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The deformation of a nearly straight thread in a shearing flow with weak Brownian motions

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As a model of an almost fully extended macromolecule, a small, flexible, inextensible, nearly straight thread in a shearing flow with weak Brownian motions is considered. The hydrodynamic resistance to motion is included using the slender-body theory for Stokes flow. The variation of the small transverse displacements along the thread is expressed as a truncated sum of Fourier components, with appropriately chosen modal functions. A diffusion equation is derived in the Fourier space and solved. The expected deformation of the thread is then given for axisymmetric and two-dimensional straining flows. The transverse displacement of the ends and the small shortening of the projected length of the thread are both found to be sensitive to the truncation of the Fourier representation, although it becomes clear on physical grounds that the ratio of the shortening to the typical transverse distortion should increase with the number of degrees of freedom. In simple shear flow the deformation increases as the thread aligns with the flow, until the analysis breaks down when the entire thread is no longer in the extensional quadrants. The influence of the 2 : 1 ratio of the resistance coefficients from the slender-body theory is found to be a small numerical factor.

1. Introduction

A flexible nearly straight thread performing weak Brownian motions is presented as a model of an almost fully extended polymer molecule. The dynamics of the distortion of an isolated long-chain macromolecule by a bulk straining motion are complicated, and simple models help in an understanding of the many different features. When Brownian motions are strong, the backbone of the polymer executes a random walk with an overall linear dimension much smaller than the length along the backbone. As first hinted by Takserman-Krozer's (1963) study of the bead-and-spring model in a pure straining flow, the random walk is substantially distorted (in almost all flow types, but not including simple shear) if the velocity gradient exceeds a critical value proportional to the strength of the Brownian motions. In supercritical flows the distortion is limited by the inextensibility of the backbone, so long as the flow is not so strong that it breaks the molecular bonds of the backbone. Studying an inextensible flexible thread in a shearing flow, Hinch (1976) concluded that the thread would rapidly straighten through a tension induced in it by the flow. Except for the complication of knots inherent in the initial random walk, one is led to speculate that the macromolecule will adopt an almost straight configuration when it is in a supercritical flow for sufficient time. In dilute solutions of polymers the transition from the small random coil to the much larger extended configuration could be reflected in the solution viscosity changing from a value a few per cent larger than that of the solvent to a value several orders of magnitude larger.

In this paper an almost fully extended macromolecule is modelled by a nearly straight, inextensible, flexible thread. The strength of the flow is allowed to be less than in the case of the first inextensible-thread model, so that now Brownian motions can no longer be neglected. Weak Brownian motions acting on a straight thread will cause small transverse distortions, which can be investigated by including a diffusion process in the earlier linear theory of a nearly straight thread. The diffusion equation is best tackled in the Fourier space generated by the eigensolutions from the earlier linear theory, and its solution yields the r.m.s. transverse distortion together with the associated small shortening of the projected length of the inextensible thread. These calculations will provide a measure of the strength of the flow needed to maintain the polymer in its almost fully extended configuration.

The continuum thread fails to represent the discrete nature of the small but finite bond of the polymer backbone. When the Brownian motions are neglected, there is little difference between the continuum and the discrete system with many degrees of freedom. When the thermal agitations are included, however, there is an ultraviolet catastrophe unless the number of degrees of freedom is kept finite. To make such a restriction the distortion of the thread is represented by a truncated Fourier series. Some results (including the r.m.s. distortion except near the ends) will prove to be insensitive to the truncation, while other results (including, clearly, those reflecting the total energy of the system) will depend critically on the truncation. A careful molecular interpretation of the truncation is necessary before any implication of the sensitive results can be given for the polymer molecule.

2. The Fourier space

This section recalls the relevant results of the earlier paper, Hinch (1976). The basic description of the flexible, inextensible, nearly straight thread is given together with the evolution of the distortion in a shearing flow with no Brownian motions. Brownian motions will be introduced in the following section. The linearized motion for the nearly straight thread can be described in terms of some eigensolutions which generate a Fourier space to be used later.

