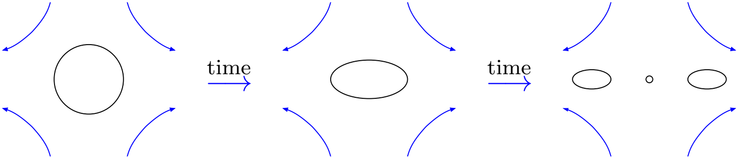

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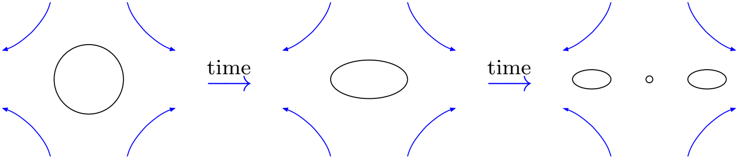
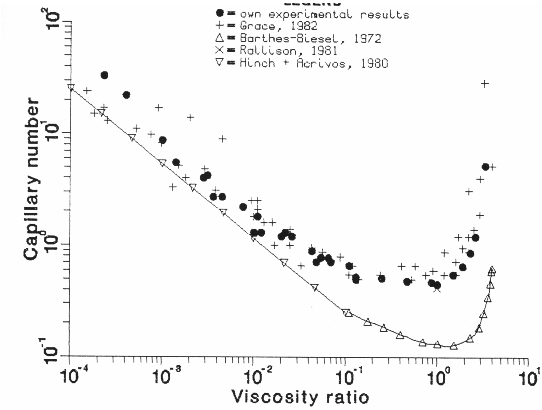


Irreversible reduction in size to $a_* = T/\mu_{\text{ext}}E$, as coalescence very slow.

Rupture in shear flow

$$\frac{T}{\mu_{\mathrm{ext}} Ea}$$



$$\frac{\mu_{\mathrm{int}}}{\mu_{\mathrm{ext}}}$$

Experiments: de Bruijn (1989) (=own), Grace (1982)

Theories: Barthes-Biesel (1972), Rallison (1981), Hinch & Acrivos (1980)

Rupture difficult if $\mu_{\mathrm{int}} \ll \mu_{\mathrm{ext}}$

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$$\mu_{\text{ext}} E > \frac{T}{a} \begin{cases} 0.54 \left(\mu_{\text{ext}}/\mu_{\text{int}}\right)^{2/3} & \text{simple shear} \\ & \end{cases}$$

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but tip-streaming with mobile surfactants (makes rigid end-cap)

$$\mu_{\mathrm{ext}} E > \frac{T}{a} 0.56$$

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- until can rupture when $\mu_{\rm int} \leq 3\mu_{\rm ext}$

Theoretical studies: small deformations

Small ellipsoidal deformation

$$r = a\,(1 + \mathbf{x}\cdot\mathbf{A}(t)\cdot\mathbf{x} + \quad \text{higher orders})$$

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Stokes flow with help of computerised algebra manipulator

$$\frac{D\mathbf{A}}{Dt} - \Omega\cdot\mathbf{A} + \mathbf{A}\cdot\Omega = 2k_1\mathbf{E} + k_5(\mathbf{A}\cdot\mathbf{E} + \mathbf{E}\cdot\mathbf{A}) + \dots$$
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k_1 inefficiency of rotating by straining

Inefficiency of rotating by straining

Student Exercise

Consider the constitutive equation

$$\sigma = -pI + 2\mu_0 E + GA$$

$$\frac{DA}{Dt} - \Omega \cdot A + A \cdot \Omega - \alpha \left(E \cdot A + A \cdot E \right) = -\frac{1}{\tau} \left(A - I \right),$$

$$\text{in flow} \quad u = (\Omega + E) \cdot x.$$

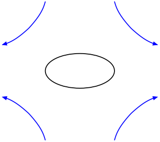
Solve for σ in steady simple shear, finding the shear viscosity and normal stress differences.

