Electronic Supplementary Material (ESI) for Soft Matter

Calculations of flow-induced orientation distributions for analysis of linear dichroism spectroscopy

James R. A. McLachlan,[a] David J. Smith,[b] Nikola P. Chmel,[c] and Alison Rodger*[c]

[a] *Molecular Organisation and Assembly in Cells Doctoral Training Centre, University of Warwick, Coventry CV4 7AL, UK.*
[b] *School of Mathematics, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK.*
[c] *Warwick Centre for Analytical Science and Department of Chemistry, University of Warwick, Coventry CV4 7AL, UK. E-mail: A.Rodger@warwick.ac.uk*

A Derivation of equation (8)

The material time constant, λ, is given by $1/(6D_r)$ [1], where D_r is the rotational diffusion coefficient. Since $D_r = k_BT/f_r$,where f_r is the rotational frictional coefficient, k_B the Boltzmann constant and T the temperature, we have

$$\lambda = \frac{f_r}{6k_BT}. \tag{A.1}$$

For a prolate spheroid,

$$f_r = 8\pi\eta R_e^3 F_r, \tag{A.2}$$

where η is the dynamic fluid viscosity, the equivalent radius R_e is $(ab^2)^{1/3}$ (a and b are defined in section 2.1.2), and F_r is the frictional coefficient for rotation around the bth axis relative to a sphere of radius R_e [2]. Combining equations (A.1) and (A.2), we obtain

$$\lambda = \frac{4F_r\pi\eta ab^2}{3k_BT}, \tag{A.3}$$

which is equation (8).

B Solving equation (7)

The orientation distribution function, $\psi(t)$, is the solution to the governing Fokker–Planck equation (equation (7)). By expanding ψ in the basis of spherical harmonics [3], we obtain

$$\psi(\theta,\phi,t) = \frac{1}{4\pi}\sum_{n=0}^{N}\sum_{m=0}^{n}\{A_{0n}^{m}(t)P_{n}^{m}(\cos\theta)\cos(m\phi) + A_{1n}^{m}(t)P_{n}^{m}(\cos\theta)\sin(m\phi)\}, \tag{B.1}$$

where N is the expansion order, the $P_n^m(\cos\theta)$ are the associated Legendre polynomials with argument $\cos\theta$, and the amplitudes $A_{in}^m(t)$ are unknown functions of time. We define $A_{1n}^0(t)$ as zero. The normalisation condition, equation (5), is satisfied if and only if $A_{00}^0(t) = 1$. Since the particle is symmetric, we require $\psi(\theta,\phi,t) = \psi(\theta,\phi+\pi,t) = \psi(\theta+\pi,\phi,t)$. If m is odd, then $\cos(m\pi) = -1 \neq \cos(m\cdot 0)$, which violates the first condition unless $A_{0n}^m = A_{1n}^m = 0$. If n is odd, then by the above we need only consider the case when m is even. The associated Legendre polynomial P_n^m is an odd function under these circumstances, so $P_n^m(\cos\pi) = P_n^m(-1) = -P_n^m(1) = -P_n^m(\cos 0)$, which violates the second condition unless $A_{0n}^m = A_{1n}^m = 0$ again.

Following the procedure of Strand *et al.* [1], we find that solving equation (7) reduces to solving the following linear system of $((N/2+1)^2 - 1)$ ordinary differential equations:

$$\frac{dA_{0q}^{p}}{d\tau} = -\frac{q(q+1)}{6}A_{0q}^{p} - P_\lambda\sum_{n=0}^{N}\sum_{m=0}^{n}A_{1n}^{m}a_{nq}^{mp}, \tag{B.2a}$$

$$\frac{dA_{1q}^{p}}{d\tau} = -\frac{q(q+1)}{6}A_{1q}^{p} + P_\lambda\sum_{n=0}^{N}\sum_{m=0}^{n}A_{0n}^{m}a_{nq}^{mp}, \tag{B.2b}$$

for $q = 0, 2, ..., N$ and $p = 0, 2, ..., q$. The dimensionless time $\tau = t/\lambda$, where λ is the material time constant, and the dimensionless quantity P_λ is the Péclet number. The coefficients a_{nq}^{mp} are given in Table B.1. For a given Péclet number and expansion order, the orientation distribution function (equation (B.1)) can be obtained from the solution to equations (B.2).

