Large-Eddy Simulations of turbulent flows with polymer additives

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June 2016

Abstract

A new subgrid-scale (SGS) model is developed for large-eddy simulations (LES) of viscoelastic flows represented by the FENE-P model. The model for the filtered conformation tensor transport equation is based on the self-similarity of the polymer stretching terms, and on a local equilibrium of the trace of the conformation tensor, which is proportional to the elastic elastic stored in the polymer molecules, while the SGS stresses are modelled with the classical Smagorinsky model. The new SGS model is assessed in direct numerical simulations (DNS) of forced isotropic turbulence using classical \textit{a priori} tests, and in \textit{a posteriori} (LES) showing excellent agreement with all the exact (filtered DNS) results. The new model is simple to implement and computationally inexpensive and provides a major progress in the numerical simulation of turbulent Newtonian flows with diluted polymer molecules.

Keywords: Homogeneous Isotropic Turbulence, Direct Numerical Simulations, Large-Eddy Simulations, Viscoelastic Turbulence, FENE-P

1. Introduction

In 1948, it was discovered that the addition of long chained polymers at low concentrations (tens of parts per million) into a turbulent Newtonian solvent, can reduce the skin friction drag on a stationary surface by up to 80 percent. Since usually the polymer is non-toxic and cheaply available, this technology has been successfully used to reduce the pumping costs and heat transfer losses for oil pipelines and district heating/cooling, to increase flow rate in fire fighting hoses and to help irrigation and drainage. The first studies were essentially empirical and experimental, trying to explain the onset of Drag Reduction (DR) caused by polymers. Although the capability to numerically simulate turbulent flow of dilute polymers is relatively new, over the past 20 years, these tools have gained an important role in the research of this field [1]. However, highly detailed numerical simulations of these flows, using Direct Numerical Simulations (DNS) have a very high computational cost which is unaffordable for the flows present in most industrial applications. They are one order of magnitude more expensive than the Newtonian counterparts, because it is necessary to solve at the same time a model to simulate the behavior of the dilute polymers. In search of a more suitable numerical method, Large-Eddy Simulations (LES) are a compromise between accuracy and computational cost. LES were first used in 1963 to study meteorological phenomena, becoming an important tool for the study of environmental and engineering turbulent flows [2]. With a LES model capable of reproducing the phenomenology of DR by polymers additives, it will be possible to acquire data that will provide advances in this area, leading to improved and expanded practical applications and increasing our understanding of fluid turbulence and its control.

2. Governing Equations for Dilute Polymer Solutions

The fluid flow is governed by the incompressible momentum transport equations in a generalised form of the Navier-Stokes equations (continuity and momentum equations respectively):

\[
\frac{\partial u_i}{\partial x_i} = 0; \quad \frac{\partial u_i}{\partial t} + u_k \frac{\partial u_i}{\partial x_k} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + 2\nu^{[s]} \frac{\partial S_{ij}}{\partial x_j} + \frac{1}{\rho} \frac{\partial \sigma_{ij}^{[p]}}{\partial x_j},
\]

where \(u_i(x,t)\) is the velocity vector, \(\rho\) is the fluid density, and \(p\) is the pressure and \(\nu^{[s]}\) is the (Newtonian) kinematic viscosity of the solvent. \(S_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2\) is the rate-of-strain tensor and \(\sigma_{ij}^{[p]}\) is
the polymer stress tensor given by $\sigma_{ij}^{[p]} = \frac{\rho \nu^{[p]}}{\tau_p} [f(C_{kk}) C_{ij} - \delta_{ij}]$, where $C_{ij}$ is a continuous conformation tensor field representing an ensemble of polymer chains, where each chain is represented by two dumbbells connected by a non-linear spring and $\nu^{[p]}$ the zero shear-rate polymeric viscosity. Apart from the viscosity ratio $\beta = \nu^{[p]} / (\nu^{[v]} + \nu^{[s]})$, i.e., the ratio between the solvent and the total zero-shear-rate viscosity of the solution, the FENE-P model uses also the longest relaxation time of the polymer molecules $\tau_p$, and the Peterlin function defined by $f(C_{kk}) = [L^2 - 3]/[L^2 - C_{kk}]$, where $\sqrt{C_{kk}}$ is the (normalised) extension length and $L$ is the maximum extensibility of the polymer chains (non-dimensional). Finally, the conformation tensor is governed by the following transport equation,

$$\frac{\partial C_{ij}}{\partial t} + u_k \frac{\partial C_{ij}}{\partial x_k} = C_{jk} \frac{\partial u_i}{\partial x_k} + C_{ik} \frac{\partial u_j}{\partial x_k} - \frac{1}{\tau_p} [f(C_{kk}) C_{ij} - \delta_{ij}], \tag{2}$$

where the first two terms in the right-hand side of Eq. 2 represent production due to velocity-polymer interactions, (polymer stretching term), while the last term represents a polymer dissipation.

