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Large-eddy simulations of forced isotropic turbulence with viscoelastic fluids described by the FENE-P model

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A new subgrid-scale (SGS) model developed for large-eddy simulations (LES) of dilute polymer solutions, described by the finitely extensible nonlinear elastic constitutive equation closed with the Peterlin approximation, is presented. In this distortion similarity model (DSIM) the filtered conformation tensor evolution equation is based on the self-similarity of the polymer stretching terms, and on a global equilibrium of the trace of the conformation tensor, which is proportional to the elastic energy stored in the polymer molecules, while the SGS stresses are modelled with the classical Smagorinsky model. The DSIM closure is assessed in direct numerical simulations (DNS) of forced isotropic turbulence using classical a priori tests, and in a posteriori (LES) showing very good agreement with all the exact (filtered DNS) results. The DSIM model is simple to implement and computationally inexpensive and represents a major step forward in the numerical simulation of turbulent flows of Newtonian fluids with polymer additives. Published by AIP Publishing.

I. INTRODUCTION

Turbulent flows of viscoelastic fluids based on polymeric and surfactant additives have industrial applications in flows of smart thermal fluids in district heating and cooling systems,1 in pipeline oil transport,2 and in oil and gas well-drilling. Turbulent duct flows of such fluids may show significant reductions in friction and heat transfer and this has motivated extensive research,3 but modern predictive techniques associated with viscoelastic constitutive equations are almost exclusively based on Reynolds-averaged Navier-Stokes equations (RANS) calibrated for wall flows.4

However, it is well known that these models present inherent limitations in many engineering flows involving, e.g., strong curvature, large-scale unsteadiness, or rotation.5 Consequently, in complex new situations for which no calibration has been carried out, RANS models may result in a substantial deviation from the actual flow statistics.5 Moreover, some important flow data such as the dominating flow frequencies are not accessible in RANS.5 For these reasons large-eddy simulations (LES) have been increasingly employed in engineering applications. In LES the largest energetic scales of motion are explicitly simulated, and the effect of the smallest scales on the large scales is modelled by using a subgrid-scale (SGS) model. Today, LES is the most advanced and accurate method for the simulation of turbulent flows of Newtonian fluids for engineering applications,6 but the possibility of using LES for non-Newtonian viscoelastic fluids remains elusive, as attested by the extremely small number of LES studies in such flows7 and under a limited range of flow conditions. Moreover, some of these early attempts are extremely complex, computationally expensive, and have only been calibrated for wall flows, and their behavior in wall-free turbulent flows is unknown for practical purposes.7 Thus, no SGS models are available today for routine engineering LES with non-Newtonian viscoelastic fluids.

Arguably, the most important feature that any subgrid-scale model must represent is the kinetic energy flux from the resolved (or grid-scales) to the unresolved (or subgrid) scales.5 In Newtonian...
fluids the development of subgrid-scale models is largely based on the Richardson-Kolmogorov energy cascade concept, according to which the smallest scales of motion are essentially isotropic, statistically universal, dynamically passive, and simply dissipate whatever kinetic energy is injected into them from the large scales. This simple concept, which describes well the interscale interactions in turbulent Newtonian flows away from solid walls, explains much of the success of classical SGS models. A key ingredient of this picture is the so-called equilibrium assumption, which states that all the kinetic energy transferred from the large into the smallest scales of motion is balanced (on average) by the viscous dissipation acting on the smallest scales. However, when dealing with non-Newtonian fluids, one is immediately confronted with a much more challenging situation, because of the extremely complex SGS interactions arising there. Investigations of turbulent flow behavior of viscoelastic fluids have focused on the Finitely Extensible Non-Linear Elastic constitutive model with Peterlin’s approximation (FENE-P), a basic constitutive equation for viscoelastic fluids that displays the main ingredients of an elastic fluid model. Fluid elasticity is associated with the deformability and orientation of some of the constituents of a fluid and their interactions with the turbulent structures significantly changes the energy distribution across scales. The present understanding of the physical mechanisms of these interactions is very limited, and even the most solid facts about the dynamics of the small scales are not observed in non-Newtonian inertio-elastic turbulence. For example, in a dilute solution of long polymer molecules, an important fraction of the kinetic energy transferred into the small scales is dissipated by the polymer and in some cases one may observe the formation of a polymer-induced energy cascade that competes with the classical energy cascade. Any future SGS model applied to non-Newtonian fluids will need to cope with this complex interplay between the existing scales of motion and the fluid rheology. Recently, much of this complexity was studied through a detailed analysis of the large/small scale interactions in a viscoelastic flow, by using new direct numerical simulations (DNS) of isotropic turbulence for the FENE-P model.

The existing attempts for developing SGS closures for LES of elastic fluids have been mainly concerned with wall flows, because of their practical engineering applications. However, we contend here that this strategy is not very effective, and that one should first study simpler flows before addressing the difficulties associated with LES of wall flows. Indeed, even for Newtonian flows the near wall region is challenging for LES since there the large energetic scales are quite small and the main premise of LES, that the more energetic scales of motion have to be explicitly resolved, is often not met. Additionally, other requirements such as a clear separation of scales are only met partially. Consequently, most LES of wall flows require that the flow be either fully resolved (i.e., DNS resolution near the wall) or that some sort of near wall adjustment needs to be included in the model to handle these difficulties.

Thais et al. proposed what is probably the first SGS model for viscoelastic fluids, using temporal LES of channel flows. The SGS quantities were modelled using an approximate deconvolution method for the momentum and conformation tensor equations. However, the resulting model is extremely complex and is only active near the wall, where the level of SGS activity is necessarily limited, making it impossible to assess whether the model will perform well in high Reynolds number configurations. Moreover, the deconvolution procedures are intrinsically known to rely only on mathematical properties, without potential to add any physical input from the complex GS/SGS/viscoelastic fluid interactions, which could be a limitation given the unusual small scale physical complexity associated with fluid/polymer interactions, particularly when the SGS activity is very important, such as away from walls or in high Reynolds number configurations. Other recent non-Newtonian LES investigations include the work of Wang et al. on forced homogeneous isotropic turbulence (HIT) of FENE-P fluids, using also an approximate deconvolution method, and Ohta et al. on turbulent channel flow of power law inelastic fluids, with the SGS stresses modelled by a modified Smagorinsky closure. Again, these early LES models are all rather restricted in that little if any information regarding the complex physics of GS/SGS/rheology interactions is included in the models.

The goal of the present work is to develop and test, both in a priori and LES, a new subgrid-scale closure for FENE-P fluids (the distortion similarity model—DSIM), without the problems raised by the presence of solid walls. The ideal flow case to develop this work, and which is used
here, consists of statistically stationary (forced) HIT, where moreover large-scale inhomogeneities, such as caused by mean shear, are also absent. Furthermore, many important flow quantities such as the three-dimensional kinetic energy spectrum are naturally and easily accessed in HIT and not in other flows where inhomogeneities are present, such as in wakes or jets. Naturally, future developments, outside the scope of this paper, will include the assessment of the effects of inhomogeneities and of the presence of walls.

This paper is organised as follows. Section II introduces the governing equations and the new subgrid-scale model developed for FENE-P fluids, while Section III details the reference DNS and numerical quantities analysed in the subsequent discussion. Section IV thoroughly assesses the new model in classical \textit{a priori} tests, and Section V discusses the performance of the new model in LES. Section VI closes the work with an overview of its main results and conclusions.

II. GOVERNING EQUATIONS FOR DILUTE POLYMER SOLUTIONS

This section reviews the main equations governing the fluid flow, consisting in a Newtonian fluid (solvent) to which a small fraction of long chain polymers is added. The resulting fluid is simulated here by using the Finely Extensible Non-Linear Elastic constitutive model with Peterlin’s approximation (FENE-P).\cite{Peterlin78} Therefore, the filtered momentum and conformation tensor equations, together with the explicit polymer stress definition, are the starting point for the viscoelastic large-eddy simulations studied here. The new (unknown) “subgrid-scale” terms arising from the filtering operation that require new modelling closures are described.

A. The “FENE-P” fluid governing equations

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),

\begin{equation}
\frac{\partial u_i}{\partial x_i} = 0, \tag{1}
\end{equation}

\begin{equation}
\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{1}{\rho} \frac{\partial \sigma_{ij}}{\partial x_j}, \tag{2}
\end{equation}

where \(u_i(\mathbf{x}, t)\) is the velocity vector, \(\rho\) is the fluid density, and \(p(\mathbf{x}, t)\) is the pressure. The stress tensor \(\sigma_{ij}\) is the sum of the Newtonian solvent and the stresses resulting from the polymer molecules,

\begin{equation}
\sigma_{ij} = \sigma_{ij}^{[s]} + \sigma_{ij}^{[p]}. \tag{3}
\end{equation}

The Newtonian stresses are given by

\begin{equation}
\sigma_{ij}^{[s]} = 2 \rho v^{[s]} S_{ij}, \tag{4}
\end{equation}

where \(v^{[s]}\) is the (Newtonian) solvent kinematic viscosity, \(S_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2\) is the rate-of-strain tensor, and \(\beta = v^{[s]}/(v^{[p]} + v^{[s]})\) is the ratio between the solvent and the total zero-shear-rate viscosity of the solution.

The additional polymer stresses are computed using the FENE-P model,

\begin{equation}
\sigma_{ij}^{[p]} = \frac{\rho v^{[p]}}{\tau_p} \left[ f(C_{kk} C_{ij} - \delta_{ij}) \right], \tag{5}
\end{equation}

where \(C_{ij}\) is a continuous conformation tensor field representing the rheological behaviour of an ensemble of polymer chains (\(\delta_{ij}\) is the Kronecker delta). The ensembles are represented by coarse-grained models, notably by dumbbells in which two beads are connected by a non-linear spring, while the beads represent subsets of chains and the spring accounts for their interactions. Specifically, the conformation tensor is defined as

\begin{equation}
C_{ij} = \frac{\langle r_i r_j \rangle}{\langle R^2 \rangle_0}, \tag{6}
\end{equation}

where \langle \cdot \rangle_0 \) denotes the ensemble average.
i.e., the second moment of the end-to-end vector of the dumbbells representing the entire polymer chains, normalised by the square of its equilibrium radius \( \langle R^2 \rangle _0 \). Apart from the polymer contribution to the zero shear kinematic viscosity \( \nu ^{[p]} \), the FENE-P model uses also the longest relaxation time of the polymer molecules \( \tau _p \), and the Peterlin function is defined by

\[
f(C_{kk}) = \frac{L^2 - 3}{L^2 - C_{kk}}, \tag{7}
\]

where \( \sqrt{C_{kk}} \) is the (normalised) extension length and \( L \) is the normalised maximum extensibility of the polymer chains. Finally, the conformation tensor is governed by the following evolution equation:

\[
\frac{\partial C_{ij}}{\partial t} + u_k \frac{\partial C_{ij}}{\partial x_k} = C_{jk} \frac{\partial u_i}{\partial x_k} + C_{ik} \frac{\partial u_j}{\partial x_k} - \frac{1}{\tau _p} \left[ f(C_{kk})C_{ij} - \delta _{ij} \right], \tag{8}
\]

where the first two terms on the right-hand side of Eq. (8) represent production due to velocity-polymer interactions (polymer stretching/distortion term), while the last term is associated with the storage of elastic energy by the polymer molecules. In the following, the trace of the above equation will be used:

\[
\frac{\partial C_{ii}}{\partial t} + u_k \frac{\partial C_{ii}}{\partial x_k} = 2C_{ik} \frac{\partial u_i}{\partial x_k} - \frac{1}{\tau _p} \left[ f(C_{kk})C_{ii} - \delta _{ii} \right]. \tag{9}
\]

Since the trace of the conformation tensor \( C_{kk} \) is proportional to the elastic energy within the polymer molecules, the terms on the left-hand-side of Equation (9) are proportional to the temporal and convective variation of the elastic energy, while the first term on the right-hand-side represents a source of elastic energy caused by the stretching of polymer molecules by the flow, and the last term is proportional to the elastic energy stored within the polymer molecules.

