Stretching of Polymers in Isotropic Turbulence: A Statistical Closure

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We present a new closure for the mean rate of stretching of a dissolved polymer by homogeneous isotropic turbulence. The polymer is modeled by a bead-spring-type model (e.g., Oldroyd B, FENE-P, Giesekus) and the analytical closure is obtained assuming the Lagrangian velocity gradient can be modeled as a Gaussian, white-noise stochastic process. The resulting closure for the mean stretching depends upon the ratio of the correlation time for strain and rotation. Additionally, we derived a second-order expression for circumstances when strain and rotation have a finite correlation time. Finally, the base level closure is shown to reproduce results from direct numerical simulations by simply modifying the coefficients.

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The dynamics of an isolated polymer molecule in a turbulent flow field is of both fundamental and practical significance. Turbulence provides a mixture of flow types (from rotation to strain) and the response of the polymer is very sensitive to the nature of the underlying flow. Moreover, turbulent flows vary rapidly in space and time, and this, combined with the elasticity of the polymer, produces very complex memory effects. The prime motivation to understand polymer-turbulence interactions is their potential use as drag reducing agents. Since the pioneering work of Toms [1], this technology is routinely used in oil pipelines to reduce pumping costs [2]. The notion of using polymer additives to reduce the drag around ships and submarines has been around for decades, but has yet to be demonstrated on a full-scale system. Early approaches based on trial and error were not successful. Prediction of drag reduction on a complex surface moving at high Reynolds number requires generalized turbulence models (e.g., k-ϵ, Reynolds stress) capable of describing non-Newtonian fluids. Of course, the reliability of these models will depend strongly on the assumptions used to model the higher-order terms.

Direct numerical simulation (DNS) has recently emerged as an important tool for analyzing drag reduction in channel flows [3–6], boundary layers [7,8], and homogeneous turbulence [9–11]. The advantage DNS has over laboratory experiments is that it yields information about the polymer orientation and the flow simultaneously, making it easier to understand the mechanism(s) of turbulent drag reduction and how they depend upon the polymer parameters. However, despite the successes of DNS, it is clear that it will not be a useful tool for designing large-scale systems at realistic Reynolds numbers.

In this Letter, we present a systematic closure approximation for the stretching term in the equation for the mean polymer conformation. This term plays an important role in non-Newtonian turbulence by establishing the mean stretch of the polymer due to turbulent fluctuations. The closure is obtained by assuming the velocity gradient in the Lagrangian frame of reference (i.e., frame of reference moving with the polymer molecule) is Gaussian and short correlated. In that limit, the stretching term takes on an analytic form. We compare the result to stochastic simulations of the velocity gradient and find agreement in the limit as the correlation time approaches zero, as would be expected. For finite correlation times, the form of the closure approximation still appears to hold, but the coefficients must be adjusted. From simple fits, we obtain expressions for the coefficients as functions of the correlation time. Furthermore, we make comparisons with DNS of Newtonian turbulence with polymer and obtain optimized coefficients for this case.

We consider a dilute solution of polymers described by the finite extensible nonlinear elastic model with the Peterline closure (FENE-P). Conservation of mass and momentum take the form

$$\boldsymbol{\nabla}\cdot\mathbf{u}=0, \tag{1}$$

$$\frac{D\mathbf{u}}{Dt}\equiv\frac{\partial\mathbf{u}}{\partial t}+\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u}=-\frac{1}{\rho}\boldsymbol{\nabla}p+\frac{1}{\rho}\boldsymbol{\nabla}\cdot\mathbf{T}^{[s]}+\frac{1}{\rho}\boldsymbol{\nabla}\cdot\mathbf{T}^{[p]}, \tag{2}$$

where $\mathbf{u}(\mathbf{x},t)$ is the velocity vector, ρ is the constant fluid density, $p(\mathbf{x},t)$ is the local pressure, $\mathbf{T}^{[s]}(\mathbf{x},t)$ is the Newtonian stress due to the solvent, and $\mathbf{T}^{[p]}(\mathbf{x},t)$ is the polymer stress. Note that vectors are designated by bold, lower case letters and rank 2 tensors are designated by bold, upper case letters. The Newtonian and polymer stresses, respectively, are given by $\mathbf{T}^{[s]}=2\mu^{[s]}\mathbf{S}$ and $\mathbf{T}^{[p]}=(1-\beta)\mu[f(r)\mathbf{C}-\mathbf{I}]/\tau_p$, where $\mathbf{S}\equiv\frac{1}{2}(\boldsymbol{\Delta}+\boldsymbol{\Delta}^T)$ is the rate-of-strain tensor, $\boldsymbol{\Delta}\equiv\boldsymbol{\nabla}\mathbf{u}$, $\mu^{[s]}$ is the solvent molecular viscosity, $\beta\equiv\mu^{[s]}/\mu$ is the ratio of the solvent viscosity to the solution viscosity at zero shear, τ_p is the polymer relaxation time, $\mathbf{C}$ is the conformation tensor, $r\equiv\sqrt{\mathrm{Tr}(\mathbf{C})}$ is the end-to-end distance of the polymer chain,