We numerically solved equations (B.2) for $\tau \in [0, 10]$ (*i.e.*, $t \in [0, 10\lambda]$) using the “ode45” function in MATLAB (The MathWorks, Inc.) with $N = 12$ and initial conditions corresponding to an isotropic orientation distribution: $A_{00}^0(0) = 1$, $A_{iq}^p(0) = 0$ otherwise.

Table B.1 The a_{nq}^{mp} in equations (B.2).

$$a_{n,n-2}^{m,m-2} = \frac{(n-2)(n+m)!(1-\delta_{m0})}{4(2n+1)(2n-1)(n+m-4)!}$$

$$a_{n,n}^{m,m-2} = \frac{3(n-m+2)!(n+m)!(1-\delta_{m0})}{4(2n-1)(2n+3)(n+m-2)!(n-m)!}$$

$$a_{n,n+2}^{m,m-2} = -\frac{(n+3)(n-m+4)!(1-\delta_{m0})}{4(2n+1)(2n+3)(n-m)!}$$

$$a_{n,n}^{m,m} = -m/2$$

$$a_{n,n-2}^{m,m+2} = -\frac{(n-2)(1+\delta_{m0})}{4(2n+1)(2n-1)}$$

$$a_{n,n}^{m,m+2} = -\frac{3(1+\delta_{m0})}{4(2n-1)(2n+3)}$$

$$a_{n,n+2}^{m,m+2} = \frac{(n+3)(1+\delta_{m0})}{4(2n+1)(2n+3)}$$

All other a_{nq}^{mp} are zero

C Calculation of mean shear rate for a rectangular flow channel

As given by Pozrikidis [4], unidirectional flow in the x-direction through a rectangular microchannel with cross section $-a < y < a$ and $-b < z < b$ is described by the velocity profile

$$u(y,z) = \frac{Gb^2}{2\eta}\left[1 - \left(\frac{z}{b}\right)^2 + 4\sum_{n=1}^{\infty}\frac{(-1)^n}{\alpha_n^3}\frac{\cosh(\alpha_n y/b)}{\cosh(\alpha_n a/b)}\cos\left(\alpha_n\frac{z}{b}\right)\right], \tag{C.1}$$

with η the dynamic viscosity of the fluid, G the pressure gradient driving the flow, and the constants α_n being defined by $\alpha_n = (2n-1)\pi/2$. Without loss of generality we shall take $a \leqslant b$.

Equation (C.1) can be rewritten as $u(y,z) = (Gb^2/\eta)\hat{u}(\hat{y},\hat{z})$, where hatted variables are dimensionless, $\hat{y} = y/a$, and $\hat{z} = z/b$. Integrating equation (C.1) over the square cross-section and noting that $\sin(\alpha_n) = (-1)^{n+1}$, we have that the volume flow rate is,

$$Q = 4ab\left(\frac{Gb^2}{\eta}\right)\hat{q}(a/b). \tag{C.2}$$

The dimensionless factor $\hat{q}$, which depends on a and b only through their ratio, is given by

$$\hat{q} = \frac{1}{3} - 2\frac{b}{a}\sum_{n=1}^{\infty}\frac{\tanh(\alpha_n a/b)}{\alpha_n^5}. \tag{C.3}$$