A thin thread of length $2L$ with a slowly varying cross-section which typically has a thickness 2ρ ($\rho \ll L$) is considered. The deformed shape is restricted to have curvatures comparable with the length rather than the thickness. Arc length along the thread is measured by s, $-L \leqslant s \leqslant L$. A suitable kinematic description of such a deforming thread is to specify the centre-line of the cross-section. The thread is placed in a time-dependent shearing flow with a velocity-gradient tensor $\nabla\mathbf{U}(t)$. From the slender-body theory ($\rho \ll L$) for Stokes flow ($|\nabla\mathbf{U}|\, L^2/\nu \ll 1$) the drag per unit length is in the leading approximation related locally to the slip of the undisturbed flow relative to the moving thread. The friction coefficient is $2\pi\mu/\ln(2L/\rho)$ for motion parallel to the thread and twice this for transverse motion.

The nearly straight thread is taken to be approximately in the direction of the rotating unit vector $\mathbf{p}(t)$, an orthonormal triad being completed by $\mathbf{q}(t)$ and $\mathbf{r}(t)$. The centre-line of the thread can then be specified as

$$\mathbf{p}(t)\,s+\mathbf{q}(t)\,x_{(1)}(s,t)+\mathbf{r}(s,t)\,x_{(2)}(s,t),$$

with the small distortion $\mathbf{x}(s,t)$, a two-dimensional vector function. A straight thread, $\mathbf{x}\equiv 0$, has a tension

$$\mathsf{T}=\frac{\pi\mu}{\ln 2L/\rho}\,\mathbf{p}\,.\,\nabla\mathbf{U}\,.\,\mathbf{p}(L^2-s^2)$$

and rotates according to

$$\dot{\mathbf{p}}=\mathbf{p}\,.\,\nabla\mathbf{U}-\mathbf{p}(\mathbf{p}\,.\,\nabla\mathbf{U}\,.\,\mathbf{p}).$$

These two results will serve as an adequate approximation for the nearly straight thread. It is convenient to choose the rotation of the remainder of the orthonormal triad to be given by

$$\dot{\mathbf{q}}=-\mathbf{p}(\mathbf{q}\,.\,\dot{\mathbf{p}}),\quad \dot{\mathbf{r}}=-\mathbf{p}(\mathbf{r}\,.\,\dot{\mathbf{p}}).$$

The local tangent to the nearly straight thread is

$$\mathbf{p}+\mathbf{q}x'_{(1)}+\mathbf{r}x'_{(2)},$$

where the dashes denote differentiation with respect to the arc length. Using this expression for the tangent, the slip of the undisturbed shearing flow relative to the moving thread can be resolved into tangential and normal components. Written in the two-dimensional space, the normal components of slip are

$$\mathbf{v}=\begin{pmatrix}\mathbf{q}\,.\,\nabla\mathbf{U}\,.\,\mathbf{q} & \mathbf{r}\,.\,\nabla\mathbf{U}\,.\,\mathbf{q}\\ \mathbf{q}\,.\,\nabla\mathbf{U}\,.\,\mathbf{r} & \mathbf{r}\,.\,\nabla\mathbf{U}\,.\,\mathbf{r}\end{pmatrix}\mathbf{x}-s\mathbf{x}'(\mathbf{p}\,.\,\nabla\mathbf{U}\,.\,\mathbf{p})-\dot{\mathbf{x}}.$$

The normal force equation requires that the frictional resistance to this slip should balance the tension multiplied by the curvature:

$$\frac{4\pi\mu}{\ln(2L/\rho)}\,\mathbf{v}+\mathsf{T}\mathbf{x}''=0.$$

Substituting the expressions for $\mathbf{v}$ and T yields the evolution equation for the small distortions.

The evolution equation for the small distortions can be solved by decomposing the distortion into Fourier components. The appropriate modal functions are

$$f_n(s)=P'_n(s/L)\,[Ln(n+1)]^{-\frac{1}{2}},$$

which have been normalized such that

$$\int_{-L}^{L} f_n^2\,ds=1.$$

The modal functions are not orthogonal without a weighting function. They have adjoints

$$f_n^+ = \frac{2n+1}{2}\left(1-\frac{s^2}{L^2}\right)f_n = \frac{n(n+1)}{2}\left[\frac{1}{2n+3}(f_n-f_{n+2})+\frac{1}{2n-1}(f_n-f_{n-2})\right].$$