and $f(r) = L^2/(L^2 - r^2)$ is a nonlinear entropic force. Note that the function $f(r)$ diverges as $r \to L$, preventing the polymer from extending beyond L. To complete the model, a transport equation for the conformation tensor $\mathbf{C}$ is required

$$\frac{D\mathbf{C}}{Dt} = \mathbf{C}\cdot\boldsymbol{\Delta} + \boldsymbol{\Delta}^T\cdot\mathbf{C} - \frac{1}{\tau_p}[f(r)\mathbf{C} - \mathbf{I}]. \quad (3)$$

If we apply a Reynolds average to Eq. (3), we obtain the following exact equation

$$\frac{\bar{D}\,\bar{\mathbf{C}}}{Dt} - \bar{\mathbf{C}}\cdot\bar{\boldsymbol{\Delta}} - \bar{\boldsymbol{\Delta}}^T\cdot\bar{\mathbf{C}} = \underbrace{\overline{\mathbf{C}\cdot\boldsymbol{\Delta}' + \boldsymbol{\Delta}'^T\cdot\mathbf{C}}}_{\boldsymbol{\Lambda}/\tau_p} - \frac{1}{\tau_p}\underbrace{\left[\overline{f(r)\mathbf{C}} - \mathbf{I}\right]}_{\mathbf{P}}, \quad (4)$$

where the overbar denotes the average over the statistics of the flow and the prime indicates the zero-mean, fluctuating part of the concerned tensor. The terms on the right-hand side of Eq. (4) are not closed. The focus of this Letter is to derive a closed expression for $\boldsymbol{\Lambda}$, the dimensionless stretching term.

The appropriate reference frame to consider deformation of a dissolved polymer molecule is the Lagrangian frame [12]. Under the assumption that the molecular extension of the polymer chain is small compared to the Kolmogorov length, the velocity increment between the two beads of the chain is given by the local velocity gradient dotted into the separation vector. Hence, polymer dynamics are controlled exclusively by the time history of the velocity gradient in the Lagrangian frame, $\boldsymbol{\Delta}'(t)$. We adopt the model for $\boldsymbol{\Delta}'(t)$ introduced by Brunk *et al.* [13]. The gradient is decomposed into the sum of the rate of strain, $\mathbf{S}' \equiv \frac{1}{2}(\boldsymbol{\Delta}' + \boldsymbol{\Delta}'^T)$, and rate of rotation, $\mathbf{R}' \equiv \frac{1}{2}\times(\boldsymbol{\Delta}' - \boldsymbol{\Delta}'^T)$, tensors that each satisfy a Langevin equation of the form

$$d\mathbf{S}' + \frac{\mathbf{S}'}{\tau_S}dt = \mathbf{A}\,d\mathbf{W}, \quad (5)$$

$$d\mathbf{R}' + \frac{\mathbf{S}'}{\tau_R}dt = \mathbf{B}\,d\tilde{\mathbf{W}}, \quad (6)$$

where τ_S and τ_R are the correlation times for the strain and rotation components, respectively, and $\mathbf{W}$ and $\tilde{\mathbf{W}}$ are independent, tensor Wiener processes. The fourth-order, constant matrices $\mathbf{A}$ and $\mathbf{B}$ are defined to satisfy the symmetries of the two tensors, incompressibility, and to be consistent with $\overline{\mathbf{S}'(t):\mathbf{S}'(t)} = \overline{\mathbf{R}'(t):\mathbf{R}'(t)} = \tau_\eta^{-2}$, where $\tau_\eta \equiv (\nu/\epsilon)^{1/2}$ is the Kolmogorov time scale, ϵ is the turbulent energy dissipation rate, and ν is the kinematic viscosity of the solution.

