Dynamics of filaments: modelling the dynamics of driven microfilaments

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We describe a method for simulating the inertialess dynamics of a flexible filament immersed in a fluid. Typically, this regime is appropriate for filaments a few micrometres or less in size (flagella that propel micro-organisms for example). We apply the model to two systems; a filament that is wiggled at one end and planar swimming motion characteristic of simple spermatozoa. For the former we find qualitative agreement with theory. The shape is determined by a balance between bending and viscous forces and there is an optimal balance that maximizes the propulsion generated by this mechanism. Quantitatively we find less satisfactory agreement. For the spermatozoa, assuming a relatively naive bending mechanism in the form of a travelling force quadrupole wave, the model generates waveforms in very good agreement with experiment. This is only true, however, if the bending forces acting on the filament are large compared with the viscous forces. Experimental measurements of the tail stiffness imply this should not be the case. We discuss the implications of this observation in the context of the sperm's swimming mechanism.

Keywords: computer simulation; filaments; spermatozoa; motility

1. INTRODUCTION

As pointed out by Purcell in his lecture 'life at low Reynolds numbers' (Purcell 1977), micro-organisms experience an environment quite different from our own. Notably, because of their small size (of the order of micrometres), inertia is, to them, essentially irrelevant. We are all familiar with the concept of inertia. It is the tendency of things in motion to remain in motion. If, for example, you tore this page from the journal (hopefully having read it first), screwed it up into a ball and threw it, you would expect to propel it a few metres. Inertia keeps it moving until the friction exerted by the air (or the floor once it has landed) brings it to a halt. Let us now keep our physical size fixed at a couple of metres and see what would happen if we experienced the same environment as the micro-organism. As long ago as the nineteenth century, Reynolds showed that, as far as the dynamics of a fluid are concerned, scaling down a problem (decreasing the characteristic length scale) is, in dimensionless terms, equivalent to increasing the viscosity. That is, if we wanted to repeat our paper throwing experiment in a world parametrically equivalent to that of the micro-organism we would have to immerse ourselves in a fluid a million times more viscous than air. If we further take into account that we (and our projectile) are much denser than air, whereas a micro-organism is typically equivalent in density to its surroundings, we find the following. Transforming the microscopic world to our macroscopic dimensions and repeating the experiment, we could propel our projectile *ca.* 10^{-9} m. That is, we could throw the screwed up paper

a few atomic distances. In an inertialess world it is hard to shake off your environment.

The fact that inertia is irrelevant for micro-organisms makes it difficult for them to move. Many propulsive mechanisms that are perfectly viable on our scale will not work in a micro-environment. This is because of some particular properties of inertialess systems. First, by definition the mass of an object becomes irrelevant. Second, the equations of motion governing the motion of the surrounding fluid become time reversible. This means that any reciprocal motion produces no net propulsion. Purcell (1977) termed this the 'scallop theorem'. A scallop uses a reciprocal motion, opening and closing its shell, so it could not propel itself if it were micrometres, rather than centimetres, in size. Another oft quoted example is that of the stiff one-armed swimmer. He or she tries to move by waving a stiff appendage back and forth. However, in the absence of inertia any net force generated by one half of the stroke will be equal and opposite to the force generated during the remainder. The total will be zero and the stiff one-armed swimmer, in the absence of inertia, falls foul of the scallop theorem and goes nowhere. There are two obvious strategies for avoiding this problem. One is to introduce flexibility. If the one-armed swimmer has a flexible arm the shape need not be reciprocal during a cycle. Net propulsion can be generated. Another solution is to have an appendage execute some non-reciprocal motion. That is, to generate motion with some 'handedness'. The classic example of this, and the one used by most bacteria, is to rotate a chiral tail (Berg & Anderson 1973). Rotation of a chiral tail again breaks the symmetry of one cycle and has the potential to generate net motion.

