An ALE-based finite element model of flagellar motion driven by beating waves: A parametric study

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A B S T R A C T

A computational model of flagellar motility is presented using the finite element method. Two-dimensional traveling waves of finite amplitude are propagated down the flagellum and the swimmer is propelled through a viscous fluid according to Newton's second law of motion. Incompressible Navier-Stokes equations are solved on a triangular moving mesh and arbitrary Lagrangian–Eulerian formulation is employed to accommodate the deforming boundaries. The results from the present study are validated against the data available in the literature and close agreement with previous works is found. The effects of wave parameters as well as head morphology on the swimming characteristics are studied for different swimming conditions. We have found that the swimming velocities are linear functions of finite amplitudes and that the rate of work is independent of the channel height for large amplitudes. Furthermore, we have also demonstrated that for the range of wave parameters that are often encountered in human sperm motility studies, the propulsive velocity versus the wavelength exhibits dissimilar trends for different channel heights. Various head configurations were analyzed and it is also observed that wall proximity amplifies the effects induced by different head shapes. By taking non-Newtonian fluids into account, we present new efficiency analyzes through which we have found that the model microorganism swims much more efficiently in shear-thinning fluids.

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1. Introduction

Microscale propulsion has been one of biologists’ main areas of interest for many years, since motility of these small swimmers plays a profound role in biosystems. Those particular types of bacteria that exhibit motility can move in the direction of the concentration gradient of food molecules to provide nutrition or to avoid repellants. The biology of reproduction is significant for many years, since motility of these small swimmers is propelled through a viscous fluid according to Newton’s second law of motion. Incompressible Navier-Stokes equations are solved on a triangular moving mesh and arbitrary Lagrangian–Eulerian formulation is employed to accommodate the deforming boundaries. The results from the present study are validated against the data available in the literature and close agreement with previous works is found. The effects of wave parameters as well as head morphology on the swimming characteristics are studied for different swimming conditions. We have found that the swimming velocities are linear functions of finite amplitudes and that the rate of work is independent of the channel height for large amplitudes. Furthermore, we have also demonstrated that for the range of wave parameters that are often encountered in human sperm motility studies, the propulsive velocity versus the wavelength exhibits dissimilar trends for different channel heights. Various head configurations were analyzed and it is also observed that wall proximity amplifies the effects induced by different head shapes. By taking non-Newtonian fluids into account, we present new efficiency analyzes through which we have found that the model microorganism swims much more efficiently in shear-thinning fluids.

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Numerical simulations of flagellar and also non-flagellar motility have been proven to be powerful tools to gain better insight into the underlying physics of such motions. Also, the emergence of microrobots and synthetic swimmers which are believed to have great potential in biomedical applications, have rendered computational tools even more important by providing invaluable data for improving and optimizing their design. The Study of microswimmers hydrodynamics was first initiated by the pioneering work of Taylor [1], who analyzed swimming of an infinite sheet subject to planar beating waves with small amplitudes, analogous to the beating flagellum of spermatozoa. As inertia is unimportant at microscales and the Reynolds number is quite small, Stokes equations were used in Taylor’s analysis. Using the same method, Tuck [2] studied this case of swimming by taking inertia into account. Through his perturbation analysis of an infinite sheet swimming near boundaries, Katz [3] demonstrated that both the propulsive velocity and the rate of work by the sheet increase as the wall separation distances are reduced. Hancock [4] introduced the slender-body theory (SBT) by utilizing the distribution of “Stokeslets” in order to model the flow resulting from the beating of a flagellum. Gray and Hancock [5] developed a model that represents the flagellum by a series of cylinders, translation of which gives rise to resistive forces. These forces were considered to be proportional to the relative velocity; a...
fundamental assumption that forms the basis of what is known today as the resistive-force theory (RFT). Numerous studies concerning flagellar fluid dynamics have ever since made use of either of SBT or RFT. Subsequently, boundary-element method was successfully applied to flagellar hydrodynamic problems. Phan-Thien et al. [6] analyzed the swimming of a microorganism by the propagation of helical waves along its flagellum using boundary-element method and found that the results from this method were in excellent agreement with experimental observations and also with those of the slender-body theory. Smith et al. [7] developed a hybrid boundary-integral/slender-body algorithm for modeling flagellar cell motility to investigate the accumulation of human spermatozoa near plane boundaries. Planar and three-dimensional helical waveforms were prescribed and various near-wall behaviors of flagellated cell, such as trapping and deflection were studied.