The truncated Fourier decomposition will be taken to run from $n = 2$ to $n = N$. The $n = 1$ mode is a translating straight thread and does not enter the deformation problem. The first mode included, $n = 2$, is a rotating straight thread and this does contribute to the rheology of a suspension of threads. With

$$\mathbf{x}(s,t) = \sum_{n=2}^{N} \mathbf{x}_n(t) f_n(s),$$

the Fourier amplitudes obey equations

$$\dot{\mathbf{x}}_n = -\mathbf{A}_n(t).\mathbf{x}_n,$$

where
$$\mathbf{A}_n = \mathbf{p}.\nabla\mathbf{U}.\mathbf{p}\frac{n^2+n-2}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - \begin{pmatrix}\mathbf{q}.\nabla\mathbf{U}.\mathbf{q} & \mathbf{r}.\nabla\mathbf{U}.\mathbf{q}\\ \mathbf{q}.\nabla\mathbf{U}.\mathbf{r} & \mathbf{r}.\nabla\mathbf{U}.\mathbf{r}\end{pmatrix}.$$

In any particular flow $\nabla\mathbf{U}(t)$, the equation for the rotation of unit vector $\mathbf{p}(t)$ is solved first. Then the equations for the remainder of the orthonormal triad can be integrated. Finally, with the triad substituted in the expression for $\mathbf{A}_n$, the amplitude equations can be solved. This procedure was followed in three examples given in the earlier paper.

In other models of macromolecules in solution the hydrodynamic resistance to motion is often poorly treated. A common prescription is to calculate the drag on representative spheres neglecting the hydrodynamic interaction between the spheres. For the thread this would lead to friction coefficients of $3\pi\mu$ for parallel and transverse slip. The change from the true slender-body theory with the 2 : 1 ratio of friction coefficients to the isotropic relation produces small detailed changes in the above. The modal functions become the self-adjoint Legendre functions $P_{n-1}(s/L)\,[(2n+1)/2L]^{\frac{1}{2}}$, $n = 2, \ldots, N$, and in the expression for $\mathbf{A}_n$ the factor $\frac{1}{4}(n^2+n-2)$ is replaced by $\frac{1}{2}(n^2-n)$.

3. The diffusion equation

The Brownian motions are now introduced via a diffusion process in the Fourier space. When there are Brownian motions the distortion of the thread must be described statistically. Let $\Psi(\mathbf{x}_2, \ldots, \mathbf{x}_N; t)$ be the probability distribution function of the Fourier amplitudes. The probability distribution satisfies the conservation equation

$$\frac{\partial\Psi}{\partial t} + \sum_{n=2}^{N}\frac{\partial}{\partial\mathbf{x}_n}.(\Psi\dot{\mathbf{x}}_n) = 0,$$

where the velocity components $\dot{\mathbf{x}}_n$ include, in addition to the straightening term from the shearing flow derived in the last section, a term representing the migrational motion from the diffusion.

The migrational motion can be derived by considering the chemical potential $kT\ln\Psi$. In a small change in the configuration $\{\delta\mathbf{x}_n\}$, the change in the chemical potential will be equal to the work done against a transverse entropic force $\mathbf{F}(s)$ distributed along the thread:

$$\delta(-kT\ln\Psi) = \int_{-L}^{L} \mathbf{F}(s) . \sum_{n=2}^{N} \delta\mathbf{x}_n f_n(s)\, ds.$$

The entropic force is therefore

$$\mathbf{F}(s) = -kT \sum_{n=2}^{N} \frac{\partial \ln \Psi}{\partial \mathbf{x}_n} f_n^+(s).$$

The migrational motion which this force drives can then be calculated using the transverse friction coefficients. The contribution to the velocity component $\dot{\mathbf{x}}_n$ from the diffusion is thus

$$-\sum_{m=2}^{N} D_{nm} \frac{\partial \ln \Psi}{\partial \mathbf{x}_m},$$

where $$D_{nm} = \frac{kT\ln(2L/\rho)}{4\pi\mu} \int_{-L}^{L} f_n^+ f_m^+\, ds.$$

This result does not depend on the form of the modal functions. The alternative isotropic friction law would thus have produced the last expression multiplied by the factor $4/3\ln(2L/\rho)$.

