Simulation of Auto-propulsion Mechanism of Microorganism inside Microchannel

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Abstract: The maneuvers of appendage enabled bacteria displays a lot of intriguing fluid dynamic behavior in the viscosity dominated world, which has fascinated the researchers over the time. Till date ample of enthralling results have been reported by different analytical and computational studies supported by experimental investigations. Stepping ahead, the present study manifests about the several ground breaking flow phenomena arising out of hydrodynamic interactions between two microorganisms swimming inside a microchannel with close proximity. The results theorized in the present investigation scrutinizes the varying behavior of the bacteria while moving inside a micro-capillary at different Reynolds number (Re). At high Re the two swimming microorganisms tend to lock at anti-phase configuration while at low Re an in-phase configuration is attained as a consequence of hydrodynamic interaction alone. Computational fluid dynamic framework with fluid structure interaction (FSI) interface is adopted for experimentation in which the motion of fluid (solid) is described in Eulerian (Lagrangian) framework. All the numerical computations are performed in finite element method based commercial software COMSOL Multiphysics.

Keywords: Fluid-structure interaction (FSI), multiphysics, synchronized swimming, phase locking, auto-propulsion, microorganism

1. Introduction

Auto-propulsion of microorganisms such as the bacterial locomotion in the human gut, auto-propulsion of spermatozoa inside fallopian tube, the algal migrations, or the protozoan movements in the water bodies have been able to capture the attention of researchers over the years. Different varieties of stimulus can induce motions in the living microorganisms such as chemotaxis, phototaxis, geotaxis and etc. The cilia and flagella enabled propulsion is the most commonly observed swimming technique for micro

swimmer involves rotation of helical flagellum besides the passing of the lateral waves at the downstream of the bacterial body to produce the required thrust for the motion. The physics governing the swimming strategies are significantly different if the movements of the microorganisms are considered inside the macroscopic and microscopic domains. Thanks to size and shape of the microorganisms the viscous force dominates significantly over the inertia force [1].

The pioneering work of Taylor [2] on waving sheet problem first demonstrated about the hydrodynamics of microswimmer analytically. The waving sheet immersed in fluid resembles flagellum, through which a lateral wave is propagated down the body. As consequence, the travelling wave gives rise to viscous stress and produce net displacement in forward direction. Till date numerous fundamental aspects of hydrodynamics of swimming microorganism have been studied on the testbed of waving sheet by many researchers analytically [3-5] Due to the higher computing cost and tedious calculation in analytical works, numerical tools came to picture to assist it.

Invention of computational fluid dynamics (CFD) added a new chapter to the study on motility of microorganisms. In this field fluid structure interaction (FSI), immersed boundary method (IBM), boundary element method (BEM) serve as cutting edge tool to predict the hydrodynamics of micro swimmer. Subsequent numerical studies revealed about several interesting flow phenomena such as near wall attraction, phase locking, synchronized swimming and etc. [6-8].

In order to understand the nature's complicacy and miracle, it is indispensable to approach the problem precisely and accurately. In this study fluid structure interaction (FSI) interface is adapted for investigation using finite element method (FEM) based commercial software COMSOL Multiphysics. The phase locking and unlocking mechanism between two

microorganisms swimming in upstream direction inside a micro capillary will be investigated in this paper. The report describes about the two cases of swimming configuration i.e. parallel swimming and approached swimming and its dependency on *Re*.

2. Problem Formulation

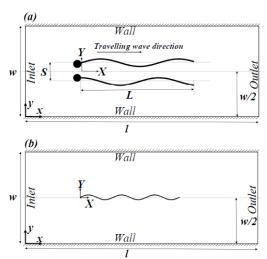


Figure 1: Schematic diagram of the computational domain in which a microorganism with a flagellum swims across a microchannel. The width and the length of the microchannel are denoted by w = 0.4 mm and l = 1.3 mm, respectively.