Find the condition on the parameters for the shear stress to be a monotonic increasing function of the shear-rate (non-shear-banding).

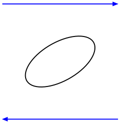
Theoretical studies: small deformations 2

Equilibrium shapes before rupture

extension



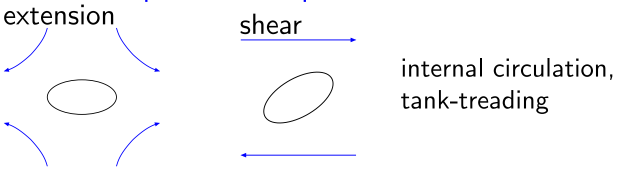
shear



internal circulation,
tank-treading

Theoretical studies: small deformations 2

Equilibrium shapes before rupture

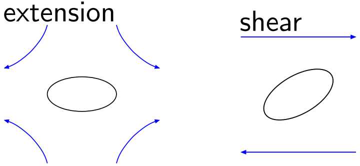


Rheology before rupture

Small strain-hardening, small shear-thinning, $N_1 > 0$, $N_2 < 0$.

Theoretical studies: small deformations 2

Equilibrium shapes before rupture



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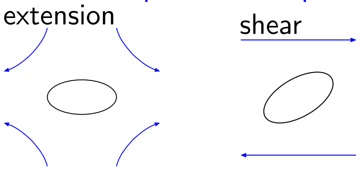

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Form of constitutive equation

$$\frac{d}{dt}(\text{state}) \quad \& \quad \sigma \qquad \text{linear in} \quad \mathbf{E} \quad \& \quad \frac{T}{\mu_{\text{ext}} a}$$

Numerical studies: boundary integral method

deformation

angle

σ_{xy}

$N_1, \; N_2$

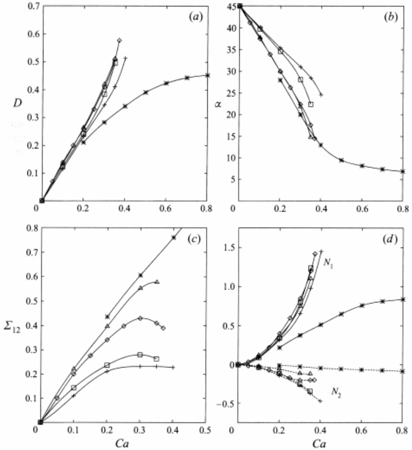

FIGURE 12. Steady-state results as a function of capillary number for $\phi = 10\%$; (*a*) average steady-state drop deformation, (*b*) drop orientation, (*c*) shear stress contribution of drops, and (*d*) contribution of drops to normal stresses: first normal stress difference (solid curves), second normal stress difference (dashed curves); $\lambda = 0$ (+), $\lambda = 0.2$ (□), $\lambda = 1$ (◇), $\lambda = 2$ (△), $\lambda = 5$ (*).

Different λ. No rupture for $\lambda = 5$ (*)

Flexible thread – deformable microstructure

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Position $\mathbf{x}(s,t)$, arc length s, tension $T(s,t)$

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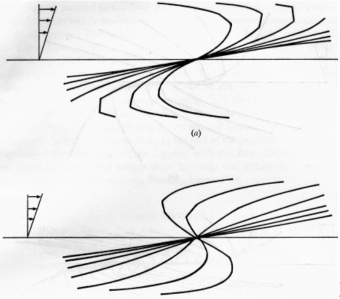

Snap straight

Electrical double layer on isolated sphere

– another deformable microstructure

Electrical double layer on isolated sphere

– another deformable microstructure

- Charged colloidal particle.

Electrical double layer on isolated sphere

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- $\longrightarrow$ very small change in Einstein $\frac{5}{2}$.

