Large-Eddy Simulations of turbulent flows with polymer additives

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"Thus, the task is not so much to see what no one yet has seen, but to think what nobody yet has thought about that which everybody sees." - Arthur Schopenhauer
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"Are your Thesis already finished?"

Now, I can finally answer: "Don’t worry, it’s done!"
Resumo

Um novo modelo de sub-malha é desenvolvido para simulação das grandes escalas de escoamentos viscoelásticos, representados pelo modelo constitutivo reológico FENE-P. O modelo para a equação de transporte do tensor de conformação filtrada é baseado na *auto-semelhança* dos termos de extensão polimérica, e no *equilíbrio local* do traço do tensor de conformação, que é proporcional à energia elástica armazenada nas moléculas de polímero, enquanto as tensões de sub-malha são modeladas usando o modelo clássico de Smagorinsky. O novo modelo de sub-malha é testado em simulações numéricas directas de turbulência isotrópica forçada usando testes *a priori*, e *a posteriori* mostrando uma excelente concordância com os resultados provenientes das simulações numéricas directas filtradas. Este novo modelo é fácil de implementar, com baixo custo computacional e representa um enorme progresso nas simulações numéricas de escoamentos turbulentos de um solvente newtoniano com aditivos poliméricos.

**Palavras-chave:** Turbulência Homogénea Isotrópica, Simulações Numéricas Directas, Simulações de Grandes Escalas, Turbulência Viscoelástica, FENE-P
Abstract

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

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

Acknowledgments ................................................................. v
Resumo ........................................................................ vii
Abstract ........................................................................ ix
List of Tables ...................................................................... xv
List of Figures ..................................................................... xvii
Nomenclature ..................................................................... xxi

1 Introduction ........................................................................ 1
  1.1 Motivation ................................................................. 1
  1.2 Turbulence ................................................................. 2
    1.2.1 Homogeneous Isotropic Turbulence ......................... 5
  1.3 Numerical Simulations of Turbulent Flows ....................... 6
    1.3.1 Direct Numerical Simulations (DNS) ......................... 6
    1.3.2 Large-Eddy Simulations (LES) ................................. 8
  1.4 Turbulence in Dilute Polymer Solutions ......................... 8
    1.4.1 First Experiments and Observations ....................... 8
    1.4.2 Onset of Drag Reduction ...................................... 9
    1.4.3 Maximum Drag Reduction ................................... 10
    1.4.4 Turbulence Structure .......................................... 11
    1.4.5 Computational Modelling .................................... 13
  1.5 Objectives ................................................................. 16
  1.6 Main Contributions ................................................... 16
  1.7 Thesis Outline .......................................................... 16

2 Governing Equations and Subgrid-Scale Modelling .......... 19
  2.1 Velocity Field .......................................................... 19
  2.2 The FENE-P Constitutive Model .................................. 19
  2.3 Filtering Operator ...................................................... 21
  2.4 Filtered Governing Equations ...................................... 23
  2.5 Eddy Viscosity Models .............................................. 24
    2.5.1 The Boussinesq Hypothesis ................................. 24
Appendix: A priori tests

A.1 Tables for the local equilibrium of the polymeric elastic energy assumption: H42 . . . . . A.1
List of Tables

4.1 Physical and computational parameters of the reference (Newtonian) DNS: Taylor based Reynolds number ($Re_\lambda$); turbulent kinetic energy ($K$); solvent dissipation ($\varepsilon_s$); Taylor micro-scale ($\lambda$); integral scale ($\ell$); maximum effective wavenumber ($k_{max}$) normalised by the Kolmogorov micro-scale. SI units have been used for all dimensional quantities.  

4.2 Physical and computational parameters of the reference DNS: non-dimensional viscosity ratio ($\beta$); Polymer relaxation time normalised by the Kolmogorov time-scale ($Wi_0$); Weissenberg number ($Wi$); Deborah number ($De$); Taylor based Reynolds number ($Re_\lambda$); turbulent kinetic energy ($K$); solvent dissipation ($\varepsilon_s$); polymer dissipation ($\varepsilon_p$); Taylor micro-scale ($\lambda$); integral scale ($\ell$); 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 $\nu = 0.003 \text{m}^2\text{s}^{-1}$, and $\beta = 0.8$. The input power forcing has the same characteristics as the Newtonian reference simulation, e.g. $P = 3.3 \text{m}^3\text{s}^{-2}$. SI units have been used for all dimensional quantities.

4.3 Correlation coefficients between the trace of the subgrid-scale polymer stretching terms at filter sizes $\Delta$ and $2\Delta$, $\gamma_{ii}$ and $G_{ii}$, respectively, for all the reference DNS used in the present work and for filter sizes $\Delta/\Delta x = 2, 4, 8,$ and $16$.

4.4 Root-mean-square (Rms) of $\gamma_{ii}$ and $G_{ii}$ using the reference DNS with $De = 0.11, 0.38,$ and $0.91$ with filter sizes $\Delta/\Delta x = 4$ and $16$.

4.5 Correlation coefficients between the polymer stretching and dissipation terms, $C_p$ and $C_d$, respectively, for all the reference DNS used in the present work and for filter sizes $\Delta/\Delta x = 2, 4, 8,$ and $16$.

4.6 Drag reduction ($DR$) obtained with the several LES compared with the corresponding filtered DNS (DNS) and with simulations without any model (−) for the polymer dynamics. The Smagorinsky model is used in the momentum equations in all the LES and the simulations use the same parameters as described in table 4.2 (e.g. $\nu_s = 0.003 \text{m}^2\text{s}^{-1}$ and $\beta = 0.8$) and $N = 48^3$ collocation points.
A.1 Mean and Root-mean-square (Rms) of terms from the *a priori* analysis using the reference DNS with $De = 0.11$, with four filter sizes ($\Delta/\Delta x = 2, 4, 8, 16$). Terms from the trace of the conformation tensor $C_{ii}$ governing equation: temporal variation ($C_t$), convection ($C_a$), polymer stretching ($C_p$), and dissipation ($C_d$). $\gamma_{ii}$ and $G_{ii}$ are the (exact) traces of the subgrid-scale stretching terms at scales $\Delta$ and $2\Delta$, respectively.

A.2 Mean and Root-mean-square (Rms) of terms from the *a priori* analysis using the reference DNS with $De = 0.38$, with four filter sizes ($\Delta/\Delta x = 2, 4, 8, 16$). Terms from the trace of the conformation tensor $C_{ii}$ governing equation: temporal variation ($C_t$), convection ($C_a$), polymer stretching ($C_p$), and dissipation ($C_d$). $\gamma_{ii}$ and $G_{ii}$ are the (exact) traces of the subgrid-scale stretching terms at scales $\Delta$ and $2\Delta$, respectively.

A.3 Mean and Root-mean-square (Rms) of terms from the *a priori* analysis using the reference DNS with $De = 0.91$, with four filter sizes ($\Delta/\Delta x = 2, 4, 8, 16$). Terms from the trace of the conformation tensor $C_{ii}$ governing equation: temporal variation ($C_t$), convection ($C_a$), polymer stretching ($C_p$), and dissipation ($C_d$). $\gamma_{ii}$ and $G_{ii}$ are the (exact) traces of the subgrid-scale stretching terms at scales $\Delta$ and $2\Delta$, respectively.
# List of Figures

1.1 The Trans-Alaska Pipeline System is an example of application of this technology [source: http://www.alaskacenters.gov/the-alyeska-pipeline.cfm] .......................... 2
1.2 Leonardo da Vinci sketch of turbulent flows (1500) ............................................ 2
1.3 Illustration of the energy cascade mechanism [28] ..................................................... 3
1.4 Energy Spectrum at high $Re$ under Kolmogorov hypothesis. Flow scales are expressed as Log of the wavenumber, $k = 1/l$. $l_0$ is the characteristic size of the largest eddies and $\eta$ the Kolmogorov scale. $l_{EI}$ marks the beginning of the inertial sub-range and $l_{DI}$ of the dissipation sub-range [30] ................................................................. 4
1.5 Turbulent flow past a grid. The left picture corresponds to the near field, while on the right we can observe the far field [35] ................................................................. 6
1.6 Intense vorticity iso-surfaces in direct numerical simulation with $4096^3$ grid points and $Re_\lambda = 1131$ of Homogeneous Isotropic Turbulence. The field consists of clouds of a large number of small eddies and void regions [36] ................................................................. 7
1.7 Aspects of the polymeric regime: Effect of the pipe diameter. Pipe I.D. 2.92, 8.42, and 32.1 mm, temperature 35°C, solvent distilled water, polymer solution PEO, $M = (0.66 \pm 0.1) \times 10^6$, $c = 250 \pm 50$ wppm [9] ................................................................. 9
1.8 A schematic illustrating the onset and different trajectories of polymer drag reduction. The dashed line represents the case in which $Re$ is fixed (at the value at which the onset of drag reduction is first observed) and polymer concentration, $C$, is increased. The dotted line represents the case which $C$ is fixed and $Re$ is increased [6] ............................................................. 11
1.9 Numerical simulation of EIT in a channel flow: (a) Contours of pressure fluctuations on the bottom wall and polymer stretch in vertical planes ($Re = 750$) (b) Isosurfaces of regions of slightly rotational (orange) or extensional (cyan) nature ($Re = 750$), as identified by the second invariant of the velocity tensor $Q$ [53] ................................................................. 12
1.10 Elastic dumbbell with configuration given by vector $\mathbf{R}$ [60] ........................................ 14
1.11 One-dimensional schematic of a shock (thick, solid line). Black dots represent the grid points. Thick dashed line is an ideal representation of the shock on the grid. A spectral representation, without an artificial stress diffusivity, would look like the thin dashed line, with overshoots and undershoots (Gibbs phenomenon). The dotted line indicates the effect of adding the stress diffusivity to the spectral representation [63] ................................................................. 15
2.1 (a) Example of a physical space function $\phi(x)$. (b) Grid-scale part $\phi(x)$. (c) Subgrid-scale part $\tilde{\phi}(x)$. [75] .......................... 22

2.2 Box filter. a) Physical space representation. b) Fourier space representation. [39] .......................... 23

2.3 Dynamics of the kinetic energy in the spectral space. The energy is injected at the rate $P$. The kinetic transfer rate through the cut-off, located wavenumber $k_c$, is denoted $\Pi$. The dissipation rate due to viscous effects is denoted $\varepsilon$. The local equilibrium hypothesis is expressed by the equality $P = \Pi = \varepsilon$. [39] .......................... 25

2.4 Spectral subdivisions for double sharp-cutoff filtering. $\Pi$ is the resolved field in the sense of the test filter, $\pi'$ the test field, and $u'$ the unresolved scales in the sense of the initial filter. [39] .......................... 27

2.5 Spectral decomposition based on the extended scale similarity hypothesis. [39] .......................... 27

3.1 Sketch of the computational box. For HIT $L_x = L_y = L_z = 2\pi$ .......................... 31

4.1 Kinetic energy spectral $E(k)$ for the Newtonian DNS. .......................... 42

4.2 Spectral energy budget showing the spectral forcing function $F(k)$, non-linear energy transfer within the solvent $\Pi(k)$, normalised by the dissipation $\varepsilon$ for the Newtonian DNS. .......................... 44

4.3 Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{rms}$) corresponding to a threshold equal to $Q/Q_{rms} = 7$ for the Newtonian DNS. .......................... 44

4.4 Kinetic energy spectral $E(k)$ for all viscoelastic DNS with two filter sizes $\Delta/\Delta x = 4$ and 16. (the vertical dashed line represents the wavenumber corresponding to the Lumley scale). .......................... 47

4.5 Spectral energy budget (Eq. 4.22) for all viscoelastic DNS, showing the spectral forcing function $F(k)$, non-linear energy transfer within the solvent $\Pi(k)$, and kinetic/elastic energy transfers between the solvent and the polymer molecules $\Pi^{[\phi]}(k)$, normalised by the total power input $P$. The filter sizes $\Delta/\Delta x = 4$ and 16 are also shown. (the dashed vertical line represents the wavenumber corresponding to the Lumley scale). .......................... 48

4.6 Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{rms}$) corresponding to a threshold equal to $Q/Q_{rms} = 7$ for all DNS. 49

4.7 Smagorinsky constant ($C_S$) computed with Eq. (4.28) for filter sizes $\Delta/\Delta x = 2, 4, 8$ and 16 and all the reference simulations used in this work. .......................... 50

4.8 Probability density function (PDF) of $\varepsilon_d = \frac{f(C_{kk})C_{ii}}{C_{kk}}$ and $C_D = f(C_{kk}C_{ii})$ normalised by their root-mean-square, for the DNS with $De = 0.11, 0.38$ and 0.91 and filter size $\Delta/\Delta x = 16$. .......................... 51

