

# Dynamics of individual Brownian rods in a microchannel flow

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*Summary by Faustine Gomand*

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## 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  $\lambda$ ,
- The shear rate  $\dot{\gamma}$ ,
- The Jeffery constant  $C$  such as defined in the figure below:

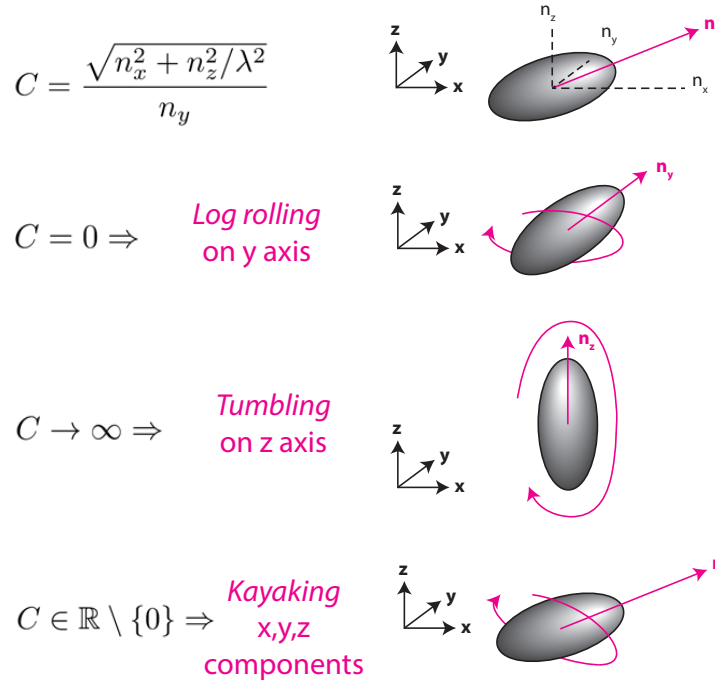


Figure 1: Different Jeffery orbits for an ellipsoidal particle depending on its Jeffery constant value  $C$ .

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;  $\lambda$  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,  $\xi$  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  $\xi_r$  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**  $\tau$ . This time can be compared to the **rotational diffusion time**  $\tau_r$ , which can be calculated in the ideal case using:

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

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**  $\tau$ ,
2. Comparing  $\tau$  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  $\tau_r$  with the Jeffery reorientation time  $t_J$  and  $f(\lambda)$  the shape function with  $\lambda$  aspect ratio.

$$\begin{cases} \text{Pe} = \frac{\tau_r}{t_J} = \frac{f(\lambda)\dot{\gamma}}{D_r} \\ f(\lambda) = (4\pi(\lambda + \lambda^{-1}))^{-1} \end{cases} \quad (5)$$

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,  $\tau$  is smaller than the rotational diffusion time  $\tau_r = 1/2D_r = 2.38$  and that  $\tau$  approaches  $\tau_r$  for really small  $\dot{\gamma}$ . Consequently, in their case Jeffery orbits can only be observed at large shear rates ( $\dot{\gamma} \geq 10^2 \text{ s}^{-1}$ ).