2.1. Filtered ‘FENE-P’ fluid governing equations: subgrid-scale terms for the FENE-P fluid

In LES each flow variable $\phi(x, t)$ is decomposed into a resolved (or large-scale) $\phi(x, t)$, and a unresolved (or subgrid-scale) $\phi'(x, t)$, scales of motion: $\phi(x, t) = \phi(x, t) + \phi'(x, t)$. In the present work, a box filter is used to separate the resolved and unresolved scales of motion. Application of this filtering operation to the equations of motion for a FENE-P fluid yields the filtered FENE-P fluid equations, consisting on the filtered continuity, momentum equation, and conformation tensor transport equations,

$$\frac{\partial \tau_{ij}}{\partial t} = 0; \quad \frac{\partial \tau_{ij}}{\partial t} + u_k \frac{\partial \tau_{ij}}{\partial x_k} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu^{[s]} \frac{\partial^2 \tau_{ij}}{\partial x_i \partial x_j} - \frac{\partial \psi_{ij}}{\partial x_j} + \frac{1}{\rho} \frac{\partial \sigma_{ij}^{[p]}}{\partial x_j}, \tag{3}$$

and,

$$\frac{\partial C_{ij}}{\partial t} + u_k \frac{\partial C_{ij}}{\partial x_k} = \frac{\partial \tau_{ij}}{\partial x_i} C_{kk} + \frac{1}{\tau_p} [f(C_{kk}) C_{ij} - \delta_{ij}] - \psi_{ij} + \gamma_{ij}, \tag{4}$$

respectively, where $\tau_{ij} = \frac{\partial \tau_{ij}}{\partial x_i} C_{kk}$ is the subgrid-scale stresses tensor, describing the effect of the subgrid-scale stresses in the evolution of the resolved velocity field. Notice that the new term arising in the filtered momentum equation (3), and that is not present in the filtered Navier-Stokes equations, given by $\sigma_{ij}^{[p]} = \frac{\rho \nu^{[p]}}{\tau_p} [f(C_{kk}) C_{ij} - \delta_{ij}]$. The new terms requiring modelling are the subgrid-scale advection conformation tensor, and the subgrid-scale polymer stretching (non-symmetric) tensor, respectively,

$$\psi_{ij} = u_k \frac{\partial C_{ij}}{\partial x_k} - \tau_{ij} \frac{\partial C_{kk}}{\partial x_k}; \quad \gamma_{ij} = \left[ \frac{\partial u_i}{\partial x_k} C_{ik} - \frac{\partial \tau_{ij}}{\partial x_k} \right] \frac{1}{\tau_p} [f(C_{kk})] + \left[ \frac{\partial u_i}{\partial x_k} C_{ik} - \frac{\partial \tau_{ij}}{\partial x_k} \right]. \tag{5}$$

Similarly, since the trace of the conformation tensor $C_{kk}$ is proportional to the elastic energy within the polymer molecules, the filtered transport equation for the trace of the conformation tensor $C_{ii}$ it is presented,

$$\frac{\partial C_{ii}}{\partial t} + u_k \frac{\partial C_{ii}}{\partial x_k} = 2C_{ik} \frac{\partial u_i}{\partial x_k} - \frac{1}{\tau_p} [f(C_{kk}) C_{ii} - \delta_{ii}], \tag{6}$$

2.2. A subgrid-scale model for large-eddy simulations of ‘FENE-P’ fluids for steady isotropic turbulence

To develop a subgrid-scale model for viscoelastic fluids modelled by the FENE-P model, one needs to close the subgrid-scale stresses in the momentum equations $\tau_{ij}$ (Eq. 3), the subgrid-scale advection $\psi_{ij}$, and the subgrid-scale polymer stretching $\gamma_{ij}$ (Eq. 4). Additionally, it is needed to approximate the term $f(C_{kk}) C_{ij}$ that appears in both equations. Before describing how to deal with these terms, the subgrid-scale modelling of the momentum equation where the subgrid-scale stresses tensor $\tau_{ij}$ needs to be computed, must be briefly discussed. In the present work, for simplicity and ease of implementation and testing, the classical Smagorinsky model is used to compute the subgrid-scale stresses arising in the momentum equations, although in principle any other model could be used for this purpose. This model uses an eddy viscosity assumption, $\tau_{ij} = \frac{1}{2}\tau_{kk} \delta_{ij} = -2\nu_t \delta_{ij}$, where $\nu_t$ is the turbulent viscosity which is in the case of the Smagorinsky model $[2]$ is given by $\nu_t = (C_S \Delta)^2 \overline{S}$ where $\overline{S} = (2S_{ij} S_{ij})^{1/2}$ is the norm of the resolved rate-of-strain tensor, $\Delta = (\Delta x \times \Delta y \times \Delta z)^{1/3}$ is the filter size and $C_S$ is the Smagorinsky constant. The remaining of this section is therefore restricted to the analysis to the modelling of terms.
$\psi_{ij}$ and $\gamma_{ij}$. We start with the modelling of the source term in the $C_{ij}$ transport equation. The following approximation will be used (H1), $f(C_{kk})C_{ij} \approx f(C_{kk}) C_{ij}$. This assumption is justified by results obtained previously obtained using a priori tests in wall bounded flows [3, 4]. Secondly, the subgrid-scale advection of the filtered conformation tensor transport equation is neglected (H2), $\psi_{ij} \approx 0$ which is justified by the small local magnitude of this term compared with the other terms in equation (4) as described in e.g. [3, 4]. Finally, self-similarity of the subgrid-scale polymer stretching term is assumed, by which this term is equal at two nearby filter sizes, apart from a constant of order $O(1)$. Specifically, the subgrid-scale polymer stretching tensor at filter size $\Delta = 2\Delta$ is defined by,