Methods involving direct solution of Navier-Stokes equations have gained more and more popularity in recent years, since they do not pose any restrictions on the geometry or physics of the problem. The immersed boundary method which was proposed by Peskin [8] to model blood flow in heart valves is a versatile direct numerical methodology to handle moving boundaries, particularly those encountered in biological flows. In this method, rather than considering the moving boundary as an actual flow boundary, it is represented by a singular source term in Navier-Stokes equations and thus the no-slip condition is imitated. Fauci and Peskin [9] modeled the locomotion of aquatic animals using immersed boundary method, treating the organism as a massless, elastic boundary immersed in a viscous fluid. In a similar analysis, Qin et al. [10] used a feedback law to calculate the interaction forces between the swimmer and the fluid, and analyzed the swimming of a computational organism in a channel. Among the direct methods, an alternative approach to flagellar propulsion is to apply finite element method to solve the governing equations, with the deformations taken into account through arbitrary Lagrangian–Eulerian formulation. Temel and Yesilyurt [11] simulated microrobots swimming in circular channels and made a comparison of the data obtained from CFD model and experimental work involving a robot of almost the same size. In another study, Acemoglu and Yesilyurt [12] investigated the effects of geometric parameters on swimming of a microorganism with a single helical flagellum in circular channels using finite element method.

The techniques discussed up to this point have all taken advantage of a known sinusoidal beating wave-form based on experimental observations. However, the true nature of flagellar beating waves is an emergent property of the fluid dynamics and flagellum structural response. The action of internal molecular dynein motors, forces due to the passive structure of the flagellum and the hydrodynamic drag induced by the ambient fluid constitute a fully coupled physical system [13]. The curvature control theory was proposed by Brokaw [14] and helical waves were shown to be generated in simulations based on this theory [15]. Lindemann [16,17] developed the geometric clutch hypothesis and attributed the activation of dynein motors to the specific internal geometric structure of the flagellum. Recently, Gadêlha et al. [18] have developed a model based on passive flexible filaments in shear flow which takes the geometric nonlinearities into consideration in spermatozoon flagellum. They have concluded that nonlinear model predicts buckling behavior and complicated waveforms, and that curved swimming trajectories are possible without requiring asymmetric forces with such a model. Utilizing the active elastic model of Gadêlha et al. [18], nonlocal SBT, boundary-element and regularized stokeslets, Montenegro-Johnson et al. [19] have lately devised an approach to analyze the phenomenon of sperm scatter near geometric features which has promising applications in cell sorting through their individual motility characteristics. They have indicated that sperm scattering depends nonlinearly on the ratio of viscous and elastic forces: a simple backstep produces attractive or repulsive scattering of cells considering different values for specific parameters reflecting the effects of such a critical ratio.

In the present work, flagellar motion of a model microorganism with the characteristic planar beat patterns of human sperm is explored. A two-dimensional finite element model is established and the time-varying, incompressible Navier-Stokes equations are solved on an arbitrarily moving mesh to allow for the displacements of the boundaries due to the motion of the flagellum. Simulations are then validated against the previous analytical and numerical works reported in the literature and the effects of various geometric parameters including amplitude, frequency, wavelength of the traveling waves as well as size and shape of the head and near-wall swimming behaviors of the swimmer are studied. In addition, swimming in non-Newtonian fluids is also investigated and discussed in this paper, owing to the widespread occurrences of such fluids in biological flow problems.

2. Methodology

2.1. Governing equations

Inertia can be ignored for very small Reynolds numbers (Re<1) and the two-dimensional flow field around the microswimmer can be described by the Stokes equations. However, to allow local inertial effects and hence imposing no restriction on the Reynolds number, the full incompressible Navier-Stokes equations are solved and arbitrary Lagrangian–Eulerian scheme is employed

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} - \mathbf{u}_{\text{mesh}}) \cdot \nabla \mathbf{u} \right) = \nabla \cdot \mathbf{\tau}$$

$$(1) \quad \nabla \cdot \mathbf{u} = 0$$

where $\mathbf{u}^T$ shows the transpose of a matrix, $\mathbf{u} = \{u, v\}$ the velocity vector, $t$ the time, $\rho$ the density, $\mathbf{\tau}$ the total stress tensor and $\mathbf{u}_{\text{mesh}}$, the velocity vector of the deforming mesh. The total stress tensor for a generalized Newtonian fluid is defined by

$$\mathbf{\tau} = -p \mathbf{I} + \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right)$$

$$(2)$$

where $p$ shows the pressure, $\mathbf{I}$ the identity tensor and $\mu$ the viscosity function. In the ALE formulation, mesh velocity is calculated from the propagation of the moving boundary displacement throughout the domain and hence, a smooth mesh deformation can be obtained. Here, it is done by solving the time-dependent version of Laplace smoothing PDEs subject to appropriate boundary conditions

$$\frac{\partial^2 \mathbf{u}}{\partial t^2} + \mathbf{\nabla} \cdot \frac{\partial \mathbf{u}}{\partial t} = 0$$

$$\text{(4)}$$

where $\mathbf{u} = \{x, y\}$ and $\mathbf{X}_m = \{X_m, Y_m\}$ are the spatial and material coordinates. Thus the mesh velocity would be