Deformations

- Emulsions
  - Rupture
  - Theories
  - Numerical
- Flexible thread
- Double layer

Microstructural studies for rheology

- Micro & macro views
- Einstein viscosity
- Rotations
- Deformations
- Interactions
- Polymers
- Others

Interactions

- Hydrodynamic
  - Dilute
  - Experiments
  - Numerical
- Electrical double-layer
  - Concentrated
- van der Waals
- Fibres
- Drops
  - Numerical

Hydrodynamic interactions for rigid spheres

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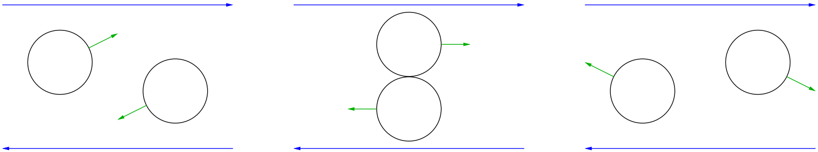

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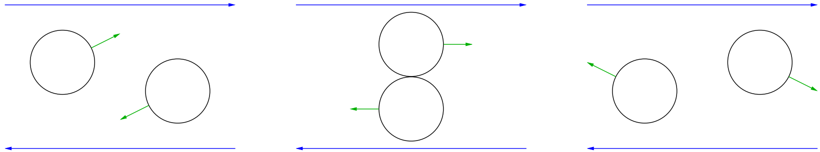

Reversible (spheres + Stokes flow) $\rightarrow$ return to original streamlines

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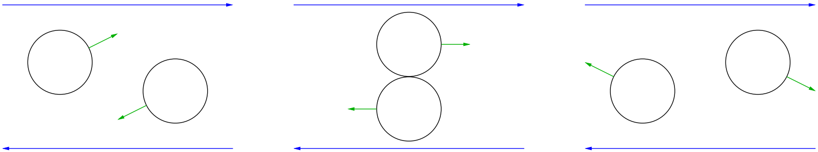

Reversible (spheres + Stokes flow) $\rightarrow$ return to original streamlines

But minimum separation is $\frac{1}{2}\,10^{-4}$ radius $\rightarrow$ sensitive to roughness (typically 1%) when do not return to original streamlines.

Summing dilute interactions

Divergent integral from $\nabla \mathbf{u} \sim \dfrac{1}{r^3}$

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- 7.6 for strong extensional flow

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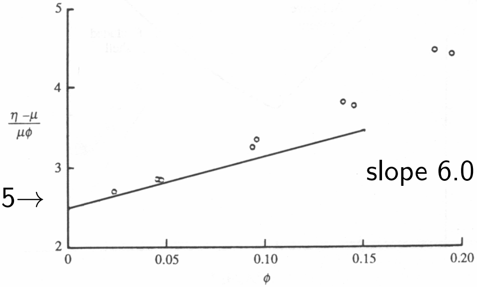
Small strain-hardening, small shear-thinning

Test of Batchelor ϕ^2 result

$$\mu^* = \mu \left[1 + 2.5\phi + 6.0\phi^2\right]$$

Fig. 14.17. Low shear viscosity for dilute suspensions of hard spheres (Russel, 1980): ○, data for polystyrene latices ($a = 42$, 87 nm) in water (Saunders, 1961); ——, theory of Batchelor (1977).

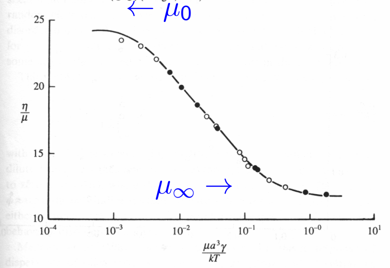


Russel, Saville, Schowalter 1989

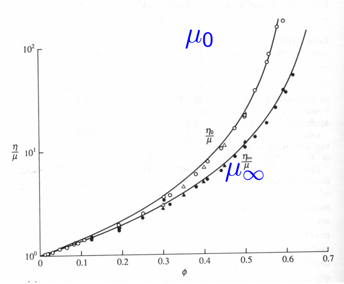
Experiments – concentrated

Effective viscosities in shear flow

Fig. 14.3. Relative steady shear viscosity as function of Peclet number for polystyrene latices of radii listed in Table 14.3 dispersed in water (——) and benzyl alcohol or meta-cresol (○ ●) (Krieger, 1972).