Since this term behaves as a “sink” in Equation (9), in this work we will label it as the “dissipation of elastic energy”; however, it is important to bear in mind that this term does not represent a typical dissipation mechanism since the storage of elastic energy is a reversible process, unlike a typical dissipation term, e.g., the viscous dissipation of kinetic energy.

**B. Filtered “FENE-P” fluid governing equations: Subgrid-scale terms for the FENE-P fluid**

In LES each flow variable \( \phi (\vec{x}, t) \) is decomposed into a resolved (or large-scale) \( \overline{\phi}(\vec{x}, t) \) and an unresolved (or subgrid-scale) \( \phi'(\vec{x}, t) \) components,

\[
\phi(\vec{x}, t) = \overline{\phi}(\vec{x}, t) + \phi'(\vec{x}, t), \tag{10}
\]

by the application of a spatial (low pass) filtering operation defined as

\[
\overline{\phi}(\vec{x}, t) = \int _{\Omega} \phi(\vec{x}', t) G_\Delta (\vec{x} - \vec{x}') d\vec{x}', \tag{11}
\]

where \( G_\Delta (\vec{x}, t) \) is a filter satisfying \( \int _{\Omega} G_\Delta (\vec{x}) d\vec{x} = 1 \), with filter width equal to \( \Delta \), and \( \Omega \) is the computational domain. In the present work a box filter is used to separate the resolved and unresolved scales of motion, defined (in the one-dimensional case) as

\[
G_\Delta (x) = \begin{cases} 
\frac{1}{\Delta} & \text{if } |x| < \frac{\Delta}{2}, \\
0 & \text{otherwise}.
\end{cases}
\]

Other filter sizes commonly used in LES studies comprise the sharp spectral (or spectral cutoff filter) and the Gaussian filter. The main difference between the three filter types has to do with the localisation in the physical and Fourier spaces. The box/cutoff filter is localised/non-localised in the physical space and non-localised/localised in the Fourier space, while the Gaussian filter is local both in the physical and Fourier spaces. In the present work only results for the box filter are discussed because this filter is formally equivalent to a discretisation using finite volume or
finite differences schemes, and our plan is to develop a subgrid-scale model for engineering applications, where Fourier methods present well known limitations.\textsuperscript{5} Another reason to use the box filter has to do with the self-similarity concept used in modelling the polymer stretching term (see below), because some self-similar model formulations are not effective when the filter is a Reynolds operator, (e.g., cutoff filter)\textsuperscript{6}.

Application of a low pass filtering operation to the equations of motion for a FENE-P fluid yields the filtered FENE-P fluid equations, consisting on the filtered continuity, filtered momentum, and filtered conformation tensor transport equations,

\[ \frac{\partial \vec{u}_i}{\partial x_i} = 0, \quad (12) \]

\[ \frac{\partial \vec{u}_i}{\partial t} + \vec{u}_k \frac{\partial \vec{u}_i}{\partial x_k} = -\frac{1}{\rho} \frac{\partial \vec{p}}{\partial x_i} + \gamma^{(s)} \frac{\partial^2 \vec{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{1}{\rho} \frac{\partial \sigma_i^{[p]}}{\partial x_j}, \quad (13) \]

and,

\[ \frac{\partial \vec{C}_{ij}}{\partial t} + \vec{u}_k \frac{\partial \vec{C}_{ij}}{\partial x_k} = \frac{\partial \vec{u}_i}{\partial x_k} \vec{C}_{jk} + \frac{\partial \vec{u}_j}{\partial x_k} \vec{C}_{ik} - \frac{1}{\tau_p} \left[ f(C_{kk}) \vec{C}_{ij} - \delta_{ij} \right]. \quad (14) \]

respectively, where \( \tau_{ij} = \vec{u}_i \vec{u}_j - \vec{u}_k \vec{u}_k \) is the subgrid-scale stress tensor, describing the effect of the subgrid-scale stresses in the evolution of the resolved velocity field. The first two terms on the right-hand side of Eq. (14) are the filtered polymer stretching, and the last term is the filtered polymer dissipation, and both are unavailable in the LES grid. Notice that the new (last) term arising from the filtered momentum equation (13),

\[ \frac{\partial \sigma_i^{[p]}}{\partial x_j} = \frac{\rho \gamma^{[p]}}{\tau_p} \left[ f(C_{kk}) \vec{C}_{ij} - \delta_{ij} \right], \quad (15) \]

is closely related to the last term in Equation (14) through the definition of polymer stress in Equation (5) leading to the filtered polymer stress in Equation (15). It is convenient to write Equation (14) in a form allowing to isolate for all the new terms arising from the filtering operation, the resolved from the corresponding subgrid-scale quantity,

\[ \frac{\partial \vec{C}_{ij}}{\partial t} + \vec{u}_k \frac{\partial \vec{C}_{ij}}{\partial x_k} = \frac{\partial \vec{u}_i}{\partial x_k} \vec{C}_{jk} + \frac{\partial \vec{u}_j}{\partial x_k} \vec{C}_{ik} - \frac{1}{\tau_p} \left[ f(C_{kk}) \vec{C}_{ij} - \delta_{ij} \right] - \psi_{ij} + \gamma_{ij}. \quad (16) \]

The new terms requiring modelling are the subgrid-scale conformation advection tensor,

\[ \psi_{ij} = u_k \frac{\partial \vec{C}_{ij}}{\partial x_k} - \vec{u}_k \frac{\partial \vec{C}_{ij}}{\partial x_k}, \quad (17) \]

and the subgrid-scale polymer stretching tensor,

\[ \gamma_{ij} = \left[ \frac{\partial u_i}{\partial x_k} C_{jk} - \frac{\partial \vec{u}_i}{\partial x_k} \vec{C}_{jk} \right] + \left[ \frac{\partial u_j}{\partial x_k} C_{ik} - \frac{\partial \vec{u}_j}{\partial x_k} \vec{C}_{ik} \right]. \quad (18) \]

Similarly, the filtered transport equation for the trace of the conformation tensor \( \vec{C}_{ii} \) is

\[ \frac{\partial \vec{C}_{ii}}{\partial t} + \vec{u}_k \frac{\partial \vec{C}_{ii}}{\partial x_k} = 2 \vec{C}_{ik} \frac{\partial \vec{u}_i}{\partial x_k} - \frac{1}{\tau_p} \left[ f(C_{kk}) \vec{C}_{ii} - \delta_{ii} \right]. \quad (19) \]

which can be rewritten as

\[ \frac{\partial \vec{C}_{ii}}{\partial t} + \vec{u}_k \frac{\partial \vec{C}_{ii}}{\partial x_k} = 2 \vec{C}_{ik} \frac{\partial \vec{u}_i}{\partial x_k} - \frac{1}{\tau_p} \left[ f(C_{kk}) \vec{C}_{ii} - \delta_{ii} \right] - \psi_{ii} + \gamma_{ii}. \quad (20) \]
C. Relevant subgrid-scale quantities for large-eddy simulations of “FENE-P” fluids in stationary isotropic turbulence

To develop a subgrid-scale model for viscoelastic fluids described by the FENE-P constitutive equation, one needs to close the subgrid-scale stresses $\tau_{ij}$ in the momentum equations (Eq. (13)), the subgrid-scale advection $\psi_{ij}$, and the subgrid-scale polymer stretching $\gamma_{ij}$ in Eq. (16). Additionally, we also need to approximate the term $f(C_{kk})C_{ij}$ that appears in Equations (14) and (15).

Before we describe how to deal with these terms, we must briefly discuss the subgrid-scale closure of the momentum equation, where the subgrid-scale stress tensor $\tau_{ij}$ needs to be computed.

In the present work, for simplicity and ease of implementation and testing, and low computational cost, we have used the classical Smagorinsky\(^\text{15}\) model to compute the subgrid-scale stresses, although in principle any other model could be used for this purpose. This model uses an eddy viscosity assumption,

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2 \nu_t \delta_{ij},$$

(21)

where $\nu_t$ is the turbulent viscosity which in the case of the Smagorinsky model is given by

$$\nu_t = (C_S \Delta)^2 | \mathbf{S} |.$$

(22)

Here $| \mathbf{S} | = (2 \tilde{S}_{ij} \tilde{S}_{ij})^{1/2}$ 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 remainder of this section is therefore restricted to the analysis to the modelling of terms originating from the constitutive equation.

We start with the modelling of the sink term in the $C_{ij}$ transport equation. The following approximation will be used (H1):

$$\overline{f(C_{kk})C_{ij}} \approx f(\overline{C_{kk}}) \overline{C_{ij}}.$$

(23)

This assumption is justified by results previously obtained using $a$ priori tests in wall bounded flows,\(^\text{7,16}\) in which the corresponding subgrid-scale quantities were found to be negligible. Notice moreover that the properties of the filtering operation imply that $\overline{f(C_{kk})} = f(\overline{C_{kk}})$.

Secondly, we also neglect the subgrid-scale advection of the filtered conformation tensor evolution equation (H2),

$$\psi_{ij} \approx 0,$$

(24)

which is justified by the small local magnitude of this term compared with the other terms in Equation (16) as described in, e.g., Refs. 7 and 16.

Finally, we assume self-similarity of the subgrid-scale polymer stretching term. In short we assume that the unknown subgrid-scale polymer stretching stresses (Eq. (18)) are structurally similar at two different near sized filter scales. Self-similarity is the hallmark of turbulent flows and is manifested in many ways when the range of scales considered is within the so called inertial range of the energy cascade. The main assumption made here regarding the subgrid-scale polymer stretching term is that, like the subgrid-scale stresses, this term is also self-similar and can be modelled in a similar way. The self-similarity concept was used extensively in the development of some of the very first subgrid-scale models for Newtonian turbulence.\(^\text{17}\)

We base our closure for the subgrid-scale polymer stretching tensor on the Liu-Meneveau-Katz model\(^\text{18}\) for the subgrid-scales stresses, which is a variant of the original Bardina model.\(^\text{19}\) According to this model the subgrid-scale stresses are approximated by

$$\tau_{ij} = \overline{C \left( \tilde{u}_i \tilde{u}_j - \tilde{\bar{u}}_i \tilde{\bar{u}}_j \right)},$$

(25)

where $C$ is a model constant of order $O(1)$, and $\tilde{\bar{u}}$ represents filtering at a larger filter size than the original filter $\Delta$.