$$\mathbf{u}_{\text{mesh}} = \frac{\partial \mathbf{X}}{\partial t}$$

$$\text{(5)}$$

As the mesh distorts over time, remeshing is done once the mesh quality falls below a certain criterion already defined in the model. A new mesh is generated for the current configuration and the values of the dependent variables are mapped onto the new mesh. The behavior of non-Newtonian fluids can be described by a constitutive relation of the form

$$\mathbf{\tau} = f(\gamma(\mathbf{u}))$$

$$\text{(6)}$$

where $\tau$ is the deviatoric stress tensor and $\gamma$ is the strain rate tensor. The rheological equation of state for generalized Newtonian fluids is given by

$$\tau = \mu’(\gamma)\gamma = |\gamma(u)| = |\nabla u + (\nabla u)^T| = \sqrt{\frac{1}{2} L_2}$$  \hspace{1cm} (7)

where $L_2$ is the second invariant of the strain rate tensor. Stress is proportional to strain rates for Newtonian fluids, hence $\mu’(\gamma) = \text{constant}$. For non-Newtonian fluids, the model of Carreau [21] is chosen for the viscosity function. As will be elucidated later, this constitutive model has also been used by Montenegro-Johnson et al. [22] and Vélez-Cordero and Lauga [23] in their studies on flagellar motility in non-Newtonian fluids. The viscosity function in Carreau’s model has the form

$$\mu’(\gamma) = \mu_\infty + \frac{\mu_0 - \mu_\infty}{1 + (\lambda \gamma)^n}$$ \hspace{1cm} (8)

where $\mu_0$ and $\mu_\infty$ are the low and high shear limiting viscosity, $\lambda$ is the relaxation time and $n$ is the power-law index ($n < 1$). As the flagellum undergoes deformations in time, local interaction forces develop. Also, these forces exert a torque which rotates the head. The net force and torque exerted on the swimmer can be expressed as follows:

$$F = \int_{\text{swimmer}} (n \Delta \vec{a}) dA$$ \hspace{1cm} (9)

$$M_z = \int_{\text{swimmer}} (x - x_s) \times (n \Delta \vec{a}) dA$$ \hspace{1cm} (10)

where $F = [F_x, F_y]^T$ is the interaction force vector, $M_z$ is the moment of the interaction forces about the mass center, $x_s = [x_s, y_s]^T$ the instantaneous position vector for the mass center of the swimmer, $A$ the surface area and $n$ the normal to that surface. The values of the net force and torque obtained from the above relations are then used to solve the following differential equations

$$\frac{d\dot{x}_s}{dt} = F / m$$ \hspace{1cm} (11)

$$\frac{d\dot{\theta}_s}{dt} = \frac{M_z}{I_z}$$ \hspace{1cm} (12)

In the above set of equations, $x_s = [\dot{x}_s, \dot{y}_s]^T$ denotes the instantaneous swimming velocity vector, $m$ the mass of the swimmer, $\theta_s$ the swimmer’s instantaneous angular velocity, $I_z$ the moment of inertia about the normal axis to the swimmer’s center of mass and $\dot{\theta}_s$ the instantaneous angular position with reference to the channel centerline. These equations are added to the model as global equations and solved for each timestep.

2.2. Boundary conditions

The flow domain consists of a two-dimensional rectangular area in which the swimmer is immersed. Open boundary conditions are specified at the left and right boundaries of the domain which are sufficiently away from the swimmer:

$$[-p I + \mu' (\nabla u + (\nabla u)^T)] n = 0 \text{ at } x = 0 \text{ and } x = L$$ \hspace{1cm} (13)

which describes boundaries in contact with large volumes of fluid. The top and bottom boundaries of the domain that represent the channel walls are subject to no-slip conditions:

$$u = 0 \text{ at } y = \pm h$$ \hspace{1cm} (14)

The required boundary conditions for the swimmer surface are imposed in a reference frame which is fixed relative to the mass center and aligned with the centerline of the swimmer (Fig. 1). A sinusoidal wave-form that imitates realistic beating waves of spermatozoa is prescribed for the displacement of the flagellum in $Y$-direction as follows:

$$v(X, t) = A_m(X) \sin \left[ \frac{2\pi}{T} \left( \frac{X - X_s}{\lambda} \right) \right]$$ \hspace{1cm} (15)

where $(X_b, Y_b)$ is the position vector of the boundary point $b$, $X$ the mean longitudinal position of boundary point $b$, $A_m(X)$ the amplitude, $T$ the period and $\lambda$ the wavelength of the traveling waves. The $Y$-component of velocity vector of the points on the flagellum surface can be found by taking the derivative of the above equation with respect to time in the body frame as follows

$$v(X, t) = \frac{2\pi}{T} A_m(X) \cos \left[ \frac{2\pi}{T} \left( \frac{X - X_s}{\lambda} \right) \right]$$ \hspace{1cm} (16)

For the flagellum to be inextensible, Taylor [1] arrived at the following velocity boundary conditions in the $X$-direction for the flagellum in the body frame of reference. Ignoring those terms of orders higher than 2 we have

$$u(X, t) = \frac{2\pi}{4T} A_m(X)^2 \left( \frac{2\pi}{\lambda} \right) \cos \left[ \frac{2\pi}{T} \left( \frac{X - X_s}{\lambda} \right) \right]$$ \hspace{1cm} (17)

The above relation, although an approximation to the real inextensible flagellum, is a sufficiently accurate boundary condition for the presented range of parameters. These boundary conditions correctly exhibit figure of eight motions in the body frame which is a physical characteristic of an inextensible flagellum.