While we have concentrated above on a specific class of microfilaments, flagella, the problem is in fact more general. The cytoskeletal filaments actin and microtubules,

for example, also fall into the same category. For any microscopic filament the factors that determine its dynamic behaviour are the same. Namely, the equations of motion will be essentially inertialess. The motion itself will be determined by a balance between forces driving the filament, friction forces exerted as the surrounding fluid opposes the motion and the bending forces trying to restore the equilibrium state. For relatively simple model systems, there has recently been theoretical progress in solving analytically the ‘hyperdiffusion’ equation that, in the limit of small amplitude motion, describes the movement, of such a filament. Wiggins & Goldstein (1998) considered the motion of a single filament driven at one end by an external perturbation. Their analysis emphasized that there are two very different regimes, one where bending forces dominate and the filament behaves like a rigid rod, and a second where the viscous damping of the fluid has the effect of suppressing the propagation of elastic waves. For the one-armed swimmer, this leads to an optimal set of parameters that maximize either the swimming speed or swimming efficiency. The same analysis gives predictions for the shape of such a wiggled filament that can be compared with experimentally observed responses in, for example, micro-manipulation experiments. In these experiments, optical tweezers are used to oscillate one end of a filament (Riveline *et al.* 1997). By comparing experimental results with theory, structural properties of the filament can be inferred.

With the aid of a numerical model we can calculate the dynamics of a driven filament without the restriction of small amplitude motion. There is also greater scope to specify the type of active forces driving the motion and the boundary conditions applicable for a given physical situation. With such a model, we can test theoretical predictions and also study more complex problems where no analytic solution is available. In this paper, we describe such a numerical model and apply it to both classes of problem, namely, the dynamics of a wiggled filament, where we can compare with theoretical results, and the swimming motion of simple spermatozoa, where we have only experimental results with which to compare.

2. DESCRIPTION OF THE MODEL

To study the dynamics of a micro-filament numerically, we need to develop a model that simulates a thin flexible filament of mass m , immersed in a fluid. We further need to impose the condition that inertia is negligible. To do so, it is useful to consider this flexible filament as a set of N rigidly connected beads. The rigid connections between beads impose the condition that the total length of the filament is constant. Experiments show that compared to bending, stretching is negligible (unsurprisingly, as the latter would require the stretching of the microtubules that make up the tail). Using rigid links imposes this condition on the model. The force on one of the individual beads should reflect the forces acting on a segment of length $\Delta l = l/(N - 1)$ of real filament with total length l . The forces on the i th bead can be characterized as follows.

- (i) A tension force, $\mathbf{F}_{iT}$, associated with the resistance of the filament to stretching.
- (ii) A bending force, $\mathbf{F}_{iB}$, associated with the resistance of the filament to bending.

- (iii) An active bending force, $\mathbf{F}_{iA}$, that induces movement.
- (iv) A viscous force, $\mathbf{F}_{iv}$, exerted by the fluid on the filament.

The equation of motion for the i th bead can thus be written

$$m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_{iT} + \mathbf{F}_{iB} + \mathbf{F}_{iA} + \mathbf{F}_{iv}, \quad (2.1)$$

where the bead mass $m_i = m/N$. Our first task is to specify how we approximate these forces and subsequently calculate them.

(a) Tension forces

The tension forces are calculated using a procedure commonly employed in molecular dynamics (Allen & Tildesley 1987), namely, the use of rigid constraints between the beads that keep their relative separation fixed. This is achieved by introducing equal and opposite constraint (or tension) forces directed along the links between beads. The magnitude of the forces can be calculated by imposing the condition that at time $t + \Delta t$ the distance between each connected pair of beads is fixed at the value Δl . For a linear chain (which we have here) this simply involves the trivial business of inverting a tridiagonal matrix. More complete details are given by Lowe & de Leeuw (1999).

(b) Bending forces

The approach we follow here is an extension of the model elastic filament developed by Lowe (Lowe 2001). We consider the set of N particles i , with $n = N - 1$ rigid links connecting particle i to particle $i + 1$ and introduce a bending potential, that is, a three body potential between groups of three connected beads. The two rigid links connecting three consecutive beads, $i - 1$, i and $i + 1$, define an angle θ_i ,

$$\cos(\theta_i) = \frac{1}{\Delta l^2} (\mathbf{r}_i - \mathbf{r}_{i-1}) \cdot (\mathbf{r}_{i+1} - \mathbf{r}_i), \quad (2.2)$$

and one unique circle will pass through all three points. From the cosine rule, it follows that the radius of this circle, which we interpret as the radius of curvature, R_i , at the position of bead i , is given by

$$\left(\frac{1}{R_i}\right)^2 = \frac{2}{\Delta l^2} (1 - \cos(\theta_i)). \quad (2.3)$$