It is useful to introduce the parameters $\Omega \equiv \tau_S/\tau_\eta$ and $a \equiv \tau_R/\tau_S$. From DNS [14] we know that $\Omega \approx 2.3$ and $a \approx 3.1$ [14] at $R_\lambda = 90$, where R_λ is the Reynolds number based on the Taylor microscale. In order to make analytical progress, though, we first consider the limit $\Omega \to 0$ while keeping fixed the ratio a and the Weissenberg number defined in this limit as $\mathrm{We}_\Omega = \tau_p\tau_S/\tau_\eta^2$. This latter condition ensures that the level of polymer stretching remains constant as $\Omega \to 0$. To compute the limit of small Ω, we extend Dekker's perturbation method to tensorial stochastic differential equations [15]. An expansion of $\boldsymbol{\Lambda}$ in powers of Ω can be derived by exploiting the formula for Gaussian integration by parts, expanding the response function of $\mathbf{C}(t)$ under variations of $\boldsymbol{\Delta}'(s)$ around the point $t = s$, collecting the terms of the same order in Ω, and resuming the coefficients of these latter as convergent infinite series. The first term in the expansion for $\boldsymbol{\Lambda}$, corresponding to the white-noise limit, reads (summation over repeated indexes is understood)

$$\Lambda_{ij} = \frac{\tau_p}{2}(M_{ikjl}\bar{\mathbf{C}}_{kl} + M_{ikkl}\bar{\mathbf{C}}_{jl} + M_{jkil}\bar{\mathbf{C}}_{kl} + M_{jkkl}\bar{\mathbf{C}}_{il}), \quad (7)$$

where $M_{ijkl} = 2\tau_S S_{ijkl} + 2\tau_R R_{ijkl}$ and the fourth-order matrices S_{ijkl} and R_{ijkl} are defined such that: $\overline{S'_{ij}(s)S'_{kl}(s+t)} = S_{ijkl}\exp(-t/\tau_S)$ and $\overline{R'_{ij}(s)R'_{kl}(s+t)} = R_{ijkl}\exp(-t/\tau_R)$. Equation (7) holds for a general stationary, Gaussian velocity gradient. If we now impose isotropy on the model, the above expression simplifies to

$$\boldsymbol{\Lambda} = \alpha_1\mathrm{We}_\Omega\,\mathrm{Tr}(\bar{\mathbf{C}})\mathbf{I} + \beta_1\mathrm{We}_\Omega\bar{\mathbf{C}}, \quad (8)$$

where $\alpha_1 = (3 + 5a)/30$ and $\beta_1 = (11 - 15a)/30$. Note that when $\tau_R = \tau_S$ (i.e., $a = 1$), Eq. (8) reduces to the expression derived in Ref. [16]. However, with this restriction, the model does not capture some key aspects of the phenomenology. For example, when $a = 1$, $\Lambda_{11} > 0$ for all We_Ω, which is not consistent with DNS [11]. The discrepancy arises from the fact that the rate-of-strain and rate-of-rotation tensors have distinct correlation times in the Lagrangian frame of reference. Equation (8) is also similar to the expression derived in Ref. [17], although we do not predict an explicit dependence of $\boldsymbol{\Lambda}$ on the kinetic energy. Comparisons with DNS (not shown) do not support the inclusion of this term.

The second-order expression for $\boldsymbol{\Lambda}$ is given by

$$\begin{aligned}\boldsymbol{\Lambda} = {} & \alpha_2\mathrm{We}_\Omega\,\mathrm{Tr}(\bar{\mathbf{C}})\mathbf{I} + \beta_2\mathrm{We}_\Omega\bar{\mathbf{C}} \\ & - \gamma\mathrm{We}_\Omega\tau_\eta[2(\bar{\mathbf{C}}:\bar{\mathbf{S}})\mathbf{I} - \mathrm{Tr}(\bar{\mathbf{C}})\bar{\mathbf{S}} - \bar{\boldsymbol{\Delta}}^T\cdot\bar{\mathbf{C}} - \bar{\mathbf{C}}\cdot\bar{\boldsymbol{\Delta}}] \\ & + \delta\mathrm{We}_\Omega\tau_\eta(\bar{\mathbf{C}}\cdot\bar{\boldsymbol{\Delta}}^T + \bar{\boldsymbol{\Delta}}\cdot\bar{\mathbf{C}}) \\ & - \phi\mathbf{I} - \chi\overline{[3\mathbf{C}\cdot\mathbf{C} - \mathrm{Tr}(\mathbf{C})\mathbf{C}]f'(r)}, \end{aligned} \quad (9)$$