$$\mathcal{G}_{ij} = \left[ \frac{\partial \tilde{u}_i}{\partial x_k} \frac{\partial \tilde{u}_j}{\partial x_k} \right] + \left[ \frac{\partial \tilde{u}_i}{\partial x_k} C_{ik} - \frac{\partial \tilde{u}_j}{\partial x_k} C_{ik} \right]$$ (7)

which denotes the test subgrid-scale polymer stretching tensor and that is available at the LES grid of size $\Delta$. Using a Bardina type [2] closure the subgrid-scale polymer stretching tensor is approximated by (H3),

$$\gamma_{ij} = C_\gamma \mathcal{G}_{ij}$$ (8)

where $C_\gamma$ is a constant. To compute this constant the hypothesis of equilibrium of the elastic energy within the polymer molecules is used. Given that this energy is proportional to the trace of the (filtered) conformation tensor $C_{ii}$ (Eq. 6) this hypothesis is equivalent to admit that the temporal variation and convective transport are negligible in this equation, when compared with the other terms. A global (H41) or local (H42) equilibrium assumptions can be written as follows,

$$\left\langle 2C_{ik} \frac{\partial \tilde{u}_i}{\partial x_k} \right\rangle = \left\langle \frac{1}{\tau_p} \left[ f(C_{kk})C_{ii} - \delta_{ii} \right] \right\rangle; \quad 2C_{ik} \frac{\partial \tilde{u}_i}{\partial x_k} = \frac{1}{\tau_p} \left[ f(C_{kk})C_{ii} - \delta_{ii} \right]$$ (9)

respectively, where the brackets $\langle \rangle$ denote an averaging operation. Using the global elastic equilibrium assumption (H41) and equation $\gamma_{ij} = C_\gamma \mathcal{G}_{ij}$, together with assumptions H1, and H3 the constant $C_\gamma$ can be computed as,

$$C_\gamma = \left\langle \frac{1}{2\tau_p} \left[ f(C_{kk})C_{ii} - \delta_{ii} \right] - \frac{\tilde{u}_i}{\partial x_k} C_{ik} \right\rangle \left[ \frac{\tilde{u}_i}{\partial x_k} C_{jk} \right],$$ (10)

which closes the model. This model is extensively tested in both a priori and a posteriori (LES) tests.

3. Numerical Methods

This section describes the numerical methods used in the present investigation, which are the same as described in Valente et al. [5]. For the momentum equation classical pseudo-spectral schemes are used for spatial discretisation, 3rd-order Runge-Kutta scheme is used for temporal discretisation and de-aliasing is done with the 2/3 rule. The simulations are carried out in a three-dimensional periodic box with equal sizes $L_{box} = 2\pi$ and the domain is discretised in the physical space using $N$ uniformly spaced grid points in each direction, resulting in a mesh size $\Delta x = \Delta y = \Delta z = L_{box}/N$, with a total of $N^3$ grid points. An artificial forcing to sustain the turbulence is used, which is uncorrelated with the velocity field, and delta correlated in time. In the present work the forcing described in Alvelius [6] is used. The spectral schemes are not suitable for solving the conformation tensor equation (2) as it cannot cope with numerical discontinuities arising in these equations. Therefore, a central differences algorithm proposed by Vaithianathan et al. [7] based on the Kurganov-Tadmor method is used instead. This method insures that the conformation tensor remains symmetric and positive definite avoiding the need to add artificial diffusion in Eq. 2.

4. Results

4.1. Physical and computational parameters of the reference direct numerical simulations

A set of 6 DNS reference viscoelastic simulations were carried out. The simulations use $N = 384^3$ collocation points, kinematic viscosity equal to $\nu = 0.003 \text{ m}^2\text{s}^{-1}$, $\beta = 0.8$ and the forcing $f(k, t)$ is concentrated in the first 4 wavenumbers, with a gaussian profile centred in wavenumber $k = 3$ with a total power input equal to $P = 3.3 \text{ m}^2\text{s}^3$. All the integral flow quantities are computed directly from the spherical-shell of radius $k = |k|$ averaged kinetic energy spectrum $E(k)$, i.e., the turbulent
kinetic energy \( K = \sum_{k} E(k) \), the viscous solvent dissipation rate \( \varepsilon^{[s]} = \sum_{k} k^2 E(k) \). The integral, Taylor and Kolmogorov micro-scales are given by \( \ell = (\pi/(2K)) \sum_{k} E(k) k^{-1} \), \( \lambda = \sqrt{10\nu^2 K/\varepsilon^{[s]}} \) and \( \eta = (\nu^{[s]}/\varepsilon^{[s]})^{1/4} \) respectively. Notice that due to stationarity, the power of the input forcing balances the viscous dissipation and polymer dissipation rate \( P = \varepsilon^{[s]} + \varepsilon^{[p]} \). Finally, the Reynolds number based in the Taylor micro-scale is defined by \( Re_{\chi} = \sqrt{2\varepsilon^{[s]} \lambda / \nu^{[s]}} \). Notice that the integral scale, indirectly imposed through the input forcing, is always 10 times smaller than the size of the computational box, in order to prevent confinement effects in the simulation. Table 1 lists the physical and computational parameters of these 6 simulations, which differ mainly in the maximum relaxation time of the polymer molecules, taking the values \( \tau_p = [0.025, 0.05, 0.1, 0.2, 0.4, 0.6] \), which is accounted for in the Deborah and Weissenberg (non-dimensional) numbers, \( De = \tau_p/\sqrt{\nu} \) and \( Wi = \tau_p/\tau_0 \) that represent the ratio between the relaxation time of the polymer molecules with an eddy turnover and Kolmogorov time scales, respectively \( (\tau_\eta = (\nu^{[s]}/\varepsilon^{[s]})^{1/2}) \). Finally, we also computed Lumley’s length scale \( r_L = \sqrt{\varepsilon^{[s]} \nu^{[s]}} \), defined as the scale below which the turbulent eddies within the solvent are affected by the polymer, together with its corresponding wavenumber \( k_L = r_L^{-1} \).