If we consider our filament as ‘ideally’ elastic, that is, its bending energy (for all deflections) to be given by continuum elasticity theory (Landau & Lifshitz 1986), then the total bending energy is

$$U_B = \frac{G}{2} \int_0^l \frac{1}{R(s)^2} ds, \quad (2.4)$$

where G is the bending modulus, $R(s)$ the local radius of curvature and s a coordinate that follows the centreline of the filament. Taking a bending potential U_i between the links of the form

$$U_i = A(1 - \cos(\theta_i)), \quad (2.5)$$

the total bending energy for the model will be

$$U = \sum_{i=2}^n U_i = A \sum_{i=2}^n (1 - \cos(\theta_i)). \quad (2.6)$$

Discretizing the integral (equation (2.4)) as follows

$$U = \frac{G}{2} \Delta l \sum_{i=2}^n \left(\frac{1}{R_i^2} \right)^2, \quad (2.7)$$

and equating this with the energy of the model system, we find

$$A = \frac{G}{\Delta l}. \quad (2.8)$$

A more sophisticated approach (Ohm *et al.* 2002), where we map the problem onto the worm-like chain model of Kratky & Porod (1949), leads to a slightly different expression for A ,

$$A = (n - 1/2) \frac{G}{l}. \quad (2.9)$$

These two expressions are equivalent in the limit $N \rightarrow \infty$, but differ for the finite number of beads used in the model. In fact, the latter converges to results independent of the number of beads much more rapidly than the former, so this is the method we prefer (Ohm *et al.* 2002). The bending force on particle i is then obtained by taking (analytically) the spacial derivative of the potential with respect to its coordinates,

$$\mathbf{F}_{iB} = -\nabla_i (U(\theta_{i-1}) + U(\theta_i) + U(\theta_{i+1})). \quad (2.10)$$

(c) Viscous forces

The viscous forces are particularly complex. They are dependent on the instantaneous shape of the filament and are also time dependent (Landau & Lifshitz 1959). They can be incorporated at the ‘steady-state’ level using Stokesian dynamics (Sierou & Brady 2001), or even keeping the time dependence, using lattice Boltzmann techniques (Ladd 1994). We are currently applying both approaches, but the work described here neglects both. It is a simple approximation, consistent with tractable theoretical models. Specifically, we simplify the calculation of the viscous forces by introducing a bead friction tensor such that the equation of motion reduces to a simple Langevin equation,

$$m_i \frac{dv_i}{dt} = \mathbf{F}_{iT} + \mathbf{F}_{iB} + \mathbf{F}_{iA} - \gamma_i \cdot v_i, \quad (2.11)$$

with

$$\gamma_i = \gamma_i^{\parallel} \hat{\mathbf{p}}\hat{\mathbf{p}} + \gamma_i^{\perp} \hat{\mathbf{n}}\hat{\mathbf{n}}. \quad (2.12)$$

Here $\hat{\mathbf{p}}$ and $\hat{\mathbf{n}}$ are, respectively, unit vectors parallel and perpendicular to the filament. Physically we are representing the viscous force by means of a parallel ($\gamma^{\parallel}$) and perpendicular ($\gamma^{\perp}$) friction coefficient. It should be noted that it is not true to say that the degree of sophistication with which one treats the viscous forces does not influence the results. It does. It does not, however, significantly influence our general conclusions. We will therefore restrict ourselves to this simple hydrodynamic model. Furthermore, equations (2.11) and (2.12) assume the shape of the tail is axisymmetric. Given the symmetry of the

arrangement of the nine outer microtubules that make up the outer skeleton of the flagella, this is a very good approximation. The parallel and perpendicular friction coefficients for an infinitely slender cylinder are known analytically (Cox 1970)

$$\begin{aligned} \gamma_0^{\perp} &= \frac{4\pi\eta\Delta l}{\ln(l/a)}, \\ \gamma_0^{\parallel} &= \frac{\gamma^{\perp}}{2}, \end{aligned} \quad (2.13)$$