The amplitude function is defined as

$$A_m(X) = A_{\text{max}} (X - X_s) / L$$ \hspace{1cm} (18)

$$A_m(X) = A_m$$ \hspace{1cm} (19)

where $A_{\text{max}}$ denotes the maximum amplitude experienced by the flagellum at its distal end, $X_s$ the $X$ position of the head and flagellum junction, $L$ the length of the flagellum and $A_m$ the value of the constant amplitude. The velocity vector which also describes the wall boundary condition on the surface of the flagellum would be

$$u_{\text{wall}} = X_s + \omega \times (X - X_s) + u_p$$ \hspace{1cm} (20)

where $\omega = \partial_t \vec{e}_s$ is the angular velocity vector and $u_p$ is the velocity vector of the points on the flagellum relative to the moving frame. In order to account for the effects of different head geometries, a head is attached to the flagellum of the model swimmer. Since the head undergoes rigid-body translations with the same translational velocity as the flagellum, the following boundary condition is imposed:

![Fig. 1. An illustration of the laboratory frame and the moving frame which is fixed to the swimmer’s mass center and aligned with the flagellum centerline.](image-url)
\( \mathbf{u}_{\text{wall}} = \mathbf{x}_s + \mathbf{\omega} \times (\mathbf{x} - \mathbf{x}_s) \) on the head  \( (21) \)

noting that \( \mathbf{u}_p = 0 \) here because the head is stationary with respect to the moving frame.

The ALE-Laplace set of PDEs in Eq. (4) smoothly deform the mesh, given the constraints placed on the boundaries to obtain the desired mesh displacements and velocities. The outer boundaries of the mesh are fixed and their displacements are set to zero at all times, regardless of whether being channel walls or open boundaries

\( \mathbf{u}_{\text{mesh}} = 0 \) at \( x = 0 \) and \( x = L_c \) and \( y = \pm h \) \( (22) \)

The mesh boundaries which correspond to the flagellum surface and the microorganism’s head should move according to the swimmer’s net motion as follows

\( \mathbf{u}_{\text{mesh}} = \mathbf{x}_s + \mathbf{\omega} \times (\mathbf{x} - \mathbf{x}_s) + \mathbf{u}_p \) on the flagellum surface \( (23) \)

\( \mathbf{u}_{\text{mesh}} = \mathbf{x}_s + \mathbf{\omega} \times (\mathbf{x} - \mathbf{x}_s) \) on the head \( (24) \)

3. Results and discussion

The governing equations are discretized on unstructured triangular meshes and solved using COMSOL Multiphysics© version 4.4 [24] commercial finite element package. An example of the computational mesh is given in Fig. 2. P2+P1 elements were chosen for the discretization of the fluids. The solution evolves in time using variable-order, variable-stepsize BDF method with a maximum order of two. At any timestep, PARDISO direct solver is employed here as described in [10]. Furthermore, the current finite element model, the same nondimensionalization strategy is employed here as described in [10].

For all the test cases, the swimmer is placed along the centerline of the channel. The velocity vector is set to zero at the beginning of the calculations throughout the domain. A step function is used to smoothly initiate the wave motion of the flagellum, and the swimmer is assumed to be neutrally buoyant in all calculations. After starting the simulation, a transient phase is seen to occur after which a periodic steady-state ensues. The mean swimming velocity of the computational organism is obtained by taking the average of instantaneous \( x \)-direction velocity, \( s_x \) over at least two periods, after steady swimming conditions have been established. As the flagellum undergoes deformations and the swimmer propels itself steadily, the resulting interaction forces produce a torque that rotates the head and the swimmer also experiences displacements in the transverse direction. However, for confined swimming as is the case for the present simulations the rotation and transverse displacements are negligibly small. Unless the swimmer’s position is offset from the centerline of the channel, the average \( y \)-displacement remains zero, barely affecting the swimming velocity.