Employing the same concept to the computation of the subgrid-scale polymer stretching tensor (Eq. (18)) consists in assuming that this contribution, computed at two nearby filter sizes, is equal apart from a constant of order $O(1)$. Specifically, we define the subgrid-scale polymer stretching
tensor at filter size $\Delta = 2\Delta$

$$G_{ij} = \begin{bmatrix} \partial u_i/\partial x_k C_{jk} - \partial u_j/\partial x_k C_{ik} \\ \partial u_j/\partial x_k C_{ik} - \partial u_i/\partial x_k C_{jk} \end{bmatrix}$$

(26)

which we denote as $G_{ij}$. This is a test subgrid-scale polymer stretching tensor which is available at the LES grid (of size $\Delta$). Using a Bardina type closure, the subgrid-scale polymer stretching tensor is approximated by

$$\gamma_{ij} = C_\gamma G_{ij},$$

(27)

where $C_\gamma$ is a constant. To compute this constant we use the trace of the (filtered) conformation tensor $\overline{C}_{ii}$ (Eq. (19)) and note that in statistically steady isotropic turbulence ensemble averaging this equation in the whole computational domain leads to

$$\langle 2C_{ik} \partial u_i/\partial x_k \rangle_{box} = \frac{1}{\tau_p} \left[ f(C_{kk}) C_{ii} - \delta_{ii} \right]_{box},$$

(28)

where the brackets $\langle \rangle_{box}$ denote the averaging operation carried out in the whole computational box. Equation (28) thus implies that in steady HIT the polymer stretching rate is balanced by the polymer relaxation, so that the polymers are at a steady state of stretching. Since $\overline{C}_{ii}$ is proportional to the elastic energy stored in the polymer molecules we designate Eq. (28), which is always valid in steady HIT, as the global elastic equilibrium assumption (H41). Similarly, if the “local” temporal variation and convective transport terms in Eq. (19) are negligible we can write a “local” elastic equilibrium assumption (H42),

$$2C_{ik} \partial u_i/\partial x_k = \frac{1}{\tau_p} \left[ f(C_{kk}) C_{ii} - \delta_{ii} \right],$$

(29)

where Eq. (29) is valid at each point of the flow domain.

Using the global elastic equilibrium assumption (H41) and Equation (27), together with assumptions H1 and H3, the constant $C_\gamma$ can be computed as

$$C_\gamma = \frac{\langle 1/\tau_p [ f(C_{kk}) C_{ii} - \delta_{ii} ] \rangle_{box} - \langle \partial u_j/\partial x_k C_{jk} \rangle_{box}}{\langle \partial u_j/\partial x_k C_{jk} - \partial u_j/\partial x_k C_{jk} \rangle_{box}}$$

(30)

which closes the model. This model will be extensively tested in Sections IV and V in both a priori and a posteriori (LES) tests.

III. DIRECT NUMERICAL SIMULATIONS OF ISOTROPIC TURBULENCE WITH VISCOELASTIC FLUIDS

This section describes the numerical methods used in the present investigation, which are the same as described in the work of Valente et al.,11 and the several DNS data banks used in the subsequent analysis.

A. Numerical methods

For the momentum equation, classical pseudo-spectral schemes are used for spatial discretisation and a 3-stage, 3rd-order Runge-Kutta scheme is used for temporal discretisation; 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. The momentum equations are transformed into the Fourier space by using the
three-dimensional (direct) Fourier transform,
\[
\tilde{u}_i(\vec{k},t) = F\{u_i(\vec{x},t)\} = \frac{1}{N^3} \sum_{\vec{x}} u_i(\vec{x},t) \exp \left(-i\vec{k} \cdot \vec{x}\right),
\]
and the inverse transform is defined by,
\[
u_i(\vec{x},t) = F^{-1}\{\tilde{u}_i(\vec{k},t)\} = \sum_{\vec{k}} \tilde{u}_i(\vec{k},t) \exp \left(+i\vec{k} \cdot \vec{x}\right),
\]
where \(\vec{x}\) and \(\vec{k}\) are the discrete coordinates in the physical space and the discrete wavenumbers, with components \(k_i = \pm n_j = 0,1,2,\ldots,N/2, \ i = 1,2,3\), respectively, with \(\Delta k = 2\pi/L_{box} = 1\) (i is the imaginary unit). Temporal evolution of the Fourier coefficients of the velocity field are given by the transformed momentum equation,
\[
\frac{d\tilde{u}_i}{dt} + \nu^{[s]}|k^2 & \tilde{u}_i = -\left(\delta_{ij} - \frac{k_i k_j}{k^2}\right)\tilde{N}_j + \frac{1}{\rho} \frac{\partial \sigma_{ij}^{[p]}}{\partial x_j} + \tilde{\eta}_i,
\]
where \(\tilde{N}_i(\vec{k},t) = i k_i u_j \tilde{u}_j(\vec{k},t)\) is the non-linear term from the Navier-Stokes equations, and \(\tilde{\eta}_i(\vec{k},t)\) is an artificial forcing to sustain the turbulence.

The spectral schemes are not suitable for solving the conformation tensor equation (8) as they cannot cope with numerical discontinuities arising in these equations. Therefore, a central differences algorithm proposed by Vaithianathan et al.,\(^{20}\) based on the Kurganov-Tadmor method,\(^{21}\) is used instead. This method ensures that the conformation tensor remains symmetric and positive definite and avoids the need to add artificial diffusion in Eq. (8).

### B. Physical and computational parameters of the reference direct numerical simulations

Table I lists the physical and computational parameters of the reference Newtonian DNS. The simulation uses \(N = 384^3\) collocation points and the kinematic viscosity equal to \(\nu^{[s]} = 0.003\ m^2 s^{-1}\). All the integral flow quantities are computed directly from the kinetic energy spectrum defined by
\[
E(k) = 4\pi k^2 \left\{ \frac{1}{2} \tilde{u}_i(\vec{k},t) \tilde{u}_i(\vec{k},t) \right\}_{\vec{k}},
\]
where """" represents a complex conjugate and \(\left\langle \phi \right\rangle_{\vec{k}}\) denotes the spherical-shell average of the quantity \(\phi\), i.e.,
\[
\left\langle \tilde{\phi}(\vec{k},t) \right\rangle_{\vec{k}} = \frac{1}{N_k} \sum_{k = \Delta k/2 < k < k + \Delta k/2} \tilde{\phi}(\vec{k},t).
\]

<table>
<thead>
<tr>
<th>(\nu^{[s]}) (m(^2) s(^{-1}))</th>
<th>(Re_\lambda)</th>
<th>(K) (m(^2) s(^{-2}))</th>
<th>(\varepsilon^{[s]}) (m(^2) s(^{-3}))</th>
<th>(\ell) (m)</th>
<th>(\lambda) (m)</th>
<th>(k_{max}) ((-))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.003</td>
<td>104</td>
<td>4.00</td>
<td>3.27</td>
<td>0.45</td>
<td>0.19</td>
<td>1.2</td>
</tr>
</tbody>
</table>
Here the summation is carried over all the $N_k$ modes within a shell, of thickness $\Delta k = 1$, centred at $k = |\vec{k}|$. The turbulent kinetic energy and viscous (solvent) dissipation rate are computed as

$$\begin{align*}
K &= \sum_{k_{\text{min}}}^{k_{\text{max}}} E(k) \\
\varepsilon^{[s]} &= 2\nu^{[s]} \sum_{k_{\text{min}}}^{k_{\text{max}}} k^2 E(k),
\end{align*}$$

respectively, while the integral, Taylor, and Kolmogorov micro-scales are given by,

$$\begin{align*}
\ell &= \left( \frac{\pi}{2K} \right) \sum_{k_{\text{min}}}^{k_{\text{max}}} \frac{E(k)}{k}, \\
\lambda &= \sqrt{\frac{10\nu^{[s]} K}{\varepsilon^{[s]}},}
\end{align*}$$

and

$$\eta = \left( \frac{\nu^{[s]}}{\varepsilon^{[s]}} \right)^{1/4}$$

respectively.

The total power input $P$ due to the forcing is computed by adding the averaged input forcing function $f(k)$,

$$P = \sum_{k_{\text{min}}}^{k_{\text{max}}} f(k),$$

which is computed with the artificial forcing field $\tilde{\vartheta}_i(\vec{k}, t)$ through

$$f(k) = 4\pi k^2 \left( \frac{1}{2} \left( \tilde{\vartheta}_i^*(\vec{k}, t) \tilde{u}_i(\vec{k}, t) + \tilde{\vartheta}_i(\vec{k}, t) \tilde{u}_i^*(\vec{k}, t) \right) \right)_{|k|}. $$

In the present work the forcing described in the work of Alvelius$^{22}$ is used, where the artificial forcing field $\vartheta_i(x, t)$ is uncorrelated with the velocity field, and delta-correlated in time,

$$\langle \vartheta_i(x, t) \vartheta_i(x, \tau) \rangle = P \delta(t - \tau)$$

(the brackets without subscript represent a simple ensemble averaging operation). The input forcing function was chosen in order to have the power input concentrated in the low wavenumber range, while at the same time assuring that the box size is always much larger than the integral scale. Specifically, the input forcing function is imposed on the first 4 wavenumbers, using a Gaussian profile centred at wavenumber $k = 3$, with a total power input equal to $P = 3.3$ m$^2$/s$^3$. As shown by Valente et al.$^{23}$ this was enough to provide results independent of the forcing. Due to stationarity in the reference Newtonian simulation, the power of the input forcing balances the viscous dissipation rate $P = \varepsilon^{[s]}$. This forcing function $f(k)$ is a part of the energy budget as discussed below in relation to Eqs. (47) and (51).

Finally, the Reynolds number based on the Taylor micro-scale is defined by

$$Re_\lambda = \sqrt{\frac{2K}{3} \frac{\lambda}{\nu^{[s]}}}. $$

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. Similar precaution was taken in the viscoelastic simulations (see below).
A set of 6 DNS reference viscoelastic simulations was also carried out with the same number of collocation points of the reference Newtonian simulation \((N = 384^3)\), same kinematic viscosity of the solvent \((\nu[k] = 0.003 \text{ m}^2 \text{s}^{-1})\), and the same input forcing characteristics, \((e.g., P = 3.3 \text{ m}^2 \text{s}^{-3})\). Table II 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 \(\tau_p = [0.025, 0.05, 0.1, 0.2, 0.4, 0.6] \text{ s}\). The relaxation time is accounted for in the Deborah and Weissenberg dimensionless numbers defined as

\[
De = \frac{\tau_p \sqrt{K}}{\ell} \tag{45}
\]

and

\[
Wi = \frac{\tau_p}{\eta} \tag{46}
\]

respectively. They represent the ratio between the relaxation time of the polymer solution and the eddy turnover time and Kolmogorov time scale \((\tau_\eta = (\nu[k]/\nu[k])^{1/2})\), respectively.

Finally, we also computed Lumley’s length scale \(r_L = \sqrt{\nu[k] \tau_p} \), defined as the scale below which the turbulent eddies within the solvent are affected by the polymer, together with its corresponding wavenumber \(k_L = r_L^{-1} \), following the work of de Angelis et al.\(^{25}\)

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 studied in great detail by Valente et al.,\(^{11}\) by using the scale-by-scale kinetic energy budget in wavenumber space, analysed through a Lin-type equation\(^{26,27}\) which has been modified to include the kinetic energy transfer between the solvent and the polymers,

\[
\frac{\partial E(k,t)}{\partial t} = T(k,t) - T^{[p]}(k,t) - 2\nu[k]k^2E(k,t) + f(k,t), \tag{47}
\]

where \(E(k,t)\) is the kinetic energy spectrum and \(2\nu[k]k^2E(k)\) is the viscous dissipation within the solvent at wavenumber \(k\), respectively, while \(f(k,t)\) is the spherical-shell averaged input forcing function defined in Eq. (42). \(T(k,t)\) 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/larger than \(k\) into wavenumbers larger/smaller than \(k\), while positive/negative values of \(T^{[p]}(k,t)\) represent transfers of kinetic energy into/from the polymer molecules.