Bringing together the two contributions to the velocity $\dot{\mathbf{x}}_n$ and substituting into the probability conservation equation produces the diffusion equation

$$\frac{\partial \Psi}{\partial t} - \sum_{n=2}^{N} \frac{\partial}{\partial \mathbf{x}_n} . (\Psi \mathbf{A}_n . \mathbf{x}_n) = \sum_{n,m=2}^{N} D_{nm} \frac{\partial^2 \Psi}{\partial \mathbf{x}_n . \partial \mathbf{x}_m}.$$

This diffusion equation with a linear advection field is solved by a time-dependent Gaussian distribution

$$\Psi(\mathbf{x}_2, \ldots, \mathbf{x}_N; t) = \frac{[\det\{\mathbf{B}_{nm}\}]^{\frac{1}{2}}}{(2\pi)^N} \exp -\tfrac{1}{2} \sum_{n,m=2}^{N} \mathbf{x}_n . \mathbf{B}_{nm}^{-1} . \mathbf{x}_m,$$

where the variances

$$\mathbf{B}_{nm}(t) = \langle \mathbf{x}_n \mathbf{x}_m \rangle = \int \mathbf{x}_n \mathbf{x}_m \Psi\, d^2x_2 \ldots d^2x_N$$

satisfy the following equation for each n and m:

$$\dot{\mathbf{B}}_{nm} + \mathbf{A}_n . \mathbf{B}_{nm} + \mathbf{B}_{nm} . \mathbf{A}_m^T = D_{nm}\, \mathbf{I}.$$

This is the fundamental result of the paper. Its implications are explored for particular flows in the next section.

4. Results

Axisymmetric straining motion

The first particular flow to be considered is steady axisymmetric straining motion which has a velocity-gradient tensor

$$\nabla \mathbf{U} = E \begin{pmatrix} 2 & & \\ & -1 & \\ & & -1 \end{pmatrix}, \quad E > 0.$$

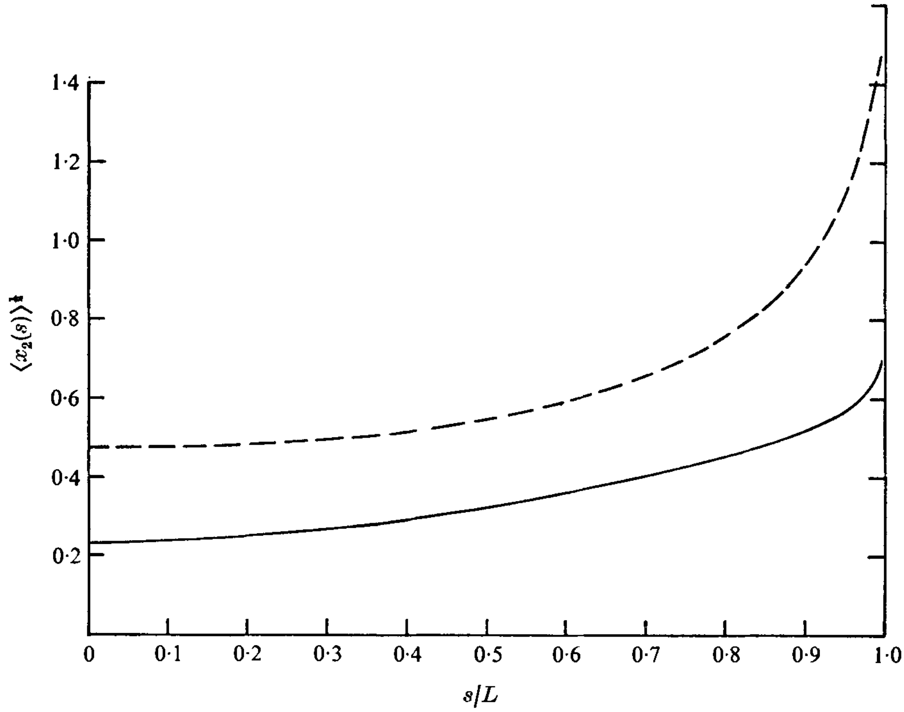

FIGURE 1. The r.m.s. distortion in axisymmetric flow. The units of $\langle x^2(s)\rangle^{\frac{1}{2}}$ are $(kT \ln (2L/\rho)/\pi\mu EL)^{\frac{1}{2}}$ for the 2:1 slender-body theory (solid curve) and $(4kT/3\pi\mu EL)^{\frac{1}{2}}$ for the 1:1 isotropic friction (dashed curve).

