Morphological transitions of flexible filaments in viscous flows

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Flexible fibers and fiber suspensions

**Biological objects**

- Credit: Dartmouth College

**Flow sensors, valves**

- Attia et al (2009)
- Alvarado Nature Physics 2017

**Industrial applications**

- Schlumberger

Lost circulation problems in oil wells

Interactions between flexible fibers and flows present in numerous situations
Understanding of freely transported fibers and suspension properties still uncomplete.
Aim of the present study

I. Understand microscopic particle dynamics

II. Understand macroscopic suspension properties

Our experimental model system
Flexible Brownian filaments

Actin filament

$L \sim 4 - 40 \mu m$
$d \sim 8nm$
$\epsilon = d/L \ll 1$
Forces at play and dimensionless numbers

\[ \epsilon = \frac{d}{L} \ll 1 \]

Viscous drag force
\[ \sim \mu \gamma L^2 \]

Elasto-viscous number
\[ \bar{\mu} = \frac{\text{viscous force}}{\text{elastic force}} \]

Elastic restoring force
\[ \sim \frac{B}{L^2} \]

Slenderness
\[ c(\epsilon) \]

Stokes equation

Filament-fluid interactions
\[ Re \ll 1 \]

Brownian effect
\[ \ell_p \]

Brownian forces
\[ \sim \frac{k_B T}{L} \]

L ~ 10 \mu m

Elastic force
\[ \frac{\ell_p}{L} = \frac{\text{elastic force}}{\text{Brownian forces}} \]
Actin filaments – wide spread biopolymer

Well controlled assembly in the laboratory – stabilized and fluorescently labelled

Pointed end (−)

Barbed end (+)

Actin monomers
Brownian motion

Spontaneous nucleus

(−) (+)

Actin monomer

Alexa 488 Phallloidin

(−) (+)
Persistence length of actin filaments

Persistence length
\[ \ell_p = 17 \pm 1 \mu m \]

Bending rigidity:
\[ B = \ell_p \times k_B T \]
\[ \sim 7 \times 10^{-26} \text{N} \cdot \text{m}^2 \]
Filaments in shear flow

**Combination of tumbling and periodic deformation**

**Theory**

Becker & Shelley, 2001  
Also Tornberg & Shelley 2004,  
Nguyen & Fauci, 2014

**Experiments**

Forgacs & Mason, 1959, Harasim et al, 2013

See also Du Roure, AL, Shelley et al, ARFM, 2019

Complete picture of the dynamics still missing.
Experimental set-up

- Elasto-viscous number
  \[ \bar{\mu} = 8\pi \dot{\gamma} \mu L^4/B \sim 10^3 - 10^7 \]

- Slenderness
  \[ c \sim 14 \pm 2 \]

- Brownian effect
  \[ \frac{\ell_p}{L} \sim 0.5 - 6 \]
Experimental observations

Rodlike tumbling

$L = 4.9 \mu m$
$\dot{\gamma} = 2.7 s^{-1}$

S bending snake turn

$L = 26.6 \mu m$
$\dot{\gamma} = 1.8 s^{-1}$

C shape buckling and tumbling

$L = 5.5 \mu m$
$\dot{\gamma} = 3.8 s^{-1}$

$L = 6.2 \mu m$
$\dot{\gamma} = 1.3 s^{-1}$

U bending snake turn

$L = 33.5 \mu m$
$\dot{\gamma} = 1.5 s^{-1}$
Experimental observations

<table>
<thead>
<tr>
<th>Tumbling</th>
<th>C buckling</th>
<th>U snake Turn</th>
<th>S snake turn</th>
<th>Complex dynamics</th>
</tr>
</thead>
</table>

Increase elasto-viscous numer $\bar{\mu} \sim \dot{\gamma}L^4$
Comparison with numerical simulations

\[ \mathbf{r}_t - \bar{\mu} \mathbf{U}_0(\mathbf{r}) = - (\Lambda(c) + K) \left[ \mathbf{r}_{ssss} - (\sigma \mathbf{r}_s)_s + \sqrt{\frac{L}{l_p \zeta}} \right] \]