where η is the viscosity of the fluid. However, as noted elsewhere (Hancock 1953; Purcell 1977), the friction coefficients of an infinitely slender rod differ significantly from those of a ‘quite’ slender rod. Therefore, rather than take the theoretical values for these friction coefficients (equations (2.13)) we have calculated them numerically. For a rod with $a/l = 1/50$ (something reasonably flagella-like) we find that

$$\begin{aligned} \gamma^{\perp} &= 0.93\gamma_0^{\perp}, \\ \gamma^{\parallel} &= 1.16\gamma_0^{\parallel}. \end{aligned} \quad (2.14)$$

Apart from taking numerical values for the friction coefficients, this approximation, first formulated by Gray & Hancock (1955), is known as ‘resistive force theory’. It is known to give values for the swimming speed of spermatozoa in good agreement with experiment *if* the shape of the tail is assumed (Brennen & Winet 1977). However, in the model we describe here the shape will not be specified. We will input the active bending forces. As pointed out by Wiggins & Goldstein (1998), the shape of the filament will then result from the force balance implied by equation (2.11).

(d) Active forces

The only force left to specify is the active force. This is not of course generic, but depends on the particular physical system one has in mind. For the one-armed swimmer, Wiggins & Goldstein (1998) consider various forms of external driving (although the results are at least qualitatively independent of this). We concentrate here on the case where the filament is driven by an external torque, T_x of the form

$$T_x = B \sin(\omega t), \quad (2.15)$$

applied at one end of the filament. Here, the prefactor B determines the magnitude of the applied torque. This will naturally determine the amplitude of the swimming motion for any given values of the other parameters. What we really want to do is specify the amplitude itself. This is done by adjusting B iteratively, over a number of cycles, until the desired value is achieved.

For the spermatozoon, the active forces present a greater difficulty because we have to second guess what the organism is doing. The only things to guide us are physical principles and experimental observations. Accordingly, we choose to specify the active forces in terms of a local force quadrupole. That is, we apply a torque T_i at a point midway between bead $i - 1$ and bead i and a torque $-T_i$ between bead i and $i + 1$. It is by means of such a force quadrupole that you would, for example, bend your elbow. The reason we assume the organism generates deformations by this means is because

it introduces no local forces or torques. According to Newton's third law spontaneous torques and forces are impossible. Specifying an active bending mechanism of this form, this condition will be satisfied automatically. We need not invoke a special structure to impose the condition that the total force and torque are zero. It is known experimentally (Brokaw & Gibbons 1973) that no such structure exists because short fragments of flagella still display the ability to bend. While the preceding argument is quite general, we now need to be more specific. To specify a plausible form of the force quadrupole we need information about how a particular organism swims. Here, we will concentrate on spermatozoa. They propagate a travelling wave along their tail. One simple means by which a spermatozoon might do this is by generating a force quadrupole in the form of a sinusoidal travelling wave. That is, in terms of the model,

$$T_i(s_i)\hat{\mathbf{z}} = M_0 \sin k(s_i - ct)\hat{\mathbf{z}}, \quad (2.16)$$

where $s_i = \Delta l/2 - i\Delta l$ is the (discrete) internal coordinate, k a wave vector and c a wave speed. The amplitude M_0 will determine the amplitude of the quadrupole and hence the amplitude of the filament motion. By directing the torques along the $\hat{\mathbf{z}}$ direction, motion will only be generated in the $x - y$ plane. Whereas the model applies quite happily in three-dimensions, we have now, with this choice of bending mechanism, specialized to planar motions typically used by the spermatozoa of simple organisms. This makes it simpler to compare with experiment.

3. RESULTS

(a) Tests of the model

Before applying the model we should of course test it. The strictest tests are as follows. The bending energy, for a given shape, should approach the continuum value (equation (2.4)). The bending forces, derived from the bending energy, can be checked by running the model without dissipation ($\gamma_{\parallel} = \gamma_{\perp} = 0$), in which case total energy should be conserved. The parallel and perpendicular friction coefficient of the model should be simply N times the bead friction coefficient and this should correspond, in both the perpendicular and parallel directions, to the value we set. The model passes all these tests.