A straight thread quickly aligns in the direction of stretching, so the orthonormal triad is chosen to coincide with the co-ordinate axes, i.e. $\mathbf{p} = (1, 0, 0)$, $\mathbf{q} = (0, 1, 0)$ and $\mathbf{r} = (0, 0, 1)$. Now the stretching matrices $\mathbf{A}_n$ can be evaluated and substituted into the equation for the variances. The steady solution for the variances is

$$\langle \mathbf{x}_n \mathbf{x}_m \rangle = \mathbf{I} \frac{kT \ln (2L/\rho)}{\pi\mu E} \frac{n(n+1)}{4[n(n+1)+m(m+1)]} \begin{cases} -(2n+3)^{-1} & \text{for} \quad m = n+2, \\ +(2n+3)^{-1} + (2n-1)^{-1} & \text{for} \quad m = n, \\ -(2n-1)^{-1} & \text{for} \quad m = n-2, \\ 0 \quad \text{otherwise.} \end{cases}$$

Using this result several properties of the distorted thread can be studied.

The r.m.s. distortion as a function of position along the thread is

$$\langle x^2(s)\rangle^{\frac{1}{2}} = L\left(\frac{kT\ln(2L/\rho)}{\pi\mu EL^3}\right)^{\frac{1}{2}} \left[\sum_{n,\,m=2}^{N} \left(\frac{n(n+1)}{m(m+1)}\right)^{\frac{1}{2}} \frac{1}{2[n(n+1)+m(m+1)]} \times \begin{Bmatrix} n \\ m \end{Bmatrix} P_n'\left(\frac{s}{L}\right) P_m'\left(\frac{s}{L}\right)\right]^{\frac{1}{2}},$$

where the curly bracket containing m and n is the same as in the preceding expression for the variances. The sum converges as $N \to \infty$ except at the ends $s = \pm L$. Within a small region near the ends, $1 - |s|/L = O(N^{-2})$, the sum behaves asymptotically like $\frac{1}{16}N[1-\frac{1}{2}N^2(1-|s|/L)+\ldots]$. The r.m.s. distortion with the converged sum is plotted against arc length in figure 1. There is less distortion in the centre because the tension is larger there and this straightens the fluctuating distortions faster. At the ends, where the tension vanishes, the distortion is $O(N^{\frac{1}{2}})$ larger. The r.m.s. integral distortion is

$$\left\langle \frac{1}{2L}\int_{-L}^{L} x^2(s)\,ds \right\rangle^{\frac{1}{2}} = 0.372L\left(\frac{kT\ln(2L/\rho)}{\pi E\mu L^3}\right)^{\frac{1}{2}}.$$

The analysis for the nearly straight thread requires that the distortions, their tangents and their curvatures should all be small. The distortions can be kept small if the non-dimensional group $kT\ln(2L/\rho)/\mu EL^3$ is made small.

In addition to the r.m.s. distortion for the true slender-body theory, also plotted in figure 1 is the r.m.s. distortion for the alternative friction law. The integral distortion is $1{\cdot}5[\ln(2L/\rho)]^{-\frac{1}{2}}$ smaller for the alternative law, although this is merely a factor of 0·53 for $L/\rho = 10^3$ and 0·38 for $L/\rho = 10^6$. Compared with the distortions for the alternative form, those for the true slender-body theory are slightly narrower.

When the inextensible thread is distorted by a small amount $O(x)$, the projection of the thread in the main $\mathbf{p}$ direction must be slightly reduced from $2L$ by $O(x^2/L)$. This shortening is important in the rheology of a suspension of the threads. For an inextensible thread, the derivative with respect to s of the position of the thread should remain the local unit tangent as the thread distorts. The derivative given in the second section of the paper was not of unit length, but had an $O(x^2/L^2)$ error. Correcting this error up to an accuracy of $O(x^4/L^4)$, the unit tangent is

$$\mathbf{p}(s-\tfrac{1}{2}x'^2)+\mathbf{q}x'_{(1)}+\mathbf{r}x'_{(2)}.$$

The total shortening of the thread in the p direction is thus seen to be

$$\left\langle \int_{-L}^{L} \tfrac{1}{2}x'^2\,ds \right\rangle = L\left(\frac{kT\ln(2L/\rho)}{\pi\mu EL^3}\right)\left[\frac{N^3}{96}+\frac{N^2}{16}+O(\ln N)\right],$$

the neglected terms giving an error of less than 1 % when $N > 10$. The shortening diverges as the number of modes is increased. The leading-order $[O(N^3)]$ contribution to the shortening comes from the small end regions $O(N^{-2}L)$.