Experience with the present model reveals that a careful choice of mesh eliminates the need for remeshing entirely for the cases of small amplitude oscillations, or delays it significantly. For instance, with a minimum allowable mesh quality of 0.2 (the mesh element quality which is a numerical value between 0 and 1, is based on the ratios of the inscribed and circumscribed circles’ or spheres’ radii for the simplex corresponding to each corner of the element. 0 for element quality represents a degenerated element and 1 represents the best possible element [25]), establishing steady swimming takes 2–10 times of remeshing for a specified minimum and maximum element size; depending on the wave amplitude, channel height, etc. Since the Reynolds number is vanishingly low, high Reynolds number phenomena such as the development of boundary layers do not occur and steep gradients of dependent variables are unlikely. Thus there is no need for extreme mesh refinement especially with the high order elements employed, and this allows for larger displacements of the boundaries relative to the element sizes before any condition for remeshing is met. It should be noted however that the likelihood of singular velocity and pressure fields makes it necessary to locally refine around the tip region of the flagellum.

We should be very well aware of the fact that the conformity of such a two-dimensional model microorganism with the real-world three-dimensional phenomenon is at best qualitative. As Katz [3] pointed out in his paper, such models can only be an effective representation of a large number of nearby swimmers moving in phase. Nonetheless, a two-dimensional model can reflect most of the trends present in the actual hydrodynamic problem, and several studies have been devoted to study the two-dimensional models so far. For instance, Dillon and Fauci [26] presented a two-dimensional model of an individual ciliun which incorporated discrete representation of the dynein arms and the passive elastic structure of the axoneme including the microtubules and nexin links. In another two-dimensional study, Riedel-Kruse et al. [27] concluded that the beat in eukaryotic flagella is an oscillating pattern of propagating bends generated by dynein motor proteins and they addressed the question regarding the coordination of these motors using a two-dimensional model of the flagellum. Recent investigations of flagellar motility in non-Newtonian fluids which have been carried out by Vélez-Cordero and Lauga [23], Montenegro-Johnson et al. [22], Riley and Lauga [28] and Yi Man and Lauga [29], have all been conducted in a two-dimensional framework.

3.1. Validation

The present model of flagellar propulsion is validated against a number of previous analytical and numerical studies. As pointed out earlier, Katz [3] carried out a biharmonic perturbation analysis for a confined infinite waving sheet assuming very small amplitude relative to the separation distance between the sheet and the walls. Qin et al. [10] reconstructed the same case using the immersed boundary method and compared their numerical results with the perturbation method. To demonstrate the validity of the current finite element model, the same nondimensionalization strategy is employed here as described in [10].
numerical results are presented for comparison with the dimensional cases studied by Fauci and Peskin [9] and the asymptotic analyzes put forward by Taylor [1] and Tuck [2].

### 3.1.1. Effects of wall proximity

The reported swimming velocities from previous works and the present study are shown versus the channel half heights in Fig. 4. The augmented viscous stresses induced by wall proximity cause a corresponding increase in velocity and the average rate of work per unit length. The latter is defined by

\[ E = \frac{1}{S} \int_S \mathbf{u} \cdot \mathbf{F} \, dS = \int_S \mathbf{n} \cdot \mathbf{r} \, dS \]  

(25)

where \( \mathbf{F} \) is the interaction forces acting on \( S \), the surface of the organism. It is apparent that the calculations of the present study compare well with the analytical as well as other numerical studies.

### 3.1.2. Effects of wavelength and wave amplitude

Another series of simulations were conducted to study the effects of the wavelength on the swimming velocity, and to compare the data from the present study with other data available in the literature. Results from immersed boundary method and the finite element model are in close agreement, and the data from both methods depart from that of the analytical calculations due to the fact that the flagellum length is taken to be finite in both numerical models, as pointed out in [10]. The results plotted in Fig. 5(b) are performed on a
dimensional basis, in order to compare the results with the cases tested by Fauci and Peskin [9].

3.2. Parametric studies

Vera et al. [30] examined the sperm motion through experimental observations and characterized the sperm motility by wave parameters. Based on their data, we define a number of base parameters and perform parametric studies by varying one parameter at a time while keeping the rest intact. The base parameters are presented in Table 1, while their corresponding geometrical representation can be seen in Fig. 3. To account for the effects of the head, an elliptic piece resembling the shape of the sperm head is attached to the flagellum which is defined by its major and minor semi-axes.

3.2.1. Effects of wave amplitude

The effects of wave amplitude were studied for two different channel heights and for constant as well as linearly increasing amplitudes. The pressure fields and streamlines for both cases of constant and linearly increasing amplitudes are presented in Fig. 6. For very small amplitudes, effects of wall on swimming velocity become negligible as expected, while for larger amplitudes the effect is more amplified for both cases of constant and linearly increasing amplitude. It is also noteworthy that in contrast to the case of very small amplitude oscillations examined by the perturbation analysis, swimming velocity varies almost linearly for large amplitudes. It is apparent from Fig. 7 that as the wave amplitude approaches the channel height, it becomes difficult to distinguish between the forward velocities of a swimmer with head or without it. The reason may be due to the amplification of the viscous forces that eventually makes the additional drag caused by the presence of head insignificant.

