



Modeling and numerical simulations of polymer degradation in a drag reducing plane Couette flow



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A B S T R A C T

Mechanical molecular scission is the main problem of polymeric drag reducers. The ability to reduce the drag is notably decreased as the molecules break down step by step as time goes on. A number of researchers have given a large part of their time to attempts to further understand the role that some important features play in polymer degradation. Until now, all efforts have been in experimental approaches. This paper is the first attempt to take into account the effect of molecular scission on a drag reducing flow by a direct numerical simulation. We analyse a turbulent plane Couette flow of a FENE-P fluid. Our degradation model is based on the maximum polymer extension length L . Unlike the standard FENE-P model, in which L is a constant, the polymer extension here is a spatio-temporal field $L(x, y, z, t)$. When the molecules are highly stretched, which is measured by the trace of the conformation tensor, their maximum length is locally reduced and, consequently, so is their ability to reduce drag. The degraded L spreads within the domain by means of a transport equation. We show here that with such a simple idea we are able to predict the main aspects of mechanical degradation in the flow, such as the change of the turbulent structures and velocity field, and, consequently, the fall of the drag reduction over time.

1. Introduction

Drag reducing polymers have been studied for over 70 years. The number of their practical uses is enormous, including the transport of liquid in pipelines, firefighting operations, and medical applications. The main aspects of the phenomenon, as the role played by the polymer concentration, molecular weight, temperature, Reynolds number, and the quality of the solvent, have been much analysed (see [12,26]). Researchers have also devoted a lot of time to attempts to describe the mechanism of drag reduction (DR). The two main ideas were first proposed by Lumley [11] (the viscous theory) and Tabor and de Gennes [22] (the elastic theory). Recently, some authors have used both the viscous and elastic concepts in an effort to describe in detail the mechanism of DR based on a coil–stretch cycle of the polymer near the wall (see [6,7,9,15,17–19]). However, many aspects of the problem are still under investigation, such as the role played by mechanical degradation in such a coil–stretch cycle. Perhaps a new mechanism should consider a cycle consisting of a coil–stretch followed by a scission, i.e. a coil–stretch–scission cycle.

The focus here is the polymer degradation. It is the consensus that

the mechanical molecular scission is the main problem in the attempt to conceive a highly efficient drag reducer. Such a problem has received deserved attention over the years and many authors have contributed to interpreting the role played by the many features of the problem in the polymer degradation in turbulent flows. The role played by the concentration, molecular weight, temperature, Reynolds number, and quality of the solvent in the resistance of the solution can be found in [1,14,16,20,21], who conducted a detailed analysis of degradation using different water soluble materials (PEO, PAM and XG) and showed that the shear resistance increases with the concentration and molecular weight. It is worth noting that the molecules break step by step in a drag reducing flow, but this process stops after a long enough time, when the polymer mean molecular weight reaches an asymptotic value. Hence, it is also to be expected that there will be a certain steady state of a DR larger than zero, [10,16,21,25]. Obviously, here we are not considering biological degradation, which can take the DR to zero, see [4].

As far as we know, our paper is the first attempt to provide a computer model of mechanical molecular scission in drag reducing flows. In fact, there have been a number of important numerical

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investigations of DR. Most of them use direct numerical simulations of the standard FENE-P model (see [7,8,15,23]), in which the maximum molecular length L is a constant. Unlike the approaches commonly used, we consider L as a spatio-temporal field, namely, $L(x, y, z, t)$. Conceptually, from the FENE-P model, L can be clearly related to the mean polymer molecular weight. In fact, we use a criterion based on the polymer stretching, computed by the trace of the conformation tensor, to change the values of L point by point. The degraded L is spread within the domain by means of a transport equation. By doing so, the domain has at each point in time a distribution of L , which resembles a distribution of molecular weights from an experimental point of view.

This paper is organized into 5 sections. In Section 2 we present the physical formulation, which is divided into two parts: A) The main governing equations and B) the mechanical degradation model. The numerical method is briefly presented in Section 3. Our results are in Section 4 and, finally, the concluding remarks are in Section 5.

