

Dynamics of individual Brownian rods in a microchannel flow

Andreas Zöttl, Kira E. Klop, Andrew K. Balin, Yongxiang Gao, Julia M. Yeomans, and Dirk G. A. L. Aarts

Summary by Faustine Gomand

Abstract

This paper deals with the orientational dynamics of microrods ($\sim 3 \mu\text{m}$) in a horizontal Hele-Shaw channel (*i.e.* Poiseuille flow in xz plane). Highlights are:

- Rotational diffusion impacts particles' orbits
 - Persistence of Jeffery orbits is quantified using temporal correlation functions
 - The rods lose their memory of their initial configurations after half a Jeffery period.
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1. THE JEFFERY ORBIT

Jeffery described in 1922 that single, non-Brownian ellipsoidal rods undergo in a simple shear flow a period motion on what is called "the unit sphere" (sphere of radius 1 centered on the object).

The orbit of a particle is determined by:

- Its aspect ratio λ ,
- The shear rate $\dot{\gamma}$,
- The Jeffery constant C such as defined in the figure below:

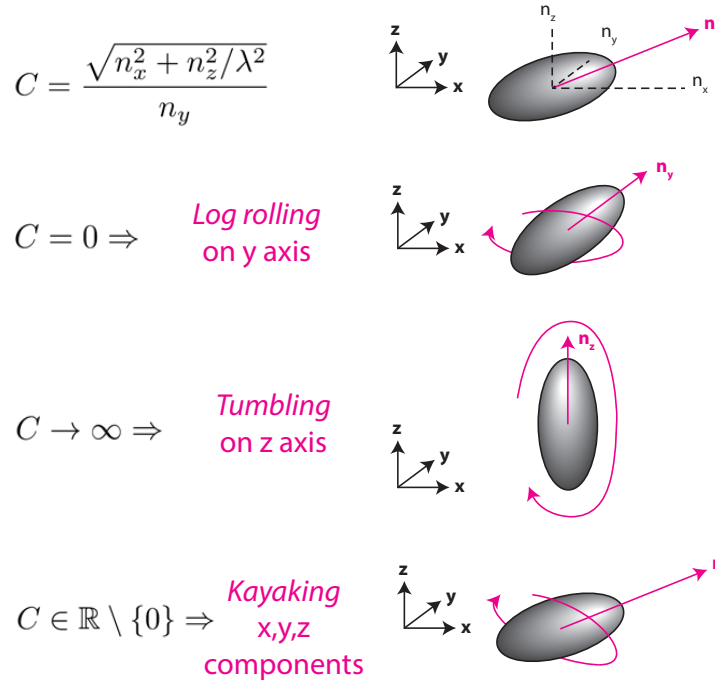


Figure 1: Different Jeffery orbits for an ellipsoidal particle depending on its Jeffery constant value C .

The *reproducibility* and *longevity* of the orbits may be affected by many experimental parameters:

- deviations,
- proximity to the walls,
- inertia,
- viscoelasticity of the shearing fluid,
- Brownian noise (neglectable for $l \sim 30\mu\text{m}$).

At small scale ($l \sim 3 - 30\mu\text{m}$), the orientational state undergoes a **fast decorrelation** due to a **competition between the Jeffery rotation and the rotational Brownian motion**.

2. EXPERIMENTS AND SIMULATIONS

Setup and input parameters	Output parameters
Hele-Shaw horizontal cell S-shape channel (2 bends) Plasma-cleaned channel Bright field Img series of 1,000 frames, 10 fps	Times and positions Orientation in xy plane Length L_p projected to the xy plane Velocity (distance travelled in a frame) Angle in xy $\phi = \arctan(n_y/ n_x)$ Angle in xz $\theta = \arcsin(n_z) = \arcsin\left(\frac{\lambda L_p/(L-1)}{\lambda-1}\right)$

Table 1: Experimental setup and output parameters recorded by Zöttl et al., 2019; λ aspect ratio, L average rod length.

- Most rods were able to **change sign of \mathbf{n}_y** and tumble in the xy plane *i.e.* perform **kayaking** which is not possible for non-Brownian objects,
- Simple Jeffery motion in xz was **not observed**,
- Dynamics seem **aperiodic**: apparent random jumping between orbits characterized by different values of the Jeffery constant C .