where

$$\alpha_2 = \alpha_1 - \Omega^2\frac{243 - a[25a(a-3)(a+4) - 723]}{3600(a+1)},$$

$$\beta_2 = \beta_1 - \Omega^2\frac{a[25a(a-3)(a+4) - 83] - 3}{1200(a+1)},$$

$$\gamma = \Omega(3 + 5a^2)/60, \qquad \delta = \Omega(12 - 10a^2)/60,$$

$$\phi = 2\Omega^2/3, \qquad \chi = 2\Omega^2/15,$$

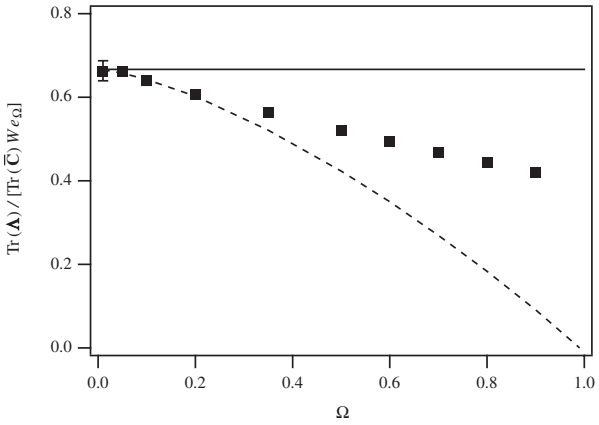

FIG. 1. Plot of $\mathrm{Tr}\,(\mathbf{\Lambda})/[\mathrm{Tr}\,(\bar{\mathbf{C}})\mathrm{We}_\Omega]$ vs Ω at fixed $\mathrm{We}_\Omega = 10$. Straight horizontal line is white-noise prediction: $3\alpha_1 + \beta_1 = 2/3$, and the dashed line corresponds to Eq. (9). Symbols are Brownian dynamics simulations; error bars indicate 1 standard deviation, except where they are smaller than the symbol.

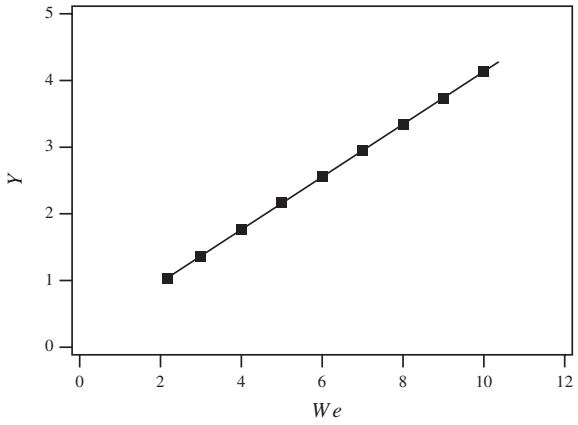

FIG. 2. Plot of $Y \equiv \mathrm{Tr}\,(\mathbf{\Lambda})/[\mathrm{Tr}\,(\bar{\mathbf{C}})]$ vs We from direct numerical simulations. The solid line is a fit through the data ($Y = 0.1822 + 0.3952\mathrm{We}$).

and $f'(r) \equiv df/dr$. Even though Eq. (9) is closed only for the Oldroyd-B model [i.e., $f(r) = 1$], it suggests the form of the terms that arise from the finite correlation time for strain and rotation, including terms that involve all available combinations of $\bar{\mathbf{C}}$ and $\bar{\mathbf{\Delta}}$ with proper symmetry.

We first compare the model predictions to stochastic simulations with $\bar{\mathbf{\Delta}} = 0$. Numerical simulations of Eqs. (5) and (6) were repeated to create an ensemble of trajectories that were used to obtain average polymer properties. Figure 1 shows a normalized plot of the trace of $\mathbf{\Lambda}$ as a function of Ω. The horizontal line at $3\alpha_1 + \beta_1 = 2/3$ corresponds to the white-noise prediction (8). Notice the simulations agree well with the theory in the limit $\Omega \to 0$. The prediction of the second-order theory is accurate for $\Omega < 0.2$; however, at larger values of Ω, it diverges from the simulations. This is most likely due to the truncation of the perturbation expansion. Given the complexity of the series, it is not practical to extend the expansion to higher order.