### Table II. Physical and computational parameters of the reference viscoelastic DNS: Deborah number (De); Weissenberg number (Wi); Taylor micro-scale based Reynolds number (ReA); Turbulent kinetic energy (K); solvent dissipation (\(\nu[k]\)); polymer dissipation (\(\nu[p]\)); integral scale (\(\ell\)); Taylor micro-scale (\(A\)); maximum effective wavenumber normalised by the Kolmogorov micro-scale (\(k_{max}\)); fraction of maximum polymer extension \((\langle C_{ii}\rangle/L^2)\). All the simulations use \(N = 384^3\) collocation points, kinematic viscosity of the solvent \(\nu[k] = 0.003 \text{ m}^2 \text{s}^{-1}\), \(\beta = 0.8\), and \(L^2 = 100^2\). The input power forcing has the same characteristics as the Newtonian reference simulation, \((e.g., P = 3.3 \text{ m}^2 \text{s}^{-3})\). SI units have been used for all dimensional quantities.

<table>
<thead>
<tr>
<th>(De)</th>
<th>(Wi)</th>
<th>(ReA)</th>
<th>(K)</th>
<th>(\nu[k])</th>
<th>(\nu[p])</th>
<th>(\ell)</th>
<th>(A)</th>
<th>(k_{max})</th>
<th>(\langle C_{ii}\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>
The non-linear kinetic energy transfer within the solvent at wavenumber \( k = |\vec{k}| \) is given by the kinetic energy transfer function \( T(k,t) \),

\[
T(k,t) = 4\pi k^2 \left\langle \tilde{T}(\vec{k},t) \right\rangle_{|\vec{k}|},
\]

obtained by spherical shell-averaging the non-linear kinetic energy transfer at wavenumber \( \vec{k} \), which is given by

\[
\tilde{T}(\vec{k},t) = \Re \left\{ \tilde{u}_i^* (\vec{k},t) \tilde{N}_i (\vec{k},t) \right\},
\]

where \( \Re \) denotes the real part of the term inside brackets. Similarly, \( T^{[p]}(k,t) \), describing the kinetic energy transfer between the solvent and the polymer molecules is given by,

\[
T^{[p]}(k,t) = 4\pi k^2 \left\langle \tilde{S}_{ij}^p (\vec{k},t) \tilde{\sigma}_{ij}^{[p]} (\vec{k},t) + \tilde{\Gamma}_{ij}^{[p]} (\vec{k},t) \right\rangle_{|\vec{k}|},
\]

\[
= 8\pi k^2 \left\langle \Re \left\{ \tilde{S}_{ij}^p (\vec{k},t) \tilde{\sigma}_{ij}^{[p]} (\vec{k},t) \right\} \right\rangle_{|\vec{k}|}.
\]

Due to the statistical stationarity of the flow, Equation (47) becomes

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

and after integrating each term in Eq. (51) (from 0 to \( k \)) we get

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

where each term still represents the same physical mechanism as in Eq. (51), but now integrated up to wavenumber \( k \), e.g., \( T^{[p]}(k) \equiv \int_0^k T^{[p]}(k')dk' \) (note the sign swap of the term \( \Pi(k) \equiv -\int_0^k T(k')dk' \), so that it is a positive quantity). These definitions can be used to compute the total solvent and polymer dissipations,

\[
e^{[s]} = D(k_{max})
\]

and

\[
e^{[p]} = \left\langle \epsilon^{[p]} S_{ij} \right\rangle_{\text{box}} = \sum_{k_{min}}^{k_{max}} T^{[p]}(k),
\]

respectively, so that statistical stationarity implies that the total power input from the forcing is equal to the sum of the solvent and polymer dissipations,

\[
P = e^{[s]} + e^{[p]}.
\]

To characterise the new simulations and to illustrate the challenges behind subgrid-scale modelling in the context of viscoelastic flows, Figs. 1(a)-1(c) show the kinetic energy spectra \( E(k) \) for the simulations with \( De = 0.11 \), \( De = 0.62 \), and \( De = 1.23 \), respectively, with the vertical lines representing Lumley’s inverse length scale \( k_L \) (dashed), and two filter sizes used in the subsequent analysis with sizes equal to \( \Delta / \Delta x = 4 \) and 16 (solid).

In all the three spectra one can clearly discern the effect of the forcing in the low wavenumber range \( k \leq 4 \), followed by an inertial range region, which deviates from the classical \(-5/3\) slope for intermediate \( De \) numbers,\(^{11}\) followed by a dissipative range region. The shape of the kinetic energy spectrum and particularly the slope of the inertial range and inertial-elastic ranges varies with the Deborah number. An extensive study of this topic was recently reported in Ref. 23. The two filter sizes are clearly associated with different regions of the energy spectrum. Whereas the filter \( \Delta / \Delta x = 16 \) is placed at the inertial range region, where the classical subgrid-scale models are expected to be operating, the filter \( \Delta / \Delta x = 4 \) on the other hand is at the dissipative range i.e., this filter size is already at very small scales, where LES tends to DNS and therefore where the classical subgrid-scale models (at least for the momentum equation) are designed to naturally “switch off.”

While Lumley’s scale is below 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. Recall that an accurate modelling of the kinetic energy transfer between resolved and unresolved
FIG. 1. Kinetic energy spectra $E(k)$ for the DNS at increasing Deborah numbers. The vertical solid green and blue lines correspond to filter sizes $\Delta/\Delta x = 4$ and 16 and the vertical red dashed line represents the wavenumber corresponding to the Lumley scale. A curve with a slope of $-5/3$ is also shown to highlight the inertial-range region in the spectra (when present). (a) $De = 0.11$. (b) $De = 0.62$. (c) $De = 1.23$.

scales is crucial in LES. It is therefore likely that in the latter case the non-linear energy flux, from the resolved into unresolved scales of motion, will be largely affected by the dynamics of the solvent/polymer interactions, thus potentially creating additional difficulties for LES, since the non-linear energy cascade flux modelling has to take into account possible polymer effects originating from smaller, and thus unavailable scales.

Worse still, in this respect, is the situation corresponding to $De = 1.23$, where Lumley’s scale is right at the forcing wavenumber range, implying that the polymer effects will be felt on the entire range of scales of motion i.e., the non-linear kinetic energy cascade flux will be affected by the polymer dynamics in the entire wavenumber region.

Figures 2(a)-2(c) show the spectral energy budgets with the spectral forcing function $F(k)$, the non-linear energy transfer within the solvent $\Pi(k)$, and the kinetic/elastic energy transfers between the solvent and the polymer molecules $\Pi[p](k)$, respectively, for the same DNS of Fig. 1, corresponding to $De = 0.11$, $De = 0.62$, and $De = 1.23$. These budgets have been extensively studied in Valente et al. and will be analysed below in the context of subgrid-scale modelling of viscoelastic turbulence. The three figures detail a quite different energy cascade picture for different $De$ numbers, as anticipated above: whereas in Newtonian turbulence the total energy input from the forcing equals the maximum non-linear energy transfer and the total viscous dissipation,

$$P = F(k_{max}) = \max \{\Pi(k)\} = D(k_{max}),$$

FIG. 2. Spectral energy budget (Eq. (52)) for the DNS at increasing Deborah numbers, showing the spectral forcing function $F(k)$, the non-linear energy transfer within the solvent $\Pi(k)$, and the kinetic/elastic energy transfers between the solvent and the polymer molecules $\Pi[p](k)$, normalised by the total power input $P$. The filter sizes $\Delta/\Delta x = 4$ and 16 are also shown as solid lines, and the dashed vertical line represents the wavenumber corresponding to the Lumley scale. (a) $De = 0.11$. (b) $De = 0.62$. (c) $De = 1.23$. 
(i.e., $P = \varepsilon^{[s]}$), in the viscoelastic simulations the total kinetic energy dissipation is assured both by the (solvent) molecular dissipation, and by the polymer molecules through an increase of their elastic/internal energy i.e.,

$$P = F(k_{\text{max}}) = D(k_{\text{max}}) + \Pi^{[p]}(k_{\text{max}}),$$

so that $P = \varepsilon^{[s]} + \varepsilon^{[p]}$ (see the work of Valente et al.$^{11}$). Notice that $\Pi^{[p]}(k)$ describes not only the direct dissipation by the polymer molecules but also the energy cascade dynamics associated with the interaction between the solvent and the polymer molecules, comprising possibly (i) (additional) energy dissipation within the solvent and/or (ii) (additional) energy input into the solvent, at a given wavenumber $k$. These are features that are highly dependent on the flow Deborah number.

In contrast to the case with $De = 0.11$ (Fig. 2(a)), where most of the dissipation is assured by the solvent ($\varepsilon^{[p]} < \varepsilon^{[s]}$), in $De = 0.62$ (Fig. 2(b)) the dissipation is already largely caused by the polymer molecules $\varepsilon^{[p]} > \varepsilon^{[s]}$. Moreover, for $De = 0.62$ the Lumley scale corresponds to a wavenumber that is smaller than the wavenumbers associated with most of the viscous dissipation, where $D(k) \approx D(k_{\text{max}})$ is approximately constant. Therefore the viscous dissipation of kinetic energy at this $De$ is surely affected by the solvent/elastic energy interactions.

The case with $De = 1.23$ suggests an even more complex situation regarding the solvent/polymer interactions since even the $\Pi(k)$ peak, which is equal to the amount of energy flux into the small scales, is already severely affected by the presence of the polymers. Notice moreover that in this case the filter size corresponding to $\Delta/\Delta x = 16$ is placed at a wavenumber ($k_{16}$) that is much smaller than the peak of dissipation $D(k_{\text{max}})$ i.e., $k_{16} < k_{\text{max}}$, thus making the direct computation of the solvent dissipation very hard if not impossible.

The DNS results discussed above illustrate well some of the challenges facing any subgrid-scale model aimed at simulating turbulent viscoelastic flows, and possibly explain why few if any subgrid-scale model for these flows has ever been developed successfully.

Finally, Figs. 3(a)-3(c) show iso-surfaces of the second invariant of the velocity gradient tensor $Q = \frac{1}{2} (\omega_{ij} \omega_{ij} - 2S_{ij}S_{ij})$, where $\omega_{ij}$ is the vorticity vector, for the three simulations, $De = 0.11$, 0.62, and 1.23, respectively. It is well known that the flow structures from viscoelastic flows are markedly different from those of Newtonian turbulence, notably with a tendency for originating “sheet-like” structures, for high $De$ or $Wi$ numbers,$^{31}$ instead of the typical “worm-like” vorticity structures from Newtonian turbulence. However, since we will be also interested in assessing the capability of subgrid-scale models to describe these structures it is important to analyse them, even if no detailed investigation of these structures will be undertaken here as in Ref. 32.

For $De = 0.11$ the iso-surfaces of $Q > 0$, associated with a predominance of enstrophy over strain show typical “worm” or tube-like structures, which are very similar to Newtonian isotropic turbulence, while for $De = 0.62$ and $De = 1.23$ the iso-surfaces of $Q > 0$ displays both tube and sheet like structures, or only sheet-like regions structures, respectively.$^{33}$ An accurate subgrid-scale model for viscoelastic flows will need to capture the different flow topologies for different $De$.

![Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by the root-mean-square $Q_{\text{rms}}$) corresponding to a threshold equal to $Q/Q_{\text{rms}} = 7$ for the DNS at increasing Deborah numbers. (a) $De = 0.11$. (b) $De = 0.62$. (c) $De = 1.23$.](image-url)
numbers, as these structures are strongly linked with the solvent/polymer interactions, and with the solvent dissipation reduction mechanism\(^{39}\) here, and drag reduction in wall bounded flows. Drag reduction in viscoelastic wall bounded turbulent flows has been linked with the polymer stresses and the torque acting on the streamwise vortices near the wall;\(^{34–36}\) however, it is important to stress that the structures arising in viscoelastic isotropic turbulence are typically different from the structures observed in wall turbulence, and the typical horseshoe or hairpin vortices described in the work of Yarin\(^{37}\) are absent from HIT.

IV. A PRIORI TESTS: DNS OF ISOTROPIC VISCOELASTIC TURBULENCE

In this section we describe the results obtained using classical \textit{a priori} tests conducted in the reference simulations detailed above. The aim of these tests is to assess the several subgrid-scale hypotheses that have been used in the new subgrid-scale model for viscoelastic flows proposed in the present work.

A. Modification of the Smagorinsky model constant $C_S$ in viscoelastic flows

As described above the proposed subgrid-scale model for viscoelastic flows relies on the classical Smagorinsky closure to quantify the subgrid-scale stresses in the momentum equation $\tau_{ij}$. In order to appreciate the influence of the Deborah number and filter size on the Smagorinsky model constant $C_S$ we used the DNS data banks to compute this constant using classical \textit{a priori} tests. Following the work of Meneveau\(^{17}\) we compute

$$C_S^2 = \frac{\langle \tau_{ij} \rangle_{box}^2}{2\sqrt{2} \Delta^2 \langle \tilde{S}_{ij} \rangle_{box}^{3/2}},$$

where additionally to the box average we perform time averages for each simulation to improve the convergence of the results. Figure 4 shows $C_S$ obtained with Equation (58) for all the reference simulations used and for filter sizes $\Delta/\Delta x = 2, 4, 8$ and 16. The Newtonian case is also shown for comparison and it is interesting to see that in this case $C_S$ also increases with the filter size, but remains within 0.14 and 0.17. For the Newtonian case this variation is only due to finite Reynolds number effects.\(^{38}\) Recall that for Newtonian isotropic turbulence and by assuming an inertial range energy spectrum $E(k) = C_K (\epsilon^{1/3} k^{-5/3})$, the Smagorinsky constant is given by

$$C_S = \frac{1}{\pi} \left( \frac{3C_K}{2} \right)^{-3/4} = 0.16$$

FIG. 4. Smagorinsky constant ($C_S$) computed with Eq. (58) for filter sizes $\Delta/\Delta x = 2, 4, 8$, and 16 and all the reference simulations used in this work.
for a value of the Kolmogorov constant ($C_K$) of 1.6. Thus, the present values of $0.14 \leq C_S \leq 0.17$ are close to the “exact” value of $C_S = 0.16$. In the viscoelastic simulations the constant exhibits the same trend of increasing $C_S$ with the filter size; however, $C_S$ tends to decrease (for a particular filter size $\Delta$), with the Deborah number. This was expected from the reduction in subgrid-scale stresses and enhanced polymer stresses as $De$ increases and it also reflects the depletion of kinetic energy flux into the subgrid-scales of motion described above (see also Appendix A). In particular for $De = 1.23$ the constant is $C_S \approx 0.102$ which is smaller than the classical value and suggests that corrections to this constant may be needed for viscoelastic LES calculations. However, as shown in Appendix A, this is not the case at least for (forced) isotropic turbulence for the range of $De$ numbers used in the present work. Indeed as shown in the a posteriori tests (Section V) and in Appendix A very good LES results are obtained while using $C_S = 0.16$.

B. Sink of the filtered conformation tensor transport equation: H1

We start with the first hypothesis used in the present model and described in Equation (23). Figures 5(a)-5(c) show the joint probability density function (JPDF) between the two sides from this equation for the simulations with $De = 0.11$, 0.38, and 0.91, respectively, for filter size $\Delta/\Delta x = 16$. It is clear that the two quantities are in all cases very strongly correlated, and with closely matching magnitudes, even if a slight decrease in the correlation is observed for higher Deborah numbers. The same result was observed for the other simulations and filter sizes and a similar result was obtained by Masoudian et al.\textsuperscript{16} in DNS of turbulent viscoelastic channel flows described by the FENE-P fluid. Given the soundness of assumption H1 this hypothesis was used in the remaining of this work.

C. Subgrid-scale conformation tensor advection term: H2

We now turn into the modelling of the subgrid-scale advection of the conformation tensor ($\psi_{ij}$) defined in Eq. (17). In the present model this term is essentially neglected as described in assumption H2 and stated in Eq. (24). In order to assess the accuracy of this assumption we analyse the evolution equation for the filtered trace of the conformation equation (60) written as

\[
\frac{\partial \overline{C}_{ii}}{\partial t} + \frac{\partial \overline{C}_{ii}}{\partial x_k} = 2 \overline{C}_{ik} \frac{\partial \overline{u}_i}{\partial x_k} - \frac{1}{\tau_p} \left[ f(C_{kk}) \overline{C}_{ii} - \delta_{ii} \right] - \psi_{ii} + \gamma_{ii},
\]

where the approximation H1 (Eq. (23)) has been used. The terms on the left-hand side of Equation (60) are the temporal variation ($C_t$) and advection of $\overline{C}_{ii}$ ($C_a$), respectively, while the terms on the right-hand side represent the production ($C_p$) and dissipation of $\overline{C}_{ii}$ ($C_d$). These terms are followed by the unknown subgrid-scale terms associated with the convection, $\psi_{ii}$, and polymer stretching, $\gamma_{ii}$, respectively.

Since due to isotropy the mean value of the subgrid-scale advection is zero $\langle \psi_{ii} \rangle_{box} = 0$, the only way to assess the relevance of this term is by comparing its local/instantaneous value with the

\[
\overline{C}_{ii} = f(C_{kk}) \overline{C}_{ii},
\]

for the DNS at increasing Deborah numbers, and filter size $\Delta/\Delta x = 16$. (a) $De = 0.11$. (b) $De = 0.38$. (c) $De = 0.91$. 

FIG. 5. Probability density function (PDF) of $c_d = f(C_{kk})C_{ii}$ and $C_D = f(C_{kk})C_{ii}$ normalised by their root-mean-square,
other terms in Eq. (60). For this purpose Figs. 6(a)-6(c) show the probability density functions of \( \gamma_{ii} \) and \( \psi_{ii} \) for \( \Delta/\Delta x = 16 \) and for the DNSs with \( De = 0.11, 0.38 \) and 0.91. Clearly the skewness of \( \gamma_{ii} \) is much higher than that of \( \psi_{ii} \) (notice that \( \gamma_{ii} \) is not zero), with a very low probability (~0.01%) associated with events with \( \psi_{ii} \gg \gamma_{ii} \). Similar results were observed for the other simulations and filter sizes thus strongly supporting assumption H2. Note also that similar results were obtained by Masoudian et al.\textsuperscript{16} using DNS of turbulent channel flows based on the FENE-P constitutive model. However, the present results are for a flow away from solid boundaries and at a much higher Reynolds number; therefore, it can be seen as a more general result, since a lower Reynolds number and the inhibitive effect on turbulence caused by the presence of a wall in the work of Masoudian et al.\textsuperscript{16} could somehow attenuate the “energy” typically associated with advective terms in turbulence transport equations. The PDFs also suggest that the skewness of \( \gamma_{ii} \) increases with \( De \). Note that \( \gamma_{ii} < 0 \) contributes to increase the resolved stretching term in Eq. (60), and a tendency for more frequent (eventually becoming dominant) events of \( \gamma_{ii} < 0 \) consistent with the establishment of a polymer induced kinetic energy cascade at high \( De \) as observed in Ref. 23. The explanation is that at low \( De \) the instantaneous kinematic events distort the dumbbells through weak normal strains which contribute positively to \( \gamma_{ii} \), but as \( De \) increases there is an increasing stretch with positive and negative normal shear contributions and this has a strong impact on the energy cascade mechanism as we described in detail in Valente et al.\textsuperscript{23}

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

The scale-similarity of the subgrid-scale polymer stretching term (\( \gamma_{ij} \)) used by the present model is described together with Eqs. (18), (26), and (27). In order to assess this approximation Figures 7(a)-7(c) and 8(a)-8(c) show joint probability density functions (JPDFs) 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 \( \Delta/\Delta x = 4 \) to 16. Since these correlations are always quite high, these JPDFs are a first indication that the scale-similarity assumption may be a good starting point for a model of the subgrid-scale polymer stretching term in Eq. (16). A note of warning is needed here for the highest \( De \) number \( (De = 1.23) \) because the joint PDFs and correlations also showed that for this case the self-similarity assumption is not as strong as in the other cases (see Appendix B). For instance the correlation between \( \gamma_{ii} \) and \( G_{ii} \) for filter sizes \( \Delta/\Delta x = 4 \) and \( \Delta/\Delta x = 16 \) is equal to 43%, which is substantially lower than in the other cases. This may be explained by the challenging large-scale/subgrid-scale interactions arising in elasto-inertial turbulence discussed in Section III B associated with this particular simulation and also studied in detail by Valente et al.\textsuperscript{23} However as will be shown latter in Section V, the deterioration of this assumption will have a negligible impact.
Next we show that $\gamma_{ii}$ and $G_{ii}$ exhibit closely similar statistical characteristics, in terms of the range of existing magnitudes and their distributions. To show this, Figures 9(a)-9(c) show the probability density functions of $\gamma_{ii}$ and $G_{ii}$ for $\Delta/\Delta x = 4$ and for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. The similarity between the two quantities is indeed remarkable. The same is true for the other simulations and filter sizes.

To emphasise this point, Table III lists the root-mean-square (rms) of $\gamma_{ii}$ and $G_{ii}$ which is a measure of the “energy” of the agitation of both terms, for several simulations and filter sizes. The rms of the two quantities is indeed very similar in all the cases considered, which further confirms that the quantity $G_{ii}$ is indeed a good candidate to use as surrogate to approximate the unknown subgrid-scale polymer stretching term $\gamma_{ii}$.

During the course of the work it was checked that $C_{\gamma_{11}}$, $C_{\gamma_{22}}$, and $C_{\gamma_{33}}$ are statistically equivalent, as expected, and likewise $C_{\gamma_{12}}$, $C_{\gamma_{23}}$, and $C_{\gamma_{32}}$ are also (statistically) equivalent; however, a question that naturally arises when facing the model definition in Eq. (27) is whether the model constant $C_\gamma$ is “isotropic” i.e., given the well known possible anisotropy of the polymer stresses one might be tempted to extend the present model by using an anisotropic version of the model constant $C_{\gamma_{ij}}$, defined as

$$\gamma_{ij} = C_{\gamma_{ij}} G_{ij} \text{ (no summation).} \quad (61)$$

To clarify this issue Figures 10(a)-10(c) and 11(a)-11(c) show several joint probability density functions (JPDFs) involving the quantities $C_{\gamma_{11}}$, $C_{\gamma_{22}}$, and $C_{\gamma_{12}}$ for filter size $\Delta/\Delta x = 4$, and for the reference DNS with $De = 0.11$, $De = 0.38$, and $De = 0.91$, defined by

$$C_{\gamma_{11}} = \frac{\gamma_{11}}{G_{11}}, \quad (62)$$

$$C_{\gamma_{22}} = \frac{\gamma_{22}}{G_{22}}, \quad (63)$$

FIG. 7. 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 at increasing Deborah numbers. (a) $De = 0.11$. (b) $De = 0.38$. (c) $De = 0.91$.