- **Hydrodynamics:**
  - Non-local slender body theory
- **Flexibility:**
  - Euler–Bernoulli beam elasticity
- **Brownian force distribution**
  - Fluctuation-dissipation theorem

Simulations: Chakrabarti B. & Saintillan D.

\[ \bar{\mu} = 2.0E6 \quad c = 14.6 \quad \ell_p/L = 0.83 \]
Filament dynamics and morphologies

- Tumbling
- C Buckling
- U Turn
- S Turn
- Transitional

\[ \frac{\ell_p}{L} \]

\[ \mu/c \]

- \( \approx 250 - 300 \)
- \( \approx 1500 - 2000 \)

Liu, AL et al. PNAS 2018
First transition: buckling instability

Linear stability analysis: $\bar{\mu}/c = 304.6$
Becker and Shelley, 2001
AL and Shelley, Elastic fibers in flows, 2015

Numerical simulations

Experimentally observed in straining flows
Kantsler et al, (2012)
Quennouz, AL, Shelley et al., JFM, 2015
Young and Shelley, PRL, 2007

First observation in shear flow

Becker and Shelley, 2001
Second transition: U-turn

Buckling
J shape

Force Balance
Torque Balance
Energy conservation

J shape only exists above \( \bar{\mu}/c \approx 1700 \)

Liu, AL et al. PNAS 2018
The elastic energy is a measure of the integrated filament curvature and the conformation dynamics are obtained from the gyration tensor.

Microscopic properties are expected to dictate macroscopic behavior.
Filaments in straining flows

*Stagnation point*

Long residence time in homogeneous straining flow
Hyperbolic flow to provide homogeneous strain rate

Optimized microfluidic flow geometry

**Flow focusing**

with M. Oliveira, K. Zografos, J. Fidalgo, U Strathclyde

Zografos K, et al., Biomicrofluidics, 2016
Liu, Zografos, AL et al. in preparation
Optimized microfluidic flow geometry

Velocity profile

\[ u / \bar{u} \]

Strain rate profile

\[ \dot{\epsilon} / (\bar{u} / W_u) \]
Motorized stage to track filaments

- Keep filaments in frame
- Limit image blur

Image blur $\leq \pm 0.5 \mu m$

Keep filament in frame

$\Delta t = 50 ms$

$\Delta u \cdot \Delta t \leq 0.01 \mu m$
Experimental observations
Comparison with simulations

With Brownian fluctuations

Chakrabarti, AL, et al, Nature Physics, 2020
Comparison with simulations

With Brownian fluctuations

Without Brownian fluctuations (simulations)

Simulations J. Lagrone, L. Fauci, R. Cortez, Tulane University
Linear stability analysis

Helicoidal shape can be explained by linear stability analysis: odd and even, in and out of plane modes grow simultaneously -> helicoidal shape is obtained.
Weakly non-linear stability analysis

In and out of plane modes couple in weakly non-linear analysis -> helicoidal shape is always obtained.

Chakrabarti, AL, et al, Nature Physics, 2020
Helix shape – time evolution

Radius and length evolution

Compression rate

What about the final radius?
Helix shape – radius

Radius as a function of length

Radius as a function of the elasto-viscous length

Two length scales in the problem:
Filament length and **elasto-viscous length**

\[ R \sim \left( \frac{B}{\mu \dot{e}} \right)^{1/4} \]
Formation of helicoidal shapes

**Under compression**

Chelakkot et al., 2012

Mercader et al., 2010

Allende et al., 2018

**In shear**

Nguyen & Fauci, 2014

Pieuchot et al., 2015

Very general phenomenon, only requires strong enough compression, mostly overlooked so far.
Suspension rheology – flexible fiber suspensions

Tornberg and Shelley, 2004

Becker and Shelley, 2001

Perazzo, PNAS, 2017

Kirchenbuechler et al., 2014
See also Huber et al, 2014

No experimental results in the dilute regime. No simulations of flexible Brownian fibers in 3D.
Suspension rheology – 2D predictions (non-Brownian)

**Sharp onset of non-Newtonian properties at buckling threshold**

**First normal stress difference**

- Starts to grow at buckling threshold

**Shear viscosity**

- Buckling induces shear thinning
**Suspension rheology – 3D Brownian**

Brownian rotational noise induces shear thinning as well as normal stress differences already for rigid rods.