2. Physical formulation

We detach this section into two parts. At first, in Section 2.1, we show the standard equations for the flow a FENE-P fluid in parallel plates. In the second part, in Section 2.2, we give the details of our mechanical degradation model.

2.1. The main governing equations

Following our previous paper [15], we consider a turbulent plane Couette flow of an incompressible dilute polymer solution. The flow is driven by both the top and the bottom plates, which have the same magnitude of the velocity in the streamwise direction (U_h), but opposite senses. The streamwise direction is $x_1 = x$, the spanwise direction is $x_2 = y$, and the wall-normal direction is $x_3 = z$. The instantaneous velocity field is $(u_x, u_y, u_z) = (u, v, w)$ and is solenoidal ($\nabla \cdot \mathbf{u} = 0$, where \mathbf{u} denotes the velocity vector). Wall scaling is used and is based on zero-shear rate variables with the length and time scaled by ν_{tot}/u_τ and ν_{tot}/u_τ^2 , where $\nu_{tot} = \nu_N + \nu_{p0}$ is the total (solvent + polymer) zero-shear viscosity, and u_τ is the zero-shear friction velocity. Using this scaling, the dimensionless momentum equations are

$$\frac{\partial u_i^+}{\partial t^+} + u_j^+ \frac{\partial u_i^+}{\partial x_j^+} = -\frac{\partial p^+}{\partial x_i^+} + \beta_0 \frac{\partial^2 u_i^+}{\partial x_j^{+2}} + \frac{\partial \Xi_{ij}^+}{\partial x_j^+}. \quad (1)$$

In Eq. (1), the superscript ‘+’ indicates the wall unit normalization, p^+ is the pressure, and β_0 is the ratio of the Newtonian solvent viscosity (ν_N) to the total zero-shear viscosity (ν_{tot}). The extra-stress tensor components are denoted by Ξ_{ij}^+ . The formalism of Eq. (1) includes the assumption of a uniform polymer concentration in the dilute regime which is governed by the viscosity ratio β_0 , where $\beta_0 = 1$ yields the limiting behaviour of the Newtonian case. The extra-stress tensor components (Ξ_{ij}^+) in Eq. (1) represent the polymer’s contribution to the tension of the solution. This contribution is accounted for by a single spring–dumbbell model. We employ here the FENE-P kinetic theory [3]. This model employs the phase-averaged conformation tensor $C_{ij} = \langle q_i q_j \rangle$, where the q_i are the components of the *end-to-end vector* of each individual polymer molecule. The components of the extra-stress tensor, Ξ^+ , are then $\Xi_{ij}^+ = \alpha_0 (f\{tr(C)\} C_{ij} - \delta_{ij})$ with $\alpha_0 = (1 - \beta_0)/Wi_{\tau_0}$, where $Wi_{\tau_0} = \lambda u_\tau^2 / \nu_{tot}$ is the friction Weissenberg number representing the ratio of the elastic relaxation time (λ) to the viscous timescale. Additionally, δ_{ij} is Kronecker’s delta and $f\{tr(C)\}$ is given by the Peterlin approximation $f\{tr(C)\} = \frac{L^2 - 3}{L^2 - tr(C)}$, where L is the maximum polymer molecule extensibility and $\{tr(\cdot)\}$ represents the trace operator. This system of equations is closed with an evolution equation for the conformation tensor

$$\frac{DC_{ij}}{Dt^+} = (C_{ik} S_{kj}^+ + S_{ik}^+ C_{kj}) - (C_{ik} W_{kj}^+ + W_{ik}^+ C_{kj}) - \frac{f\{tr(C)\} C_{ij} - \delta_{ij}}{Wi_{\tau_0}}, \quad (2)$$

where $S_{ij}^+ = (\partial u_i^+ / \partial x_j^+ + \partial u_j^+ / \partial x_i^+) / 2$ and $W_{ij}^+ = (\partial u_i^+ / \partial x_j^+ - \partial u_j^+ / \partial x_i^+) / 2$ are, respectively, the terms of the rate-of-strain, \mathbf{S}^+ , and the rate-of-rotation, \mathbf{W}^+ , tensors.

