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 (~ 3 μm) in a horizontal Hele-Shaw channel (*i.e.* Poiseuille flow in xz plane). Highlights are:

- Rotational diffusion impacts particles' orbits (Brownian motion competes with Jeffery tumbling)
- Persistence of Jeffery orbits is quantifies 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 in a simple shear flow undergo a periodic motion on "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 (for a HORIZONTAL Hele-Shaw cell):

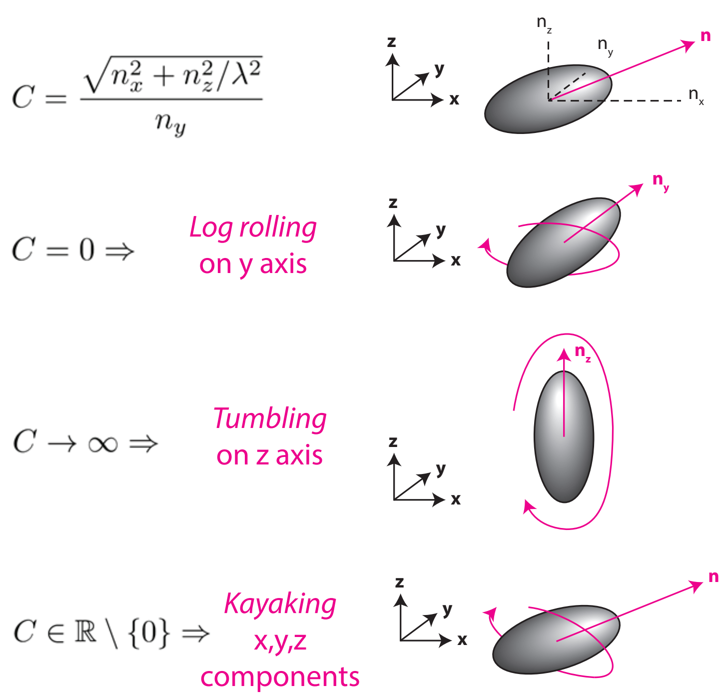

Figure 1: Different Jeffery orbits for an ellipsoidal particle depending on its Jeffery constant value C.

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 $l \sim 30\mu$m).

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

2. EXPERIMENTS AND SIMULATIONS

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

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 $\dot{\mathbf{n}}$:

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

With $\mathbf{v}_f$ Poiseuille flow (planar), v_s sedimentation velocity, $\mathscr{H}$ 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 $\dot{\gamma} = 18s^{-1}$.

3. COMPETITION BETWEEN JEFFERY ORBITS AND NOISE

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

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

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

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 (or relaxation) time** τ_r, which can be calculated in the ideal case of a sphere using:

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

Where D_r is the rotational diffusion coefficient, η the dynamic viscosity, R the sphere radius, k_B the Boltzmann constant, and T the temperature in Kelvin.

In case of elongated bodies such as prolate ellipsoids, the relaxation time τ_r of the long principal axis around the width axis can be calculated using a different rotational diffusion coefficient D_r proposed by Perrin (1936) which adapted it from the Stokes-Einstein relationship (cf. Nuris' thesis, p.47) such as:

$$D_r^* = \frac{k_B T}{6\mu V g \perp} \tag{5}$$

Where $V = \dfrac{4\pi ab^2}{3}$ is the ellipsoid volume, and:

$$g \perp = \frac{2(\lambda^4 - 1)}{3\lambda((2\lambda^2 - 1)S - \lambda)}, \tag{6}$$

$$S = \frac{1}{\sqrt{\lambda^2 - 1}} \ln\left(\lambda + \sqrt{\lambda^2 - 1}\right). \tag{7}$$

With a the half-length and b the half-width of the prolate ellipsoid, and $\lambda = a/b$ the prolate aspec ratio. 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 comparing:

1. The **Jeffery decay time** obtained from the autocorrelation function $\langle C'(t)C'(0)\rangle$,
2. The **Jeffery oscillation period** of an ideal ellipsoid $t_J = \dfrac{2\pi(\lambda + \lambda^{-1})}{\dot{\gamma}}$.

The ratio $\dfrac{\tau}{t_J}$ 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.

$$\begin{cases} \mathrm{Pe} = \frac{\tau_r}{t_J} = \frac{f(\lambda)\dot{\gamma}}{D_r} \\ f(\lambda) = \left(4\pi(\lambda + \lambda^{-1})\right)^{-1} \end{cases} \tag{8}$$

Zöttl et al. found $\dfrac{\tau}{t_J} \sim 0.5$ for rods of 3μm 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 ($\dot{\gamma} \geq 10^2$ s^{-1}).