4.9 Probability density function (PDF) of the subgrid-scale trace of the conformation tensor and polymer stretching terms normalised by their root-mean-square, for the DNS with $De = 0.11, 0.38$ and 0.91 and filter size $\Delta/\Delta x = 4$. .......................... 51

4.10 Probability density function (PDF) of the subgrid-scale trace of the conformation tensor and polymer stretching terms normalised by their root-mean-square, for the DNS with $De = 0.11, 0.38$ and 0.91 and filter size $\Delta/\Delta x = 16$. .......................... 52
4.11 Joint probability density functions between the real (exact) traces of polymer stretching terms $\gamma_{ii}$ and $\mathcal{G}_{ii}$ (normalised by their root-mean-square), at filter size $\Delta/\Delta x = 4$ for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. .................................................. 53

4.12 Joint probability density functions between the real (exact) traces of polymer stretching terms $\gamma_{ii}$ and $\mathcal{G}_{ii}$ (normalised by their root-mean-square), at filter size $\Delta/\Delta x = 16$ for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. .................................................. 53

4.13 Joint probability density functions of traces of subgrid-scale polymer stretching terms $\gamma_{ii}$ and $\mathcal{G}_{ii}$ at filter size $\Delta/\Delta x = 4$ for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. ............................... 53

4.14 Joint probability density functions of traces of subgrid-scale polymer stretching terms $\gamma_{ii}$ and $\mathcal{G}_{ii}$ at filter size $\Delta/\Delta x = 16$ for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. ............................... 54

4.15 Joint probability density functions of $C_{\gamma_{12}}$ and $C_{\gamma_{22}}$, defined in Eqs. (4.31) and (4.32), respectively, for filter size $\Delta/\Delta = 4$, and for the reference DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. .................................................. 55

4.16 Joint probability density functions of $C_{\gamma_{11}}$ and $C_{\gamma_{22}}$, defined in Eqs. (4.31) and (4.33), respectively, for filter size $\Delta/\Delta = 4$, and for the reference DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. .................................................. 55

4.17 Joint probability density functions between polymer stretching $C_p$ and dissipation $C_d$ terms from the trace of the conformation tensor transport equation (2.43), for DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$ and for filter size $\Delta/\Delta x = 4$. .................................................. 56

4.18 Joint probability density functions between polymer stretching $C_p$ and dissipation $C_d$ terms from the trace of the conformation tensor transport equation (2.43), for DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$ and for filter size $\Delta/\Delta x = 16$. .................................................. 57

4.19 Probability density function of the trace of the polymer temporal variation ($C_t$), convective transport and ($C_u$), production due to polymer stretching/distortion by the flow ($C_p$), and dissipation into potential elastic energy ($C_d$) for $\Delta/\Delta x = 4$ and for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. .................................................. 57

4.20 Probability density function of the trace of the polymer temporal variation ($C_t$), convective transport and ($C_u$), production due to polymer stretching/distortion by the flow ($C_p$), and dissipation into potential elastic energy ($C_d$) for $\Delta/\Delta x = 16$ and for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. .................................................. 58

4.21 Joint probability density functions between the trace of the polymer temporal variation ($C_t$) and convective transport and ($C_u$) (normalised by their root-mean-square), at filter size $\Delta/\Delta x = 4$ for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. .................................................. 58

4.22 Joint probability density functions between the trace of the polymer temporal variation ($C_t$) and convective transport and ($C_u$) (normalised by their root-mean-square), at filter size $\Delta/\Delta x = 16$ for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. .................................................. 58
4.23 Mean value of the model constant $C_\gamma$ defined by Eq. (2.47) and computed using Eq. (2.50) i.e. a global or box averaging defined by the brackets in this equation, or averaging the locally obtained $C_\gamma$, 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 $\Delta/\Delta = 2, 4, 8$ and $16$. 59

4.24 Probability density functions of the 'local' constant $C_\gamma$ defined by Eq. (2.47) without the volume (brackets) average for filter sizes $\Delta/\Delta = 2, 4, 8$ and $16$. 60

4.25 Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{rms}$) corresponding to a threshold equal to $Q/Q_{rms} = 4$ for the filtered reference DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$. 63

4.26 Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{rms}$) corresponding to a threshold equal to $Q/Q_{rms} = 4$ for the filtered reference DNS with $De = 0.38$ with $\Delta/\Delta x = 8$ and LES with $N = 48^3$ collocation points. 63

4.27 Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{rms}$) corresponding to a threshold equal to $Q/Q_{rms} = 4$ for the filtered reference DNS with $De = 0.91$ with $\Delta/\Delta x = 8$ and LES with $N = 48^3$ collocation points. 63

4.28 Kinetic energy spectra $E(k)$ for all the viscoelastic LES in a grid with $N = 48^3$ collocation points. The results for filtered DNS (DNS) and without polymer subgrid-scale model ((−)) are also shown. 64

4.29 Spectral energy budget for the viscoelastic LES showing the spectral forcing function $F(k)$, non-linear energy transfer within the solvent $\Pi(k)$, and kinetic/elastic energy transfers between the solvent and the polymer molecules $\Pi^{[p]}(k)$, normalised by the total power input $P$, in a grid with $N = 48^3$ collocation points. The results for filtered DNS (DNS) and without polymer subgrid-scale model ((−)) are also shown. 66

4.30 Kinetic energy spectra (ES) $E(k)$ for the reference viscoelastic DNS corresponding to $De = 0.38, 0.62$ and $0.91$ and the elasto-inertial equation (EIR) $E(k) = C_{EI} r_p^{-2} k^{-3} \log(Wi)$, with $C_{EI} = 1.5$. The dashed vertical line represents the wavenumber corresponding to the Lumley scale. 68
Nomenclature

**Acronyms**

DNS  Direct Numerical Simulations.
DR   Drag Reduction.
FENE-P  Finitely Extensible Non-linear Elastic Peterlin model.
FFT  Fast Fourier Transform.
FHIT Forced Homogeneous Isotropic Turbulence.
GS   Grid Scale.
HIT  Homogeneous Isotropic Turbulence.
KT   Kurganov-Tadmor.
LES  Large Eddy Simulation.
MDR  Maximum Drag Reduction.
PDF  Probability Density Function.
ppm  parts per million.
RANS Reynolds-Average Navier-Stokes.
SGS  Subgrid Scale.
SPD  Symmetric Positive Definite.

**Greek symbols**

$\alpha_k, \beta_k$  Runge-Kutta Coefficients.
$\beta$ Polymer Concentration.
$\Delta t$ Time step.
$\Delta$ Filter width.
$\delta_{ij}$ Kronecker's delta.
η  \quad \text{Kolmogorov length scale.}

γ_{ij}  \quad \text{SGS polymer stretching tensor.}

λ  \quad \text{Taylor microscale.}

λ_i  \quad \text{Eigenvalues of } C_{ij}.

Π  \quad \text{Kinetic Energy Transfer.}

\nu  \quad \text{Kinematic Viscosity.}

ψ_{ij}  \quad \text{SGS polymer convection tensor.}

\rho  \quad \text{Density.}

τ_\eta  \quad \text{Kolmogorov time scale.}

τ_{ij}  \quad \text{Subgrid-stress Tensor.}

τ_p  \quad \text{Zimm relaxation time of the polymer.}

\varepsilon  \quad \text{Energy dissipation rate.}

\textbf{Roman symbols}

\ell  \quad \text{Integral length scale.}

\ell_L  \quad \text{Lumley length scale.}

\textbf{C}  \quad \text{Conformation tensor.}

\textbf{H}  \quad \text{Convective flux.}

L_{ij}  \quad \text{Leonard Tensor.}

\hat{G}_i  \quad \text{Auxiliary function in the spectral space.}

C_{ij}  \quad \text{Components } i, j \text{ of the Conformation tensor.}

C_K  \quad \text{Universal Kolmogorov constant.}

C_S  \quad \text{Smagorinsky constant.}

E(k)  \quad \text{Kinetic energy density function.}

f(C_{kk})  \quad \text{Peterlin function.}

G_{\Delta}(x)  \quad \text{Spatial filter.}

K  \quad \text{Kinetic Energy.}

k  \quad \text{Wavenumber.}

L  \quad \text{Maximum polymer extension.}
Characteristic length scale.

$L_{11}$ Longitudinal integral length scale.

$L_{\text{box}}$ Size of the computation box.

$p$ Pressure.

$Re$ Reynolds Number.

**Subscripts**

$i,j,k$ Computational indexes.

$rms$ Root-mean-square.

$x,y,z$ Cartesian components.

**Superscripts**

$[p]$ Polymer.

$[s]$ Solvent.
Chapter 1

Introduction

1.1 Motivation

In 1948, it was discovered that the addition of long chained polymers at low concentrations (tens of parts per million) into a turbulent Newtonian solvent, can reduce the skin friction drag on a stationary surface by up to 80 percent [1]. After this experiment, this phenomenon caught the attention of researchers who were motivated by fundamental and engineering proposes resulting, by 1995, in 2500 papers related with this subject [2]. Since usually the polymer is non-toxic and cheaply available, this technology has been successfully used to reduce the pumping costs and heat transfer losses for oil pipelines (see figure. 1.1) and district heating/cooling, to increase flow rate in fire fighting hoses and to help irrigation and drainage [3–6].

The first studies were essentially empirical and experimental, trying to explain the onset of Drag Reduction (DR) caused by polymers. Several reviews which address the advancement in this area, were written along the second part of the 20th century [7–10]. Although the capability to numerically simulate turbulent flow of dilute polymers is relatively new [11], over the past 20 years, these tools have gained an important role in the research of this field [12–21].

However, highly detailed numerical simulations of this kind of flows have a very high computational cost which is unaffordable for the flows present in most industrial applications. They are one order of magnitude more expensive than the Newtonian counterparts, because it is necessary to solve at the same time a model to simulate the behavior of the dilute polymers.

In search of a more suitable numerical method, Large-Eddy Simulations (LES) are a compromise between accuracy and computational cost. LES were first used in 1963 to study meteorological phenomena, becoming an important tool for the study of environmental and engineering turbulent flows [22, 23].

With a LES model capable of reproducing the phenomenology of DR by polymers additives, it will be possible to acquire data that will provide advances in this area, leading to improved and expanded practical applications and increasing our understanding of fluid turbulence and its control.
1.2 Turbulence

Almost all fluid flows present in engineering applications are turbulent. Wakes around and after bluff bodies such as cars, airplanes and buildings are typical examples. Usually it is defined as the state of fluid motion which is characterized by apparently random and chaotic three-dimensional vorticity. When a flow is turbulent there are increased energy dissipation, mixing, heat transfer, and drag, which can be beneficial or prejudicial depending on the application. Therefore, in the last two centuries, scientists have made several efforts to understand the turbulence behaviour, for fundamental or engineering purposes [24].

In the end of the 15th century, Leonardo da Vinci was the first to describe turbulence (see figure 1.2). In one of his sketches, named "turbulenza", to define this kind of flows, which seems to be the origin of the word "turbulence" used nowadays.

\[
Re = \frac{UL}{\nu}
\]  
(1.1)

where \( \nu \) is the kinematic viscosity. \( U \) and \( L \) are respectively the flow characteristic velocity and length
scales. The Reynolds number expresses the balance between the viscous and inviscid forces within the flow and its value is very important to identify the transition between laminar and turbulent regimes, because small perturbations can be damped by viscosity or amplified by inviscid forces.

Another important contribution was the Reynolds decomposition [26], where the turbulent motion can be described by a mean \( \langle u \rangle \), and a fluctuating part \( u^* \):

\[
u = \langle u \rangle + u^*
\]

(1.2)

The first idea about how the energy transfer through scales was handled in turbulent flows was exposed by Richardson [27] as summarized in this poem:

"Big whirls have little whirls
That feed on their velocity,
And little whirls have lesser whirls
And so on to viscosity
(in the molecular sense)."

which introduces the concept of an “energy cascade”, suggesting the establishment of a hierarchy among the vorticity structures of turbulent flows according to their respective dimensions. The energy is transferred from the largest eddies, through processes of vortex stretching and breakup, on to smaller and smaller eddies. The energy transfer process is then mostly inviscid until the eddies reach the size where viscous effects become dominant and the energy is dissipated into heat. This idea is represented in figure 1.3

![Figure 1.3: Illustration of the energy cascade mechanism [28]](image)

Years later, this conceptual picture was made into a quantitative theory by Kolmogorov [29] who postulated three hypotheses to describe the energy transfer process (see figure 1.4):

**Hypothesis of local isotropy**: At sufficiently large Reynolds number, the small-scale turbulent motions are statistically isotropic.
**First similarity hypothesis:** In every turbulent flow at sufficiently high Reynolds number, the statistics of the small-scale motions have an universal form that is uniquely determined by viscosity and dissipation rate.

