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Numerical study on bacterial flagellar bundling and tumbling in a viscous fluid using an immersed boundary method

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ABSTRACT

The bundling and tumbling behavior of bacterial flagella in a viscous fluid has got immense significance in the field of biological fluid dynamics. In this paper we investigate the hydrodynamic interaction among two and more than two flagella in a viscous fluid based on an immersed boundary method. We model each helical flagellum by a number of triangular cross-sections with three immersed boundary (IB) points on each cross-section. Three types of elastic links are generated from each IB point to create an elastic network model of the flagellum and the first cross-section is modeled as the flagellar motor. The elastic forces are computed based on the elastic energy approach and the motor forces are obtained from the applied angular frequency of rotation of the motor. The Stokes equations governing the flow are solved on a staggered Cartesian grid system using a fractional-step based finite-volume method. It is observed that when two left-handed helical flagella rotate in the counter-clockwise direction, the resulting hydrodynamic interaction leads to bundling. When one of the flagella reverses the direction of rotation to clockwise the hydrodynamic interaction results in tumbling. During the bundling, the flagella wrap and intertwine each other, whereas during the tumbling they separate in an erratic way. There exists an exact combination of the handedness and rotational direction of the flagella to achieve the bundling. The bundling-to-tumbling behavior of the flagella is studied and it is concluded that the tumbling occurs faster than the bundling. Further, the hydrodynamic interaction among three flagella in a viscous fluid is studied for the cases of rotation in the same direction and in different directions. The bundling and tumbling behavior is well captured even for the case of multiple (more than two) flagella using the developed model.

1. Introduction

Multi-flagellated bacteria such as *Escherichia coli* (*E. coli*) use their rotating helical flagella to propel in a viscous fluid. Each flagellum is driven by a rotary motor embedded in the cell body. When all the flagellar motors rotate in the counter-clockwise direction (when viewed from behind the flagella), the flagella form a bundle and move the cell steadily in the forward direction. This behavior of bacteria is known as 'run'. When one or more of the motors reverses the rotational direction, the bundle separates and the flagella move away from one another. As a result, the bacterial cell moves erratically. This behavior is termed as 'tumble'. The 'run-and-tumble' modes alternate, allowing the bacteria to swim toward different directions in a viscous fluid [1–3]. The helical filaments of a flagellum consist of 11 protofilaments of flagellin subunits twisted together to form the compact structure. The protofilaments come in two different types, resulting in two different conformations of a straight

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filament: L-type (left-handed twist) and R-type (right-handed twist). The left-handed flagellum rotates in the counter-clockwise direction and the right-handed flagellum rotates in the clockwise direction when viewed from behind the flagellum.

Recently, an artificial microrobot employing the principle of bacterial propulsion has gained much interest among researchers in the field of microfluidics and microrobotics. The artificially developed bacterial robot can be used in the medical field to reach inaccessible areas of human body to carry out minimally invasive surgery, highly localized drug delivery and screening of diseases at early stages [4,5]. Also, a bacterial motor serving as a fluidic actuator to create local fluid motion in a microfluidic network to accomplish useful work is a novel technique which would have immense applications in microfluidic systems. This has necessitated many researchers to conduct detailed studies on the bacterial flagellum motion in a viscous fluid and the effects of various elastic and hydrodynamic parameters on the motion. A detailed review on the propulsion of flagellated bacteria based on analytical, numerical and experimental works has been presented in our previous paper [6]. Hence, in this paper the literature review will focus only on the works pertinent to the bacterial flagellar bundling and tumbling phenomena.