The rate of work varies almost quadratically for very small amplitudes. However, the trends in higher amplitudes are seen to be approximately linear, specifically for narrow channels. We have demonstrated that the effects of the walls on the rate of work done by the microorganism become negligible and the curves coincide for large amplitudes, indicating the dominance of the increased amount of power consumption due to the greater amplitudes. The linear dependence of the swimming velocity on large amplitudes in channel swimming and the overshadowing effects of relatively large amplitudes on head drag and power consumption have not been taken into consideration before.

3.2.2. Effects of period of oscillations

Fig. 8 indicates the swimming velocity values versus different periods of oscillations corresponding to the values of period seen in experimental observations [30]. The inverse dependency of the propulsive velocity on the period of oscillation as described in Taylor’s work [1] seems to be retained for the present simulations.

3.2.3. Effects of wavelength

As we can see in Fig. 5(a), the lubrication theory and the perturbation analysis lead to an almost linear dependence of swimming velocity on wavelength. However, in this study we have shown that swimming near walls with large amplitudes exhibits a totally

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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</thead>
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<tr>
<td>Amplitude</td>
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</tr>
<tr>
<td>Wavelength</td>
<td>20 [μm]</td>
</tr>
<tr>
<td>Period</td>
<td>0.3 [s]</td>
</tr>
<tr>
<td>a-semi axis</td>
<td>2 [μm]</td>
</tr>
<tr>
<td>b-semi axis</td>
<td>1 [μm]</td>
</tr>
<tr>
<td>Flagellum Length</td>
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</tr>
<tr>
<td>Viscosity</td>
<td>0.001 [Pa s]</td>
</tr>
<tr>
<td>Density</td>
<td>1000 [kg/m³]</td>
</tr>
</tbody>
</table>

Fig. 6. Pressure fields and streamlines around the swimmer for (a) constant \(A_m = 2 \mu m\) and (b) linearly increasing amplitude \(A_{max} = 3 \mu m\).
different behavior which to the authors’ best knowledge, has not been investigated before. The results in Fig. 9 indicate that the relation between swimming velocity and wavelength depends hugely on the wall separation distance for the range of data considered here. When the channel height is much smaller than the wavelength, the swimming velocity increases with wavelength almost monotonically, reaching a plateau for very large wavelengths. For wavelengths of the same order of magnitude as the channel height, the swimming velocity variations are not significant and there is also a minimum point for velocity. The swimming velocity decreases monotonically over a wide range of wavelengths and plateaus eventually for the case of large channel height.

### 3.2.4. Effects of head morphology

The effects of spermatozoa head morphology are considered to be of remarkable importance in male fertility rates: faster spermatozoa are more likely to eventually reach and fertilize the ovum and interestingly, faster sperms are those with elongated heads [31]. Higdon [32] analyzed the flagellar swimming of an organism to which a spherical head was attached and studied the effects of varying the radius of the head on the power consumption and the swimming velocity. Phan-Thien et al. [6] applied boundary-element method to investigate how a nonspherical head shape would influence important hydrodynamic parameters, and by obtaining optimal values for the parameters of head geometry they concluded that the concept of “survival of the fittest” holds for that case too. In their immersed boundary analysis, Fauci and McDonald [33] studied a model microorganism with an attached cell body and showed that the presence of the head results in a smaller swimming velocity, without any specific regard to the impacts of variation of the geometric parameters. Gillies et al. [34] conducted numerical simulations of flagellar propulsion by the method of regularized stokeslets, accompanied by sperm kinematics measured by digital microscopy. They addressed the issue of mechanical effects of the head morphology in their simulations and performed parametric studies to capture the variations of the swimming velocity and efficiency. Nevertheless; the effects of head

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**Fig. 7.** Swimming velocity plotted against wave amplitude for (a) constant amplitude and (b) linearly increasing amplitude, and (c) effects of wave amplitude on the rate of work done by the swimmer for different channel half heights.
morphology on swimming velocity in presence of walls have not been considered before, so here a model organism is simulated with multiple head geometries and the relevant variables of interest are measured for different channel heights. In Fig. 10(a) the size of the head is varied to find out how a mere enlargement of the head affects the swimming characteristics near walls. The major and minor semi-axes are lengthened with the same factor, so that the aspect ratio remains unchanged. The swimming velocity always decreases with increasing the size of the head, and wall proximity causes a corresponding steeper reduction. It is notable however, that a specific size exists with which the swimming velocity is not sensitive to channel height. For this configuration the “neutral” shape of the head is an ellipse with $a / b = 7.5 / 3.75 \mu m$. This is due to the fact that there are two competing effects here: the increase in velocity as a result of swimming in a narrower channel, and a reduction of velocity induced by larger heads. For relatively normal heads the effects of narrower channels are dominant and we observe higher swimming velocities for smaller values of $h$; however, for large heads the significantly increase drag force accounts for lower velocities in thinner channels.