An alternative approach is to use the form given by Eq. (8), but tune the coefficients to match DNS. The adjusted coefficients will account for higher-order and nonclosed terms in the Ω expansion for $\mathbf{\Lambda}$. We performed decaying isotropic DNS of Eqs. (1)–(3) using the algorithm described in Ref. [18] with $L^2 = 3000$ and initial Weissenberg number $\mathrm{We} \equiv \tau_p/\tau_\eta = 10$ for Cases 1 and 2, and 20 for Case 3. In Navier-Stokes turbulence $\mathrm{We}_\Omega \approx 2.3\mathrm{We}$, where We is the Weissenberg number definition commonly adopted in DNS. The polymer was initially unstretched in Case 1, while Cases 2 and 3 were forced until the polymer equilibrated with the fluid before the decay study was begun. We focus our comparisons on decaying turbulence so as to avoid any unphysical stretching of the polymer by the forcing term. Figure 2 shows $Y \equiv \mathrm{Tr}\,(\mathbf{\Lambda})/[\mathrm{Tr}\,(\bar{\mathbf{C}})]$ for Case 1 that Eq. (8) predicts to be a linear function of We. The behavior is quadratic at low values of We; however, for $\mathrm{We} > 2$, the behavior is very nearly linear. Finite-time correlation effects are expected to be negligible at large We, as polymer relaxation is very slow compared to the decorrelation rate of turbulence. A least squares fit of the linear portion of the curve yields $Y = 0.1822 + 0.3952\mathrm{We}$. Introducing general coefficients into Eq. (8) yields

$$\mathbf{\Lambda} = \tilde{\alpha}_1 \mathrm{We}\,\mathrm{Tr}(\bar{\mathbf{C}})\mathbf{I} + \tilde{\beta}_1 \mathrm{We}\bar{\mathbf{C}}. \tag{10}$$

Figure 3 compares Eq. (10) with $3\tilde{\alpha}_1 + \tilde{\beta}_1 = 0.3952$ (symbols) to the DNS (lines) for the three cases we performed. Overall the model predictions and DNS are in very good agreement.

In summary, we have developed a theoretical expression for the stretching tensor $\mathbf{\Lambda}$ by considering the dynamics of a polymer chain in a stochastic model of the velocity gradient. By considering the limit of small correlation time for the rate-of-strain and rate-of-rotation tensors, it was possible to derive an analytical closure for $\mathbf{\Lambda}$. The result was found to be in excellent agreement with stochas-

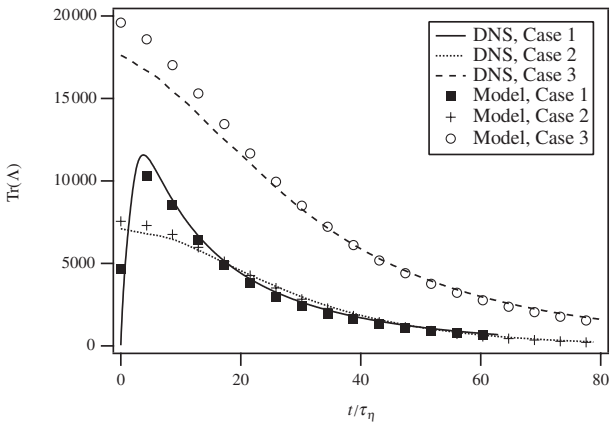

FIG. 3. Plot of $\mathrm{Tr}\,(\mathbf{\Lambda})$ vs t/τ_η, where τ_η is the Kolmogorov time scale. The lines are from direct numerical simulations and the points are Eq. (10) with the tuned coefficients.

tic simulations of the same model in the limit $\Omega \to 0$. However, Navier–Stokes turbulence has a correlation time $\Omega \approx 2.3$. Extending the perturbation expansion to higher order is very difficult. Instead, we were able to modify the white-noise expression to match DNS by adjusting the coefficients. Thus, the analytical work mainly provided the form for $\mathbf{\Lambda}$ and DNS was used to tune the coefficients.

We are extending the model to homogeneous turbulent shear flow. Recent DNS [11,18,19] can be used for comparisons. The second-order theory (9) may suggest the form of the contributions coming from the mean shear. Additionally, we are seeking a closure for the mean restoration term. In this case, knowledge of the distribution of polymer stretch [20] can be used to obtain an approximate closure.

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