**Second similarity hypothesis:** In every turbulent flow at sufficiently high Reynolds numbers, the statistics of the motions of the scale $l$ in the range of $l_0 >> l >> \eta$ have a universal form that is uniquely determined by dissipation rate and independent of the viscosity.

Using the first similarity hypothesis, and performing a dimensional analysis, one obtains the unique length, time and velocity scales for the Kolmogorov's scale.

$$
\eta \sim \left( \frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}} \quad \tau_\eta \sim \left( \frac{\nu}{\varepsilon} \right)^{\frac{1}{2}} \quad u_\eta \sim (\nu \varepsilon)^{\frac{1}{4}}
$$

(1.3)

Figure 1.4: Energy Spectrum at high $Re$ under Kolmogorov hypothesis. Flow scales are expressed as Log of the wavenumber, $k = 1/l$. $l_0$ is the characteristic size of the largest eddies and $\eta$ the Kolmogorov scale. $l_{EI}$ marks the beginning of the inertial sub-range and $l_{DI}$ of the dissipation sub-range [30].

Using Kolmogorov’s assumption that at the inertial sub-range viscous effects are negligible, becoming only function of dissipation and the eddies length scale, $l$, the energy spectrum at the inertial scales can be expressed by,

$$
E(k) = C_K \varepsilon^\frac{5}{2} k^{-\frac{5}{2}}
$$

(1.4)

for $k_{EI} < k < k_{DI}$ where $C_K \approx 1.4 – 1.7$ is the Kolmogorov constant [31].

The Taylor microscale is found in multiple turbulence physical phenomena. This scale is located within the inertial range of turbulence, incorporating contributions both small and large scales of motion:
\[ \lambda^2 = 2 \times \frac{\langle u_{rms}^2 \rangle}{\langle \left( \frac{du}{dx} \right)^2 \rangle} \]  

(1.5)

Reynolds Number based in Taylor microscale is defined as,

\[ Re_\lambda = \frac{u_{rms} \lambda}{\nu} \]  

(1.6)

As Kinetic Energy \( K \) is dissipated at small viscous eddies, assuming the equilibrium hypothesis and in statistically steady turbulence, the Dissipation Rate \( \varepsilon \) is imposed by the large scales of the flow and, in stationary turbulence is equal to the Energy Transfer across the scales \( \Pi \):

\[ \varepsilon = \Pi \sim K^{3/2} \]  

(1.7)

In experimental investigations, \( \ell \) is typically taken to be the longitudinal integral length scale, \( L_{11} \) and is typically measured with single hot-wire anemometers. In DNS \( \ell \) is an averaged integral-length scale derived from the spherical shell averaged three-dimensional energy spectra \( E(k) \) \cite{32}:

\[ \ell = \frac{\pi}{2} \frac{\int_0^\infty k^{-1} E(k) dk}{\int_0^\infty E(k) dk} = \frac{\pi}{2K} \int_0^\infty k^{-1} E(k) dk \]  

(1.8)

In homogeneous isotropic turbulence, the following relations can be derived:

\[ \ell = \frac{2}{3} L_{11} \quad u_{rms} = \left( \frac{2}{3} K \right)^{1/2} \]  

(1.9)

### 1.2.1 Homogeneous Isotropic Turbulence

The Homogeneous Isotropic Turbulence (HIT) could be considered the simplest case of a "turbulent flow". A turbulent flow can be considered Homogeneous if the statistical properties do not change with spatial translation. The flow is Homogeneous and Isotropic if also these statistics are independent of rotations and reflections. From such definition follows that in HIT the mean velocity field has to be equal to zero.

The study of HIT is a central tool against which most turbulence theories are put to test. Numerically, these flows can be simulated by using a cubic computational domain with periodic boundary conditions along all spatial directions. The fact that the boundaries are periodic makes possible the use of pseudo-spectral methods, which give place to extremely compact, fast and efficient numerical schemes, while providing extreme accuracy \cite{33}.

Although three-dimensional isotropy is an idealization that was never actually found in nature, the use of such a turbulent field to study turbulence at high \( Re \) is in accordance with Kolmogorov’s theory \cite{31}, that the small-scale statistics of turbulence at sufficiently high \( Re \) far away from flow boundaries are locally isotropic, in the sense that its statistics are insensitive to the details of the large-scale flow conditions. Although it is not strictly isotropic at large scales, HIT is suitable for exploring universality in the sense of Kolmogorov’s theory.
Unlike in experimental setups, where the HIT is continuously fed by the initial instabilities generated by a grid until it decays at very large distances (see figure 1.5), in numerical simulations the turbulence has to be maintained artificially by the action of a Forcing Scheme. This scheme balances the loss of turbulent kinetic energy by the viscous dissipative action at the smallest scales of the flow, that in an actual flow is naturally achieved by the action of large eddies as they feed from the mean field inhomogeneities. The forcing term should be applied to the small wavenumbers in the energy spectrum, by providing a continuous source of energy, which is then transferred down to the small scales through vortex breakup and stretching [34].

![Turbulent flow past a grid.](image1.png)

Figure 1.5: Turbulent flow past a grid. The left picture corresponds to the near field, while on the right we can observe the far field [35].

### 1.3 Numerical Simulations of Turbulent Flows

#### 1.3.1 Direct Numerical Simulations (DNS)

Direct Numerical Simulations (DNS) consist in computing the Navier-Stokes equations without any turbulence model. In the 1970s, after it was demonstrated its feasibility [33], DNS has grown to become one of the most useful tools in turbulence fundamental research and in the evaluation of modelling techniques used in other types of numerical simulations, because of its accuracy and because it gives a full description of the flow features (see figure 1.6 for an example).

One of the main requirements of DNS, is that the computational mesh has to account for all turbulent flow scales, specifically, it is needed a sufficiently fine grid, of the order of the Kolmogorov length scale $\eta$. If we use a coarser grid, the energy dissipation is not fully resolved, and there is an accumulation of energy at the small scales, leading to numerical divergence. The computational cost increases rapidly with the Reynolds number, so only moderate $Re$ numbers can be simulated, and not the high $Re$ found in flows of the natural world or of engineering interest. High-accuracy discretization schemes, as pseudo-spectral schemes, can be employed, reducing the computational effort for a DNS and thus allowing for a higher Reynolds number calculation, but such discretization methods are restricted to simple flow geometries.

For the case of **Homogeneous Isotropic Turbulence**, using a pseudo-spectral method [37], some estimations can be made about the specific requirements needed. For the simulations, first, the grid size has to be chosen. With uniform spacing, the maximum wavenumber is obtained from:
Figure 1.6: Intense vorticity iso-surfaces in direct numerical simulation with $4096^3$ grid points and $Re_\lambda = 1131$ of Homogeneous Isotropic Turbulence. The field consists of clouds of a large number of small eddies and void regions [36].

$$k_{max} = \frac{\pi}{\Delta x} = \frac{\pi N}{L_{box}}$$ \hspace{1cm} (1.10)

of where, $N$ is the number grid nodes in each direction and $L_{box}$ is the size of the box. Usually the size is $L_{box} = 2\pi$. The grid spacing is computed as:

$$\Delta x = \frac{L_{box}}{N} = \frac{\pi}{k_{max}}$$ \hspace{1cm} (1.11)

Furthermore, to reduce the effect of a finite box size, some authors consider that should be used [38],

$$\frac{L_{box}}{L_{11}} \geq 8$$ \hspace{1cm} (1.12)

Since the dissipation spectrum is extremely small beyond $k\eta = 1.5$ a good resolution of the small scales is:

$$k_{max}\eta \geq 1.5$$ \hspace{1cm} (1.13)

Finally, it is possible to assume that the number of points within the computational domain must be of the order of,

$$N^3 \sim \left( \frac{L_{box}}{\eta} \right)^3 \sim Re_{L}^{9/4}$$ \hspace{1cm} (1.14)

From Eq. 1.14, it can be concluded that DNS simulations are restricted to flows at low to moderate Reynolds numbers, not being able to cope with the requirements of high Reynolds number of industrial flows.
1.3.2 Large-Eddy Simulations (LES)

Large-Eddy Simulations (LES) is a technique where only the energy-containing motions are resolved and the effects of the unresolved modes are modelled. The main motivation for this approach is the fact that a vast majority of the wavenumber modes are in the dissipative range and usually for engineering applications only the large scales are of primary interest. In DNS, over 99% of the computational cost is devoted to the dissipative scales, and using the assumption that the smaller scales have an universal character, they can be represented by simple models, while the large-scale motions, which are affected by the flow geometry and are not universal, are computed explicitly, which extend the range of applicability to flows of higher Reynolds numbers. As a consequence, one can in principle expect to obtain more reliable results from LES than from Reynolds Average Navier-Stokes (RANS) procedures, for which the whole range of turbulent scales has to be modelled. Some of the disadvantages of LES are its demanding computational effort when compared to RANS methodologies and the simulation of flows where small scales are extremely relevant, which is the case of flows in the surroundings of solid walls. Although, this kind of simulation was pioneered to compute meteorological flows in the 1960s [22, 23], the first LES was obtained in the early 1970s for plane channel flows [39].

Large-Eddy Simulations will be the focus of this Thesis, therefore further details of this method will be discussed in the following chapters.

1.4 Turbulence in Dilute Polymer Solutions

1.4.1 First Experiments and Observations

Since its discovery 70 years ago, several experiments were done and some theories were proposed to try to explain the mechanisms behind drag reduction by dilute polymers. To avoid confusion, initially this phenomenon was defined as the reduction of skin friction in turbulent flows below that of the solvent alone [7]. It was proved that the drag reduction occurs in thermodynamic dilute solutions of long flexible, expanded high-molecular-weight linear polymers, as stated in the first experiments done in pipe flow with water, toluene and benzene solutions. The Polyethylene Oxide (PEO) in water became the most common solution because it is inexpensive, easy to handle, and effective since a 33% reduction in skin friction over that water alone is possible by the addition of 18 parts per million (ppm) of PEO of molecular weight of $0.76 \times 10^6$ [7, 40] (see figure 1.7). Nevertheless some experiments show that a polymer having a flexible helical structure is an even more effective drag reducing agent than a flexible linear polymer [41].

It was observed that the laminar pipe flow of dilute polymer solutions shows no significant differences in the skin-friction compared with laminar pipe flows of Newtonian fluids, and did not show any kind of Non-Newtonian characteristics like shear thinning. Also it was proved that the transition from laminar to turbulent is not delayed and the DR equally occurs over both rough and smooth surfaces [40]. However, it recently was observed through experimental data and theoretical predictions that, if same polymer solution is used, the drag reduction (DR) in roughened pipes becomes smaller relative to smooth pipe.
flows at the same Reynolds number [42].

The extent of drag reduction in a given pipe is a universal function of concentration, flow rate and molecular weight. The inertial subrange was absent in the energy spectrum taken on the pipe axis in the polymer solution [40]. The number of monomer units are a more important factor than molecular weight and as a chain length increases the relative concentration required for a given effect decreases [7].

Most polymer solutions are shear thinning so the viscosity to be used for turbulent flow cannot be found from laminar flow experiments at low shear rates, although the best drag reducers are used in such low concentrations that this viscosity change can be neglected [10].

### 1.4.2 Onset of Drag Reduction

**Time Criterion**

The first theory that tried to explain the phenomenon of Drag Reduction is based on the viscous effects in the flow: when the relaxation time of the polymers is greater than the time scale of near wall turbulence, frequently named in the literature by the "time criterion", the fluctuating strain causes the coil-stretch transition of polymers in the buffer layer of the log-law increasing the effective extensional viscosity. The extent of the expansion of the polymers depends on the concentration. This phenomenon suppresses turbulent fluctuations and the small scale eddies, but does not affect the viscosity deep in the viscous sublayer where the molecules are not expanded. Due to decreased intensity of the small eddies, the reduced Reynolds Stresses at the buffer layer, delays the reduction of mean profile thereby thickening this layer, reducing the wall friction [9, 41].

When Drag Reduction is exhibited, the turbulence structure tends to follow the extensional viscosity
model towards the wall, but this model does not follow in the central core of the pipe. In particular, on the axis the turbulence intensity is higher than Newtonian [40].

The onset wall shear stress is essentially independent of pipe diameter, polymer concentration and solvent viscosity [9].

**Elastic Theory**

Although years later, experiments were made with polymers injected far from the walls [43, 44], and the "time criterion" was criticized in that the coil-stretch does not occur in turbulent flow with randomly fluctuating strain rates. This strain rates although high, fluctuate both in time and space and can produce only partial stretching of the polymers. Furthermore, drag reduction initiates as polymer enters lower inertial wall layer from above or below suggesting that the source of the underlying polymer-turbulence dynamics lies within the lower inertial range [45, 46]. Also data obtained using monodisperse polymers clearly demonstrate that the onset of DR depends systematically on polymer concentration [47]. It follows that for predictive purposes more detailed explanations are required.