We must also show that inertialessness is satisfied. That is, show that we can make the dynamics independent of mass. Furthermore, there should be no 'numerical' swimming, due to accumulated errors in the simulation. This we can show by setting $\gamma^{\parallel} = \gamma^{\perp} = \gamma$. The model should then generate no net motion. The reason for this is that, by definition, the sum over all beads of the bending, tension and active forces is zero. In this case, equation (2.11) clearly implies that the velocity summed over all N beads should also be zero (Cosentino Lagomarsino *et al.* 2002). There will be no net movement. Any individual bead should execute a cyclic motion with a period $\tau = 2\pi/kc$. In figure 1 we have plotted the head position for the sperm model over one cycle (that is, the position of the first bead), at equal intervals of time, for a chain of 50 beads with total length unity. The dimensionless wave vector $k^* = kl$ was equal to 3π , a value typical for the tails of spermatozoa. The ratio of the characteristic time for positional change, $\tau_S = 1/c$, and the inertial time $\tau_{\gamma} = m_i/\gamma$, which we

Figure 1. The head position at 20 equally spaced time intervals during one cycle of the model. The ratio γ/mkc characterizes the ratio of the inertial time-scale to the shape time-scale. Spacial x and y coordinates are measured in units of the chain length. For this simulation the parallel and perpendicular friction coefficients are equal. Dotted line, $\gamma/mkc = 256$; filled circles, $\gamma/mkc = 64$; crosses, $\gamma/mkc = 4$.

define as $\alpha = \tau_S/\tau_{\gamma} = \gamma/m_i ck$, was varied by changing the total mass of the chain. Increasing the value of α (decreasing the mass, everything else fixed) implies that the inertial time (the time it takes an equation with the form of equation (2.11) to reach a steady state) is reduced relative to the time it takes the chain to change shape. As figure 1 shows, as we increase α the results rapidly become independent of α . While the results for $\alpha = 4$ differ slightly from the results for $\alpha = 256$, the results for $\alpha = 64$ differ by less than 0.1%. That is, so long as we satisfy the condition $\alpha \sim 100$, to a high degree of accuracy we have reached the inertialess limit in which we are interested. Regardless of the value of α , the trajectory of the head forms a closed loop over one cycle (almost to machine accuracy). Thus, over one cycle the net movement of this bead, or any other of the beads making up the chain, is zero. The model therefore satisfies the second criterion that, if $\gamma^{\perp} = \gamma^{\parallel}$, there is no propulsion.

(b) The one-armed swimmer

We will discuss our results for the one-armed swimmer in the context of the theoretical analysis of Wiggins and Goldstein. The prefactor B is adjusted to produce a maximum angle at the driven end of 60° . Note that this violates the small angle approximation of Wiggins & Goldstein (1998), but is more consistent with the head deflections found in practice for swimming organisms. A detailed comparison for the case of small angle deflection (where the theory should be more valid) will be described elsewhere (Cosentino Lagomarsino *et al.* 2002). Suffice it to say here, the conclusions are broadly the same. Where they differ this will be pointed out. Once B , and the ratio of the parallel and perpendicular friction coefficients (equation (2.14)) are fixed, the remaining variables can be expressed in terms of one dimensionless quantity, Sp , defined

Figure 2. Speed and efficiency of the one-armed swimmer, rocked back and forth by an external torque applied at one end, as a function of the sperm number. Circles and dotted line, speed; squares and dotted line, efficiency.

$$Sp = \left(\frac{l^4 \omega \gamma^+}{G} \right)^{\frac{1}{4}}. \quad (3.1)$$

This ‘sperm number’ characterizes the relative magnitudes of the viscous and bending forces. A low value implies that bending forces dominate, a high value that viscous forces dominate.

To summarize the theory, we expect, as we vary the sperm number, to see the following.

- (i) The swimming speed and efficiency (defined as the amount of energy consumed, relative to the amount of energy required to simply drag a passive filament through the fluid at the same velocity), go to zero as Sp goes to zero. This is the stiff limit where bending is negligible and the ‘scallop’ theorem applies.
- (ii) At a sperm number $Sp \sim 2$ there is a maximum in both the swimming speed and efficiency (although not at exactly the same value).
- (iii) At high sperm numbers a plateau region where the speed and efficiency become independent of Sp , albeit at values lower than the peak.