$\mu a^3 \gamma / kT$



ϕ

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Stokesian Dynamics

– (mostly) pairwise additive hydrodynamics

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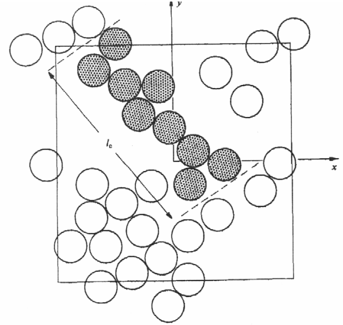
Jamming/locking – clusters across the compressive quadrant



Brady & Bossis (1985)

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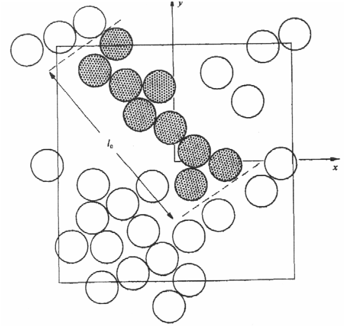
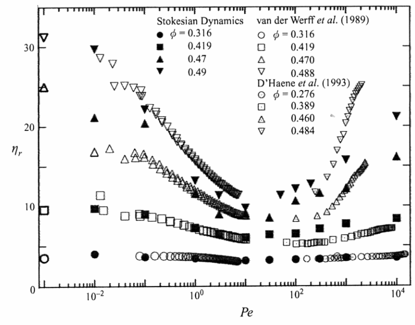


Brady & Bossis (1985)

Fragile clusters if include soft repulsion or Brownian motion

Stokesian Dynamics 2

Effective viscosity in shear flow



Foss & Brady (2000)

'Stokesian Dynamics' Brady & Bossis
Ann. Rev. Fluid Mech. (1988)

Electrical double-layer interactions

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Interaction distance r_*:

$$6\mu\mu a\gamma r_* = \frac{\epsilon\zeta^2 a^2\kappa}{r_*} e^{-\kappa(r_* - 2a)}$$

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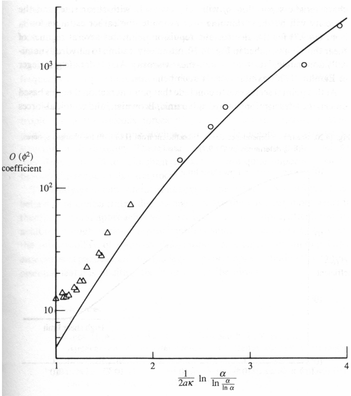
ϕ^2 coefficient as function of $\frac{r_*}{a}$



Experiments – concentrated

Stress as function of shear-rate at different pH.
Suspension of $0.33\mu m$ aluminium particles at $\phi = 0.3$

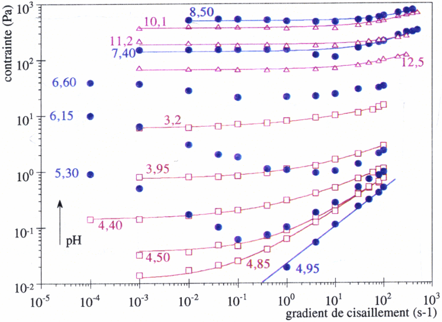


***Fig.3** : Courbes d'écoulement de suspensions d'alumine P772SB, en fonction du pH,*
ϕ_v=0,30.

Ducerf (Grenoble PhD 1992)