Experiments in homogeneous turbulence at large Reynolds Number, away from the wall explain that, this "time criterion" is a necessary but not a sufficient condition for polymer effects. The elastic theory postulates that the elastic energy stored by the partially stretched polymers is an important variable for DR and the increase in the effective viscosity is small and inconsequential. The onset of DR occurs when the cumulative elastic energy stored by the partially stretched polymers becomes comparable with the kinetic energy in the buffer layer. The small scales will be terminated at some scale larger and this leads to a buffer layer increase and reduced drag. The polymer concentration is included in the onset criterion because the cumulative elastic energy of the polymers is a function of the concentration [45, 48]. This original theory was built upon homogeneous isotropic turbulence but, years later, it was extended the framework to pipe flows and demonstrated it could predict qualitatively much of phenomenology of drag reduction [6, 46].

**Recent Results**

Recently, in experiments with fully developed three dimensional turbulence that do not support convincingly elastic theory. It was proposed a "energy flux theory" that postulates that the turbulence energy flux in the cascade process is gradually reduced by the energy transfer into the elastic motion of polymers, which becomes dominant in the small scales. Some experiments proved that this theory is supported quantitatively [49].

1.4.3 **Maximum Drag Reduction**

An interesting discovery, was that from different experiments involving different polymer concentrations, molecular weights, chemical identities, channel or pipe sizes all collapse, to a good approximation, to a curve of Prandtl-von Kármán form but with different constants than Newtonian flow. It was observed
that for a given Reynolds number, Drag Reduction (DR) for a turbulent pipe flow initially increases with polymer concentration but saturates beyond a certain value and appears bounded between two universal asymptotes: the Prandtl-Karman Law for Newtonian fluids and a Maximum Drag Reduction (MDR) asymptote [40] (see figure 1.8). There are two explanations in the literature for this phenomenon: MDR occurs when the effects of polymers are felt over all scales, causing the buffer layer thickness to extend across the entire boundary layer [9, 46]; the MDR occurs when the Reynolds stresses are strongly diminished and the mechanisms that sustain turbulence are primarily driven by the fluctuating polymer stresses, which has the implication that the polymers produce rather than dissipate turbulent kinetic energy [14, 50].

There are some contradictions to this theories: polymer injection experiments have shown large DR (near MDR) with polymers primarily within the near-wall region of the boundary layer; furthermore, the polymers effect on the turbulence in the outer portion of the boundary layer (at which there are few or no polymers) is relatively weak compared with the effect on the near-wall region [43]. Some studies found polymer stress work to dissipate (and not produce) turbulent Kinetic Energy [51].

1.4.4 Turbulence Structure

It is well known that turbulent polymer solutions have a different turbulent structure that its Newtonian counterparts [46].

Turbulent polymer solutions are viscoelastic flows, which are distinguished from viscous flows by the existence of non-zero normal stress differences in a simple shear flow and an apparent variable viscosity which typically decreases in shear flows and increases, often by several orders of magnitude,
in extensional flows. Hence, the proposed mechanisms of drag reduction are typically based on the enhanced macromolecular resistance to extensional motions or elastic memory/relaxational effects.

This specific nature of polymer solution flow is also observed at low $Re$, where the velocity field randomly fluctuates in space and time due to elastic instability, it is called Elastic Turbulence (ET), which is used to enhance mixing in micro-channels [52].

Recently, a new-state of turbulence was reported, named the Elasto-Inertial Turbulence (EIT) [53]. Both EIT and ET, operate in a cycle where velocity fluctuations induce polymer stress fluctuations, which in turn sustain velocity fluctuations. EIT exists by creating its own extensional flow patterns at sub-critical $Re$, or by exploiting extensional flow topologies at High $Re$, and unlike ET, doesn’t require curved streamlines to occur [53, 54] (see figure 1.9). This behaviour support the phenomenon of "early turbulence", described as the onset of turbulence in the presence of diluted polymer additives at Reynolds numbers significantly smaller than in the absence of polymers, and the existence two-way energy transfers between turbulent kinetic energy of the flow and elastic energy of polymers at small scales, resulting in the overall modification of the turbulence energy cascade [46, 48].

![Numerical simulation of EIT in a channel flow: (a) Contours of pressure fluctuations on the bottom wall and polymer stretch in vertical planes ($Re = 750$) (b) Isosurfaces of regions of slightly rotational (orange) or extensional (cyan) nature ($Re = 750$), as identified by the second invariant of the velocity tensor $Q$ [53].](image)

When considering the polymer effect on wall-bounded turbulent flows, it is important to note that the details of the interaction between the fluid motion and polymer dynamics depend on distance from the wall. In the near-wall region, the streamwise vortices stretch the polymers in the buffer layer, increasing the viscosity, which suppresses the turbulent fluctuations, increasing the buffer-layer thickness, leading to drag reduction [41].

Far from the wall, the interaction between the polymers and fluctuating local velocity gradient give rise to strong modifications of the small scale properties of turbulence, such as strain and enstrophy [55, 56]. Also the statistical nature of the dissipation range and the inertial-range scales are modified [16, 57]. A recent study of grid turbulence in dilute polymer solutions showed that the energy spectrum changes abruptly from the Kolmogorov $k^{-5/3}$ inertial sub-range to a $k^{-3}$ elastic sub-range, in which the rate of strain is maintained constant by the polymers. This new spectral region is separated from the
inertial cascade by the Lumley scale $\ell_L = 1/k_L$ [58]. Ultimately, a $k^{-3}$ elastic sub-range can be related with the EIT, since this two features all give support to the energy transfer between polymers and the flow.

One of the last studies on the effect of viscoelasticity in the turbulent energy spectrum, defined the Deborah Number as the ratio between the polymer relaxation time $\tau_p$, and the eddy turnover time:

$$De = \frac{\tau_p \sqrt{K}}{\ell},$$  

(1.15)

If $De \approx 1$, the polymer extract most of the energy from the large scales and transfer energy back to the solvent at the small scales giving origin to a polymer-induced energy spectrum [21].

### 1.4.5 Computational Modelling

Over the past 20 years, Direct Numerical Simulations (DNS) have played an increasingly important role in the research of turbulent drag reduction by polymer additives, particular for wall-bounded turbulent flows. DNS accuracy is limited by the model for polymer stress, inability to resolve all relevant polymer scales and numerical instability. However, DNS has the advantage over laboratory experiments of describing the average orientation of the polymer micro-structure in addition to the velocity field and Reynolds Stresses, providing additional insight into the mechanisms responsible for low versus high DR and the Maximum Drag Reduction (MDR) limit. With DNS it is possible to isolate the effects of the polymer relaxation time, polymer concentration and maximum polymer length.

Usually, numerical simulations use constitutive equations derived from modelling of the polymer molecules, using two beads connected by an elastic spring. The polymer dynamics are then entirely described by the evolution of the end-to-end vector connecting two beads (see figure 1.10), using constitutive equations as Oldroyd-B and FENE-P [59]. The polymer orientation in most models is then represented as a continuous second-order tensor field, the so-called conformation tensor, which is defined as the normalised second moment of the end-to-end vector of the dumbbell separation $R$, described as:

$$C_{ij} = \frac{\langle R_i R_j \rangle}{\frac{1}{3} \langle R^2 \rangle_{eq}}$$  

(1.16)

The conformation tensor $C_{ij}$ is a variance-covariance matrix, whose elements in the diagonal are the variance of the vector $\langle R_i R_j \rangle$ and the elements in the $i, j$ position are the covariance between the $i^{th}$ and $j^{th}$ elements. Therefore, since the variance of any real random variable is non-negative, the elements in the diagonal are also non-negative. Moreover, since $\langle R_i R_j \rangle = \langle R_j R_i \rangle$ the tensor is also symmetric. The constraint $\langle R_i R_i \rangle > 0$ leads to positive values for all elements in the diagonal, making the tensor symmetric and positive definite (SPD). This implies that the eigenvalues of $C_{ij}$ should always remain greater than zero.

Early attempts at numerical simulation of viscoelastic turbulence were plagued by Hadamard instabilities that resulted from the numerical loss of the SPD property. One way to overcome these instabilities was by introducing a stress diffusion term into the equation for the conformation tensor [61].
In the beginning, variations of this approach were used by most investigators. In 1997, the first DNS of channel flow [11], were able to show a phenomenon of Drag Reduction, although the Reynolds numbers used in simulations were lower than the corresponding to the conditions under which Drag Reduction is experimentally observed with dilute polymers. The DNS also showed that drag reduction is accompanied by a reduction of Reynolds shear stress in the buffer layer. Also the reduction in the streamwise vorticity fluctuations was further attributed to the extensional viscosity of the polymer solution. Also, a correlation between an increase in the spanwise spacing of the streamwise streaks and the degree of drag reduction was discussed. Some years later, other DNS in channel flow were made to evaluate other characteristics that lead to drag reduction like the budgets of the Reynolds stress, turbulent kinetic energy, and streamwise enstrophy [13].

Further investigations, exploited the SPD property of $C_{ij}$ to derive independent equations for the eigenvectors and eigenvalues of the conformation tensor [62]. In this formulation, besides remain greater than zero, the eigenvalues of $C_{ij}$ should comply with the finite extensibility of the polymer:

$$\lambda_1 + \lambda_2 + \lambda_3 \leq L^2$$

(1.17)

where $\lambda_i$ are the eigenvalues of $C_{ij}$ and $L$ is the maximum polymer extension (non-dimensional). However this implicit formulation guarantees that Eq. 1.17 is satisfied, the compact finite-difference method that was used did not guarantee the eigenvalues remain positive. Instead, realizability was enforced by setting the negative eigenvalues to zero before constructing the conformation tensor, ensuring numerical stability. However, the uncontrolled, spatially distributed adjustments of the eigenvalues destroyed overall conservation of the conformation tensor, and spatial averages of the conformation tensor contained spurious contributions from the convective term. Thus the decomposition applied guaranteed stability (by providing easy access to the eigenvalues), but did not guarantee conservation.

The problem can be traced in part to the hyperbolic nature of the equation for $C_{ij}$ in the Oldroyd-B, FENE-P and Giesekus models, which admits shocks (discontinuities) in the polymer stress tensor. Discontinuities in the polymer stress cannot be fully resolved by a grid, and so the main responsibility of the numerical scheme is to correctly predict the jump magnitude. Jumps in the conformation tensor should satisfy the overall conservation balance to guarantee correct elastic wave propagation. Consider, for example, the schematic shown in figure 1.11.
The solid line indicates a jump in the polymer stress tensor across a discontinuity. The other curves illustrate the equivalent numerical representation based on a finite-difference and spectral scheme. The Gibbs phenomenon observed in the spectral representation can be attenuated by introducing an artificial diffusivity. However, artificial diffusion can also reduce the magnitude of the jump. There are more sophisticated approaches to filtering the spectral modes so as to (just) eliminate the ringing, but they are still at a relatively early stage of development [64].

More recent approaches have overcome these shortcomings while still preserving the simplicity of implementation and robustness. Due to these difficulties, was developed an algorithm based on the method of Kurganov and Tadmor (KT) [63, 65]. This second-order scheme guarantees that a positive scalar will remain so at all points and it was generalized to guarantee that a SPD tensor also remains SPD. Besides, the limitation with numerical dissipation suffered by some central difference schemes, that cause severe smearing in the limit $\Delta t \to 0$ is also overcome by the central difference scheme of KT. Furthermore, the method dissipates less elastic energy than methods based on artificial diffusion, resulting in stronger polymer–flow interactions. This approach as been successfully used in DNS of Shear Flow, Decaying and Forced HIT [21, 56, 66], and will be used in this dissertation.

Regarding the DNS of forced HIT with polymer additives, there are two important requirements: the use of double precision in all calculations, to guarantee that the simulation attains a statistically stationary state [21] and the use of resolution condition much more stringent than of the velocity field for adequate computation of the FENE-P model [67]. Nevertheless, some recent works proved that a resolution of $k_{\text{max}} \eta \geq 1.3$ is sufficient to compute correctly this equations [19, 21, 66].