In figure 2 we have plotted the swimming speed and efficiency, calculated from the model, as a function of sperm number. Clearly the essential features predicted are indeed present. Both approach zero for small sperm numbers, but with increasing sperm number display a single maximum. It should be noted however that there are significant differences. First, the maximum comes at $Sp \sim 1$ rather than $Sp \sim 2$ as the theory predicts. This may seem a rather small difference. However, in the definition of the sperm number all quantities except the length enter to the power $1/4$. This would correspond to a discrepancy of a factor of 2^4 if we were, for example, trying to extract the bending modulus from experimental results. Note also that we should in principle be able to make a quantitative comparison with theory but the expression for the swimming speed derived by Wiggins & Goldstein (1998) is clearly erroneous. It involves only the transverse friction coefficient, whereas we know that if the transverse and longitudinal friction coefficients are equal the swimming

speed must be zero. No expression involving only one coefficient can be right. This result can, in fact, be corrected (Cosentino Lagomarsino *et al.* 2002).

The second notable area of disagreement is at high values of the sperm number ($Sp \gg 1$) where we do not find a plateau but a slow and steady drop in both speed and efficiency. This effect is, we believe, a consequence of the large amplitude of the motion. At smaller amplitudes a plateau is indeed reached. This is a limitation of the theory, one respect in which large amplitude motions differ from the small amplitude limit. We should conclude with a few comments. Notably, the peak efficiency of *ca.* 0.7% seems very low. However, this depends strongly on the amplitude of the motion. If we go above the 60° limit we have imposed here, it is possible to reach values of 2% before the motion becomes unstable. This is similar to the efficiency typical for both the helical screw mechanism and the sperm motion that we will discuss later. Thus, the one-armed swimmer operating at peak efficiency is a plausible and not especially inefficient entity. Nonetheless, we have not been able to identify a single organism that actually uses this mechanism. Perhaps the most interesting question surrounding the one-armed swimmer is why he or she does not exist.

(c) *Spermatazoon*

To model the swimming motions of spermatozoa we need to specialize the values of the parameters used in the model to those found in practice. First, we will stick to the planar motion generated by a driving quadrupole of the form given by equation (2.16). The wavelength $\lambda (= 2\pi/k)$ associated with these flagellae varies significantly from species to species (Brennen & Winet 1977). However, a typical value is $\lambda = l^*/1.25$, where l^* is the ‘apparent’ length of the tail. By apparent length we mean the end-to-end length for a tail in motion. This is equal to the actual tail length l in the limit of small amplitude motion, but for large deflections, l^* is less than l because of the bending. The value $\lambda = l^*/1.25$ thus implies a tail propagating 1.25 waves. To induce this characteristic wavelength in our model, it would seem sensible to set $k = 2.5\pi/l$. This should induce the required number of bends. For the work reported here we have specialized to this case. As pointed out earlier, the amplitude M_0 will determine the amplitude of the motion and will have to be varied to match typical experimental values. Once M_0 , k and the ratio of the parallel and perpendicular friction coefficients (equation (2.14)) are fixed, the remaining variables can again be lumped together to define a sperm number,

$$Sp = \left(\frac{l^4 c k \gamma^+}{G} \right)^{\frac{1}{4}}, \quad (3.2)$$

characterizing the relative magnitudes of the viscous and bending forces.

We begin by considering low values of the sperm number. That is, the case where bending forces dominate. In figure 3 we have shown a typical example of the waveform we obtain in this regime ($Sp = 1$). Note that, although we input a sinusoidal force quadrupole, the waveform we get out has a number of non-sinusoidal features. Most notably, the amplitude of the first half wave (A1) is not equal to the second (A2), and the first half wavelength

Figure 3. A typical waveform generated by the model at low values of the sperm number ($Sp = 1$). The angle ϕ is by definition the shear angle.

Figure 4. Comparison of the model waveform shown in figure with a video image of a sea slug spermatozoon (Pacey *et al.* 1994). The scale bar represents $20\text{ }\mu\text{m}$.