Figure 1(a) shows the schematic diagram of the computational domain with dimensions employed for the numerical simulations. The swimmers are placed at equidistant from neighboring walls with a separation distance of S. While the microfluidic flow is represented in a spatial coordinate system (x, y), the motion of the microorganisms is solved in the material coordinate system (X, Y), as shown in the figure. The microorganisms are composed of a circular head of diameter D = 0.01 mm and a wavy flexible tail of length L = 0.3 mm. In the simulations, the fluid in the microchannel is kept stationary and the wavy tails of the microorganisms are allowed to move in Y-direction to engender forward motion towards negative X direction. The oscillatory waves on the tails of the microorganisms travelling towards the positive Xdirection, which eventually provides the necessary thrust for the motion in the negative Xdirection, is defined as,

$$y(X,t) = b\sin(kX - \omega t)\min(t,T) \tag{1}$$

Where b, t, k, ω is the amplitude, time period, wavenumber and angular frequency, respectively. The parameters k and ω is defined as $2\pi/\lambda$ and $2\pi/T$ respectively.

1.1 Governing Equations

The flow induced by the beating of the tail is governed by incompressible Navier-Stokes equation as follows,

$$\nabla \cdot \mathbf{u}^f = \mathbf{0} \tag{2}$$

$$\rho^f \left(\frac{\partial \mathbf{u}^f}{\partial t} + \left(\mathbf{u}^f \cdot \nabla \right) \mathbf{u}^f \right) - \nabla \cdot \mathbf{\sigma}^f = \rho^f \mathbf{f}^f \quad (3)$$

Where ρ is density, \mathbf{u} is velocity vector, $\mathbf{\sigma}$ is stress tensor and \mathbf{f} is volume force vector. The swimmer body is considered as structural part, which is governed by the conservation of linear momentum, a constitutive relation which relates stress, strain and some kinematic relations. In order to solve large structural deformation, a nonlinear description of kinematics is required. However, a linear constitutive law for the material is assumed. The equilibrium equations for structure is,

$$\rho^{S} \frac{d\mathbf{u}^{S}}{dt} = \nabla \cdot \mathbf{\sigma}^{S} + \rho^{S} \mathbf{f}^{S} \tag{4}$$

In the above equation \mathbf{u}^s , $\mathbf{\sigma}^s$, \mathbf{f}^s , ρ^s denote velocity, Cauchy stress tensor, body force and density of the solid, respectively.

1.2 Boundary Conditions

In the present simulation, the top and bottom wall are defined with no-slip boundary condition.

$$\begin{bmatrix} u(x,0,t) \\ v(x,0,t) \end{bmatrix} = \begin{bmatrix} u(x,w,t) \\ v(x,w,t) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
 (5)

The inlet velocity is set to 0.1 mm.s^{-1} while at outlet the default pressure outlet boundary condition is given. The tail, which need to move for generation of propulsive thrust, is enforced with moving boundary condition as a function of material coordinate system (X, Y).

$$u(X,t) = 0 (6)$$

$$v(X,t) = \frac{-b\omega\cos(kX - \omega t)\min(t,T)}{+b\sin(kX - \omega t)\frac{\partial(\min(t,T))}{\partial t}}$$
(7)

The fluid enclosed within the channel is initialized with zero values and the velocity components and pressure, all are set to zero value at t = 0.