Now the truncated Fourier series was introduced to represent the finite number of bonds along the backbone of the polymer molecule. As all the bonds are roughly the same size, the shortest length to be resolved is $2L/N$. Thus the contributions from the smaller-scale end regions, $O(LN^{-2})$, should be ignored. When at large n the end contributions to the integrals from P'^2_{n-1} and P''^2_{n-1} are ignored, the shortening is predicted as $O(N)$, although the precise value depends on how the end contributions are ignored. Ignoring the end contributions to the normalization integrals does not affect the results for the r.m.s. distortion, except near the ends.

In order that the analysis for a nearly straight thread should be valid, the shortening must be kept small. Thus the non-dimensional group must be further restricted such that $kT\ln(2L/\rho)/\mu EL^3 \ll N^3$ or, when ignoring the end regions, $\ll N$. Within this limitation, however, it is clear that the shortening can be larger than the distortions when the number of degrees of freedom $2N-2$ becomes large. Essentially each degree of freedom brings an amount $\frac{1}{2}kT$ of stored potential energy. In the stretched thread the potential energy is mainly stored as the shortening weighted by the tension:

$$\left\langle \int_{-L}^{L} \mathrm{T}x'^2\, ds \right\rangle = \tfrac{1}{2}kT[2{\cdot}5N - 3\ln N - 1 + O(N^{-1})].$$

A small amount of energy is also stored by the transverse displacement against the adverse inward flow. As the weighted shortening increases with the number of degrees of freedom, so also does the unweighted shortening. When the unrealistic contributions from the end regions, where the tension is vanishing, are included, the unweighted shortening increases more rapidly.

The final property of the thread to be evaluated is its r.m.s. curvature, which must be kept small for the application of the slender-body theory. The integral r.m.s. distortion is

$$\left(\frac{1}{2L}\int_{-L}^{L} \langle x''(s)^2\rangle\, ds\right)^{\frac{1}{2}} = \frac{1}{L}\left(\frac{kT\ln(2L/\rho)}{\pi\mu EL^3}\right)^{\frac{1}{2}} 0{\cdot}01976N^{\frac{7}{2}}\left(1+\frac{2{\cdot}446}{N}+O\left(\frac{1}{N^2}\right)\right),$$

the neglected terms giving an error of less than 3 % when $N > 10$. As in the shortening problem, the dominant contributions to the integrals at large n come from small $[O(Ln^{-2})]$ end regions. If these regions are excluded the leading-order term in the integral r.m.s. curvature becomes $O(N^{\frac{3}{2}})$ rather than $O(N^{\frac{7}{2}})$, although the precise value depends on how the end regions are ignored. The requirement for the slender-body theory that the curvature be not too large thus further restricts the non-dimensional group such that $kT\ln(2L/\rho)/\mu EL^3 \ll N^7$ or, when the end effects are ignored, $\ll N^3$.

The use of the alternative friction law instead of the true slender-body theory does not drastically change the predictions of the properties of the macromolecule. Ignoring the end regions, the shortening is $O(NkT/\mu EL^2)$ and the integral r.m.s. curvature is $O[(N^3kT/\mu EL^5)^{\frac{1}{2}}]$. When the end effects are included, the N in the shortening becomes N^2 and the N^3 in the curvature becomes N^6, which are both an order of magnitude smaller than with the correct friction.

As the estimates of the shortening and the curvature of a macromolecule depend critically on the crude representation by the continuum thread of the finite number of bonds, a study of the more representative discrete version of the theory would be useful. In such a study the restriction on the curvature could be lifted by using the Oseen hydrodynamic interaction between the bonds.

Two-dimensional straining motion

A stretching flow similar to axisymmetric straining motion is the two-dimensional flow

$$\nabla\mathbf{U} = E\begin{pmatrix}1 & & \\ & -1 & \\ & & 0\end{pmatrix}, \quad E > 0.$$

In this flow a straight thread would quickly align in the stretching direction, so as in the preceding case the orthonormal triad is chosen to coincide with the