Table 1. Comparison between waveform characteristics (defined in figure 3) obtained from the model and experimental values (figure 4).

	model	experiment
$A1/l$	0.20	0.20
$A2/l$	0.27	0.26
$L1/l$	0.31	0.30
$L2/l$	0.35	0.34

($L1$) is (slightly) different from the second ($L2$). In figure 4 we have superimposed this waveform onto a video image of a spermatozoon of *Arenicola marina* (blow lug, belonging to the lugworm family Arenicolidae), taken at a matching point in the swimming cycle (Pacey *et al.* 1994). Clearly the agreement is very good. Most notably, the non-sinusoidal features displayed by the model are also present for the real spermatozoon. Values for $A1$, $A2$, $L1$ and $L2$ calculated from the model waveform and the video image are compared in table 1. Given the simplicity of the model and the surprisingly good agreement with experiment, it may be useful to point out that, having fixed k and taken a low value of Sp , the only parameter we have adjusted is the amplitude of the force quadrupole, M_0 . In figure 5 we have plotted the shear angle ϕ as a function of the (absolute) distance from the head, x , at 10 sequential time intervals during one cycle. Both x and ϕ are defined in figure 3. The waveform clearly consists of circular arcs (a linear relation between x and ϕ) separated by

Figure 5. The shear angle ϕ as a function of the distance from the head x at low values of the sperm number ($Sp = 1$). The 10 curves correspond to equally spaced time intervals during one cycle. The dotted curve is the first in the sequence.

a relatively narrow transition region. The maximum shear angle is, furthermore, relatively insensitive to the position along the tail. Again this is very typical of the non-sinusoidal waveforms observed experimentally (Brokaw 1965). Before we move on to higher values of the sperm number, we should point out that the waveforms we have discussed here are not specific to this particular value of the sperm number (unity). If we make the value lower an almost identical waveform is observed. In figure 4 we could equally well have shown the results for any value $Sp < 1$; the difference would have been hardly discernible. The reason for this is that, in this regime, viscous forces are negligible and do not influence the shape. The shape is determined by the balance between tension, resistance to bending and the active bending mechanism. These forces do not depend on the velocity and the waveform is thus independent of Sp .

Moving to higher values of the sperm number, where the velocity dependent viscous forces start to play a role, we find a marked change. The typical waveforms we observe become quite different. An example, for $Sp = 14$, is illustrated in figure 6. Here, we show the waveform at five equal time intervals during one cycle. Note that the circle indicating the head position is only drawn to indicate that the wave propagates from left to right. The effects of any real head are not included in the simulations reported here. In contrast to the low sperm number result, this waveform is atypical of sperm tails. Notably, the amplitude of the motion has a pronounced maximum at the two ends and is significantly suppressed in the middle. The shear angle as a function of the distance from the head is plotted in figure 7 and makes the point more quantitatively. Typical values for the shear angle halfway along the tail are less than one-tenth those at the ends. There is a marked similarity here with the behaviour of a flexible rod being waved about at one end (Wiggins & Goldstein 1998). At high values of Sp the oscillations only propagate a certain penetration depth into the rod. This penetration depth, a result of viscous damping, is related to the reciprocal of the sperm number.

Figure 6. Typical waveforms generated by the model at high values of the sperm number ($Sp = 14$), shown at five equally spaced time intervals during one cycle. The circle indicates the head end, in the sense that the wave propagates from left to right.

Figure 7. The shear angle ϕ as a function of the distance from the head x at high values of the sperm number ($Sp = 14$). The 10 curves correspond to equally spaced time intervals during one cycle. The dotted curve is the first in the sequence.

Not surprisingly, the swimming speeds we obtain in these two different regimes also differ significantly. In figure 8 we have plotted the swimming speed v_s as a function of the sperm number. The swimming speed we define as the ratio of the net displacement of the chain in one cycle to the time for one cycle. We have made this quantity

Figure 8. Dimensionless swimming speed as a function of sperm number. The two sets of data correspond to motion with a maximum shear angle, ϕ_m , of 45° (circles) and 60° (squares). The dashed lines are guides to the eye. Also shown are experimental values for the dimensionless swimming speed of spermatozoa executing planar motion of the form described in the text (Brennen & Winet 1977).