Macnab [7] explored the behavior of multiple rotating helices leading to quantitative relationship among the interaxial separation, phase difference and intertwisting using a working model. He concluded that the bundle formation and function are perfectly compatible with a rotational mechanism of the individual flagellum. Kim et al. [3] studied the bundling process using a macro-scale model consisting of stepper-motor driven polymer helices rotating in a highly viscous silicon oil. They observed the flagellar bundling for the counter-clockwise rotation of left-handed helices. They also reported that the motor frequency controls the initial rate of bundling. Later, Kim et al. [8] extended their study to measure the flow induced by rigid and flexible rotating helices employing the particle image velocimetry technique (PIV). They concluded that the rotational component of the flow due to the fully developed bundle is close to the flow generated by a single rotating rigid helix. Flores et al. [9] presented a computational study based on regularized Stokeslets and rotlets and a network of springs modeling the flagellum to study the flagellar motion and their hydrodynamic interaction. In their work, a constant magnitude torque was applied at the base of each flagellum to represent the rotary motor. They addressed the bundling and tumbling behavior of three flagella each driven by a constant torque. Watari and Larson [10] simulated the run-and-tumble motion of a multi-flagellated bacterium using a bead-spring model. Using the developed model they reproduced the experimentally observed behaviors of *E. coli*, namely, a three-dimensional random-walk trajectory in run-and-tumble motion and steady clockwise swimming near a wall. They also addressed the stress-induced polymorphic behavior of the flagellum during the tumbling motion. Using a mathematical model Janssen and Graham [11] explored the bundling process between a pair of flexible flagella each driven by a constant torque motor. They reported that the hydrodynamics plays a pivot role in the initial stage of bundling but the final state is a result of nontrivial balance between the hydrodynamics and elasticity. Also, the coexistence of tight and loose bundle states was observed in their study. Recently, Lim and Peskin [12] studied the fluid-mechanical interaction of flexible bacterial flagella using the generalized immersed boundary (IB) method combined with the Kirchoff rod theory. In their work, the flagella are modeled by using Kirchoff theory of thin rods. They consider helical flagellar filaments rotating at a specified frequency and investigated their behavior in a viscous fluid. They addressed the hydrodynamic interaction between two flagella. They concluded that the fluid-mechanical interplay between the two flagella may result in flagellar bundling, depending on the handedness of the helices and the direction of rotation of the flagellar motors.

The hydrodynamic interaction of bacterial flagella with the surrounding fluid is complex because of the interplay of hydrodynamics and elasticity. Recently, the immersed boundary method has become popular for solving fluid–structure interaction problems in computational fluid dynamics. In this method, a momentum forcing function is incorporated in the Navier–Stokes equation to make the presence of the immersed boundary and the entire simulation can be carried out on a regular Cartesian grid. Easiness in grid generation, and CPU and memory savings are main advantages of the method compared with unstructured grid methods. Peskin [13] firstly developed the immersed boundary (IB) method to simulate the interaction of elastic structures immersed in a viscous incompressible fluid. The IB method was originally applied to model the blood flow in the heart and heart valves [13–15]. Since then, it has been successfully implemented to simulate various problems especially in the field of biofluiddynamics where complex geometries and immersed elastic structures are present and make use of conventional computational techniques difficult. Examples include platelet aggregation in blood clotting [16], biofilm processes [17], cochlear dynamics [18], insect flight [19], dynamic instability of an elastic rod in a viscous fluid [20,21] and swimming of various aquatic animals, organisms and micro organisms including eels, leech, nematodes, sperm, biflagellated algal cells, bacterial helical flagella [22–27,6].

From the review of the literatures presented above, it becomes abundantly clear that only a few studies have been reported relevant to the bacterial flagellar bundling and tumbling. The experimental studies of Macnab [7] and Kim et al. [8] lack sufficient evidence of the actual flow field surrounding the flagella during the bundling and tumbling processes. Flores et al. [9] addressed the bundling and tumbling phenomena for the case of three flagella. Each flagellum has a motor modeled by a torque applied at the center of the first cross-section. The three flagella were placed equally-spaced on a circle in such a way that the center points of the first cross-sections of the three flagella form an equilateral triangle. This arrangement was typical to apply a counter-torque to represent the counter-rotation effect of the bacterial body. Hence their simulations were suitable only for the case of three flagella. Also, their study was based on the Stokeslets and rotlets model where the numerical result strongly depends on the numerical Stokeslets and rotlets regularization parameters, which is somewhat idealistic. The study of Watari and Larson [10] was based on a bead-spring cell model with a body and multiple flagella. Their flagella model was a one-dimensional line segment formed by a number of beads. Recent studies of Janssen and Graham [11] addressed mainly the coexistence of tight and loose bundles and did not investigate the tumbling