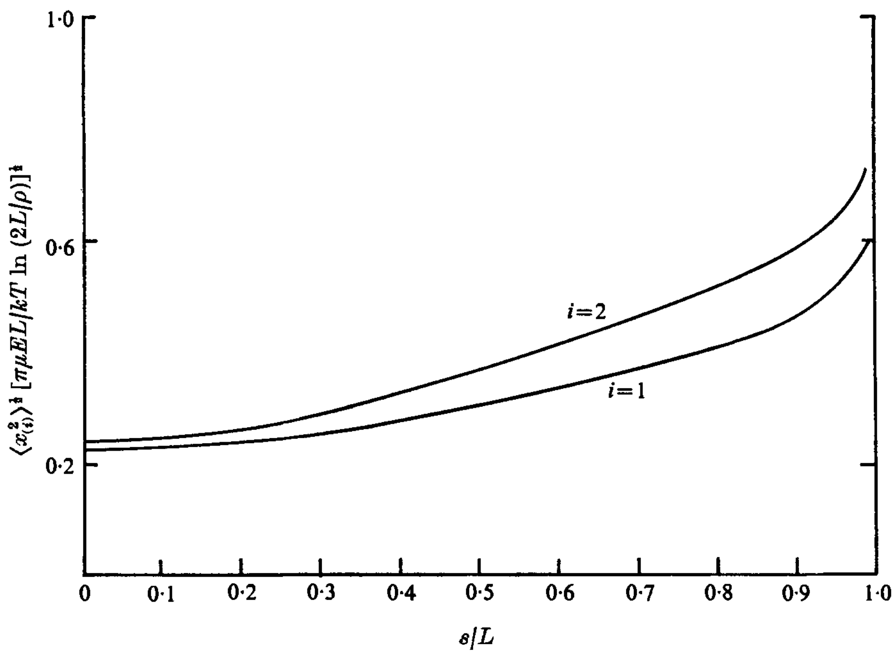

FIGURE 2. The r.m.s. distortion in the compression direction ($i = 1$) and the no-flow direction ($i = 2$) in two-dimensional straining motion.

co-ordinate axes, i.e. $\mathbf{p} = (1, 0, 0)$, $\mathbf{q} = (0, 1, 0)$ and $\mathbf{r} = (0, 0, 1)$. The steady solution for the variances of the Fourier amplitudes is, with the same curly bracket as before,

$$\langle \mathbf{x}_n \mathbf{x}_m \rangle = \frac{kT\ln(2L/\rho)}{\pi\mu E}\begin{pmatrix} (n^2+n+m^2+m+4)^{-1} & 0 \\ 0 & n^2+n+m^2+m-4)^{-1} \end{pmatrix}\frac{n(n+1)}{2}\begin{Bmatrix} n \\ m \end{Bmatrix}.$$

In the $i = 2$ or $\mathbf{r}$ direction there is only the tension straightening the distortions, while in the $i = 1$ or $\mathbf{q}$ direction the compressional inflow also reduces the distortions. Thus the thread is slighly thinner in the $\mathbf{q}$ direction compared with the $\mathbf{r}$ direction. This difference in thickness in the two directions can be seen in figure 2, in which the r.m.s. distortion is plotted as a function of position along the thread. The largest contributor to the difference is the $n = 2$ rotating straight thread mode, which explains why the difference is greatest at the ends of the thread. The r.m.s. distortion has a singularity at the ends very similar to the axisymmetric case, with the end displacement being proportional to $N^{\frac{1}{4}}$. The integral r.m.s. distortion is

$$\left\langle \frac{1}{2L}\int_{-L}^{L} x_{(i)}x_{(j)}\,ds \right\rangle^{\frac{1}{2}} = L\left(\frac{kT\ln(2L/\rho)}{\pi\mu EL^3}\right)^{\frac{1}{2}}\begin{cases} 0{\cdot}3441 & \text{for } i=j=1, \\ 0 & \text{for } i\neq j, \\ 0{\cdot}4188 & \text{for } i=j=2. \end{cases}$$

The orders of magnitude of the shortening and curvature for this flow are the same as for the axisymmetric straining motion.

Simple shear flow

The bead-and-spring models of randomly coiled macromolecules suggest that there may be no critical flow phenomenon in simple shear flow,

$$\nabla\mathbf{U} = \gamma\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Thus if the macromolecule is subjected only to simple shear of arbitrary magnitude it will probably not be greatly extended. Therefore, when the model presented in this paper is applied to simple shear it is imagined that the simple shear follows a different flow which can nearly fully extend the macromolecule, e.g. the flow down a pipe after a convergence at the entrance. As the initial configuration is determined by the preceding flow conditions, which are not under examination, an arbitrary initial configuration must be used.