Towards Large-Eddy Simulations of turbulent flows with polymer additives

The first attempt to do LES of viscoelastic flows used an approach based upon a temporal approximate deconvolution method (TADM) [68]. The approximate deconvolution methods (ADM) rely on an attempt to recover, at least partially, the original unfiltered velocity field by inverting the filtering operator. Since, the full deconvolution cannot be computed exactly, only an approximate deconvolution is used. The subgrid tensors are no longer modelled, but reconstructed using an mathematical procedure [39].
Although a good agreement between the LES and the DNS was obtained, in terms of drag reduction prediction, the grid used for these simulations are too fine to draw conclusions of the real accuracy of this method. Also the TADM is very expensive in terms of computational cost, in comparison to turbulent viscosity models like Smagorinsky Model. Recently some studies were made to understand which are the most relevant terms to the development of a subgrid model for this kind of flows. Although, a recent investigation was made to understand how the grid/subgrid-scale interactions are affected by the presence of the polymer additives in turbulent channel flow [69], the most valuable insight, was obtained in an recent work of HIT of dilute polymers, where it was concluded that it might possible to adapt the current Newtonian LES models to viscoelastic fluids, since the same scaling is retained for Newtonian and viscoelastic Flows [21].

1.5 Objectives

The main objective of this work is to extend the existing Direct Numerical Simulations data bank of Homogeneous Isotropic turbulent flows with polymers additives described by the FENE-P model, and develop a subgrid-scale model for Large-Eddy Simulations (LES) of this kind flows. Finally, the new model has to be tested \textit{a priori} using the new DNS data bank, and \textit{a posteriori} comparing the filtered DNS of the data bank with several LES in the same grid.

1.6 Main Contributions

The main contributions of this work is a new data bank of high Reynolds numbers Direct Numerical Simulations and a new subgrid-scale (SGS) model for Large-Eddy Simulations of stationary isotropic turbulence with viscoelastic fluids described by the FENE-P model. During this work several types of SGS models were tested, although only the most successful was described and its results presented. Also, an energy spectrum equation for the elasto-inertial range was deduced, which opens the possibility to create new future types of SGS models for this kind of flows.

1.7 Thesis Outline

The present work is divided in five chapters.

In the first chapter, the subject is introduced and the importance of Large-Eddy Simulations (LES) of viscoelastic turbulent flows for fundamental and industrial applications is discussed. Then, some topics about the advancements on turbulence research, classical theories, the different approaches of numerical modelling, and the literature review about drag-reducing flows of turbulent dilute polymer solutions are presented. Also, the challenges of the computational modelling of this kind flows are addressed. Finally, the objectives and main contributions of this work are highlighted.

In the second chapter, the governing equations, \textit{i.e.}, the continuity, the momentum and the transport conformation tensor equations are described with detail. Also, filtering operations, different subgrid-
scales (SGS) models based on turbulent viscosity and on scale-similarity hypothesis for LES to Newtonian Flows are discussed. Then, the proposed SGS model for the transport conformation tensor equation of the FENE-P model, is derived.

In the third chapter, the numerical algorithm, i.e., the boundary and initial conditions, the spatial discretization, and the temporal advancement for the momentum and transport conformation tensor equations are explained. Subsequently, de-aliasing, forcing, stability control methods are addressed.

In the fourth chapter, the integral quantities, the kinetic energy spectra, the energy budgets, and iso-surfaces of the second-invariant of the velocity gradient tensor obtained for the new data bank of Direct Numerical Simulations (DNS) of homogeneous isotropic turbulent Newtonian and dilute polymer solutions, for different Deborah numbers, are presented. Then, the new SGS model is tested a priori, where several hypothesis in its construction are discussed. Using the data bank of filtered DNS and LES with the same grid points, the new model is tested a posteriori. Finally, an energy spectrum equation for the elasto-inertial range, was deduced.

The conclusions are presented in the fifth chapter, as well as suggestions for future work.
Chapter 2

Governing Equations and Subgrid-Scale Modelling

2.1 Velocity Field

The first assumption is that the fluid is incompressible and satisfies the continuity and momentum equations, respectively, with an additional term related with divergence of polymer stress:

\[ \frac{\partial u_i}{\partial x_i} = 0 \]  (2.1)

\[ \frac{\partial u_i}{\partial t} + u_k \frac{\partial u_i}{\partial x_k} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + 2 \nu_s \frac{\partial S_{ij}}{\partial x_j} + \frac{1}{\rho} \frac{\partial \sigma_{ij}^{[p]}}{\partial x_j}, \]  (2.2)

where \( u_i \) is the \( i \) component of the velocity vector, \( \rho \) is the constant fluid density, \( p \) is the local pressure and \( \nu_s \) is the kinematic viscosity of the fluid. The \( S_{ij} \) is the Strain Rate Tensor defined as:

\[ S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  (2.3)

and the \( \sigma_{ij}^{[p]} \) is the Stress Tensor of the Polymer which is described in the next sub chapter.

2.2 The FENE-P Constitutive Model

Finitely Extensible Non-Linear Elastic Peterlin Model (FENE-P) it is the most used tool in the study of turbulent polymer solutions [6]. FENE-P models the polymer dynamics as an average of polymer chains, where each chain is represented by two dumbbells connected by a non-linear spring with a maximum length [59]. With this simplification the rheological parameters are reduced to the Zimm polymer relaxation time \( \tau_p \) of the polymer molecule, its maximum (squared) extensibility \( L^2 \) (which is normalised by the square of the equilibrium radius \( \langle R^2 \rangle_{eq} \) of the polymer chain), and \( \nu^{[p]} \) the zero shear-rate polymeric viscosity. \( \nu^{[p]} \) is included in the model as a non-dimensional parameter \( \beta \) which is the ratio between the
solvent and the zero-shear-rate viscosity of the solution:

$$\beta = \frac{\nu[s]}{\nu[p] + \nu[s]}$$  \hspace{1cm} (2.4)$$

The $\beta$ used in laboratory experiments can be estimated using "$\beta$ concentration" defined as:

$$c_\beta = 1 - \frac{\beta}{\beta}$$  \hspace{1cm} (2.5)$$

which is given by [67]:

$$c_\beta = \frac{ck_B T \tau_p}{\nu[p] M_p}$$  \hspace{1cm} (2.6)$$

where $c, k_B, T, M_p$ are the polymer mass fraction, Boltzmann’s constant, the temperature of the solution and mass of a single polymer molecule, respectively. As example, in the presented simulations $\beta = 0.8$ which corresponds to a $c \approx 45 \text{ ppm}$ of high polymer weight polyacrylamide (PAAm). The overlap concentration $\beta = 0.5$ corresponds to the critical concentration for the PAAm ($c^* \approx 200 \text{ ppm}$) [70]. Also $\tau_p$ and $L^2$ can be estimated as [49, 57],

$$\tau_p = \frac{R^3 G \nu[s]}{\rho k_B T}$$  \hspace{1cm} (2.7)$$

where $R_G$ is the equilibrium radius of gyration and defined as $R_G = N^{3/5}a$ where $N$ is the number of monomers and $a$ is the length of a monomer and,

$$L^2 \approx \frac{L^2_{\text{max}}}{R^2_G}$$  \hspace{1cm} (2.8)$$

where $L_{\text{max}}$ is the length of a fully extended chain.

In FENE-P, the conformation tensor follows a closed evolution equation:

$$\frac{\partial C_{ij}}{\partial t} + u_k \frac{\partial C_{ij}}{\partial x_k} = \frac{\partial u_i}{\partial x_k} C_{jk} + \frac{\partial u_j}{\partial x_k} C_{ik} - \frac{1}{\rho \nu[p]} \sigma^{[p]}_{ij}$$  \hspace{1cm} (2.9)$$

The conformation tensor transport equation is solved simultaneously with the flow equations, the polymers are deformed by the flow and in their turn influence the flow structures by exerting a polymer stress. The Stress Tensor of the Polymer $\sigma^{[p]}_{ij}$ is:

$$\sigma^{[p]}_{ij} = \frac{\rho \nu[p]}{\tau_p} [f(C_{kk}) C_{ij} - \delta_{ij}]$$  \hspace{1cm} (2.10)$$

where $\delta_{ij}$ is the Kronecker delta and $f(C_{kk})$ it is the Peterlin function described as,

$$f(C_{kk}) = \frac{L^2 - 3}{L^2 - C_{kk}}$$  \hspace{1cm} (2.11)$$

where $C_{kk} = C_{xx} + C_{yy} + C_{zz}$ is the trace of the conformation tensor, and it is proportional to the elastic energy stored by a stretched polymer [71] and it is also defined as the square of the mean separation between the beads. This function gives rise to a non-linear spring force that diverges as $\sqrt{C_{kk}} \to L$. 

$20$
Within the framework of the FENE-P model, we can interpret the effects of polymer stretch on the flow as either an elastic effect or a viscous effect. If the problem is approached from the perspective of the elastic theory of drag reduction, the transport equation for the elastic energy can be studied to understand the energy transfer between the polymers and the flow \[14\]. Alternatively, approaching the problem from the perspective of the viscous theory, it was found that an important component of the confirmation tensor is \( C_{yy} \), which appears in the momentum and kinetic energy equations as an additional viscosity \[72\].

There are some circumstances where the FENE-P model does not represent the correct physics \[73\], and although there are other models that describes the polymer molecules more precisely, the FENE-P offers a good trade-off between rheological fidelity and computational demand for turbulence research \[67\]. The main limitations are related with the closure approximation (higher-order moments are not accounted for) and the fact that a polymer molecule consisting of typically \( N \approx 10^5 \) monomers has been reduced to a single dumbbell. In addition, the model does not incorporate polymer-polymer interactions, important even for dilute polymer solutions in which polymers have been found to organize into supermolecular structures \[74\].

In the following work, use will be made of the trace of the conformation tensor transport equation which is written as,

\[
\frac{\partial C_{ii}}{\partial t} + u_k \frac{\partial C_{ii}}{\partial x_k} = 2C_{ik} \frac{\partial u_i}{\partial x_k} - \frac{1}{\tau_p} \left[ f(C_{kk})C_{ii} - \delta_{ii} \right].
\]

(2.12)

Since the trace of the conformation tensor \( C_{kk} \) is proportional to the elastic energy within the polymer molecules the terms of left-hand side of this equation are proportional to the temporal and advection 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 caused by the fluid, and the last term is proportional to the elastic energy stored within the polymer molecules.

### 2.3 Filtering Operator

In LES each flow variable \( \phi(x,t) \), using an isotropic filter, is decomposed into a resolved (or large-scale) \( \phi_0(x,t) \), and a unresolved (or subgrid-scale) \( \phi'(x,t) \), scales of motion (see figure 2.1),

\[
\phi(x,t) = \phi_0(x,t) + \phi'(x,t),
\]

(2.13)

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

\[
\phi_0(x,t) = \int_{\Omega} \phi(\xi,t)G_\Delta(x-\xi)d\xi,
\]

(2.14)

where \( G_\Delta(x,t) \) is the filter kernel of width \( \Delta \), and \( \Omega \) is the computational domain.

Any isotropic filter has to verify the following properties,

- \( \int_{\Omega} G_\Delta(x)d\mathbf{x} = 1 \)
• $\pi = a$, for any given constant $a$

• $\phi(x, t) + \varphi(x, t) = \bar{\phi}(x, t) + \overline{\varphi}(x, t)$

• $\frac{\partial \phi(x, t)}{\partial x_k} = \frac{\partial \overline{\phi}(x, t)}{\partial x_k}$

although,

• $\overline{\phi}(x, t) \neq \overline{\varphi}(x, t)$

• $\overline{\phi}(x, t)' \neq 0$

Figure 2.1: (a) Example of a physical space function $\phi(x)$. (b) Grid-scale part $\overline{\phi}(x)$. (c) Subgrid-scale part $\phi(x)'$. [75]

The most common filters are the Box or Top-hat, Gaussian and spectral Cut-off filter. The representation of the kernels in the physical $G(x)$ and spectral $\hat{G}(k)$ space for the Box filter are shown below:

$$G(x - \xi) = \begin{cases} \frac{1}{\Delta} & \text{if } |x - \xi| \leq \frac{\Delta}{2} \\ 0 & \text{otherwise} \end{cases} \quad \hat{G}(k) = \frac{\sin(k\Delta/2)}{k\Delta/2}$$

(2.15)

where $\Delta$ is the filter width. Looking for both representations of the filter (see figure 2.2), it can be seen that the Box filter is local in the physical space, but non-local in the Fourier space. The Box filter is equivalent to classical second order finite difference and finite volume discretization procedures.
Figure 2.2: Box filter. a) Physical space representation. b) Fourier space representation. [39]

Also the kernels for the cut-off filter are shown below:

\[ G(x - \xi) = \frac{\sin(k_c(x - \xi))}{k_c(x - \xi)} \]
\[ \hat{G}(k) = \begin{cases} 
1 & \text{if } |k| < k_c \\
0 & \text{otherwise}
\end{cases} \quad (2.16) \]

where \( k_c \) is the cut-off wavenumber.

