Statistical Closures for Homogeneous Shear Flow Turbulence of Dilute Polymer Solutions

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1 Introduction

Dilute polymer solutions exhibit macroscopic behaviors that distinguish them from ordinary Newtonian fluids. For example, minute concentrations of polymers (parts per million on a weight basis) can lead to impressive reductions in the drag on solid surfaces (by up to 80%) [1]. Numerical simulations of viscoelastic flows are generally based on an evolution equation for the conformation tensor of the polymer, $C_{ij} \equiv \langle r_i r_j \rangle$, where $\mathbf{r}$ is the separation vector between the ends of the molecule and angle brackets indicate the average over the Brownian configuration space of the molecule. Direct numerical simulations (DNS) of viscoelastic turbulence are able to reproduce the key phenomenology found in experiments; however, in view of the large number of degrees of freedom, they are limited to modest values of the Reynolds number [2–4]. An alternative approach is to seek a closed equation for the average configuration tensor $\overline{C}_{ij}$, where the average should now be intended over statistical realizations of the turbulent flow. That equation could then be coupled to a Reynolds averaged Navier-Stokes (RANS) solver [5]. Here, we present preliminary results based on a statistical analysis of the transport equation for C_{ij}.

Continuum models for dilute polymer solutions are based on a coarse-grained description of the polymer molecule. Within two-bead dumbbell models, the conformation tensor C_{ij} obeys the transport equation [6]:

$$\frac{\partial C_{ij}}{\partial t} + u_k \frac{\partial C_{ij}}{\partial x_k} = C_{ik} \frac{\partial u_j}{\partial x_k} + C_{jk} \frac{\partial u_i}{\partial x_k} - \frac{f(r) C_{ij} - r_0^2 \delta_{ij}}{\tau_p} , \qquad (1)$$

where r_0 is the equilibrium extension of the polymer, τ_p is its relaxation time, $\mathbf{I}$ is the identity tensor, and r^2 denotes the square of the mean

separation between the ends of the molecule: $r^2 = C_{ii}$. The function f models entropic forces restoring stretched molecules to their equilibrium configuration. In the Oldroyd-B model, the restoration force is assumed to be linear ($f(r) = 1$); this assumption is however appropriate only for weakly stretched polymers. A more realistic model is the FENE-P model, which takes into account the finite extensibility of polymers by means of an nonlinear entropic force that prevents polymers to extend beyond the maximum extension L: $f(r) = (L^2 - 3r_0^2)/(L^2 - r^2)$. The relevant nondimensional number for (1) is the Weissenberg number $We \equiv \tau_p/\tau_\eta$, where τ_η denotes the Kolmogorov time scale. The Weissenberg number measures the strength of the turbulence relative to the restoration force of the polymer.

2 Mean Polymer Conformation Equation

The possibility of introducing a RANS solver for viscoelastic turbulence depends on our ability to deduce an effective evolution equation for $\overline{C}_{ij}$. Averaging (1) over the statistical realizations of the turbulent flow yields

$$\frac{\partial \overline{C}_{ij}}{\partial t} + \overline{u_k \frac{\partial C_{ij}}{\partial x_k}} = \overline{C}_{ik} \frac{\partial \overline{u}_j}{\partial x_k} + \overline{C}_{jk} \frac{\partial \overline{u}_i}{\partial x_k} + \overline{C_{ik} \frac{\partial u'_j}{\partial x_k} + C_{jk} \frac{\partial u'_i}{\partial x_k}} - \overline{\frac{f(r) C_{ij} - r_0^2 \delta_{ij}}{\tau_p}}, \tag{2}$$

where $\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}'$. For notational convenience, we hereafter denote the velocity gradient by $\Gamma_{ij} \equiv \partial u_i / \partial x_j$ and decompose it into the sum of the mean gradient $\overline{\Gamma}_{ij}$ and zero-mean fluctuations Γ'_{ij}. When deriving a closed equation for $\overline{C}_{ij}$ from (2) under homogeneous conditions, we are faced with two closure problems. The first one deals with the contribution to the stretching term coming from fluctuations of the velocity gradient: $\Lambda_{ij} \equiv \tau_p \overline{C_{ik} \Gamma'_{jk} + C_{jk} \Gamma'_{ik}}$. The second one arises only within nonlinear models, such as the FENE-P model, and deals with the closure of the elastic term $\overline{f(r) C_{ij}}$. Here we focus on the first closure, which is more related to the description of turbulent fluctuations rather than to polymer rheology. Our goal is then to derive a closed expression for Λ_{ij} in terms of $\overline{C}_{ij}$.

The appropriate reference frame to consider the deformation of a polymer molecule is the Lagrangian frame. In applications, polymer extension is known to be smaller than the Kolmogorov scale of the flow. In this range of scales the velocity increment between two points in the flow can be assumed to depend linearly on the relative separation between these points. This means that the velocity gradient depends only on time. In order to make analytical progress, we describe the velocity gradient fluctuations $\Gamma'_{ij}(t)$ according to the model introduced by Brunk et al. [7, 8] and subsequently applied to inertial particle motion in turbulent flows [9, 10]. Velocity gradient fluctuations are assumed to be Gaussian, statistically isotropic and stationary in time. The random gradient Γ'_{ij} can be decomposed into the sum of the rate-of-strain and the rate-of-rotation. From DNS of isotropic turbulence, the autocorrelation times of

strain and rotation are known to be different and proportional to τ_η: $\tau_s = 2.3\tau_\eta$ and $\tau_r = 7.2\tau_\eta$, respectively [11]. This range of time scales cannot be solved analytically. Our approach is then to compute Λ_{ij} in the limit of very small autocorrelation times and deduce from that limit the general structure of Λ_{ij} in terms of $\overline{C}_{ij}$. The turbulent regime ($\tau_s = 2.3\tau_\eta$, $\tau_r = 7.2\tau_\eta$) could then be described by preserving the same structure of Λ_{ij} and properly tuning the coefficients appearing in that expression to match DNS.

