

Dynamics of individual Brownian rods in a microchannel flow

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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:

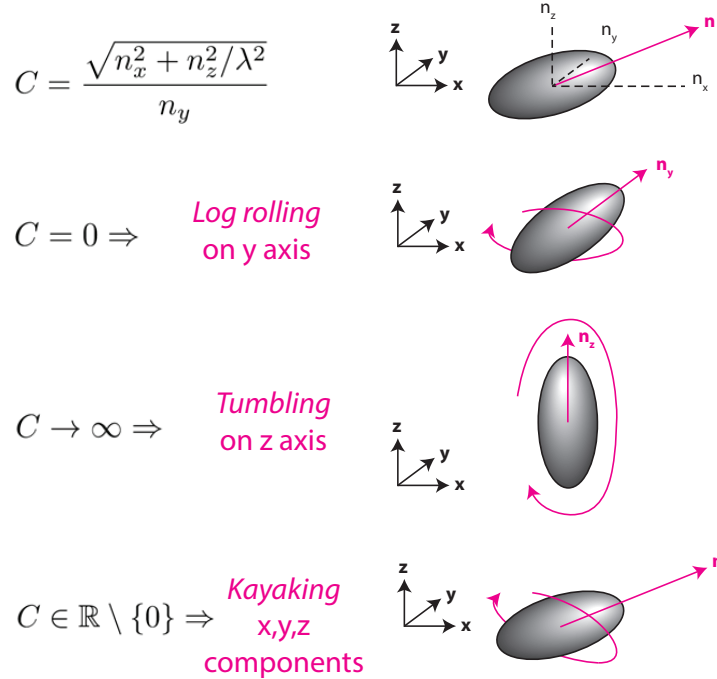


Figure 1: Different Jeffery orbits for an ellipsoidal particle depending on its Jeffery constant value C .

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, $\Omega(\mathbf{n}; z)$ 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 $\dot{\gamma} = 18\text{s}^{-1}$.

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).

4. PERSISTENCE OF A JEFFERY ORBIT

The persistence of a Jeffery orbit is determined by:

1. Computing the **autocorrelation function** $\langle C'(t)C'(0) \rangle$ 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.

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

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 ($\dot{\gamma} \geq 10^2 \text{ s}^{-1}$).