### 2.4 Filtered Governing Equations

In LES, all the existing scales of motion are decomposed into resolved, filtered or grid-scale (GS) part and a unresolved, unfiltered or subgrid-scale (SGS) part by the application of a spatial filtering operations defined by Eq. 2.13 to the Navier-Stokes (NS) equations. Since the filtering and differentiating commute, the application of a spatial filter to these equations yields,

\[
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + 2\nu \mu \frac{\partial \overline{S}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j},
\]

(2.17)

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

(2.18)

where \( \overline{S}_{ij} \) is given by,

\[ \overline{S}_{ij} = \frac{1}{2} \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) \]

(2.19)

The influence of the subgrid-scale on the grid-scale variables, appears through the subgrid-scale stresses tensor \( \tau_{ij} \):

\[ \tau_{ij} = \overline{u}_i \overline{u}_j - \overline{\overline{u}_i \overline{u}_j} \]

(2.20)

which must be modelled.
2.5 Eddy Viscosity Models

2.5.1 The Boussinesq Hypothesis

The eddy viscosity concept dates back to 1877 when French mathematician and physicist Joseph Boussinesq related the effect of turbulence to an additional source of stress similar to the viscous stress caused by molecular viscosity. The Boussinesq hypothesis states that turbulent motion creates additional "turbulent stresses", which can be described in the same way as the "normal" stresses by the molecular viscosity. The turbulent motion involves the definition of a turbulent viscosity, which has to be computed by the turbulence model. In the frame of SGS modelling these ideals are applied to the SGS tensor. This hypothesis, consists in postulating,

\[ \tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = -2 \nu_t \mathcal{S}_{ij} \] (2.21)

where \( \nu_t \) is the turbulent viscosity. Within this approach, the turbulent viscosity \( \nu_t \) has to be provided by the SGS model, in order to close the system of equations. Inserting Eq. 2.21 into Eq 2.17 leads to,

\[ \frac{\partial m_i}{\partial t} + \frac{\partial m_i m_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + 2 \frac{\partial}{\partial x_j} \left[ (\nu[I] + \nu_t) \mathcal{S}_{ij} \right], \] (2.22)

and the filtered pressure field now includes the normal SGS stresses:

\[ \bar{p}_* = \frac{\bar{p}}{\rho} - \frac{1}{3} \delta_{ij} \tau_{kk} \] (2.23)

2.5.2 Local Equilibrium assumption

The local equilibrium assumption between the large and small scales of motion in turbulent flows is one of the most frequently used in turbulence theory and modeling. In the context of LES, local equilibrium is often used to obtain mathematical relations and model constants. This assumption supposes that, at the small scales level and for statistically homogeneous turbulence, all the energy arriving from the large scales is instantaneously dissipated by molecular viscosity. The flow is in constant spectral equilibrium, so there is no accumulation of energy at any frequency and the shape of the energy spectrum remains invariant with time. Mathematically, the local equilibrium assumption translates into [39]:

\[ -\mathcal{T}_{ij} \mathcal{S}_{ij} = \nu[I] \left( \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} - \frac{\partial m_i}{\partial x_j} \frac{\partial m_i}{\partial x_j} \right) \] (2.24)

here \( \mathcal{II} \) represents the kinetic energy transfer from GS to SGS motions and \( \varepsilon \) is the viscous dissipation of the kinetic energy associated with the SGS (see figure 2.3).
Figure 2.3: Dynamics of the kinetic energy in the spectral space. The energy is injected at the rate $P$. The kinetic transfer rate through the cut-off, located wavenumber $k_c$, is denoted $\Pi$. The dissipation rate due to viscous effects is denoted $\varepsilon$. The local equilibrium hypothesis is expressed by the equality $P = \Pi = \varepsilon$.[39]

2.5.3 Smagorinsky Model

The Smagorinsky model [22, 23] is one of the most famous and still the most widely used model. The model is based on the Boussinesq hypothesis and in the local equilibrium assumption. One of most important relations of homogeneous isotropic turbulence (HIT) is the estimate:

$$\varepsilon \sim \frac{u_{rms}^3}{l}$$

in which the viscous dissipation $\varepsilon$ is related to the root-mean-square of the velocity $u$ and length $l$ scales of turbulence. Assuming the SGS viscous dissipation of Eq. 2.24 can be modelled by Eq. 2.25 and using Eq. 2.21, the turbulent viscosity $\nu_t$ in the Smagorinsky model is given by,

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

where the velocity and length scales were approximated by $u_{rms} \sim l|\mathbf{S}|$ and $l \sim \Delta$ respectively. $C_S$ is the Smagorinsky Constant, $\Delta$ is a characteristic length scale of the SGS and usually taken to be the width of the implicit grid filter $\Delta = (\Delta_x \times \Delta_y \times \Delta_z)^{1/3}$ and $|\mathbf{S}|$ is the characteristic Favre-filtered rate of strain $|\mathbf{S}| = (2\mathbf{S}_{ij}\mathbf{S}_{ij})^{1/2}$. Thus, the SGS tensor becomes:

$$\tau_{ij}^{Smag} = -2(C_S\Delta)^2|\mathbf{S}|\mathbf{S}_{ij}$$

For HIT, it is possible to deduce the theoretical Smagorinsky Constant. Assuming that the energy spectrum in the inertial subrange adopts the Kolmogorov form, $C_K \varepsilon^{2/3}k^{-5/3}$, the mean-square of $|\mathbf{S}|$ can be obtained:
Using the hypothesis \( \langle |\mathbf{S}|^{3/2} \rangle \approx \langle |\mathbf{S}| \rangle^{3/2} \), and using a spectral cut-off filter to evaluate \( \langle |\mathbf{S}|^2 \rangle \) we get the equality:

\[
\epsilon = \frac{1}{\pi^2} \left( \frac{3C_k}{2} \right)^{-3/4} \Delta^2 \langle |\mathbf{S}|^2 \rangle^{3/2} \quad (2.29)
\]

Now, using the local equilibrium hypothesis that

\[
\Pi = \epsilon \Leftrightarrow \epsilon \approx \langle \nu_t |\mathbf{S}|^2 \rangle \approx \langle \nu_t \rangle \langle |\mathbf{S}|^2 \rangle \quad (2.30)
\]

By stating at the outset that the subgrid viscosity is of the form (2.26) and using the relations (2.29) and (2.30), the Smagorinsky Constant is obtained:

\[
C_S = \frac{1}{\pi} \left( \frac{3C_K}{2} \right)^{-3/4} \approx 0.16 \quad (2.31)
\]

where \( C_K \approx 1.6 \) is the Kolmogorov constant. This coefficient is thus scale-invariant in the inertial range.

This model has some drawbacks: it is usually too dissipative, observes a poor correlation with the actual stresses and is always a pure dissipative model \( i.e. \) does not allow backscatter \(-\tau_{ij}^{Smag} \S_{ij} \geq 0\). This deficiency was originally observed from DNS data [76, 77]. Quantitatively, the correlation coefficient \( C_p(\tau_{ij}, \tau_{ij}^{Smag}) \) typically ranges from 0 - 0.25 [76, 78]. The correlation is higher \( C_p \sim (0.5 - 0.7) \) when comparing the local SGS dissipation rate \(-\tau_{ij} \S_{ij} \) with \(-\tau_{ij}^{Smag} \S_{ij} \) [76].

A priori, this model can be tested by comparing \( \langle -\tau_{ij} \S_{ij} \rangle = \Pi \) with \( \langle -\tau_{ij}^{Smag} \S_{ij} \rangle \) in the inertial range [23]. Also using the local equilibrium assumption \( P = \Pi = \epsilon \) it is obtained:

\[
\epsilon = 2^{3/2} (C_S \Delta)^2 \langle |\mathbf{S}|^2 \rangle^{3/2} \quad (2.32)
\]

which it is useful to evaluate if the model is reproducing the correct energetics of the resolved scales.

### 2.6 Scale Similarity Hypothesis

The scale similarity hypothesis consists in assuming that the statistical structure of the tensors constructed on the basis of the subgrid scales is similar to that of their equivalents evaluated on the basis of the smallest resolved scales [77]. The spectrum of the solution based on this hypothesis is therefore broken down into three bands: the largest resolved scales, the smallest resolved scales (\( i.e. \) the test field), and the unresolved scales (see figure 2.4).
The scale similarity hypothesis uses the energy cascade idea. That is, the unresolved scales and the smallest resolved scales have a common history due to their interactions with the largest resolved scales. The classical representation of the cascade defines that the effect of the largest resolved scales is exerted on the smallest resolved scales, which in turn influence the subgrid scales, which are therefore indirectly forced by the largest resolved scales, but similarly to the smallest.

Later, the scale similarity hypothesis was generalized [78] to a spectrum split into an arbitrary number of bands, as illustrated in figure 2.5. The scale similarity hypothesis is then re-formulated for two consecutive spectrum bands, with the consistent forcing being associated with the low frequency band closest to those considered. Thus the specific elements of the tensors constructed from the velocity field $u^n$ and their analogous elements constructed from $u^{n+1}$ are assumed to be the same.
2.6.1 Scale Similarity Model

In this model no eddy-viscosity assumption is used. The Bardina model was the first similarity model introduced, and the assumption of scale invariance is used in a strong and almost literal sense. It was developed to exploit the fact that there is strong correlation between the smallest grid-scale and the subgrid-scale stress \[^{[77]}\]. The subgrid tensor is computed by applying the analytical filter a second time and thereby evaluating the fluctuation of the resolved scales. Experience shows that this model is not effective when the filter is a Reynolds operator (e.g., cut-off filter), because the contribution thus computed then cancels out. The model is defined as,

\[
\tau_{ij} \equiv L_{ij} = (\overline{u_i u_j} - \overline{\bar{u}_i \bar{u}_j}) \tag{2.33}
\]

The Bardina model uses a second application of the same filter, and therefore a single cut-off scale. Years later, this model was generalized to the case of two cut-off levels as \[^{[78]}\]:

\[
\tau_{ij} = C_{sim} L_{ij}^m = C_{sim} (\overline{\tilde{u}_i \tilde{u}_j} - \overline{\tilde{\tilde{u}}_i \tilde{\tilde{u}}_j}) \tag{2.34}
\]

where the tensor \( L_{ij}^m \) is now defined by two different levels of filtering. The test filter cut-off length designated by the \( \sim \) is larger than that of the first level. Usually is done at a scale \( 2\Delta \), as it was shown that improves the original formulation. The constant \( C_{sim} \) can be evaluated theoretically to ensure that the average value of the modeled generalized subgrid kinetic energy is equal to its exact counterpart \[^{[79]}\]. This leads to the relation:

\[
C_{sim} = \frac{\langle \overline{u_k u_k} - \overline{\bar{u}_k \bar{u}_k} \rangle}{\langle \overline{\tilde{u}_k \tilde{u}_k} - \overline{\tilde{\tilde{u}}_k \tilde{\tilde{u}}_k} \rangle} \approx 1 \tag{2.35}
\]

It was found very good correlation was found between the actual and the modelled subgrid-scales stress tensor, typically as high as 80%, and these models can describe backscatter, including when the flow is anisotropic. Although, contrary to the subgrid viscosity models, these ones do not induce an alignment of the proper axis system of the subgrid tensor on those of the strain rate tensor and it was verified that these models don’t dissipate sufficient energy leading to numerical problems \[^{[80]}\].