We treat the small autocorrelation-time expansion of Λ_{ij} by generalizing the method presented in [13] to tensorial stochastic differential equations. We then let $\Omega = \tau_s/\tau_\eta$ tend to zero, while keeping $\tau_r/\tau_s = 7.2/2.3$ and $\Omega\, We$ constant. The latter condition ensures that the level of polymer stretching stays constant as Ω tends to zero.

The first term of the small Ω expansion corresponds to the white-noise limit and reads

$$\Lambda_{ij} = \Omega\, We(\alpha_0\, \overline{C}_{kk}\, \delta_{ij} - \beta_0 \overline{C}_{ij}) \tag{3}$$

with $\alpha_0 = 0.62$ and $\beta_0 = 1.20$. The above expression depends linearly on $\overline{C}_{ij}$ and explicitly shows that small-scale isotropic turbulent fluctuations make the conformation tensor isotropic. It is worth noting that the limiting expression (3) is independent of $\overline{\Gamma}_{ij}$ and the form of the entropic force $f(r)$. When $\tau_r = \tau_s$, (3) reduces to the expression derived in [14]. However, with that restriction, the model does not capture some key aspects of the phenomenology. For instance, if $\tau_r = \tau_s$, then Λ_{11} is forced to be positive for all We, which is not the case in the presence of a large mean shear.

The next order in the small Ω expansion gives

$$\begin{aligned}\Lambda_{ij} = {} & [(0.62\Omega\, We - 0.15\Omega^3\, We)\overline{C}_{kk}\delta_{ij} - (1.20\Omega\, We + 0.007\Omega^3\, We)\overline{C}_{ij}] \\ & -0.87\Omega^2[2\overline{C}_{lk}\overline{\Gamma}_{kl}\delta_{ij} - \overline{C}_{kk}(\overline{\Gamma}_{ij} + \overline{\Gamma}_{ji}) - \overline{C}_{kj}\overline{\Gamma}_{ki} - \overline{C}_{ki}\overline{\Gamma}_{kj}] \\ & +1.43\Omega^2(\overline{C}_{kj}\overline{\Gamma}_{ik} + \overline{C}_{ki}\overline{\Gamma}_{jk}) \\ & -\tfrac{2}{15}\Omega^2\, \overline{(3C_{ik}C_{kj} - C_{kk}C_{ij})f'(r)} - \tfrac{2}{3}R_0^2\Omega^2\delta_{ij}\ ,\end{aligned} \tag{4}$$

where $f'(r) = df/dr$. Although (4) is closed only for the Oldroyd-B model, it suggests that a contribution similar to that coming from the white-noise limit is present also for finite autocorrelation times of strain and rotation. Moreover, the contribution from the mean velocity gradient consists of all the possible combinations of $\overline{C}_{ij}$ and $\overline{\Gamma}_{ij}$ that give a symmetric second-order tensor. For the isotropic case ($\overline{\Gamma} = 0$) the above predictions were validated by Brownian Dynamics simulations based on the flow introduced in [7, 8] (Fig. 1). Numerical simulations were conducted by means of a second-order numerical scheme and the averages were computed both as ensemble averages over independent Lagrangian trajectories and steady-state time averages.

Even if they have been derived in the asymptotic range of small autocorrelation times, we expect that our predictions will be useful for deducing a closed equation for the mean conformation tensor in real turbulent viscoelastic flows. This result may be achieved by direct comparison with DNS.

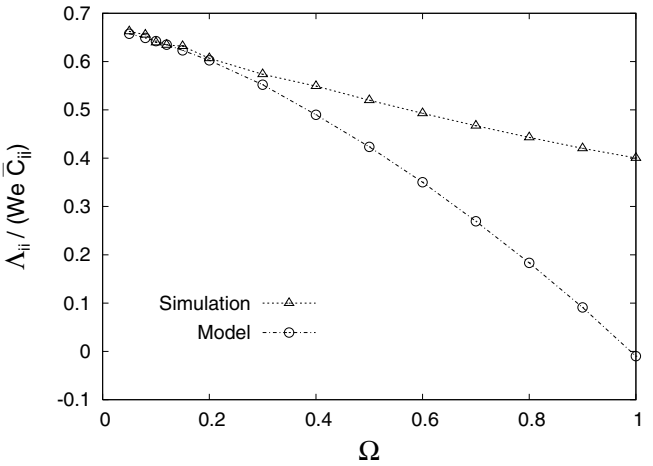

Fig. 1. Validation of the model prediction in the limit of small autocorrelation times of strain and rotation by means of Brownian Dynamics simulations ($\Omega We = 10$)

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