1.3 Solution Methodology

The computational domain is divided into 4520 numbers of triangular mesh to obtain a grid independent solution. To visualize the time evolved flow physics, the unsteady governing equations (Eq. 2-3), subjected to mentioned initial condition and boundary conditions (Eq. 6-7) are solved by Finite Element method (FEM) based commercial software COMSOL multiphysics. The inbuilt Galerkin least square (GLS) method with crosswind and streamlined stabilization technique is used for discretization of non-linear convective diffusive equation where a quadratic basis function and linear basis function is used for velocity and pressure field discretization, respectively. To determine the velocity and pressure profiles for the incompressible flow. incremental pressure correction scheme for the segregated predictor-corrector method is used. A second order accurate backward difference formulation (BDF) is used for time marching with backward Euler consistent initialization. The problems associated with the moving-deforming mesh are very often confronted with the stiffness originating from the ill conditioned matrix while re-meshing of the computational domain takes place. In order to tackle these problems during the numerical simulation automatic re-meshing feature is used with minimum element quality 0.1. The time step of size $10^{-4} - 10^{-5}$ is found to be suitable for a converged solution. The default parallel direct linear solver (PARDISO) with nested dissection multithread pre-ordering algorithm is used for all the numerical simulations.

3. Validations

The propulsion of self-oscillating sheets having infinite length and zero thickness has been employed as a model prototype to theoretically explore the movements of appendages of the microswimmer as shown in the Fig. 1(b). In one of his pioneering works, Taylor [1] term this prototype as swimming sheet problem and proposed an asymptotic solution for the speed of propulsion. Later Tuck [5] also modified the empirical formula for propulsion speed for finite. Here in this case the propulsion speed obtained by numerical simulation has been compared with Taylor (Eq. 8) and Tuck (Eq. 9) empirical relation.

$$U = \frac{1}{2}b^2k^2\left(1 - \frac{19}{16}b^2k^2\right)V + O(b^6k^6)$$
 (8)

$$U = \frac{1}{4}b^{2}k^{2}\left(1 + \frac{1}{F(Re)}\right)V + O(b^{4}k^{4})$$
 (9)
Where
$$F(Re) = \left(\frac{1 + \sqrt{1 + Re^{2}}}{2}\right)^{\frac{1}{2}}$$

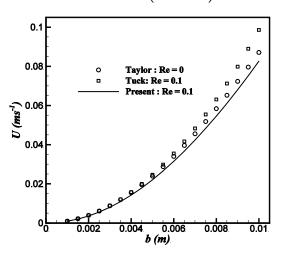


Fig 2: Variation of swimming speed (U) with amplitude (b)

It can be seen from the Fig. 2 that the analytical and numerical predictions slightly deviates from each other at higher velocity. It is worth noticing that, the analytical solutions are valid for certain order of magnitude. Hence for smaller value of amplitude it matches well and deviates at higher amplitude.

4. Results and Discussion

4.1 Case 1

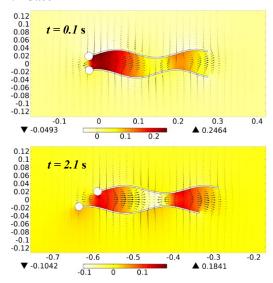
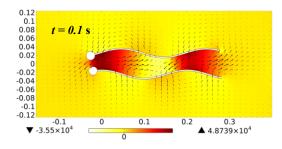


Figure 3: Anti-phase lock configuration achieved between microorganisms swimming at Re = 0.13, where contour shows the magnitude of pressure

4.2 Case 2



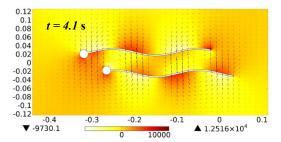
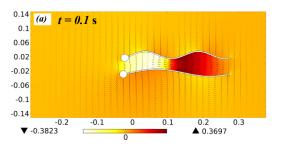


Figure 4: In-phase lock configuration achieved between microorganisms swimming at Re = 0.0003, where contour shows the magnitude of pressure

4.1 Case 3



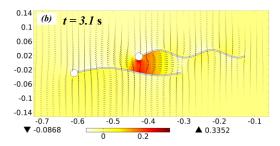
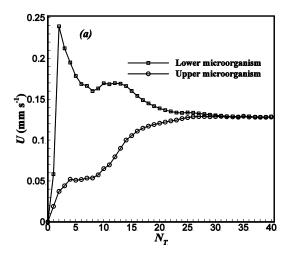