The motion of a thread without Brownian motions was discussed in the earlier paper (Hinch 1976), using the rotating orthonormal triad

$$\begin{aligned} \mathbf{p}(t) &= (\gamma t,\ 1,\ C)\,[1+C^2+\gamma^2t^2]^{-\frac{1}{2}}, \\ \mathbf{q}(t) &= (-1-C^2,\ \gamma t,\ C\gamma t)\,[(1+C^2)\,(1+C^2+\gamma^2t^2)]^{-\frac{1}{2}}, \\ \mathbf{r}(t) &= (0,\ -C,\ 1)\,[1+C^2]^{-\frac{1}{2}}, \end{aligned}$$

where C is a constant depending on the initial conditions. With this triad substituted in the expression for $\mathbf{A}_n$, the time-dependent solution for the variances $\langle \mathbf{x}_n, \mathbf{x}_m\rangle$ can be found starting from arbitrary initial conditions. As this solution is complex in detail, only the long-time asymptotic behaviour, which is simpler and sufficient for the discussion, is given. For $\gamma^2t^2 \gg 1+C^2$ and with $M = n^2+n+m^2+m$,

$$\langle \mathbf{x}_n\mathbf{x}_m\rangle \sim t\,\frac{kT\ln(2L/\rho)}{\pi\mu}\,\frac{n(n+1)}{2}\left\{\frac{n}{m}\right\}\begin{pmatrix} \dfrac{1}{M+8}\left(1+\dfrac{32C^2}{M(M+4)}\right) & \dfrac{4C}{M(M+4)} \\ \dfrac{4C}{M(M+4)} & \dfrac{1}{M} \end{pmatrix}$$

$$+a(\gamma t)^{-\frac{1}{4}(M-4)}\begin{pmatrix} C^2 & C \\ C & 1 \end{pmatrix} + b(\gamma t)^{-\frac{1}{4}M}\begin{pmatrix} 2C & 1 \\ 1 & 0 \end{pmatrix} + c(\gamma t)^{-\frac{1}{4}(M+4)}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

with an error $O((\gamma t)^{-2})$ smaller in each of the four terms. The coefficients a, b and c in the last three terms are related to the initial conditions. The asymptotics given show that, while the initial distortion decays rapidly as if there were no Brownian motions, there is a term in the variance growing linearly in time which is due to the Brownian motion. This growing part leads to a growth in the r.m.s. distortion

$$O[L(tkT\ln(2L/\rho)\,\mu^{-1}L^{-3})^{\frac{1}{2}}]$$

and a growth in the shortening

$$O[LN(tkT\ln(2L/\rho)\,\mu^{-1}L^{-3})]$$

ignoring the end regions. The form of the growing part of the variances can be explained by considering the decrease in the tension of the thread,

$$O(\mu L^2/\ln(2L/\rho)\,t),$$

as the thread aligns with the flow direction. Equating the order of magnitude of the stored potential energy in the nth mode, i.e. the product of the above tension and the shortening from the nth mode, $O(\langle x_n^2\rangle n^2/L^2)$ ignoring end effects, to the thermal activity kT yields an estimate for the variances $O(kT\ln(2L/\rho)\,t\mu^{-1}n^{-2})$. This argument must be contrasted with one in which the decreasing tension is neglected and the variances are assumed to grow only under the influence of the Brownian motions. Such an argument also yields variances growing linearly in time, but with the constant of proportionality $kT\ln(2L/\rho)\,\mu^{-1}$ now being independent of the mode. Such a growth in the variances yields a growth in the r.m.s. distortion $O[LN^{\frac{1}{2}}(tkT\ln(2L/\rho)\,\mu^{-1}L^{-3})^{\frac{1}{2}}]$ and a growth in the shortening $O[LN^3(tkT\ln(2L/\rho)\,\mu^{-1}L^{-3})]$ ignoring the end regions.

As the thread aligns with the flow its thickness grows. At some time the thickness must be comparable with the angle $\mathbf{p}(t)$ makes with the direction of the flow. A little before this time, the theory presented in this paper must break down because some terms of second order in the near-straightness become important; see the crossing problem discussed in the earlier paper. The angle between the direction of the flow and the thread is $1/\gamma t$ as $\gamma t\to\infty$. The r.m.s. distortion growing owing to the Brownian motions is $O[(tkT\ln(2L/\rho)\,\mu^{-1}L^{-1})^{\frac{1}{2}}]$ at most positions along the thread and $N^{\frac{1}{2}}$ larger at the ends. Taking for the thickness this larger distortion at the end, the theory is valid only while

$$\gamma t \lesssim \left(\frac{kT\ln(2L/\rho)}{\mu\gamma L^3}N\right)^{\frac{1}{3}}.$$

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