2.2. The mechanical degradation model

Our effort here is to build a very simple model as a first attempt to take into account the effects of the mechanical polymer degradation in drag reducing flows based on a FENE-P fluid. We deliberately modify the standard approach widely used to simulate drag reducing flows to the smallest extent possible, minimizing numerical instabilities and costs, but creating the means to further understand the polymeric DR, considering the very important mechanism of mechanical degradation. Specifically, our degradation model is focused on the maximum molecule extensibility L , which seems to be the most evident parameter that can be changed when degradation play a role. Obviously, when a molecule breaks into two pieces, the maximum length reached by each part is reduced. Hence, that is exactly what we consider here. Unlike the standard FENE-P model, here L is spatio-temporal field, which spreads within the domain by a transport equation. We are certainly conscious of the extra implications of molecule degradation for the FENE-P fluid. We mean that a more sophisticated degradation model based on the FENE-P fluid should, perhaps, also consider a spatio-temporal field of viscosity and Weissenberg number, but these modifications all together would impose a lot of numerical instabilities.

As mentioned above, we consider a spatio-temporal field of the maximum polymer extension length, $L(x, y, z, t)$, instead of the unique and constant L typically used in the standard FENE-P model. Thus, L is a molecular property that must be transported, as occurs in a real flow. In order to spread the degraded molecules within the domain, we use a transport equation for $L(x, y, z, t)$,

$$\frac{\partial L}{\partial t^+} + \left(u_x^+ \frac{\partial L}{\partial x^+} + u_y^+ \frac{\partial L}{\partial y^+} + u_z^+ \frac{\partial L}{\partial z^+} \right) = k_L \left(\frac{\partial^2 L}{\partial x^{+2}} + \frac{\partial^2 L}{\partial y^{+2}} + \frac{\partial^2 L}{\partial z^{+2}} \right). \quad (3)$$

Here, L is the local and instantaneous maximum polymer extension length and u_x^+ , u_y^+ , and u_z^+ dictate the corresponding local velocity components in the streamwise (x^+), spanwise (y^+) and wall-normal (z^+) directions. The explicit dissipative elliptic term in Eq. (3) is an artifact used to remove the unphysical high wave-number instabilities typically induced by the chaotic nature of viscoelastic turbulent flows, when computed with high-order spectral code. Hence, k_L represents a constant of artificial diffusivity. Here, this constant is quite small, $k_L = 10^{-6}$, and, as a result, the transport of L is dominated by advection. At last, in order to keep the physical consistency, the maximum polymer extension length equation (Eq. (3)) was solved following exactly the same method employed for the conformation tensor equation (Eq. (2)). More specifically, the maximum polymer extension length equation without artificial diffusivity was at first updated on the channel walls. These intermediate values were then used as boundary conditions to step forward the maximum extension length equation including artificial diffusivity (Eq. (3)). This temporal scheme proved to be stable, as explained in details by Thais et al. [24], and guarantees the positive-definiteness of $L(x, y, z, t)$.

At the beginning of the simulation, $L(x, y, z, t)$ is uniform and equal to an initial value ($L_i = 30$ in the simulations presented here). As the simulation progresses, we use a mechanical scission criterion to evaluate the new values of $L(x, y, z, t)$ within the domain. The criterion is based on the relative polymer stretching, which is taken into account by the ratio between the trace of the conformation tensor and L_i^2 , i.e. $tr(C(x, y, z, t)/L_i^2)$.

More precisely, at particular time-steps during the simulation, if $tr(C(x, y, z, t)/L_i^2) \geq \zeta$, then $L(x, y, z, t)$ is reduced by a previously determined amount. Since $L(x, y, z, t)$ is used to calculate a local Peterlin function at each time-step (which is related to the polymer forces), a decreasing $L(x, y, z, t)$ reduces the polymer’s contribution in

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