Another series of simulations were carried out to address the problem of how the aspect ratio of an elliptic head would influence the hydrodynamics of the problem. The reference geometry was chosen to be a circular head with a radius of 4 $\mu m$. In a set of runs, the width of the ellipse, i.e. the minor axis was kept constant while the length of the head was changed. These results correspond to the part of Fig. 10(b) where $a / b > 1$. In another set of computations, no changes were made to the length of the head while the width of the head was varied at the same time, pertaining to the portion of Fig. 10(b) where $a / b < 1$. It is shown in Fig. 10(b) that the swimming velocity increases rapidly as the width of the head is reduced, although the slope is steeper for when the organism swims in narrower channels. On the other hand, elongation of the head with keeping the width constant results in reduction of swimming velocity for the $a / b > 1$ range. Again, the changes are more amplified in smaller channel heights. Considering that for low Reynolds numbers drag is approximately proportional to surface area, it is obvious that wherever the head surface
are increased, velocity decreases and a reduction in the surface area results in an increased swimming velocity for the whole range of \( \frac{h}{L} \). The steep increase in velocity Fig. 10(b) (where \( \frac{h}{L} < 1 \)) may be attributed to the rapid reduction of the viscous drag exerted on the head, an effect which is much more intense when the head is almost as wide as the channel itself.

The last series of simulations regarding the effects of head morphology are devoted to a test case in which the volume of the head is preserved, so as to resemble the fact that a constant amount of the genetic material is packed in the sperm head. For this case, a geometry factor is defined and different values of this factor are used to increase the length while decreasing the width of the head, in such a way that the volume remains constant. The dashed line in Fig. 11 corresponds to an aspect ratio of around 1.65, which is reported in [34] as the mean normal aspect ratio for the human sperm head. It is shown in Fig. 11 that the effects of head elongation are considerable when the organism swims in a narrow channel, and the magnitude of such effects are not substantial when the organism is far from solid boundaries.

The trends in these numerical simulations are consistent with the results obtained by Gillies et al. [31]. They concluded that spermatozoa with high head length/width ratio have notably higher swimming velocities, but only when the length is kept fixed. As shown in the present study, elongation of the head while the width is constant actually leads to velocity reduction, and narrowing the head with constant volume causes only slight velocity increase. Hence, it can be inferred that faster spermatozoa that are observed experimentally have less width rather than being more “elongated”.

### 3.3. Swimming in non-Newtonian fluids

It is known that biological fluids, especially those encountered in female reproductive tract manifest non-Newtonian behaviors [35]. It is also reported that flagellar beat pattern changes dramatically in the mucus, exhibiting waves of smaller amplitudes confined to the distal end of the flagellum [13]. As previously mentioned in [23], a number of works have considered the effects of viscoelasticity on flagellar propulsion, while the locomotion of microorganisms in shear-dependent non-Newtonian fluids received less attention. Effects of swimming in non-Newtonian shear-dependent fluids on swimming velocity and trajectory of sperm-like swimmers have been examined in recent studies [23,36], so here we turn our attention to another important physical consideration; that is, we present efficiency analyzes of our model microswimmer in such fluids for which we believe there has been no investigation in the literature.

In this study, the Carreau model is chosen to describe the dependence of viscosity on the shear rate, with various sets of parameters to simulate the different shear-thinning and shear-thickening characteristics of non-Newtonian fluids. Inspection of the dynamic viscosity distribution in the fluid domain demonstrates that a region of relatively low viscosity, or a “thin fluid capsule” develops around the swimmer when the fluid is regarded as shear-thinning. The counterpart of this situation occurs also for the shear-thickening fluids, with the “capsule” encompassing a relatively high viscosity fluid, as shown in Fig. 12.

To assess how efficiently the microorganisms swim, efficiency is defined as the ratio of the axial resistance power of a nonbeating swimmer to the rate of work done by the swimmer on the ambient fluid. Higdon [32], Phan-Thien et al [6] and Gillies et al. defined efficiency as

\[
\eta = \frac{\frac{6\pi \mu A}{p} + \frac{2\pi \mu L}{\log \left(\frac{L}{a}\right)} U^2}{p}
\]

Fig. 11. Effects of head elongation on the swimming velocity while keeping the head volume fixed.

![Fig. 11](image)

Fig. 12. The distribution of dynamic viscosity in the fluid domain for (a) a shear-thinning fluid and (b) a shear-thickening fluid.

![Fig. 12](image)
where $\bar{A}$ is the volume equivalent radius of the head, $L$ is the flagellum length, $U$ is the average swimming velocity, $a$ is the flagellum cross-sectional radius and $\mathcal{F}$ is the average rate of work done by the swimmer. The axial resistance in Eq. (26) is obtained for Newtonian fluids however, and hence is not applicable to the non-Newtonian case. The value of axial resistance is therefore calculated here by direct simulation with a nonbeating swimmer moving with a constant velocity through the fluid.