FIG. 8. 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 $\Delta/\Delta x = 16$ for the DNS at increasing Deborah numbers. (a) $De = 0.11$. (b) $De = 0.38$. (c) $De = 0.91$. 
FIG. 9. Probability density functions of traces of subgrid-scale polymer stretching terms $\gamma_{ii}$ and $G_{ii}$ at filter size $\Delta/\Delta x = 4$ for the DNS at increasing Deborah numbers. (a) $De = 0.11$. (b) $De = 0.38$. (c) $De = 0.91$.

and

$$C_{\gamma_{12}} = \frac{\gamma_{12}}{G_{12}}.$$  \hspace{1cm} (64)

Clearly the quantities, $C_{\gamma_{11}}$, $C_{\gamma_{22}}$, and $C_{\gamma_{12}}$, are statistically independent, with the remaining component coefficients behaving similarly. Similar observations were made for filter size $\Delta/\Delta x = 16$. This supports the use of an “isotropic” constant $C_{\gamma}$ in the present model and finalises the assessment of the hypothesis $H_3$. However, the closure relies on the quantification of $C_{\gamma}$ through Eq. (30) which also relies on the hypothesis $H_{41}$ (Eq. (28)) and $H_{42}$ (Eq. (29)), investigated below. From this point on $C_{\gamma}$ is assumed to be constant and isotropic.

E. Global equilibrium of the polymeric elastic energy: $H_{41}$

The coefficient of the closure in Eq. (30) uses the assumption of global equilibrium of the polymers elastic energy described in Equation (28). It was checked that indeed the two sizes of Equation (28) 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 advective terms are zero. Therefore, this hypothesis does not need any additional discussion. It is however interesting to discuss the possibility of using instead 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. This is addressed next.

F. Local equilibrium of the polymeric elastic energy: $H_{42}$

The local equilibrium assumption defined by Equation (29) is not used in the present model, but is discussed here because of its usefulness in future model developments. The hypothesis of local equilibrium of the subgrid-scales of motion, in the momentum transport equation, is one of the main assumptions of classical subgrid-scale models, e.g., the Smagorinsky model, and a

<table>
<thead>
<tr>
<th>$\Delta/\Delta x$</th>
<th>$De = 0.11$</th>
<th>$De = 0.38$</th>
<th>$De = 0.91$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma_{11}$</td>
<td>11.8</td>
<td>21.2</td>
<td>44.4</td>
</tr>
<tr>
<td></td>
<td>258</td>
<td>584</td>
<td></td>
</tr>
<tr>
<td>$\gamma_{12}$</td>
<td>4.4</td>
<td>56.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>358</td>
<td>478</td>
<td></td>
</tr>
<tr>
<td>$G_{11}$</td>
<td>11.8</td>
<td>2.7</td>
<td>51.8</td>
</tr>
<tr>
<td></td>
<td>53.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$G_{12}$</td>
<td>11.8</td>
<td>2.7</td>
<td>51.8</td>
</tr>
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<td></td>
<td>53.3</td>
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</tr>
</tbody>
</table>
“local” equilibrium of the elastic energy (which is proportional to the trace of the conformation tensor) are in some ways similar. The local equilibrium of the subgrid-scale stresses however is a flawed hypothesis as attested by the less than 40% correlation between the kinetic energy flux at the subgrid-scale level and the viscous dissipation of kinetic energy. However, in contrast to this classical equilibrium, the hypothesis H42 is indeed strongly supported by the present data banks.

This can be appreciated in Figs. 12(a)-12(c) showing the joint probability density functions (JPDFs) of the polymer stretching ($C_p$) and dissipation ($C_d$) from the trace of the conformation tensor transport equation (19) for several Deborah numbers and filter size $\Delta/\Delta x = 16$. The correlation between $C_p$ and $C_d$ is always quite high and the JPDFs shape and correlation coefficients are relatively independent of the filter size, e.g., the correlation coefficient varies between 0.85 to 0.89 for $\Delta/\Delta x = 4$ and 16, respectively for $De = 0.38$, while slightly decreasing with increasing $De$ number, e.g., from 0.98 to 0.80 at $\Delta/\Delta x = 16$ from $De = 0.11$ to $De = 0.91$.

The strong correlation between $C_p$ and $C_d$ described above is a strong indication that these terms are approximately in equilibrium; however, the assessment of the assumption H42 is not complete without showing that the other terms in Eq. (29), terms $C_t$ and $C_a$, are negligible in relation to terms $C_p$ and $C_d$. To investigate this issue, and since the mean values of $\langle C_t \rangle$ and $\langle C_a \rangle$ are zero, Figures 13(a)-13(c) show the probability density functions of all the terms in Eq. (19) ($C_t$, $C_a$, $C_p$, and $C_d$) for $\Delta/\Delta x = 16$ and $De = 0.11$, 0.38, and 0.91, respectively. In some cases $C_t$ and $C_a$ attain much smaller magnitudes than terms $C_p$ and $C_d$, e.g., for $De = 0.11$; however, in other situations the reverse is observed, e.g., for $De = 0.91$, but in all instances one sees that the probability density functions of $C_t$ and $C_a$ are very similar, and symmetric around 0. The same is true of the other simulations and filter sizes (not shown). Therefore the only possibility for the local equilibrium assumption to hold is if $C_t$ and $C_a$ are strongly anti-correlated, so that their joint effect is cancelled and Eq. (19) is well approximated by the remaining terms, $C_p$ and $C_d$. This is indeed the case as can be seen in Figures 14(a) and 14(b) showing the joint probability density functions between $C_t$ and $C_a$ for $De = 0.11$, 0.38, and 0.91 and $\Delta/\Delta x = 16$ (similar results are observed for $\Delta/\Delta x = 4$).
Thus, the present results convincingly show that assumption $H_{42}$ is strongly supported by the DNS data, which suggests that it can probably be used in viscoelastic inhomogeneous turbulent flows, where the global elastic energy equilibrium assumption (Eq. (28)) does not necessarily hold.

G. Influence of the Deborah number and filter size on $C_γ$

Next we analyse the sensitivity of the model constant $C_γ$ to the filter size and Deborah number. We employ two procedures. In the first one the constant is computed using globally averaged quantities,

$$C_γ = \frac{⟨γ_{jj}⟩\text{box}}{⟨G_{ii}⟩\text{box}},$$

where the brackets represent a volume average which is computed for each time step of the simulations (Fig. 15(a)). In the second procedure the constant is computed locally,

$$C_γ = \frac{γ_{jj}}{G_{ii}\text{box}},$$

i.e., using the definition of the constant at each point of the flow domain and for each time step, and averaging the constant $C_γ$ thus obtained in the whole domain (Fig. 15(b)). Equations (65) and (66) thus use the “local” and the “global” elastic equilibrium assumptions, respectively.

The two figures are remarkably similar which again confirms that the local and global equilibrium assumptions $H_{41}$ and $H_{42}$ are equally valid and lead essentially to the same results. The
model constant is, as expected $O(C_γ) = 1$ and remains bounded by $0 \leq C_γ \leq 5$, with a tendency of increasing with the filter size but of decreasing with the Deborah number. The cases corresponding to $De \approx 1$ are interesting in that $C_γ$ approaches $\approx 0$. This is consistent with the depletion of the non-linear energy cascade for $De \approx 1$ observed in the work of Valente et al.,\textsuperscript{11} where almost all the energy input is dissipated by the elastic stresses from the polymers. Since a smaller subgrid-scale activity will also lead to a decrease of the polymer stretching term, it is thus natural to expect the model to automatically “switch-off” in these cases.

Finally, Figures 16(a)-16(c) show the probability density functions of the local constant $C_γ$, i.e., again computed through Eq. (30) without the averaging operation, for all the filter sizes considered in this work $\Delta/\Delta x = 2, 4, 8$, and 16. The figures show that the events corresponding to large deviations from the mean values obtained before are very rare, particularly for the larger filter sizes, again confirming that the local approximation is a good candidate to use in large-eddy simulations of inhomogeneous flows of viscoelastic fluids described by the FENE-P model. Indeed, as far as \textit{a priori} tests are concerned the results indicate that the present model can be used for simulating viscoelastic inhomogeneous flows away from solid boundaries. This completes the \textit{a priori} analysis of the present model.

In the present study the filter size used in all the \textit{a priori} and \textit{a posteriori} tests was always computed as $\Delta = (\Delta x \times \Delta y \times \Delta z)^{1/3}$, and only isotropic grids were considered $\Delta x = \Delta y = \Delta z$, however in a future study the effects of grid anisotropy should also be investigated, e.g., as in Ref. 19.

---

**FIG. 14.** Joint probability density functions between the trace of the polymer temporal variation ($C_t$) and advective transport ($C_a$) (normalised by their root-mean-square), at filter size $\Delta/\Delta x = 16$ for the DNS at increasing Deborah numbers. (a) $De = 0.11$. (b) $De = 0.38$. (c) $De = 0.91$.

**FIG. 15.** Mean value of the model constant $C_γ$ defined by Eq. (27) and computed using Eq. (65) i.e., a global or box averaging defined by the brackets in this equation, or averaging the locally obtained $C_γ$ (Eq. (66)), after it has been computed at each flow point/time step. The two procedures are carried out for all the reference DNS and for filter sizes $\Delta/\Delta x = 2, 4, 8$, and 16. (a) Global. (b) Local.
V. A POSTERIORI TESTS: LES OF ISOTROPIC VISCOELASTIC TURBULENCE

In this section we discuss the results from LES obtained with the present model. A total of 6 LES were carried out using the same physical parameters described in Table II, 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, 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. We also compare the LES with simulations using no subgrid-scale polymer stretching term i.e., by forcing \( C_\gamma = 0 \), which we name “incomplete LES model” or “no-model,” since the Smagorinsky model is always active in all the LES. Each LES goes through a transient of roughly \( 6 - 7 \) turnover times, corresponding to the build up of the enstrophy field. It is only after this transient is reached that the subgrid-scale model for the polymer stretching term is activated, whereas the Smagorinsky model is active throughout the whole transient.

A. Final set of governing equations for LES of viscoelastic isotropic turbulence: The distortion similarity model - DSIM

Denoting by an overbar (\( \overline{\cdot} \)) a quantity represented in the LES grid, the final closed system of LES equations for viscoelastic turbulence using the distortion similarity model consists in the following set: continuity,

\[
\frac{\partial \overline{u}_i}{\partial x_i} = 0, \tag{67}
\]

momentum transport,

\[
\frac{\partial \overline{u}_i}{\partial t} + \overline{u}_k \frac{\partial \overline{u}_i}{\partial x_k} = -\frac{1}{\rho} \frac{\partial \overline{p}}{\partial x_i} + 2 \frac{\partial}{\partial x_j} \left[ (\nu^f + \nu_t) \overline{S}_{ij} \right] + \frac{\partial}{\partial x_j} \left\{ \frac{\gamma^{lp}}{\tau_p} [f(\overline{C}_{kk}) \overline{C}_{ij} - \delta_{ij}] \right\}, \tag{68}
\]

and conformation tensor

\[
\frac{\partial \overline{C}_{ij}}{\partial t} + \overline{u}_k \frac{\partial \overline{C}_{ij}}{\partial x_k} = \frac{\partial \overline{u}_i}{\partial x_j} \overline{C}_{jk} + \frac{\partial \overline{u}_j}{\partial x_i} \overline{C}_{ik} - \frac{1}{\tau_p} [f(\overline{C}_{kk}) \overline{C}_{ij} - \delta_{ij}] + C_\gamma G_{ij}, \tag{69}
\]

respectively. The eddy viscosity \( \nu_t(\overline{\cdot},t) \) is computed by using the Smagorinsky model in Eq. (22) and with the Smagorinsky constant \( C_S = 0.16 \). As discussed above, the \( a \) priori tests suggest that a smaller \( C_S \) should have been used for the higher \( De \) cases. However, since constants do not differ very much, we decided to keep the same constant for all simulations, since the level of activity of the resolved rate-of-strain fields will also adjust to the modification of the small scale energy and compensate for mild deviations from the classical \( C_S = 0.16 \) value i.e., it is hoped that any small variations of the local energy flux into the unresolved scales will be compensated by a decrease...
of the resolved rate-of-strain intensity at these scales, thus decreasing the effective eddy viscosity without the need for adjusting the model constant $C_S$.