2.7 "FENE-P" Fluids - Subgrid-Scale Modelling

2.7.1 Filtered Governing Equations

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

\[
\frac{\partial \bar{m}_i}{\partial x_i} = 0, \tag{2.36}
\]
\[
\frac{\partial \bar{u}_i}{\partial t} + u_k \frac{\partial \bar{u}_i}{\partial x_k} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_i \partial x_j} - \frac{\partial \tau_{ij}}{\rho \partial x_j} + \frac{1}{\rho} \frac{\partial \sigma^{[p]}}{\partial x_j},
\]

(2.37)

and,

\[
\frac{\partial \bar{C}_{ij}}{\partial t} + u_k \frac{\partial \bar{C}_{ij}}{\partial x_k} = \frac{\partial \bar{u}_i}{\partial x_k} C_{jk} + \frac{\partial \bar{u}_j}{\partial x_k} C_{ik} - \frac{1}{\tau_p} [f(C_{kk})C_{ij} - \delta_{ij}] - \psi_{ij} + \gamma_{ij}.
\]

(2.38)

The last two terms in the left-hand side of Eq. 2.38 are the subgrid-scale polymer stretching, and the term in the right-hand side the subgrid-scale polymer dissipation. Notice that the new term arising in the filtered momentum equation (2.17), and that is not present in the filtered Navier-Stokes equations,

\[
\sigma^{[p]}_{ij} = \rho \nu \tau_p [f(C_{kk})C_{ij} - \delta_{ij}],
\]

(2.39)

is also the last term in equation (2.38). It is convenient to write equation (2.38) in a form allowing to isolate all the new terms arising from the filtering operation,

\[
\frac{\partial \bar{C}_{ij}}{\partial t} + u_k \frac{\partial \bar{C}_{ij}}{\partial x_k} = \frac{\partial \bar{u}_i}{\partial x_k} C_{jk} + \frac{\partial \bar{u}_j}{\partial x_k} C_{ik} - \frac{1}{\tau_p} [f(C_{kk})C_{ij} - \delta_{ij}] - \psi_{ij} + \gamma_{ij}.
\]

(2.40)

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

\[
\psi_{ij} = u_k \frac{\partial \bar{C}_{ij}}{\partial x_k} - \frac{\partial \bar{C}_{ij}}{\partial x_k}
\]

and the subgrid-scale polymer stretching (non-symmetric) tensor,

\[
\gamma_{ij} = \left[ \frac{\partial \bar{u}_i}{\partial x_k} C_{jk} - \frac{\partial \bar{u}_k}{\partial x_k} C_{ij} \right] + \left[ \frac{\partial \bar{u}_j}{\partial x_k} C_{ik} - \frac{\partial \bar{u}_k}{\partial x_k} C_{ij} \right].
\]

(2.42)

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

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

(2.43)

### 2.7.2 A subgrid-scale model for LES of 'FENE-P' fluids

To develop a subgrid-scale model for viscoelastic fluids modelled by the FENE-P model, one needs to close the subgrid-scale stresses in the momentum equations \( \tau_{ij} \) (Eq. 2.17), the subgrid-scale advection \( \psi_{ij} \), and the subgrid-scale polymer stretching \( \gamma_{ij} \) (Eq. 2.40). Additionally, the term \( f(C_{kk})C_{ij} \) that appears in both equations needs to be approximated.

The modelling of the Peterlin term in the \( \bar{C}_{ij} \) transport equation is first shown. The following approximation will be used (H1),

\[
f(C_{kk})C_{ij} \approx f(C_{kk}) \bar{C}_{ij},
\]

(2.44)

This assumption is justified by results previously obtained using a priori tests in wall bounded flows [68, 69].
Secondly, the subgrid-scale advection of the filtered conformation tensor transport equation is neglected \((H2)\),

\[
\psi_{ij} \approx 0,
\]  

(2.45)

which is justified by the small local magnitude of this term compared with the other terms in equation (2.40) as described in \(e.g.\) \([68, 69]\).

Finally, self-similarity of the subgrid-scale polymer stretching term is assumed, by which this term is equal at two nearby filter sizes, apart from a constant of order \(O(1)\). Specifically, the subgrid-scale polymer stretching tensor at filter size \(\tilde{\Delta} = 2\Delta\) is defined by,

\[
G_{ij} = \begin{bmatrix}
\frac{\partial \tilde{u}_i}{\partial x_k} C_{jk} - \frac{\partial \tilde{u}_i}{\partial x_k} \tilde{C}_{jk} + \frac{\partial \tilde{u}_j}{\partial x_k} C_{ik} - \frac{\partial \tilde{u}_j}{\partial x_k} \tilde{C}_{ik}
\end{bmatrix}
\]  

(2.46)

which denotes the test subgrid-scale polymer stretching tensor and that is available at the LES grid of size \(\Delta\). Using a Bardina type \([77, 78]\) closure the subgrid-scale polymer stretching tensor is approximated by \((H3)\),

\[
\gamma_{ij} = C_\gamma G_{ij},
\]  

(2.47)

where \(C_\gamma\) is a constant. To compute this constant the hypothesis of equilibrium of the elastic energy within the polymer molecules is used. Given that this energy is proportional to the trace of the (filtered) conformation tensor \(\overline{C_{ii}}\) (Eq. 2.43) this hypothesis is equivalent to admit that the temporal variation and advection are negligible in this equation, when compared with the other terms. A global \((H41)\) or local \((H42)\) equilibrium assumptions can be written as follows,

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

(2.48)

and

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

(2.49)

respectively, where the brackets \(\langle \rangle\) denote an averaging operation. Using the global elastic equilibrium assumption \((H41)\), together with assumptions \(H1\) and \(H3\), the constant \(C_\gamma\) can be computed as,

\[
C_\gamma = \frac{\left\langle \frac{1}{\tau_p} \left[ f(C_{kk})C_{ii} - \delta_{ii} \right] \right\rangle - \frac{\partial u_i}{\partial x_k} \tilde{C}_{jk} \right\rangle}{\partial u_i \tilde{C}_{jk}},
\]  

(2.50)

which closes the model. This model will be extensively tested in both \textit{a priori} and \textit{a posteriori} (LES) tests of Forced Homogeneous Isotropic Turbulence (FHIT).
Chapter 3

Numerical Methods

3.1 Boundary and Initial Conditions

Before going into the details of the numerical schemes and algorithms used in the numerical simulation code, it is important to take note of the computational domain. In simulated Homogeneous Isotropic Turbulence (HIT), the boundary conditions are periodic, which allows to use very efficient pseudo-spectral methods, which have the advantage that space derivatives can be computed accurately by algebraic operations in wavenumber space. A HIT is initialized using a ‘spectral noise’ generator to create a velocity field with the desired energy spectrum:

\[ E(k) = k^s \exp \left[ -\frac{s}{2} (k/k_0)^2 \right] \]  

(3.1)

where \( s \) is the slope of the noise spectrum at the large-scales region of the spectra and \( k_0 \) is the wavenumber location of the energy maximum. A forcing scheme is employed to maintain turbulence intensity, i.e. to conserve the global kinetic energy within the computational box (figure 3.1).

Figure 3.1: Sketch of the computational box. For HIT \( L_x = L_y = L_z = 2\pi \)
3.2 Spatial discretization

3.2.1 Navier-Stokes Equations: Pseudo-Spectral Scheme

Since using pseudo-spectral schemes ensures the best possible accuracy without numerical dispersion (to the machine precision) the numerical discretisation of the computational box was performed using a pseudo-spectral scheme along all three spatial directions. In these methods, spatial derivatives are computed with the aid of Fourier series and became computationally interesting in the early 70’s, when the Fast Fourier Transform (FFT) algorithm was invented. Furthermore, computing an one-dimensional Fourier transform, with \( N \) points, in the straightforward way would lead to a computational cost scaled with \( N^2 \), while the use of spectral schemes has a computational cost significantly lower proportional to \( N \log_2(N) \) \[81\]. Due to all this, these schemes are in a prominent position for answering DNS needs, despite the limitation to the treatment of only homogeneous directions in a flow \[37\].

Given a certain function \( u(x, t) \) in the physical space, to have the same function in the Fourier (also called spectral) space \( \hat{u}(k) \), it must be applied the direct Fourier Transform (FT):

\[
\hat{u}(k, t) = FT\{u(x, t)\} = \frac{1}{N^3} \sum_x u(x, t) \exp(-ik.x) \tag{3.2}
\]

The reverse is done with the inverse Fourier Transform (\( FT^{-1} \)):

\[
u(x, t) = FT^{-1}\{u(x, t)\} = \sum_k \hat{u}(k, t) \exp(i k.x) \tag{3.3}
\]

where \( x \) and \( k \) are the mesh points in physical space and the discrete wavenumbers with components \( k_j = \pm n_j = 0, 1, 2, \ldots, N/2, j = 1, 2, 3, \) and \( i \) is the imaginary unit.

It was shown that, the Fourier Transforms (FT) allows to represent temporal functions in terms of frequencies and spatial functions in terms of wavenumbers. One of the most important properties is the fact that the derivatives in the physical space become simple multiplications in the Fourier space.

\[
FT\left\{\frac{du(x)}{dx}\right\} = ik\hat{u}(k) \tag{3.4}
\]

This is the main reason for the high accuracy of this method and consequently its common use in spatial discretization. On the other side, multiplications turn out into convolution products, a very complex operation, reason why all products within the numerical code are performed in the physical space.

The equations to be solved, are the following:

\[
\frac{\partial u_i}{\partial x_i} = 0 \tag{3.5}
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu |h| \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{1}{\rho} \frac{\partial \sigma_{ij}}{\partial x_j}, \tag{3.6}
\]

Applying the direct Fourier transform as was exemplified in 3.4:
\[
FT \left\{ \frac{\partial u_i}{\partial x_i} \right\} = ik_i \tilde{u}_i
\]  
(3.7)

Hence, the continuity equation in the spectral space is written as follows:

\[
k_i \tilde{u}_i = 0
\]  
(3.8)

For the momentum equation, the terms in the spectral space are the following:

\[
FT \left\{ \frac{\partial u_i}{\partial t} \right\} = \frac{d \tilde{u}_i}{dt}
\]  
(3.9)

\[
FT \left\{ \nu[s] \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right\} = -\nu[s] k^2 \tilde{u}_i
\]  
(3.10)

With \( \tilde{p}(k, t) \equiv FT \{ p(x, t)/\rho \} \) being the Fourier coefficient of the dynamic pressure \((p/\rho)\), the pressure-gradient term is,

\[
FT \left\{ -\frac{1}{\rho} \frac{\partial p}{\partial x_i} \right\} = -ik_i \tilde{p}
\]  
(3.11)

The non-linear convection-term is written as:

\[
FT \left\{ \frac{\partial}{\partial x_j} (u_i u_j) \right\} = \tilde{N}_i
\]  
(3.12)

Rewriting the momentum equation, now in the Fourier space, we have:

\[
d\frac{d \tilde{u}_i}{dt} + \nu[s] k^2 \tilde{u}_i = -ik_i \tilde{p} - \tilde{N}_i
\]  
(3.13)

If we multiply the equation above by \( ik_i \), which is the same as saying to apply the divergence in the physical space, we get:

\[
k^2 \tilde{p} = ik_i \tilde{N}_i
\]  
(3.14)

From the equation the pressure can be obtained:

\[
\tilde{p} = \frac{ik_i \tilde{N}_i}{k^2}
\]  
(3.15)

Thus, adding the polymer stress contribution, the final expression for the momentum equation in the spectral space is:

\[
\frac{d \tilde{u}_i}{dt} + \nu[s] k^2 \tilde{u}_i = -\left( \delta_{ij} - \frac{k_i k_j}{k^2} \right) \tilde{N}_j + \frac{1}{\rho} \frac{\partial \sigma^{[p]}_{ij}}{\partial x_j}
\]  
(3.16)

It is important to notice that there is no pressure term in the equation above.
De-aliasing

\( \hat{G}_i \) includes a non-linear operation from the convection term of the momentum equation, that in
the physical space is transformed, into a convolution integral in the Fourier space. Since this kind of
operation is computationally costly, it is more efficient to use an inverse FFT and perform the operation
in the physical space. However, when the non-linear term is transformed back to spectral space, aliasing
errors appear. There are several ways of eliminating aliasing errors. As usual for temporal numerical
simulations, the simulation was fully dealiased using \( 2/3 \) rule in order to avoid the non-physical energy
build-up at high wavenumbers [37].

\[ k_c = \frac{2}{3} k_{\text{max}} \] (3.17)

3.2.2 Conformation Tensor Transport Equation

The spectral and high-order compact schemes are not suitable to solve the conformation tensor
transport equation, since they lose spectral convergence in the vicinity of the discontinuities [63]. Therefore,
in spatial domain, a second-order central difference scheme is adopted for the discretization, except
for the advection term.

\[ \frac{\partial C_{ij}}{\partial t} + u_k \frac{\partial C_{ij}}{\partial x_k} = \frac{\partial u_i}{\partial x_k} C_{jk} + \frac{\partial u_j}{\partial x_k} C_{ik} - \frac{1}{\rho} \frac{\sigma^p_{ij}}{\nu} \] (3.18)