dimensionless by dividing by the apparent wave-speed c^* . Again this differs from the wave speed defined in equation (2.16) because of the difference between the apparent and actual lengths i.e. $c^* = l^*/l$. The speed depends on the amplitude of the motion. We have therefore restricted ourselves to two cases: the maximum shear angle of the head being 45° and 60° . In practice, the value usually lies within this range. Along with the numerical values, we have indicated experimental values for the dimensionless swimming speed of spermatozoa that swim using this kind of mechanism (Brennen & Winet 1977). As we can see, for low values of Sp (waveforms typified by figure 3) the agreement is quite good. However, as we increase Sp (and the tail starts to take the form shown in figure 6) the speed drops significantly below experimental values. Returning to the low sperm number regime, it is noticeable that the swimming speed becomes independent of Sp . This contrasts with the flexible one-armed swimmer where, at low sperm numbers, the flexible arm starts to behave as if it were rigid. As we pointed out in § 1, without bending to generate time asymmetry, the one-armed swimmer does not move. By contrast, in our sperm model the mechanism driving the tail itself introduces the asymmetry required to generate propulsion. In the low Sp limit, the motion is simply driven by a small viscous force exerted on a particular travelling waveform. The waveform, and hence the swimming speed, become independent of Sp . The mechanism works in the same way as a rotating rigid helical screw, for example. The flexibility in itself is not important, only the asymmetry of motion.

4. DISCUSSION

We have described a method for simulating the inertialess dynamics of a flexible filament immersed in a fluid. For the one-armed swimmer, we showed that the picture suggested by Wiggins and Goldstein is essentially correct.

There is an optimal balance between bending forces and viscous forces that generates the maximum propulsion. However, in two quantitative respects our results suggest that their analysis is flawed. First, we cannot use their expression for the swimming speed: it is incorrect. Second, the peak speed and efficiency occur at a somewhat lower value of the sperm number than they predict.

Turning our attention to the results we obtained applying our model to simulate the swimming mechanism of a simple spermatozoon, we found that, using a very simple driving mechanism requiring no local force or torque, we could reproduce the essential features of the waveform observed for real spermatozoa. Furthermore, the swimming speeds we obtained were also consistent with experimental values. The problem here is the following. This was only true in the regime where the resistance of the filament to bending significantly outweighed the viscous forces exerted on the filament by the fluid. If we take experimental values for the bending modulus of the tail and calculate the sperm number, we find a value $Sp \sim 7$. This would mean that in reality viscous forces are of more importance than bending forces. The situation is, it would seem, more akin to that illustrated in figure 6 than figure 4. If one accepts that the agreement found between the model and experiment at low values of the sperm number is not coincidental, there are two possible explanations for this. The simplest is that the tail, when in use, is stiffer than current experimental measurements would suggest. The second is that the spermatozoon uses an active mechanism to generate a force to compensate almost all the viscous force. This would require a much more sophisticated mechanism than the essentially 'dumb' approach we have used here (for example the 'curvature controlled' models extensively studied by Brokaw (1972)).

While our simulations yield a lot of additional information we have not discussed here (efficiency, power requirements for the molecular motor driving the tail), the central point raised by the simulations is therefore the following. If we assume that resistance to bending determines the shape of the tail, a very simple mechanism can produce a waveform strikingly similar to that observed experimentally. If, as experiments suggest, this is not the case, we need to think of how the organism manages to generate internal forces that compensate for the viscous forces, given the constraints of the underlying structure of the tail. It is not at all easy to see how this could be achieved while keeping within the bounds of what is physically possible. It should also be noted that the viscous forces are, in general, complex functions of not just the shape of the tail, but the sperm's environment. The close proximity of an egg, for example, would significantly alter the viscous forces acting on the tail. Presumably the sperm does not want its swimming mechanism to let it down at the crucial moment. Thus, even if correcting for the viscous forces is in principle possible, the sperm would need the ability to sense the friction due to its environment, process the information and act accordingly. As it is on a kamikaze mission, one would not expect the sperm to be over endowed with brain power. The most likely explanation, it seems to us, is when it is in action a sperm's tail is simply stiffer than the experiments suggest.

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GLOSSARY

Sp : sperm number