The subgrid-scale polymer stretching term is computed directly from its definition (Eq. (26)),

\[ G_{ij} = \left[ \frac{\partial \ddot{u}_i}{\partial x_k} \Gamma_{jk} - \frac{\partial \ddot{u}_j}{\partial x_k} \Gamma_{ik} \right] + \left[ \frac{\partial \ddot{u}_i}{\partial x_k} \widetilde{\Gamma}_{jk} - \frac{\partial \ddot{u}_j}{\partial x_k} \widetilde{\Gamma}_{ik} \right]. \]

Finally, the model constant for the conformation tensor transport equations $C_\gamma$, is calculated by the following formula:

\[ C_\gamma = \frac{\varepsilon[p]}{\rho v [p]} \left( \frac{1}{f(C_{kk})} \right)_{\text{box}} - \left( \frac{\sigma_{ik} \bar{\Gamma}_{jk}}{\text{box}} \right)_{\text{box}}. \]

which was observed to be computationally more stable than its direct definition through Eq. (30).

The polymer dissipation $\varepsilon[p] = P - \varepsilon[s]$ is computed from the energy balance equation (55) since the total power input $P$ is imposed and the solvent dissipation $\varepsilon[s]$ can be computed from its definition (Eq. (37)), and the following equality has been used:\[^{11}\]

\[ \varepsilon[p] = \frac{f(C_{kk})}{2 \tau_p} \sigma_{ii}^2. \]  

For consistency, each new modelling term has been computed using the same numerical method used in its corresponding (DNS) term, e.g., $G_{ij}$ has been computed using 2nd order central finite differences.

**B. Solvent dissipation reduction and coherent structures obtained from the LES**

Table IV lists the values of the solvent dissipation 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\[^{30}\] 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 and their approximations in a reference DNS ($\varepsilon[p]$ and $\varepsilon[s]$ have been computed.

**TABLE IV.** Solvent dissipation reduction (DR) obtained with the complete LES model compared with the corresponding reference filtered DNS (DNS) and with simulations without the subgrid-scale polymer closure (−), i.e., by forcing $C_\gamma = 0$ (incomplete LES). The Smagorinsky model is used in the momentum equations in all the LES and the simulations use the same parameters as described in Table II, (e.g., $\nu[s] = 0.003$ m$^2$/s$^{-1}$ and $\beta = 0.8$) and $N = 48^3$ collocation points (the subgrid-scale stresses in the momentum equation are closed using the Smagorinsky model with $C_S = 0.16$ - even in “incomplete LES model” simulations where $C_\gamma$ is artificially set to 0).

<table>
<thead>
<tr>
<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>
</tr>
<tr>
<td>0.22</td>
<td>0.36</td>
<td>0.17</td>
<td>0.35</td>
</tr>
<tr>
<td>0.38</td>
<td>0.71</td>
<td>0.25</td>
<td>0.66</td>
</tr>
<tr>
<td>0.62</td>
<td>0.88</td>
<td>0.84</td>
<td>0.89</td>
</tr>
<tr>
<td>0.91</td>
<td>0.94</td>
<td>0.95</td>
<td>0.96</td>
</tr>
<tr>
<td>1.23</td>
<td>0.95</td>
<td>0.96</td>
<td>0.96</td>
</tr>
</tbody>
</table>
from the LES as outlined above). Even though DR is referred to as drag reduction in Ref. 30 strictly speaking there is no overall drag reduction since the forcing energy is kept constant. Instead it quantifies the relative energy dissipation by the polymer or the reduction of solvent dissipation. This latter designation is used here. The DR from the DNS data (without filtering) can be computed directly from the values in Table II and varies between 0.19 and 0.89 for De = 0.11 – 1.23. As discussed in Refs. 11 and 23 the DR values obtained here agree well with the existing numerical and experimental works.

It is important to realise that the values of De and Wi computed through Eqs. (45) and (46) during the LES simulations slightly differ from those computed from the DNS. The difference is small however, with less than ~10% error for the simulations carried out in the present work. For instance regarding De computed in the LES using Eq. (45) τp is imposed while K and ℓ are computed from the LES velocity field. The differences in ℓ computed from the DNS, filtered DNS, LES without the subgrid-scale polymer closure, and with the DSIM closure are almost imperceptible. This was expected since ℓ is mostly concentrated at the large scales which are fully captured in the LES. In regard to the turbulent kinetic energy K the effect is slightly stronger with the (unfiltered) DNS presenting slightly higher values than those of the other methods. Therefore De computed from LES (or from filtered DNS) tends to be always slightly smaller than the original De from the DNS. For example for the cases De = 0.11 and De = 0.22 the filtered DNS, no polymer closure, and the DSIM closure give identical values of De = 0.09 and De = 0.18, respectively. The differences decrease slightly with De and for De = 1.23 the filtered DNS, no polymer closure, and the DSIM closure give De = 1.15, 1.11, and 1.10 respectively.

For small to intermediate De numbers, the absence of a model for the subgrid-scale polymer stretching term (incomplete LES model - Cy = 0) leads to DR values that significantly underpredict the correct values. In contrast, inclusion of such subgrid-scale polymer stretching closure clearly allows the recovery of the DR from the simulations, which is a strong indication that the closure is indeed performing its role well. For high values of De (De ≥ 0.91) the differences between the DR obtained with DNS, and with the complete and incomplete (Cy = 0) LES models, are not very important. As we shall see below, this fact is attributed to the significant depletion of the non-linear energy cascade flux for these cases, and with the fact that almost all the energy input through the forcing is dissipated by the elastic energy dissipation term and thus no role is played by the subgrid-scale polymer stretching term. This is consistent with the elasto-inertial turbulence mechanism recently studied in detail in the work of Valente et al., 23 whereby the forward and backward energy transfers between large and small scales of motion cancel out at high De.

Figure 17 compares iso-surfaces of the second invariant of the velocity gradient tensor obtained for the LES with De = 0.91, and with the filtered DNS, using the same threshold. The flow structures are seen 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.

C. Kinetic energy spectra and spectral budgets

In order to assess the detailed spectral behavior of the present LES model Figures 18(a)-18(c) and 19(a)-19(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 LES simulations without the polymer subgrid-scale closure. Notice however that in all cases the subgrid-scale stresses in the momentum equations are closed with the classical Smagorinsky model with a constant equal to Cs = 0.16.

For the lower Deborah numbers De = 0.38 and 0.62 (Figs. 18(a) and 18(b)) the energy spectra obtained from LES closely follows the filtered DNS spectra, until a certain high wavenumber kLES c is reached. The simulations with the incomplete LES model (model without subgrid-scale polymer stretching closure) also display the same feature, however at a much lower wavenumber k(LES) c, after which the two simulations (full LES and incomplete LES for each De number) start to deviate
from the filtered DNS data, even if no particular accumulation of kinetic energy at high wavenumbers is observed. The comparison between the LES results with and without polymer stretching closure for intermediate De numbers already indicates that the present full LES model does achieve an improvement over the incomplete 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 18(c) corresponding to the case with De = 1.23. Here both the LES with and without polymer subgrid-scale closure show very similar energy spectra, which also follow closely the filtered DNS spectra until a given (approximately similar) wavenumber $k_c^{(-)} \approx k_c^{LES}$, above which the spectra carry less energy than in the filtered DNS results. As discussed above, the simulations corresponding to $De \geq 1$ are particular in that almost all the input power is dissipated by the polymer molecules and therefore there is here no need to model the subgrid-scale kinetic energy transfer, or the subgrid-scale polymer stretching, because of the power of the polymer “dissipation”/elastic energy term to cope with the power input forcing. On the contrary, the use of a subgrid-scale model in the momentum equation is likely the reason behind the slight excessive kinetic energy dissipation observed for these cases, particularly given that the Smagorinsky model coefficient used here ($C_S = 0.16$) is higher than the value suggested by the a priori tests in the form of Figure 4, where one sees that a constant of the order of $C_S \approx 0.1$ should have been used instead. However, since these cases ($De \geq 1$) are not particularly challenging, and the solvent dissipation reduction (see Table IV) and flow structures are well captured, we do not investigate them further.

![Figure 18](image-url)
The spectral budgets for the same cases $De = 0.38, 0.62,$ and $1.23,$ (Figs. 19(a)-19(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 Eq. (73) is

$$\overline{F}(k) = \overline{\Pi}(k) + \Pi^{[p]}(k) + D(k) + \Pi_{sgs}(k) + \Pi_{sgs}^{[p]}(k),$$

(73)

where the overbar “−” represents data available in the LES grid, and $\Pi_{sgs}(k)$ and $\Pi_{sgs}^{[p]}(k)$ represent the subgrid-scale contribution arising from interactions between resolved and unresolved wavenumbers, for the solvent and the polymer contributions, respectively.\(^5\)

Before analysing these results it is important to emphasise that spectral budgets are rarely analysed in LES studies, since it is very hard for a subgrid-scale model to present a perfect agreement with the filtered DNS results in the whole wavenumber range. Also, such a perfect match is not a necessary condition for a subgrid-scale model to provide excellent results in actual LES. However, the spectral budgets allows one to understand in detail the interplay between the solvent and the polymers in an actual LES model and therefore to gain further insight into the results from the present model.

From the outset it is important to stress that as expected the filtered DNS, full LES and incomplete model LES simulations, for all $De$ numbers, lead exactly to the same results for the forcing term since this term is fully imposed in the simulations, and moreover, it is imposed in the fully resolved wavenumber range, $F^{LES}(k) = F^{DNS}(k) = F^{-}(k)$.

In the simulations with $De = 0.38$ (Fig. 19(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 incomplete model simulation significantly over-predicts this quantity. The resolved solvent dissipation is well captured by both LES models, $D^{LES}(k) = D^{DNS}(k) = D^{-}(k)$ although the full LES displays a nearly perfect agreement, in contrast with the incomplete LES 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 it under-predicts $\Pi^{[p]}^{DNS}(k)$ for the remaining wavenumbers $5 < k < 24$, while the incomplete model simulation displays a very poor performance for the entire wavenumber range.

The slight under-prediction of $\Pi^{[p]}^{DNS}(k)$ for the present model for $5 < k < 24$ does not present a problem, as clearly shown in the DR value obtained for this case (see Table IV), since for this range of $De$ numbers the leading term in the spectral energy budget is the classical exchange
$\Pi_{DNS}(k)$, which is very well captured by the model, while the most energetic modes of $\Pi^{[p]DNS}(k)$ are also captured. Similar spectral budgets are observed in the simulations with similar or smaller Deborah numbers (not shown for conciseness).