For unidirectional flow, the magnitude of shear rate $\dot{\gamma} = (\mathrm{tr}\{\dot{\gamma}_{ji}\dot{\gamma}_{ij}\}/2)^{1/2}$ is given by the quantity $((\partial u/\partial y)^2 + (\partial u/\partial z)^2)^{1/2}$. Combining equations (C.1) and (C.2), we deduce the following expression for $\dot{\gamma}$ in terms of volume flow rate:

$$\dot{\gamma}(y,z) = \frac{\hat{e}(\hat{y},\hat{z})}{\hat{q}}\left(\frac{Q}{4ab^2}\right), \tag{C.4}$$

where dimensionless $\hat{e}(\hat{y},\hat{z})$ is given by

$$\begin{aligned}\hat{e}(\hat{y},\hat{z}) \quad = \quad & \left[\left(2\sum_{n=1}^{\infty}\frac{(-1)^n}{\alpha_n^2}\frac{\sinh(\alpha_n\hat{y})}{\cosh(\alpha_n a/b)}\cos(\alpha_n\hat{z})\right)^2\right. \\ & \left. + \left(\hat{z} + 2\sum_{n=1}^{\infty}\frac{(-1)^n}{\alpha_n^2}\frac{\cosh(\alpha_n\hat{y})}{\cosh(\alpha_n a/b)}\sin(\alpha_n\hat{z})\right)^2\right]^{1/2}.\end{aligned} \tag{C.5}$$

We define $\langle\hat{e}\rangle$ as the mean value of $\hat{e}$ over the scaled cross-section $-1 < \hat{y} < 1$, $-1 < \hat{z} < 1$, noting that this depends on a and b only through their ratio. We also define $\langle\dot{\gamma}\rangle$ as the mean value of the shear rate $\dot{\gamma}$ over the cross-section in physical variables $-a < y < a$, $-b < z < b$, which leads to

$$\langle\dot{\gamma}\rangle = \frac{Q}{4(ab)^{3/2}}\left(\frac{a}{b}\right)^{1/2}\frac{\langle\hat{e}\rangle}{\hat{q}}. \tag{C.6}$$

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This equation can be written in a more user-friendly form:

$$(\text{mean shear rate}) = \frac{(\text{volume flow rate})}{(\text{cross-sectional area})^{3/2}} \mathcal{E}(\text{aspect ratio}), \qquad \text{(C.7)}$$

where $\mathcal{E}(a/b)$ is defined as $2(a/b)^{1/2} \langle \hat{e} \rangle / \hat{q}$. The designation of a and b in the problem is arbitrary, with $\mathcal{E}(a/b) = \mathcal{E}(b/a)$. We plot $\mathcal{E}$ for aspect ratios varying from 0.2 to 5 in Fig. C.1.

For the present problem, $Q = 1.5$ mL min^{-1} $= 2.5 \times 10^{-8}$ m^3 s^{-1} and the channel cross-section has area 10^{-6} m^2; we also have $\mathcal{E}(1) = 4.97$ for a square channel. Hence the mean shear rate $\langle \dot{\gamma} \rangle \approx 124$ s^{-1}.

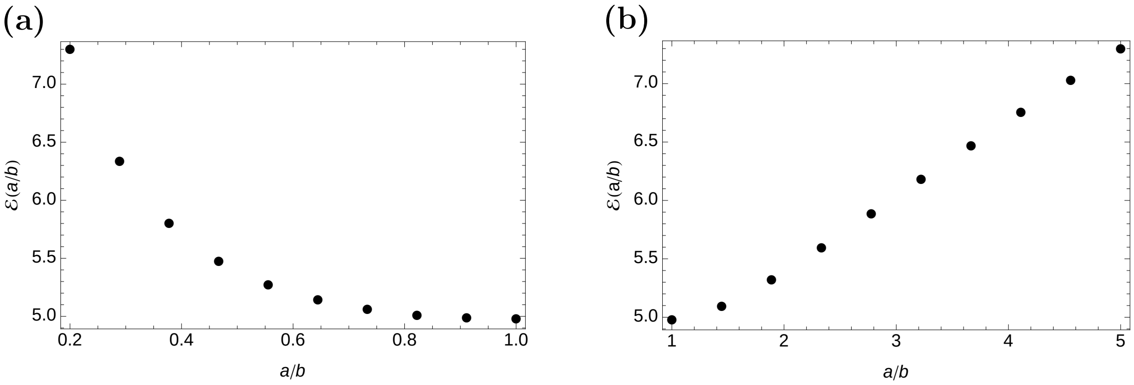

Fig. C.1 Mean shear coefficient, $\mathcal{E}$, versus aspect ratio, a/b, plotted (a) for values $a < b$ and (b) for values $a > b$. Note that $\mathcal{E}(a/b) = \mathcal{E}(b/a)$.