Brownian dynamics simulations were performed to obtain the rod velocity $\dot{\mathbf{r}}$ and the orientation rate $\dot{\mathbf{n}}$:

$$\begin{cases} \text{Translational terms: } \dot{\mathbf{r}} = \mathbf{v}_f - v_s \hat{\mathbf{z}} + \mathcal{H} \cdot \xi \\ \text{Rotational terms: } \dot{\mathbf{n}} = \Omega_J(\mathbf{n}; z) + \sqrt{2D_r} \xi_r \end{cases} \quad (1)$$

With \mathbf{v}_f Poiseuille flow (planar), v_s sedimentation velocity, \mathcal{H} translational diffusion of the rod, ξ translational Gaussian white noise, $\Omega_J(\mathbf{n}; z)$ Jeffery reorientation rate (linearly depending on the local shear rate $\dot{\gamma}_l(z) = \dot{\gamma}(1 - 2z/H)$, with H the channel height), D_r rotational diffusion coefficient, and ξ_r rotational Gaussian white noise. These simulations were in good agreement with experiments taking $\dot{\gamma} = 18s^{-1}$.

3. COMPETITION BETWEEN JEFFERY ORBITS AND NOISE

Instantaneous Jeffery constants $C(t)$ are calculated that map a **modified Jeffery constant C'** :

$$C' = \frac{\text{sign}(C)}{1 + |C|} = \frac{\text{sign}(C)}{1 + \left| \frac{\sqrt{n_x^2 + n_z^2/\lambda^2}}{n_y} \right|} \quad (2)$$

$$\begin{cases} \text{Tumbles, xz plane: } C' = 0 \Leftrightarrow C \rightarrow \infty \\ \text{Log rolls, xy plane: } C' = \pm 1 \Leftrightarrow C = 0 \end{cases} \quad (3)$$

Zöttl et al. obtained C' maxima for both simulations and experiments at $C' \pm 0.25$ (closer to Jeffery than to log rolling).

Computing the **autocorrelation function** $\langle C'(t)C'(0) \rangle$ (how fast the orbit characterized by $C'(t)$ decorrelates from the initial orbit defined by $C'(0)$) that decays at $e^{-t/\tau}$ gives out the **Jeffery decay time** τ . This time can be compared to the **rotational diffusion time** τ_r , which can be calculated in the ideal case using:

$$\tau_r = \frac{1}{2D_r} = \frac{8\pi\eta R^3}{2k_B T} \quad (\text{Einstein-Smoluchowski relation}) \quad (4)$$

In case of elongated bodies such as prolate ellipsoid, a different relationship for the rotational diffusion coefficient D_r was proposed by Perrin (1936) adapted from the Stokes-Einstein relationship such as:

$$D_r^* = \frac{k_B T}{6\pi\eta \left(\frac{(a^2 - b^2)^{1/2}}{\ln \left(\frac{a + (a^2 - b^2)^{1/2}}{b^2} \right)} \right)} \quad (5)$$

With a the half-length and b the half-width of the prolate ellipsoid. Also note that for small average length L , $\tau_r \sim L^3$.

4. PERSISTENCE OF A JEFFERY ORBIT

The persistence of a Jeffery orbit is determined by:

1. Computing the **autocorrelation function** $\langle C'(t)C'(0) \rangle$ (how fast the orbit characterized by $C'(t)$ decorrelates from the initial orbit defined by $C'(0)$) that decays at $e^{-t/\tau}$ to find out the **Jeffery decay time** τ ,
2. Comparing τ and the **Jeffery oscillation period** of an ideal ellipsoid $t_J = \frac{2\pi(\lambda + \lambda^{-1})}{\dot{\gamma}}$.

The ratio $\frac{\tau}{t_J}$ is the number of Jeffery oscillations a rod performs before losing information about its Jeffery orbit state. It depends on:

- The wall shear rate $\dot{\gamma}$: $\dot{\gamma} \uparrow \Rightarrow \tau \downarrow$,
- The rod length: $\tau_r \sim L^3$.

The fact that at both small $\dot{\gamma}$ or small L dynamics are governed by Brownian fluctuations is captured by the **rotational Péclet number**, which compares the rotational diffusion time τ_r with the Jeffery reorientation time t_J and $f(\lambda)$ the shape function with λ aspect ratio.

$$\begin{cases} \text{Pe} = \frac{\tau_r}{t_J} = \frac{f(\lambda)\dot{\gamma}}{D_r} \\ f(\lambda) = (4\pi(\lambda + \lambda^{-1}))^{-1} \end{cases} \quad (6)$$

Zöttl et al. found $\frac{\tau}{t_J} \sim 0.5$ for rods of $3\mu\text{m}$ which means that **decorrelation occurs before the completion of even one Jeffery orbit**. They also noticed that in their experiments, τ is smaller than the rotational diffusion time $\tau_r = 1/2D_r = 2.38$ and that τ approaches τ_r for really small $\dot{\gamma}$. Consequently, in their case Jeffery orbits can only be observed at large shear rates ($\dot{\gamma} \geq 10^2 \text{ s}^{-1}$).