Table 1: Physical and computational parameters of the reference DNS: SI units have been used for all dimensional quantities.

<table>
<thead>
<tr>
<th>( De )</th>
<th>( Wi )</th>
<th>( Re_\chi )</th>
<th>( K )</th>
<th>( \varepsilon^{[s]} )</th>
<th>( \varepsilon^{[p]} )</th>
<th>( \ell )</th>
<th>( \lambda )</th>
<th>( k_{max} \eta )</th>
<th>( \langle C_{ij} \rangle / L^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.11</td>
<td>0.7</td>
<td>116</td>
<td>4.01</td>
<td>2.65</td>
<td>0.61</td>
<td>0.47</td>
<td>0.21</td>
<td>1.3</td>
<td>0.0</td>
</tr>
<tr>
<td>0.22</td>
<td>1.4</td>
<td>123</td>
<td>3.96</td>
<td>2.32</td>
<td>0.90</td>
<td>0.46</td>
<td>0.23</td>
<td>1.3</td>
<td>0.0</td>
</tr>
<tr>
<td>0.38</td>
<td>2.1</td>
<td>156</td>
<td>3.73</td>
<td>1.26</td>
<td>2.00</td>
<td>0.51</td>
<td>0.30</td>
<td>1.5</td>
<td>0.6</td>
</tr>
<tr>
<td>0.62</td>
<td>2.9</td>
<td>182</td>
<td>3.03</td>
<td>0.61</td>
<td>2.73</td>
<td>0.56</td>
<td>0.38</td>
<td>1.9</td>
<td>2.7</td>
</tr>
<tr>
<td>0.91</td>
<td>4.4</td>
<td>159</td>
<td>2.04</td>
<td>0.36</td>
<td>2.94</td>
<td>0.63</td>
<td>0.41</td>
<td>2.1</td>
<td>8.9</td>
</tr>
<tr>
<td>1.23</td>
<td>6.7</td>
<td>126</td>
<td>1.65</td>
<td>0.38</td>
<td>2.93</td>
<td>0.62</td>
<td>0.36</td>
<td>2.1</td>
<td>15.9</td>
</tr>
</tbody>
</table>

Arguably, the most important role of any subgrid-scale model is the accurate modelling of the kinetic energy flux between the grid-scale and the subgrid-scales of motion. This mechanism was been studied in great detail by Valente et al. [5] in the Fourier space, by using the scale-by-scale kinetic energy budget in wavenumber space, analysed through a Lin-type equation which has been modified to include the kinetic energy transfer between the solvent and the polymers for statistically stationarity state,

\[ f(k) = - T(k) + T^{[p]}(k) + 2\nu^{[s]} k^2 E(k) \] (11)

where \( 2\nu^{[s]} k^2 E(k) \) is the viscous dissipation within the solvent at wavenumber \( k \), while \( f(k,t) \) is the spherical-shell averaged input forcing function. \( T(k,t) \) and \( T^{[p]}(k,t) \) represent transfers of kinetic energy across wavenumber \( k \) within the solvent and between the solvent and polymer molecules, respectively, with positive/negative values of \( T(k,t) \) representing kinetic energy transfers within the solvent from wavenumbers smaller than \( k \) into/from wavenumbers larger than \( k \), while positive/negative values of \( T^{[p]}(k,t) \) represent transfers of kinetic energy into/from the polymer molecules. After integrating each term in Eq. (11) (from 0 to \( k \)) one gets,

\[ F(k) = \Pi(k) + \Pi^{[p]}(k) + D(k), \] (12)