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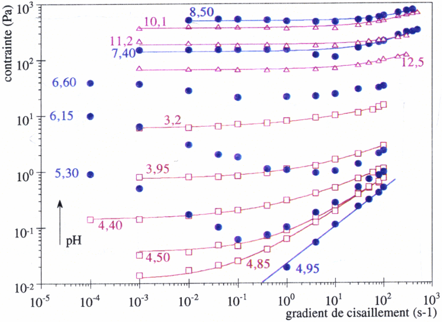

***Fig.3 :** Courbes d'écoulement de suspensions d'alumine P772SB, en fonction du pH, ϕ_v=0,30.*

Ducerf (Grenoble PhD 1992)

Note yield stress very sensitive to pH

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Breakdown of structure in rheology $\mu(\gamma)$

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but shear viscosity $\propto \phi r$ is only big if aligned.

Disk not random if $\phi \frac{1}{r} > 1$.

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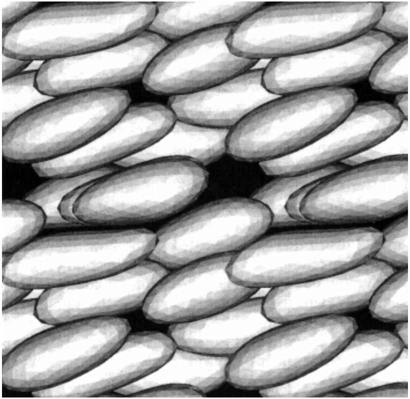
  - slippery particle, no co-rotation problems
- Faster flow $\rightarrow$ more deformed $\rightarrow$ wider gaps in collisions
- Deformed shape has lower collision cross-section

  so 'dilute' at $\phi = 0.3$, blood works!

Numerical studies: boundary integral method

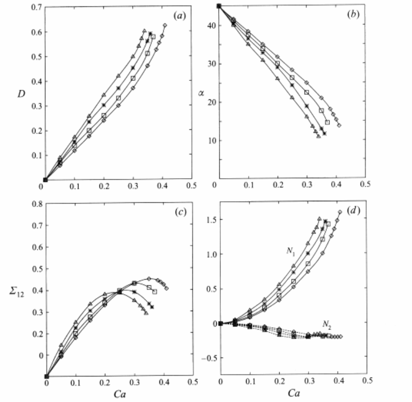


$\phi = 0.3$, $Ca = \mu_{\rm ext}\gamma a/T = 0.3$ $\lambda = 1$, $\gamma t = 10$,
12 drops, each 320 triangles.

Numerical studies: boundary integral method 3

deformation

angle



σ_{xy}

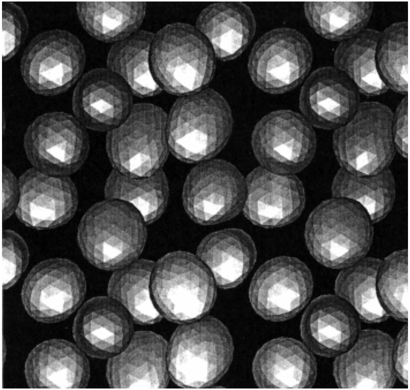
$N_1, \; N_2$

FIGURE 10. Steady-state results as a function of capillary number for $\lambda = 1$. (*a*) Average steady-state drop deformation, (*b*) drop orientation, (*c*) shear stress contribution of drops, and (*d*) contribution of drops to normal stresses: first normal stress difference (solid curves), second normal stress difference (dashed curves); $\phi = 0$ (◇), $\phi = 10\%$ (□), $\phi = 20\%$ (*), $\phi = 30\%$ (△).

$\lambda = 1$, different $\phi = 0, 0.1, 0.2, 0.3$. Effectively dilute at $\phi = 0.3$.

Numerical studies: boundary integral method 4

Reduced cross-section for collisions



into flow

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  - Dilute
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