At higher Deborah numbers, e.g., $De = 0.62$, the non-linear term $\Pi^{DNS}(k)$ is overshadowed by $\Pi^{[p]DNS}(k)$, which is now the dominating term over a significant wavenumber range (see Fig. 19(b)). Again the leading term is well captured by the full LES model, i.e., $\Pi^{[p]LES}(k) \approx \Pi^{[p]DNS}(k)$. As in Figure 18(a) the solvent dissipation is well captured both by the complete and incomplete LES models, with the former performing slightly better. The main difference between the two LES models compared to the previous $De$ number cases concerns the slightly better agreement of the incomplete model case with $\Pi^{DNS}(k)$ data, however only for $k < 5$. But at this value of $De$ this term is much less important than $\Pi^{[p]DNS}(k)$, which explains the overall better agreement of the complete LES model, as previously demonstrated in the results of $E(k)$ (Fig. 18(a)) and the numerical value of $DR$ (see Table IV).

Finally, we discuss what is arguably the least interesting case, corresponding to the simulation with $De = 1.23$ (Fig. 19(c)). As discussed before in Section III B, for this case the polymer dissipation term $\Pi^{[p]}(k)$ largely dominates the other transfer terms and is mainly governed by the fully resolved large scale motions, thus the role of the subgrid-scale contribution is less critical here than in the other cases, even considering the slightly smaller value of $\Pi^{[p]LES}(k)$ for this case associated with the excessive contribution from the Smagorinsky model term (here $C_s = 0.16$ is higher than the optimal value quantified in the a priori assessment). This is attested also by the relatively good performance of the simulations with the incomplete LES model (model without a closure for the subgrid-scale polymer stretch). It appears that in this high $De$ number simulation, the relatively small contribution of the subgrid-scales for the flow dynamics somehow compensates for the difficulty that might have been foreseen from the comparison of the Lumley scale with the smallest scale available in the LES grid discussed in Section III B and also the possible breakdown of the self-similarity assumption for $De > 1$. Paradoxically the cases with higher $De$ numbers turn out to be the less challenging because at high $De$ virtually all the kinetic energy transferred from the large into the subgrid-scales in the solvent is transferred into the polymer molecules, making the subgrid-scale model contribution negligible. The DSIM closure adapts to this situation by automatically “switching-off” as the model constant goes to $C_y \to 0$.

This concludes the analysis of the results from the LES using the present model. Overall, one sees that in all the cases the curves from the simulations using the new subgrid-scale closures for viscoelastic fluids display excellent agreement with the corresponding (filtered) DNS results, and are superior to the results obtained with an incomplete LES model which does not incorporate a subgrid-scale polymer stretch contribution to the conformation tensor transport equation.

VI. CONCLUSIONS

In this work a new set of subgrid-scale closures are developed for large-eddy simulations (LES) of Newtonian solvents carrying small amounts of long chain polymer molecules described by a coarse-grained Finitely Extensible Nonlinear Elastic continuous model closed with the Peterlin approximation (FENE-P); the distortion similarity model (DSIM).

Three direct numerical simulations using $N = 384^3$ collocation points and with Reynolds numbers ranging $116 \leq Re_k \leq 182$ and Deborah numbers ranging $0.11 \leq De \leq 1.23$ were used to conduct a priori tests by the application of a box filter to separate the scales of motion into resolved and unresolved/subgrid-scale components, using several filter sizes ranging from the dissipative range $\Delta/\Delta x = 2, 4$ to the inertial range regions $\Delta/\Delta x = 8, 16$.

The detailed analysis of the filtered momentum and conformation tensor equations showed that the only term that requires an additional closure, compared to the Newtonian fluid equations, is the subgrid-scale polymer stretching term $\gamma_{ij}$, while all the other terms of the conformation equation arising from the filtering procedure can be neglected, e.g., the subgrid-scale conformation tensor convection $\psi_{ij}$.
It is shown that the Smagorinsky constant $C_S$ associated with the dissipation of kinetic energy within the solvent should be slightly decreased for viscoelastic LES at high Deborah number flows, due to the observed decrease of the non-linear kinetic energy transfer from the resolved into the unresolved scales of motion. Appendix A provides an expression to compute $C_S$ for LES of HIT.

The new LES model essentially rests on the assumptions of scale similarity of the subgrid-scale polymer stretching mechanism and on a global equilibrium of the elastic energy within the polymers in the computational box. A “local” elastic energy equilibrium assumption for use in future inhomogeneous flows is also assessed and confirmed for the complete data bank simulations.

Finally, the new LES model is tested \textit{a posteriori} through LES of viscoelastic turbulence covering the same physical parameters of the reference DNS, but using a grid with (only) $N = 48^3$ collocation points. The LES 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.

Future work will focus on the application of the distortion similarity model into LES of free shear flows such as jets and wakes.

**ACKNOWLEDGMENTS**

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**APPENDIX A: THE SMAGORINSKY CONSTANT FOR VISCOELASTIC FLUIDS**

An approximate expression for the Smagorinsky constant $C_S$ for viscoelastic flows can be derived by using an appropriate form of the kinetic energy spectrum $E(k)$ for the inertial and elasto-inertial range, where the spectrum displays a power law range with $E(k) \sim k^p$, where $-3 \leq p \leq -5/3$, as shown in Valente et al. As suggested by an anonymous Referee, assuming that in addition to the solvent dissipation $\epsilon_s$ and wavenumber $k$, the kinetic energy spectrum also depends on the relaxation time of the polymer $\tau_p$, i.e.,

$$ E(k) = f(\epsilon_s[k], k, \tau_p), \quad (A1) $$

the only dimensionally correct possibility is

$$ E(k) = C_k'(\epsilon_s[k])^{\frac{p+3}{2}} \tau_p^{-\frac{3p+5}{2}} k^p, \quad (A2) $$

where $C_k'$ is the “viscoelastic” Kolmogorov constant, which in Newtonian turbulence reverts to the well known value of $C_k' = C_k$, which typically is $1.4 \leq C_k \leq 1.6$. Starting with the subgrid-scale dissipation $\epsilon_{sgs}$, representing, in the physical space, the local non-linear kinetic energy flux transferred from the resolved into the unresolved scales, at scale $k_c = \pi/\Delta$,

$$ \epsilon_{sgs} = -\tau_{ij} \bar{S}_{ij} = 2 \sqrt{2} (C_S \Delta)^2 \left( \bar{S}_{ij} \bar{S}_{ij} \right)^{3/2} \quad (A3) $$

where the resolved rate-of-strain product is,

$$ \bar{S}_{ij} \bar{S}_{ij} = \int_0^{\pi/\Delta} k^2 E(k) dk, \quad (A4) $$

and by using Eq. (A2) one gets the desired expression for $C_S$,

$$ C_S = \frac{1}{\sqrt{2}} \left( \frac{p+3}{\tau_p^3 \epsilon_s[k]} \right)^{3/4} \left( \frac{\Delta^2}{C_k'} \right)^{m}, \quad (A5) $$
where \( m = (3p + 5)/8 \), and it is assumed that the subgrid-scale dissipation is equal to the total solvent dissipation \( \varepsilon_{sgs} = \varepsilon_{s} \). Particular cases are obtained for \( p = -5/3 \) \((m = 0)\) when Eq. (A5) reverts into Eq. (59), and \( p = -3 \) \((m = 4/3)\), when Eq. (A5) yields \( C_S = 0 \). Equation (A5) can be used, as a dynamic model, to compute \( C_S \) during LES of FENE-P fluid flows, provided the slope \( p \) is computed during the simulation, which presents no major difficulty in simulations of HIT (notice that in general \( \varepsilon_{s} \) also needs to be computed, and that the viscoelastic and Newtonian Kolmogorov constants are assumed to be equal \( C'_{k} = C_k \)). Thus, when the non-linear energy cascade is strongly depleted by the presence of important levels of polymer dissipation the slope \( p \) will tend to deviate from \( p = -5/3 \), and this will result in a decrease of \( C_S \), and thus to an attenuation of the subgrid-scale dissipation caused by the Smagorinsky model.

However, Equation (A5) cannot in general be used in inhomogeneous LES of the FENE-P fluid, since \( E(k) \) is not in general directly available, although it could be computed, e.g., through relations to unidimensional spectra \( E_1(k_1) \). Furthermore we note that Fig. 1 actually suggests that, unsurprisingly, the viscoelastic Kolmogorov constant \( C'_{k} \) is not equal to the Newtonian Kolmogorov constant \( C_k \), but changes with \( De \) (and possibly with other flow variables). This variation is however small and is ignored in the derivation of Eq. (A5). A detailed study on the variation of \( C'_{k} \) in viscoelastic flows certainly deserves a future study.

Moreover, as shown in the work of Horiuti and Tamaki\(^{39}\) for Newtonian non-equilibrium turbulence the slope of the energy spectrum deviates significantly from the classical \(-5/3\) slope and needs to be corrected. A similar procedure to that of Horiuti and Tamaki\(^{39}\) may be also needed here to simulate non-equilibrium viscoelastic turbulent flows; however, this is outside the scope of the present work and should be assessed in a separate study.

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<th>( De )</th>
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Since in all the LES carried out in this work the Smagorinsky model constant was set to $C_S = 0.16$, instead of being prescribed to the value dictated by the \textit{a priori} tests as shown in Figure 4, we have carried out an additional LES to assess whether the particular value of $C_S$ adopted significantly affects the results.

Figure 20 shows the kinetic energy spectrum $E(k)$ obtained from the LES corresponding to $De = 1.23$, where the Smagorinsky constant was set to $C_S = 0.10$ as indicated in Figure 4 for this case, which is the case where $C_S$ is farther from the prescribed value of $C_S = 0.16$. As in the other LES runs a grid with $N = 48^3$ collocation points was used. The spectrum is compared with the spectrum previously obtained using $C_S = 0.16$ and with the filtered DNS spectra (Figure 18(c)).

As expected the kinetic energy spectrum for $C_S = 0.10$ is slightly above the one for $C_S = 0.16$, due to a smaller amount of kinetic energy dissipation prompted by the solvent \textit{i.e.}, associated with the subgrid-scale stress; however, the observed difference is very small, which indicates that corrections to $C_S$, as could be easily implemented by dynamically using Eq. (A5) in LES using the present model, are not needed for the present simulations. The need for such a dynamically computed $C_S$ for other more challenging LES of viscoelastic fluids cannot be fully discarded however.

### APPENDIX B: CORRELATION COEFFICIENT BETWEEN THE SUBGRID-SCALE STRETCH AND ITS SURROGATE

For completeness the correlation coefficient between $\gamma_{ii}$ and $G_{ii}$ for all the reference DNSs used in the present work and for filter sizes $\Delta/\Delta x = 2, 4, 8$, and 16 is shown in Table V. As described in the main text of the paper the correlation is very high for small $De$ and small filter sizes, but tends to decrease as $De$ increases. This suggests that the self-similar assumption is less suited for high $De$ than for the other cases. However as shown in the main text of the paper (Section V), this turns out not to be a problem for the DSIM closure. Interestingly the local equilibrium assumption does not seem to suffer from this apparent high $De$ number limitation, as attested by the high correlations between the polymer stretching and dissipation terms, $C_P$ and $C_d$ (see Table VI). This information may prove to be useful for future developments of the DSIM (or other) polymer stretching subgrid-scale closure.

### Table VI. Correlation coefficients between the polymer stretching and dissipation terms, $C_P$ and $C_d$, respectively, for all the reference DNSs used in the present work and for filter sizes $\Delta/\Delta x = 2, 4, 8, \text{and } 16$. 

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