where each term represents the same physical mechanism as in Eq. (11), integrated up to wavenumber \( k \), e.g. \( \Pi^{[p]}(k) = \int_k^{\Lambda} T^{[p]}(k') dk' \) (note, the sign swap of the term \( \Pi(k) = \int_0^k T(k') dk' \), so that it is a positive quantity) and these definitions can be used to compute the total solvent and polymer dissipations \( \varepsilon^{[s]} = D(k_{max}) \) and \( \varepsilon^{[p]} = \langle \sigma_{ij}^{[p]} S_{ij} \rangle = \sum_{k} T^{[p]}(k) \), respectively, so that statistically stationarity implies that the total power input from the forcing is equal to the sum of the solvent and polymer dissipations, \( P = \varepsilon^{[s]} + \varepsilon^{[p]} \). To characterise the new simulations and to illustrate the challenges behind subgrid-scale modelling in the context of viscoelastic flows figures 1 (a-c) show the Kinetic energy spectra \( E(k) \) for the simulations with \( De = 0.11, De = 0.62 \) and \( De = 1.23 \) respectively, together with Lumley’s length scale \( k_L \), and with two of the filter sizes used in the subsequent analysis with \( \Delta / \Delta x = 4 \), and 16. While Lumley’s scale is below the maximum wavenumber and the Kolmogorov micro-scale for
$De = 0.11$, it is well within the inertial range region for $De = 0.62$, where the subgrid-scale closures are supposed to be active.

Figure 1: Kinetic energy spectral $E(k)$ for the DNS corresponding to $De = 0.11$, $De = 0.62$ and $De = 1.23$ with two filter sizes $\Delta/\Delta x = 4$ and 16. (the vertical dashed line represents the wavenumber corresponding to the Lumley scale).

Figures 2 (a-c) show the spectral energy budgets with the spectral forcing function $F(k)$, non-linear energy transfer within the solvent $\Pi(k)$, and kinetic/elastic energy transfers between the solvent and the polymer molecules $\Pi^{[p]}(k)$, respectively, for the DNS corresponding to $De = 0.11$, $De = 0.62$, and $De = 1.23$. The three figures detail a quite different energy cascade picture for different $De$ numbers, as anticipated above. In contrast to the case with $De = 0.11$, where most of the dissipation is assured by the solvent ($\varepsilon^{[p]} < \varepsilon^{[s]}$), in $De = 0.62$ the dissipation is largely caused by the polymer molecules $\varepsilon^{[p]} > \varepsilon^{[s]}$.

Figure 2: Spectral energy budget (Eq. 12) for the DNS corresponding to $De = 0.11$, $De = 0.62$ and $De = 1.23$. The filter sizes $\Delta/\Delta x = 4$ and 16 are also shown. (the dashed vertical line represents the wavenumber corresponding to the Lumley scale).

5. A priori tests: DNS of isotropic viscoelastic turbulence

In this section, the results obtained using classical a priori tests conducted in the reference simulations are described. The aim of these tests is to assess the several subgrid-scale hypothesis that have been used in the new subgrid-scale model for viscoelastic flows proposed in the present work.

5.1. Modification of the Smagorinsky model constant $C_{S}$ in viscoelastic flows

As described above the proposed subgrid-scale model for viscoelastic flows relies in the classical Smagorinsky model, to compute the subgrid-scale stresses from the momentum equation $\tau_{ij}$. In order to appreciate the influence of the Deborah number and filter sizes in the Smagorinsky model constant $C_{S}$, the DNS data banks are used to compute this constant using classical a priori tests. Following Meneveau [2], $C_{S}^{2} = \langle -\tau_{ij} \rangle / 2\sigma \Delta^2 (\left\langle S_{ij} S_{ij} \right\rangle)^{3/2}$ is computed where the brackets represent time and volume averages for each simulation, for all the simulations used in this work and for filter sizes $\Delta/\Delta x = 2, 4, 8$ and 16. The results are displayed in figure 3. Recall that for Newtonian isotropic turbulence the Smagorinsky constant is given by $C_{S} = 0.16$. Therefore the present value of $0.14 \leq C_{S} \leq 0.17$ are quite close to the ‘exact’ value of $C_{S} = 0.16$. In the viscoelastic simulations the constant exhibits the same trend of
decreasing $C_S$ for the higher $De$ numbers.

Figure 3: Smagorinsky constant ($C_S$) computed following Meneveau for filter sizes $\Delta/\Delta x = 2, 4, 8$ and 16 and all the reference simulations used in this work.

5.2. Scale-similarity of the subgrid-scale polymer stretching: H3

The scale-similarity for the subgrid-scale polymer stretching term used by the present model is described by Eq. (8). In order to assess this approximation Figures 4 (a-c) show joint probability density functions (JPDF) between $\gamma_{ii}$ and $G_{ii}$ for filter sizes $\Delta/\Delta x = 4$ and 16, and for the simulations with $De = 0.11, 0.38$ and 0.91. The JPDFs show the existence of a strong correlation between the two quantities, even though the correlations decrease with increasing filter sizes and Deborah numbers e.g. the correlation coefficient between $\gamma_{ii}$ and $G_{ii}$ decreases from 0.84 to 0.76 at $\Delta/\Delta x = 4$ for $De = 0.11$ to $De = 0.91$, and from 0.84 to 0.62 at $De = 0.11$ for $\Delta/\Delta x = 4$. These JPDFs are a first indication that this assumption may be a good starting point for a model of the subgrid-scale polymer stretching term in Eq. (4).

Figure 4: Joint probability density functions between the real (exact) traces of polymer stretching terms $\gamma_{ii}$ and $G_{ii}$ normalised by their root-mean-square), at filter size $\Delta/\Delta x = 4$ for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$.

