The Physics of Morphologically Diverse Bacteria in Moving Fluids

Emma Allen

Supervisors: Dr. Tyler N Shendruk and Dr. Gavin Melaugh

Abstract

Large systems of so called "banana-shaped" particles suspended in a fluid provide an effective model for understanding the role of bacterial motion in sludge bulking seen in wastewater treatment. To analyse this system, it is useful to first understand the dynamics of a single bacterium. By modelling this bacterium as a banana-shaped particle and employing Molecular Dynamics in Multi-Particle Collision Dynamics, the rotational behaviour is studied as its curvature angle is varied from 0 to 2π.

The particle is suspended in a fluid with a constant shear flow, confined within a two-dimensional box with periodic boundary conditions applied to the vertical walls. It is found that the particle follows a Jeffery's Orbit trajectory. However, noise effects are found to have a significantly greater influence on the rotational dynamics than the curvature angle, as indicated by the Péclet number, which is calculated to be 12.91 ± 0.59. These effects cause noticeable deviations from theoretical predictions and highlights it is critical to account for noise in computational models for bacterial motion in wastewater.

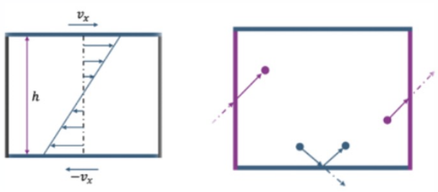

Figure 2: flow profile (left) and bounce back (right, blue) and periodic (right, pink) boundary conditions

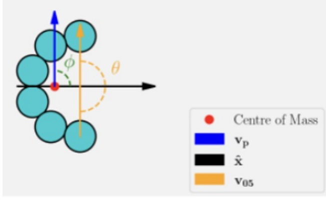

Figure 1: banana with curvature angle $\frac{\pi}{2}$

Background and Setup

A bacterium is modelled as a polymer made of six monomers with a curvature angle, θ. Its orientation angle, ϕ is defined as the angle between x direction and principal vector (Figure 1).

One banana is suspended in a fluid with a constant shear rate, confined to a 2D box. The vertical walls have periodic Boundary Conditions (BC) and the horizontal walls have reflective BC (Figure 2).

The banana rotates due to shear flow, which causes the banana to complete full rotations or diffusion (noise) which causes the banana to randomly oscillate. We can tell which one in dominating through a ratio of these quantities – the Péclet number, where shear dominates when $Pe > 1$ and diffusion when $Pe < 1$. The rotational dynamics of the banana are given theoretically by Jeffery Orbit equations [1].

Results

The angular velocity is shown to follow a trajectory predicted by Jeffery Orbits (Figure 3). Despite high levels of noise, there is a clear clustering of data, which agrees with theoretical predictions although has a slight offset to the right which indicates that noise is more prevalent as the banana rotates from a parallel to perpendicular orientation. As the curvature angle decreases, the period of rotation also decreases, shown by the cluster frequency decreasing. This period is irregular due to noise.

The calculated Péclet number (12.91 ± 0.59) indicates that, although shear flow is the primary force driving rotation, noise still substantially affects the system.

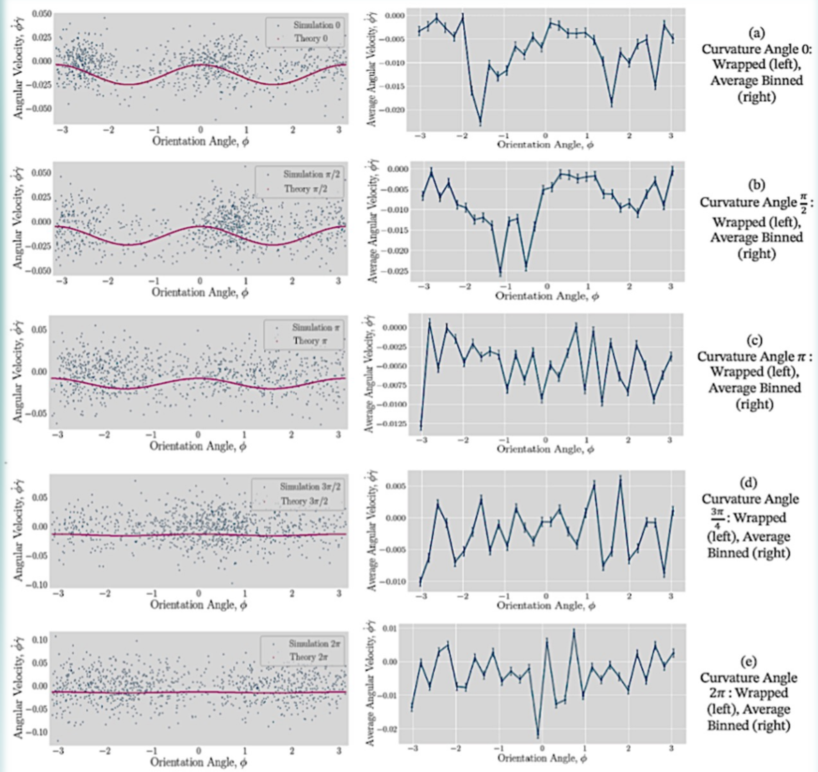

Figure 3: The first column overlays the wrapped simulation data with the theoretical predictions (pink curve), while the second column shows data binned across orientation angle and averaged over the angular velocity. Rows correspond to increasing curvature values: 0 (top), $\frac{\pi}{2}$, π, $\frac{3\pi}{2}$, 2π (Bottom). The first column demonstrate clustering in line with theoretical predictions which is clearer in the second column 0 (top), $\frac{\pi}{2}$, π, $\frac{3\pi}{2}$, 2π (Bottom)

Conclusions

These simulations demonstrate that noise plays a dominant role overshadowing the effects of curvature. The angular trajectories followed a Jeffery Orbit pattern with irregularities found to be a result of noise, causing noticeable deviations from the theoretical predictions. The calculated Péclet number (12.91 ± 0.59) supports this.

Future studies could look at the interactions between multiple bananas to understand how they interact with each other and the fluid. Here, the effects of curvature may be more pronounced, which could prove particularly useful in understanding sludge bulking.

References

[1] G. B. Jeffery. "The Motion of Elliptical Particles Immersed in a Viscous Fluid". In: Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character 102.715 (1922), pp. 161–179. doi: 10.1098/rspa.1922.0078.