D Determining the orientation of α-helices in FtsZ and M13 bacteriophage

For simplicity, we wanted an angle that represented the average direction of the transitions occurring at 210 nm with respect to the fibre axis. (For *LD* calculations, the average must be of $\cos^2\alpha$, not α.) The 210-nm region of the spectrum is dominated by the low-energy component of the first α-helix π–π^* transition, which is polarised along the long axis of the helix. Following the procedure of Löwe and Amos [5], we reconstructed a model structure of the FtsZ protofilament from the FtsZ crystal structure (PDB accession code 1FSZ [6]). We established the angles between the main axis of the protofilament and the transition vectors of each of the α-helices in FtsZ by drawing least-squares lines through the backbone nitrogen atoms of each of the α-helices and determining the angle each line made with the main axis of the FtsZ protofilament. The $\cos^2\alpha$ for each helix was then evaluated and weighted by the helix length (Table D.1) to determine an average $\cos^2\alpha$ (0.442). This average yielded an effective angle, α_{eff} (*cf.* equation (1)), of 48.3°.

The angles between the long axis of the bacteriophage filament and the transition polarisation vectors of the 210-nm π–π^* peptide sheath were established from the structure of the phage (PDB accession code 2HI5 [7]). The reconstructed cryo-EM structure introduces three additional bends into the α-helices, effectively splitting them into four α-helical units with different angles with respect to the phage main axis. The angles (Table D.2) were established by drawing least-squares lines through the backbone nitrogen atoms of each of the α-helices and the average (determined as for FtsZ) was found to be 30.8°. This contrasts with the value of 21° stated in reference [7] (our averaging of $\cos^2\alpha$ is not sufficient to account for the difference) but accords well with the values of 29° or 35°±10° from reference [8].

Table D.1 Angles α-helices in FtsZ make with the protofilament axis. Here, L is the helix length in amino acids and α the angle in degrees between the helix long axis and the main axis of the protofilament.

α-helix	L	α	$\cos\alpha$	$\cos^2\alpha$	$L\cos^2\alpha$
H0	11	82.0	0.14	0.019	0.21
H1	14	54.0	0.59	0.345	4.83
H2	5	46.4	0.69	0.476	2.38
H3	10	61.3	0.48	0.230	2.30
H4	8	44.6	0.71	0.508	4.06
H5	15	28.8	0.88	0.767	11.51
H6	3	28.6	0.88	0.771	2.31
H7	15	33.0	0.84	0.704	10.56
H8	6	86.5	0.06	0.004	0.02
H9	24	27.3	0.89	0.790	18.96
H10	10	57.0	0.54	0.296	2.96
H11	11	55.1	0.57	0.327	3.60
H12	14	75.5	0.25	0.062	0.87

Table D.2 Angles α-helical units in M13 bacteriophage make with the main axis. Here, L is the helix length in amino acids and α the angle in degrees between the helix long axis and the phage main axis.