A question that naturally arises when facing the model definition in Eq. (8) is whether the model constant $C_\gamma$ is 'isotropic' i.e. given the well known anisotropy of the polymer stresses one might be tempted to extend the present model by using an anisotropic version of the model constant $C_\gamma$, defined in by, $\gamma_{ij} = C_\gamma \gamma_{ij}$ (no summation). To clarify this issue Figure 5 (a-c) shows several joint probability density functions (JPDFs) involving the quantities $C_{\gamma_{11}}$ and $C_{\gamma_{22}}$ for filter size $\Delta/\Delta = 4$, and for the reference DNS with $De = 0.11, De = 0.38$ and $De = 0.91$, defined by $C_{\gamma_{11}} = \frac{\gamma_{11}}{\sigma_{11}}$ and $C_{\gamma_{22}} = \frac{\gamma_{22}}{\sigma_{22}}$. Clearly the quantities $C_{\gamma_{11}}$ and $C_{\gamma_{22}}$, are statistically independent, and similar observations were made for filter size $\Delta/\Delta = 16$. This supports the use of an 'isotropic' constant $C_\gamma$ in the present model and finalises the assessment of the hypothesis H3.

5.3. Global equilibrium of the polymeric elastic energy: H41

The present model uses the assumption of global equilibrium of the polymers elastic energy described in equation (9). It was checked that indeed the two sizes of equation (9) are equal to within numerical uncertainty, in all the reference DNS and for all the Deborah numbers and filter sizes used in the present work. Notice that the present DNS data bank consists of statistically stationary and homogeneous turbulence, where the averaged temporal variation, and averaged convective terms are zero. Therefore this hypothesis does not need any additional discussion. It is however interesting to discuss the possibility of using a local equilibrium approximation, with the aim of extending the present model to other flows where statistical stationarity and/or homogeneity are generally not present.
5.4. Influence of the Deborah number and filter size on $C_\gamma$

Next we analyse the sensitivity of the model constant $C_\gamma$ to the filter size and Deborah number. We employ two procedures. In the first one the constant is computed using globally averaged quantities: $C_\gamma = \langle \gamma_{ii} \rangle / \langle G_{jj} \rangle$ where the brackets represent a volume average which is computed for each time step of the simulations (see figure 6 a). In the second procedure the constant is computed locally: $C_\gamma = \langle \frac{\gamma_{ii}}{G_{jj}} \rangle$, i.e. using the definition of the constant at each point of the flow domain and for each time step, and averaging the constant $C_\gamma$ thus obtained in the whole domain (see figure 6 b). These equations thus use a "local" and a "global" equilibrium assumptions, respectively. The two figures are remarkably similar which again confirms that the local and global equilibrium assumptions $H41$ and $H42$ are equally valid and lead essentially to the same results. The model constant is, as expected $O(C_\gamma) = 1$ and remains bounded by $0 \leq C_\gamma \leq 5$, with a tendency of increasing with the Deborah number and the filter size. The cases corresponding to $De \approx 1$ are interesting in that $C_\gamma$ approaches $\approx 0$, which is connected with a depletion of the non-linear energy cascade described by Valente et al. [5], where almost all the energy input is dissipated by the elastic stresses from the polymers. Indeed, as far as a priori tests are concerned the results indicate that the present model can be used for simulating viscoelastic inhomogeneous flows away from solid boundaries.

6. $A$ posteriori tests: LES of isotropic viscoelastic turbulence

In this section, the results from LES obtained with the present model are discussed. A total of 6 LES were carried out using the same physical parameters described in table 1, but using a grid with $N = 48^3$ collocation points instead. This corresponds to an implicit LES filter with $\Delta/\Delta x = 8$ which is located in the inertial range region of the energy spectra. In order to compare the LES results with the results obtained from the reference DNS. The data fields were explicitly filtered, using a box filter with $\Delta/\Delta x = 8$, and the data fields were sampled into the corresponding (coarse) grid used in the LES.
6.1. Final set of governing equations for LES of viscoelastic isotropic turbulence

Denoting by a bar (\(\bar{\cdot}\)) a quantity represented in the LES grid, the final closed system of LES equations for viscoelastic turbulence consists in the following set of equations: continuity,

\[
\frac{\partial \bar{\rho}}{\partial x_i} = 0,
\]

momentum transport,

\[
\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{\rho} \bar{u}_i}{\partial x_j} = -\frac{1}{\bar{\rho}} \frac{\partial p}{\partial x_i} + 2 \frac{\partial }{\partial x_j} \left[ (\nu^{[p]} + \nu_t) \mathbf{S}_{ij} \right] + \frac{\partial }{\partial x_j} \left\{ \nu^{[p]} \frac{\partial (C_{kk})^G \bar{C}_{ij} - \delta_{ij})}{\tau_p} \right\},
\]

and conformation tensor transport equations

\[
\frac{\partial C_{ij}}{\partial t} + \bar{u}_k \frac{\partial C_{ij}}{\partial x_k} = \frac{\partial \bar{\rho} C_{ij}}{\partial x_j} + \frac{\partial \bar{\rho} C_{jk}}{\partial x_k} - \frac{1}{\tau_p} [f(C_{kk}) \bar{C}_{ij} - \delta_{ij}] + C_\gamma \mathbf{G}_{ij},
\]