Buckling threshold blurred due to Brownian fluctuations as well as 3D orientation distributions.

\[ \bar{\mu} = \frac{8\pi\mu\dot{\gamma}L^4}{Bc} \]
\[ Pe = \dot{\gamma}d^{-1} \]
\[ Pe_r = \frac{\mu c \ell_p}{24\ln(2r)/L} \]

Brownian rigid fibers from: EJ Hinch and LG Leal., JFM, 1972.
Suspension rheology – Gyration tensor

Average orientation

- With increasing Pe number fibers become more and more aligned with flow direction
- Initiation of U-turns lead to a sharper decrease, corresponding to folded aligned conformations
- Change in scaling observed slightly earlier for viscosity and normal stress difference indicates importance of buckling events on rheology.

Gyration tensor contribution

What about experiments?
Experimental measurements – monodisperse suspensions

Spectrin actin seed

A drop of filament suspension

Polylysine charged slide: attracting filaments to the surface

\[ \langle L \rangle = 6.4 \mu m \]
Length distribution

Short

\(L_{\text{max}} = 4 \mu m\)
\(\bar{L} = 4.3 \pm 1.2 \mu m\)
\(\varphi = 0.4\%

Middle

\(L_{\text{max}} = 8.8 \mu m\)
\(\bar{L} = 9.6 \pm 3.1 \mu m\)
\(\varphi = 7.5\%

Long

\(L_{\text{max}} = 16.1 \mu m\)
\(\bar{L} = 15.1 \pm 5 \mu m\)
\(\varphi = 23.9\%\)
Experimental measurements - rheometer

Y channel has proven to be very sensitive to small viscosity differences

\[ \frac{w_1}{w_2} = \frac{\mu_1}{\mu_2} \]

\[ W = 600\mu m \]

Gachelin, AL et al, PRL, 2013
Viscosity measurements – very preliminary

Actin filament suspension
Reference fluid
Middle
Walls
Flow rate increasing

Entangled suspension

\[ \bar{L} = 4.3 \mu m \quad \varphi = 0.4\% \]
Summary – fiber morphologies

**Fiber morphologies in shear and compressive flows flow**

- Comprehensive understanding

**Suspension properties**

- Preliminary results
  - To be continued!
**PhD students and Post-Docs**

Yanan Liu  
Brato Chakrabarti (UCSD)  
Joana Fidalgo (Strathclyde)  
John Lagrone (Tulane)

**Colleagues**

Olivia du Roure (ESPCI)  
David Saintillan (UCSD, USA)  
Ricardo Cortez (Tulane, USA)  
Lisa Fauci (Tulane, USA)  
Monica Oliveira (Strathclyde)

Biochemistry:  
Antoine Jégou & Guillaume Romet Lemonne (IJM)
Further reading

Review papers on fluid structure interactions and flexible fibers

- Fluid-Structure Interactions in Low-Reynolds-Number Flows, editors Camille Duprat and Howard Stone, RSC Soft Matter Series

Papers on which the talk was based

- B. Chakrabarti, Y. Liu, J. LaGrone, R. Cortez, L. Fauci, O. du Roure, D. Saintillan, A. Lindner, Flexible filaments buckle into helicoidal shapes in strong compressional flows, Nature Physics, 2020
- B. Chakrabarti, Y. Liu, O. du Roure, A. Lindner, and D. Saintillan, Signatures of elastoviscous buckling in the dilute rheology of stiff polymers, in preparation