It is well known that for given flagellum kinematics, the value of viscosity is unimportant as long as the swimming velocity is concerned. It turns out from the present calculations that forward velocity is not altered appreciably for swimming in shear-dependent non-Newtonian fluids. The efficiency of swimming on the contrary, is a strong function of the non-Newtonian behavior. The obtained swimming efficiencies are plotted in Fig. 13 for various values of $n$, the power-law index, and for different levels of shear-thinning and shear-thickening while keeping $\mu_\infty$ fixed. There are points of maximum and minimum efficiency for shear-thinning and shear-thickening fluids respectively through the fluid, the shear rates are considerably smaller compared to the active swimming conditions for the same non-Newtonian parameters. Furthermore, the viscosity function curves are more apart in the low shear rate limit for the same value of $\mu_\infty$. This means that the resistance forces in active swimming conditions are almost of the same magnitude for fixed values of $\mu_\infty$, while drag forces in the low shear rate limit deviate from one another greatly, hence the higher efficiencies for stronger shear-thinning fluids can be deduced. The results are presented only for the case of varying $\mu_0$, however, similar arguments are valid for other cases. The rate of work is found to be a linear function of viscosity, therefore assuming fixed values for $\lambda$ and $n$, one can predict that the efficiency remains effectively constant as long as $\mu_0/\mu_\infty$ is unchanged:

$$\eta = \frac{P_{\text{passive}}}{P_{\text{active}}} = \frac{\alpha \mu_1}{\mu_2} = \frac{\alpha + (\mu_0/\mu_\infty - 1)f(\gamma_1)}{\beta + (\mu_0/\mu_\infty - 1)f(\gamma_2)}$$

(27)

In the above relations $\mu_1$ and $\mu_2$ are some arbitrary values of viscosity function in the low and high shear rate regions respectively, $\alpha$ and $\beta$ are constants of proportionality, and $f(\gamma) = \left(1 + (\lambda \gamma)^2\right)^{-\frac{1+\gamma}{2}}$. Following the same reasoning, it is concluded that varying the viscosity in Newtonian fluids does not affect the swimming efficiency for given beat patterns. It is evident from Fig. 13 that propulsion in shear-thinning fluids is always more efficient than swimming in Newtonian or shear-thickening fluids. This is also consistent with the small amplitude analysis of Vélez-Cordero and Lauga [23] whose analytical approach confirms the same conclusion for swimming in non-Newtonian fluids.

4. Conclusion

Numerical simulation of flagellar motility of a model microorganism is presented in this paper. We conclude that finite element method can be successfully applied to simulate the phenomenon of microscale propulsion, without posing any restrictions on the magnitude of deformations or any other difficulties associated with the implementation of the method for complex geometries or flow situations. The incompressible, time-dependent Navier-Stokes equations are solved on unstructured triangular moving mesh and solved using COMSOL Multiphysics<sup>™</sup> commercial finite element package. The relative simplicity of applying high order schemes in the finite element method framework allows the usage of coarser meshes, and hence fewer remeshings are required. Navier-Stokes equations are coupled with Newton’s second law of motion to obtain the linear and angular position and velocity of the swimmer in every timestep, while deformations of the boundaries are accounted for by using ALE scheme. Results of this paper compare very well with the previous analytic works in the limits where those theories are stated to be valid, and also with the data from numerical simulations performed by immersed boundary method.

Swimming velocity is reported to be strongly correlated to male fertility [31], hence it is the parameter of interest in this study. In the very small deformations range, the swimming velocity and the rate of work preserve their quadratic dependence on the amplitude, as derived in theoretical analysis of Taylor [1]; however, our new results in this work indicate that for larger amplitudes the curves are best described as being linear. Moreover, we have also observed that for large amplitude beating, the effects of swimming in narrower channels on the power consumption become vanishingly small. Due to the lack of investigations of the effects of wavelength on forward velocity for channel swimming, we have simulated such cases and have come to an interesting observation that when the microorganism swims in narrow channels, increasing the wavelength results in significant
velocity enhancement, while it may hinder the forward motion in wider channels. Parametric studies for different geometries of head have indicated that mere elongation of the head reduces the swimming velocity if the width is kept constant. Given a constant amount of genetic material hence a constant volume of sperm head, we have shown that for an aspect ratio of 1.65 which is around the normal value for the human sperm, the elongation of the head does not change the swimming velocity appreciably except for propulsion in channels of heights less than the wavelength. As the swimming efficiency for shear-dependent fluids was not addressed before in the literature for planar beating, large amplitude propulsion, we show by simulation that propulsion in shear-thinning fluids is generally more efficient than in Newtonian or shear-thickening fluids, and that there are points of maximum and minimum when the efficiencies are plotted for different values of the power-law index, n.

Conflict of interest statement

None declared.

References