respectively. The subgrid-scale stresses tensor \(\tau_{ij}\) is computed by using the Smagorinsky model, with \(\tau_{ij} = -\frac{1}{2} \tau_{kk} \delta_{ij} = -2 \{ (C_S \Delta^2) \mathbf{S} \} \bar{S}_{ij}\) and using a model constant equal to \(C_S = 0.16\). The subgrid-scale polymer stretching term is computed directly from its definition (Eq. 7). Finally, the model constant for the conformation tensor transport equations \(C_\gamma\), is calculated by the following formula,

\[
C_\gamma = \frac{\bar{\varepsilon}^{[p]} - (1/f(C_{kk})) - \langle \frac{\partial u_j}{\delta x_k} C_{jk} \rangle}{\langle \frac{\partial u_j}{\delta x_k} C_{jk} \rangle}.
\]

which has shown to be computationally more stable than its direct definition through Eq. (10). The polymer dissipation \(\varepsilon^{[p]} = P - \varepsilon^{[s]}\) is computed from the energy balance equation since the total power input \(P\) is imposed and the solvent dissipation \(\varepsilon^{[s]}\) can be computed from its definition. The following equality was used: \(\varepsilon^{[p]} = \frac{f(C_{kk}) \bar{S}_{ij}}{2 \tau_p}\). For consistency, each new modelling term has been computed using the same numerical method used in its corresponding (DNS) term.

6.2. Drag reduction and coherent structures obtained from the LES

Table 2 lists the values of the drag-reduction (DR), defined as \(DR = \frac{\varepsilon^{[p]} + \varepsilon^{[s]}}{\varepsilon^{[p]}}\) that has been used before to characterise simulations of isotropic turbulence with polymer additives [8] and in some sense characterises the simulations as a whole since the computation of the polymer dissipation \(\varepsilon^{[p]}\) cannot be obtained in a trivial way and involves many of the large and small scale quantities with their approximations in a reference DNS (\(\varepsilon^{[p]}\) and \(\varepsilon^{[s]}\) have been computed from the LES as outlines above).

Table 2: Drag reduction (DR) obtained with the several LES compared with the corresponding reference DNS (DNS), filtered DNS (DNS) and with simulations without any model (\(-\)) for the polymer dynamics The Smagorinsky model is used in the momentum equations in all the LES and the simulations use the same parameters as described in table 1 and \(N = 48^3\) collocation points.

<table>
<thead>
<tr>
<th>(DR)</th>
<th>(De)</th>
<th>(DNS)</th>
<th>()</th>
<th>(LES)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.11</td>
<td>0.21</td>
<td>0.16</td>
<td>0.20</td>
<td></td>
</tr>
<tr>
<td>0.22</td>
<td>0.36</td>
<td>0.17</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>0.38</td>
<td>0.71</td>
<td>0.25</td>
<td>0.66</td>
<td></td>
</tr>
<tr>
<td>0.62</td>
<td>0.88</td>
<td>0.84</td>
<td>0.89</td>
<td></td>
</tr>
<tr>
<td>0.91</td>
<td>0.94</td>
<td>0.95</td>
<td>0.96</td>
<td></td>
</tr>
<tr>
<td>1.23</td>
<td>0.95</td>
<td>0.96</td>
<td>0.96</td>
<td></td>
</tr>
</tbody>
</table>

For small \(De\) numbers, the absence of a model for the subgrid-scale polymer stretching term leads to \(DR\) values that significantly underpredict the correct values. In contrast, the addition of the present model clearly allows the recovery of the \(DR\) from the simulations, which is a strong indication that the model is indeed performing well its role. For high values of \(De\) (\(De \geq 0.91\)) the differences between the
DR obtained with DNS, with and without model are not very important. Figure 7 shows iso-surfaces of the second invariant of the velocity gradient tensor obtained for the LES with De = 0.91, compared with the filtered DNS, using the same threshold. The flow structures seem to be very well captured by the present model, as the size and shape of the flow vortices see to be virtually equivalent in the two simulations. The same is true of the other simulations which again indicates that the new model is able to capture the large-scale feature of the simulations.

Figure 7: Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{rms}$) corresponding to a threshold equal to $Q/Q_{rms} = 4$ for the filtered reference DNS with De = 0.91, compared with the filtered DNS, using the same threshold. The flow structures seem to be very well captured by the present model, as the size and shape of the flow vortices seem to be virtually equivalent in the two simulations. The same is true of the other simulations which again indicates that the new model is able to capture the large-scale feature of the simulations.

6.3. Kinetic energy spectra and spectral budgets

In order to assess the detailed spectral behavior of the present model figures 8 (a-c) and 9 (a-c) show the kinetic energy spectra $E(k)$, and the spectral energy budgets, respectively, from the LES for De = 0.38, 0.62, and 1.23, compared with the reference (filtered) DNS and also with simulations without polymer subgrid-scale model.