Figure 5. Anti-phase locking at different configuration achieved between microorganisms swimming at Re = 0.13, where contour shows the magnitude of pressure. Two different wavelengths are applied to the upper and lower microorganism. $\lambda_{\text{upper}} = 0.2 \text{ mm}, \lambda_{\text{lower}} = 0.4 \text{ mm}$

As shown in the Fig. 3 and Fig. 4, the two microorganisms start swimming in parallel to each other with phase difference of $\pi/2$. But the final synchronization is different in both the cases. For high Re i.e. 0.13, the two microorganisms tend to lock at antiphase configuration and continue swimming in that configuration for rest of the swimming period, where all other wave parameters are kept constant. For low Re of 0.0003, it can be seen that both achieve the inphase configuration. The Re is calculated by the empirical formula based on lateral wave parameters passing down the tail i.e. Re = $\rho\omega/\mu k^2$. With a curiosity to investigate the synchronization phenomena, we consider another initial configuration, where the microorganisms are applied with two different type of waves which differs by wavelength. The upper one is applied with smaller wavelength and the lower one with larger wavelength. The simulations are run at Re = 0.13. Interestingly the results obtained are quite similar with previous case. At high Re, antiphase synchronization is obtained but the positioning is little different.



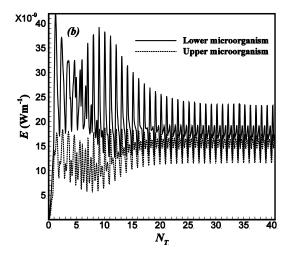


Figure 6: Evolution of (a) stabilized swimming speed (*U*) (b) Rate of dissipation of energy (*E*) with beating periods for case 3 where two microorganisms are swimming with two different wavelengths $\lambda_{\text{upper}} = 0.2 \text{ mm}$, $\lambda_{\text{lower}} = 0.4 \text{ mm}$

underlying principle responsible synchronization, can be explained on the basis of viscous force, surrounding pressure zone, vortex field and inertia force. At high Re, inertia force dominates over the viscous force. Due to lesser viscosity, the viscous dissipation will be less, which facilitates interaction between the two microorganisms hydrodynamically. The surrounding vortex field generated by two microorganisms, interact with each other and push the two microorganisms to attain resultant configuration. As a consequence, the resultant velocity field directs parallel to the swimming direction of microorganisms and both start swimming at same speed remaining in equilibrium antiphase locked configuration. But at low Re, the viscous force dominates over the inertial force. It also facilitates high viscous dissipation and creates localized high pressure zones surrounding the two microorganisms. In vicinity of the two microorganisms very high pressure zone is created. The pressure gradient tries to release out the excess pressure in vicinity of the two microorganisms by pushing both the organism to in phase configuration. In this configuration, the pressure in between of the two microorganisms is neutralized by the pressure fields created by individual microorganism. The same physics can explain well the resulting synchronization while the two microorganisms swim with different wavelength.

5. Conclusions

- In this paper, we have shown the versatility of the COMSOL Multiphysics software where a computational model is developed successfully in FSI interface in accordance to the Taylor's analytical propositions.
- 2. An interesting flow physics is revealed in terms of synchronized swimming between two microorganisms inside a micro channel.
- 3. At high *Re* (0.13), the two microorganisms attains anti-phase lock configuration in both parallel and approached swimming pattern. The synchronized swimming velocity obtained is more than un-synchronized pattern. Here in this case the rate of dissipation of energy is minimized.
- 4. Similarly, at low *Re* (0.0003), the two microorganisms attains in-phase lock configuration in both swimming pattern. But the synchronized swimming velocity obtained in this case is less than unsynchronized pattern. While the rate of energy dissipation is maximized.
- 5. We believe the results reported here will supplement significantly to enhance understanding about the auto propulsion mechanism of flagellated microorganisms.

6. References

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