α-helix	L	α	$\cos\alpha$	$\cos^2\alpha$	$L\cos^2\alpha$
H0	12	5.3	1.00	0.992	11.90
H1	10	28.6	0.88	0.771	7.71
H2	10	39.2	0.78	0.601	6.01
H3	10	42.8	0.73	0.539	5.39

E Distribution of orientation angles of particles

Calculating the proportion p of M13 bacteriophage filaments that align with $\theta_S < \vartheta$ for $\vartheta = \{10°,\ 20°,\ 30°\} \equiv \{\pi/18,\ \pi/9,\ \pi/6\}$ requires the evaluation of

$$p(\theta_S < \vartheta; t) = \int_{\frac{\pi}{2}-\vartheta}^{\frac{\pi}{2}+\vartheta} \left(\int_0^{\varphi} \psi(\theta,\phi,t)d\phi + \int_{\pi-\varphi}^{\pi+\varphi} \psi(\theta,\phi,t)d\phi + \int_{2\pi-\varphi}^{2\pi} \psi(\theta,\phi,t)d\phi \right) \sin\theta d\theta, \tag{E.1}$$

where $\varphi = \arccos\left(\frac{\cos\vartheta}{\sin\theta}\right)$. The integrals were evaluated numerically in Mathematica (Wolfram Research, Inc.) and the results are shown in Fig. E.1.

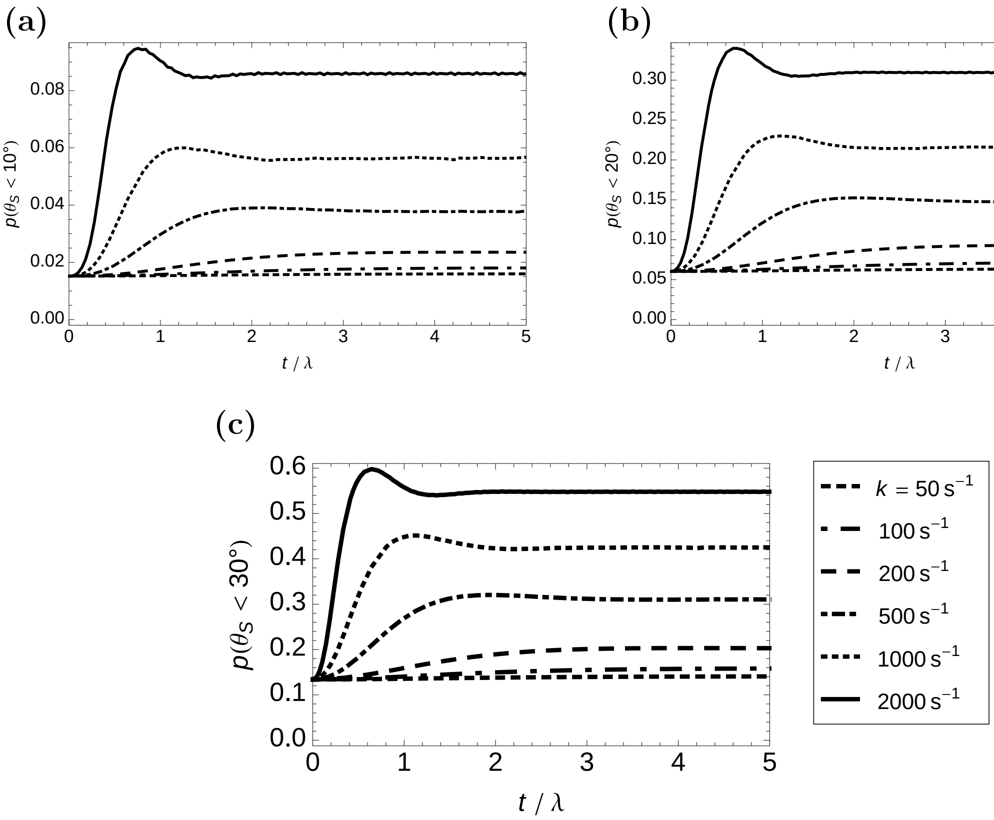

Fig. E.1 Proportion, $p(t)$, of M13 bacteriophage filaments with $\theta_S < \vartheta$ for (a) $\vartheta = 10°$, (b) $\vartheta = 20°$, (c) $\vartheta = 30°$. Shear rate, k, is a parameter. Time 0 corresponds to the onset of shear flow for an isotropic distribution of filaments.

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