Figure 8: Kinetic energy spectral $E(k)$ for the LES corresponding to De = 0.38, 0.62 and 1.23 in a grid with $N = 48^3$ collocation points. The results for filtered DNS (DNS) and without polymer subgrid-scale model ((−)) are also shown.

For the lower Deborah numbers De = 0.38 and 0.62 (figures 8 a,b) the energy spectra obtained from LES closely follows the filtered DNS spectra, until a given high wavenumber $k_c^{LES}$. The comparison between the results with and without polymer model for intermediate De numbers already indicates that the present model does achieve an improvement over the simulations without model for these cases, even though one must keep in mind that the kinetic energy dynamics is being largely handled by the Smagorinsky model. The situation is slightly different for high De numbers as shown in figure 8 (c) corresponding to the case with De = 1.23. Here both the LES with and without polymer subgrid-scale model show very similar energy spectra, which also follow closely the filtered DNS spectra until a given (approximately similar) wavenumber $k_c^{−} ≈ k_c^{LES}$, above which the spectra display less energy, than the filtered DNS spectra. The spectral budgets for the same cases De = 0.38, 0.62 and 1.23, (figures 9 a-c) detail the solvent/polymer interactions in play for these simulations and explain the shape of the kinetic energy spectra described above. Given that only results in the filtered DNS can be compared, the counterpart of the spectral budget is, $\tilde{F}(k) = \tilde{\Pi}(k) + \Pi^P(k) + \tilde{D}(k)$, where the bar "−" represents data available in the LES grid, however, for clarity the figures use the same notation as before.
From the outset it is important to stress that as expected for all De numbers the filtered DNS, LES and ‘no-model’ simulations lead exactly the same result since these term is imposed in the, moreover, fully resolved wavenumber range, \( F^{LES}(k) = F^{DNS}(k) = F^{(-)}(k) \). In the simulations with \( De = 0.38 \) (figure 9 a) the non-linear energy transfer function \( \Pi(k) \) is very well captured by the new subgrid-scale model, \( \Pi^{LES}(k) = \Pi^{DNS}(k) \), while the ‘no-model’ simulation significantly over-predicts this quantity. The resolved solvent dissipation is well captured by both simulations, LES and ‘no-model’, \( D^{LES}(k) = D^{DNS}(k) = D^{(-)}(k) \) although the LES displays a nearly perfect agreement, in contrast with the ‘no-model’ simulation at high wavenumbers. Finally, the solvent-elastic energy transfer is very well predicted by the LES model simulation for the first wavenumbers \( \Pi^{[p]LES}(k) = \Pi^{[p]DNS}(k) \) for \( k \leq 4 \), and under-predicts \( \Pi^{[p]DNS}(k) \) for the remaining wavenumbers \( 5 \leq k \leq 24 \), while the ‘no-model’ simulation displays a very poor performance for the entire wavenumber range. Similar spectral budgets are observed in the simulations with similar or smaller Deborah numbers (not shown).

For higher Deborah numbers \( De = 0.62 \) the non-linear term \( \Pi^{DNS}(k) \) is overshadowed by \( \Pi^{[p]DNS}(k) \), which is now the dominating term (see figure 9 b). Again the leading term is well captured by the LES using the present model \( i.e. \Pi^{[p]LES}(k) \approx \Pi^{[p]DNS}(k) \). As in figure 9 (a) the solvent dissipation is well captured both in the LES and ‘no-model’ simulations, the LES performing slightly better.

Finally, we discuss what is probably the least interesting case, corresponding to the simulation with \( De = 1.23 \) (figure 9 c). As described before in section 4.1 in this case the polymer dissipation term \( \Pi^{[p]}(k) \) largely dominates the other transfer terms and is largely dominated by the fully resolved large scale motions, thus, the role of the subgrid-scale models are less critical here than in the other cases, even considering that according to the \textit{a priori} tests, the Smagorinsky model constant used here \( C_S = 0.16 \) is higher than the optimal value, which is probably reflected in the slightly smaller value of \( \Pi^{[p]LES}(k) \) for this case.

7. Conclusions

In this work a new subgrid-scale model is developed for large-eddy simulations (LES) of Newtonian solvents carrying small amounts of long chain polymer molecules, simulated by the Finitely Extensible Nonlinear Elastic continuous model closed with the Peterlin approximation (FENE-P). The analysis of the filtered momentum and conformation tensor transport equations showed that the only term that requires an additional model, compared to a Newtonian simulation, is the subgrid-scale polymer stretching term \( \gamma_{ij} \), while all the other terms arising from the filtering procedure can be neglected \( e.g. \) the subgrid-scale conformation tensor convection \( \psi_{ij} \). The new model essentially rests on the assumptions of scale similarity of the subgrid-scale polymer stretching mechanics and on a global equilibrium of the elastic energy within the polymers in the computational box. Finally, the new model is tested in LES of viscoelastic turbulence covering the same physical parameters of the reference DNSs, but using a grid with (only) \( N = 48^3 \) collocation points. The LESs consistently show that the new model is able to reproduce the global flow quantities, such as the \( DR\), the flow structures, the kinetic energy spectra, and the detailed spectral budgets, thus proving that the present model presents a major progress in the numerical simulation of turbulent Newtonian flows with diluted polymer molecules.
References