Advection Term: Kurganov-Tadmor (KT) method

For the advection term, an approach based on the Kurganov-Tadmor (KT) scheme is used. This
method guarantees that a positive scalar will remain so at all points and it was generalized to do same
thing to a tensor [65]. Spatial derivatives are second-order accurate everywhere, except where it leads
to a loss of the Symmetric and Positive Definite (SPD) property. Where that occurs, the method automatically
reverts to first-order for that grid point, ensuring the SPD property is maintained. The equations
for the six independent components of \( C \) are coupled to the velocity field and must be solved simultaneously.
This scheme is used for the discretization of the advection term as follows [63]:

\[ u \cdot \nabla C = \frac{H^x_{i+1/2,j,k} - H^x_{i-1/2,j,k}}{\Delta x} + \frac{H^y_{i,j+1/2,k} - H^y_{i,j-1/2,k}}{\Delta y} + \frac{H^z_{i,j,k+1/2} - H^z_{i,j,k-1/2}}{\Delta z}, \] (3.19)

where the advection flux \( H \) in each direction is given by:

\[
\begin{aligned}
H^x_{i+1/2,j,k} &= \frac{1}{2} u_{i+1/2,j,k} (C^+_{i+1/2,j,k} + C^-_{i+1/2,j,k}) - \frac{1}{2} |u_{i+1/2,j,k}| (C^+_{i+1/2,j,k} - C^-_{i+1/2,j,k}), \\
H^y_{i,j+1/2,k} &= \frac{1}{2} v_{i,j+1/2,k} (C^+_{i,j+1/2,k} + C^-_{i,j+1/2,k}) - \frac{1}{2} |v_{i,j+1/2,k}| (C^+_{i,j+1/2,k} - C^-_{i,j+1/2,k}), \\
H^z_{i,j,k+1/2} &= \frac{1}{2} w_{i,j,k+1/2} (C^+_{i,j,k+1/2} + C^-_{i,j,k+1/2}) - \frac{1}{2} |w_{i,j,k+1/2}| (C^+_{i,j,k+1/2} - C^-_{i,j,k+1/2}).
\end{aligned}
\] (3.20)
The superscripts ‘+’ and ‘−’ on the right hand side in Eq. (3.20) refers to values of the conformation tensor at the interface obtained in the limit approaching the point of interest from the right (+) or left (−). Note that nothing is forcing the two values at a boundary to be identical, allowing the possibility of jumps in the solution. The conformation tensor \( C \) at the interface is constructed from the following second-order linear approximations:

\[
\begin{align*}
C_{i+1/2,j,k}^\pm &= C_{i+1/2 \pm 1/2,j,k} \mp \left( \frac{\Delta x}{2} \right) \frac{\partial C}{\partial x}_{i+1/2 \pm 1/2,j,k} ; \\
C_{i,j+1/2}^\pm &= C_{i,j+1/2 \pm 1/2,k} \mp \left( \frac{\Delta y}{2} \right) \frac{\partial C}{\partial y}_{i,j+1/2 \pm 1/2,k} ; \\
C_{i,j,k+1/2}^\pm &= C_{i,j,k+1/2 \pm 1/2} \mp \left( \frac{\Delta z}{2} \right) \frac{\partial C}{\partial z}_{i,j,k+1/2 \pm 1/2} .
\end{align*}
\]

(3.21)

This central difference approximation to the advection term allows to capture the potentially sharp variations in the conformation field and, by writing the advection flux with a difference formula the conservation of the mean conformation tensor is automatically satisfied [63]. To complete the expression, approximations for the spatial derivatives of the conformation tensor are required. These quantities must be defined in a way that maintains \( C^{\pm} \) each as SPD. Therefore, potential candidates to approximate the gradients are:

\[
\left( \frac{\partial C}{\partial x} \right)_{i,j,k} = \begin{cases} 
\frac{C_{i+1,j,k} - C_{i-1,j,k}}{\Delta x} \\
\frac{C_{i,j+1,k} - C_{i,j-1,k}}{\Delta y} \\
\frac{C_{i+1,j,k} - C_{i-1,j,k}}{\Delta z}
\end{cases}
\]

(3.22)

To select the correct derivative approximation, one must check if it can yield SPD results for \( C_{i-1/2}^+ \) and \( C_{i+1/2}^- \). When two or more candidates satisfy the criterion, it is selected the one which maximizes the minimum eigenvalue for these two tensors. When none of them meet this criterion, the derivative is set to zero, reducing to first-order (locally) accurate. This slope limiting procedure will ensure that all \( C^{\pm} \) are SPD.

In order to calculate the advection flux, Eq. (3.20), area-averaged velocities at the edge of the volume surrounding each grid point are required. However, by using a pseudo spectral code in the velocity update, a difficulty is the area-averaged velocities at cell edges that are not known. One could try to average the nearest grid points, but this approach would not satisfy:

\[
\frac{u_{i+1/2,j,k} - u_{i-1/2,j,k}}{\Delta x} + \frac{v_{i,j+1/2,k} - v_{i,j-1/2,k}}{\Delta y} + \frac{w_{i,j,k+1/2} - w_{i,j,k-1/2}}{\Delta z} = 0,
\]

(3.23)

which follows from the continuity equation (Eq. (3.5)). As the spectral decomposition of the velocity is known, it is possible to obtain exact expressions for the cell edge velocities:

\[
\begin{align*}
\bar{u}_{i+1/2,j,k} &= FT^{-1} \left\{ \hat{u} e^{\pm i k_y \Delta y/2} \sin(k_x \Delta x/2) \sin(k_z \Delta z/2) \right\}, \\
\bar{v}_{i,j+1/2,k} &= FT^{-1} \left\{ \hat{v} e^{\pm i k_x \Delta x/2} \sin(k_y \Delta y/2) \sin(k_z \Delta z/2) \right\}, \\
\bar{w}_{i,j,k+1/2} &= FT^{-1} \left\{ \hat{w} e^{\pm i k_z \Delta z/2} \sin(k_x \Delta x/2) \sin(k_y \Delta y/2) \right\},
\end{align*}
\]

(3.24)
where $FT^{-1}$ is the inverse fast Fourier transform, $\hat{u}(k_x, k_y, k_z)$, $\hat{v}(k_x, k_y, k_z)$ and $\hat{w}(k_x, k_y, k_z)$ are the Fourier coefficients at each grid point. Substitution of the above into shows the discrete continuity relationship is satisfied, if the continuity equation in Fourier space is also satisfied [63]:

$$k_x \hat{u}(k_x, k_y, k_z) + k_y \hat{v}(k_x, k_y, k_z) + k_z \hat{w}(k_x, k_y, k_z) = 0$$ (3.25)

**Stretching Term: Finite difference method**

The code was developed for use with a finite difference approach in which the differential equations are approximated at each point. For the stretching term was used a central difference scheme in the first derivatives, second-order accurate everywhere in space, which results in:

$$\frac{\partial u_i}{\partial x_k} C_{jk} + \frac{\partial u_j}{\partial x_k} C_{ik} = \frac{(u_i)_{m+1} - (u_i)_{m-1}}{2\Delta x_k} C_{jk} + \frac{(u_j)_{m+1} - (u_j)_{m-1}}{2\Delta x_k} C_{ik}$$ (3.26)

### 3.3 Temporal advancement scheme

This code uses a fully explicit time advancement scheme, 3$^\text{rd}$ order Runge-Kutta for the momentum equation and for the conformation tensor transport equation. The equations to be solved can be written as follows:

$$\frac{\partial \mathbf{u}}{\partial t} = N(\mathbf{u}) + L^{[s]}(\mathbf{u}) + L^{[p]}(\mathbf{C})$$ (3.27)

$$\nabla \cdot \mathbf{u} = 0,$$ (3.28)

in which, $N(\mathbf{u})$, $L^{[s]}(\mathbf{u})$ and $L^{[p]}(\mathbf{C})$ are the convective term, the viscous term due to the solvent and the viscous term due to the polymer, respectively,

$$N(\mathbf{u}) = \mathbf{u} \times \Omega - \frac{1}{\rho} \nabla p$$ (3.29)

$$L^{[s]}(\mathbf{u}) = \nu^{[s]} \nabla^2 \mathbf{u}$$ (3.30)

$$L^{[p]}(\mathbf{C}) = \nu^{[p]} \nabla \cdot \left( \frac{(C_{kk}) \mathbf{C} - I}{\tau_p} \right)$$ (3.31)

A 3$^\text{rd}$ order Runge-Kutta time stepping scheme computes each new velocity and conformation tensor at the new sub-step $\mathbf{u}^k \equiv \mathbf{u}^n$, $\mathbf{C}^k \equiv \mathbf{C}^n$ from the last two sub-steps $\mathbf{u}^{k-1}$, $\mathbf{C}^{k-1}$ and $\mathbf{u}^{k-2} \equiv \mathbf{u}^{n-1}$, $\mathbf{C}^{k-2} \equiv \mathbf{C}^{n-1}$. Hence, equation 3.27 can be rewritten:
\[
\frac{\mathbf{u}^k - \mathbf{u}^{k-1}}{\Delta t} = \alpha_k \left[ N \left( \mathbf{u}^{k-1} \right) + L^{[s]} \left( \mathbf{u}^{k-1} \right) + L^{[p]} \left( \mathbf{C}^{k-1} \right) \right] + \\
\beta_k \left[ N \left( \mathbf{u}^{k-2} \right) + L^{[s]} \left( \mathbf{u}^{k-2} \right) + L^{[p]} \left( \mathbf{C}^{k-2} \right) \right],
\]

(3.32)

and the coefficients \( \alpha_k \) and \( \beta_k \) are [82]:

\[
\begin{align*}
\alpha_1 &= \frac{8}{15} & \beta_1 &= 0 \\
\alpha_2 &= \frac{5}{12} & \beta_2 &= -\frac{17}{60} \\
\alpha_3 &= \frac{3}{4} & \beta_3 &= -\frac{5}{12}
\end{align*}
\]

(3.33)

### 3.3.1 Conformation Tensor Transport Equation

To know each new velocity at each new sub-step, it is necessary to know the conformation tensor at the previous sub-step(s). Equation 3.18 can be written in the following form:

\[
\frac{\partial \mathbf{C}}{\partial t} = N' \left( \mathbf{u}, \mathbf{C} \right) + M \left( \mathbf{u}, \mathbf{C} \right) + L^{[p]'} \left( \mathbf{C} \right),
\]

(3.34)

where \( N' \left( \mathbf{u}, \mathbf{C} \right) \), \( M \left( \mathbf{u}, \mathbf{C} \right) \) and \( L^{[p]'} \left( \mathbf{C} \right) \) are, respectively, the advection, the stretching and viscous terms:

\[
N' \left( \mathbf{u}, \mathbf{C} \right) = -\mathbf{u} \cdot \nabla \mathbf{C}
\]

(3.35)

\[
M \left( \mathbf{u}, \mathbf{C} \right) = \mathbf{C} \cdot \nabla \mathbf{u} + \nabla \mathbf{u}^T \cdot \mathbf{C}
\]

(3.36)

\[
L^{[p]'} \left( \mathbf{C} \right) = -\frac{f(C_{kk}) \mathbf{C} - \mathbf{I}}{\tau_p}
\]

(3.37)

The same process that was applied before to the Navier-Stokes Momentum equation in equation 3.32, is done here. Thus, the following is obtained:

\[
\frac{\mathbf{C}^k - \mathbf{C}^{k-2}}{\Delta t} = \alpha_k \left[ N' \left( \mathbf{u}^{k-1}, \mathbf{C}^{k-1} \right) + M \left( \mathbf{u}^{k-1}, \mathbf{C}^{k-1} \right) + L^{[p]'} \left( \mathbf{C}^{k-1} \right) \right] + \\
\beta_k \left[ N' \left( \mathbf{u}^{k-2}, \mathbf{C}^{k-2} \right) + M \left( \mathbf{u}^{k-2}, \mathbf{C}^{k-2} \right) + L^{[p]'} \left( \mathbf{C}^{k-2} \right) \right],
\]

(3.38)

where \( \alpha_k \) and \( \beta_k \) are the coefficients of equation 3.33.

It is important to notice that the Runge-Kutta step of equation 3.38 is not the same as that of the equation 3.32. In equation 3.38, \( \mathbf{C}^{k-2} \equiv \mathbf{C}^{n-2} \) and \( \mathbf{C}^k \equiv \mathbf{C}^{n-1} \), whereas in equation 3.32, \( \mathbf{C}^{k-2} \equiv \mathbf{C}^{n-1} \).
3.4 Forcing

Statistically stationary homogeneous turbulence can be obtained in DNS by artificially forcing the low-wavenumber modes, so as to supply energy to them. The energy-containing motions are, therefore, modelled and are not governed by the Navier–Stokes equations. However, since the small-scale motions are universal, useful information about them can be extracted. Without providing an artificial source of energy, the turbulence intensity and thereby the Reynolds number would rapidly decay and consequently the turbulence field would fail to reach a statistically stationary regime. As previously mentioned, the forcing is implemented by prescribing an energy spectrum that continuously provides energy preferentially at the larger scales, at each time step. The amount energy of required to balance the dissipative effects is controlled by the input power parameter, $P$, defined as the rate of change of kinetic energy $P = \frac{\partial K_{\text{force}}}{\partial t}$. At a stationary stage the input power has to balance the energy loss rate, i.e. the energy dissipation, $\varepsilon$, so that the global kinetic energy is conserved. Since the numerical solver uses a pseudo-spectral method the forcing scheme can be easily implemented in the spectral space, being directly implemented in the momentum equation [34]. Let the forcing term in spectral space be $\hat{f}$, the Navier-Stokes equation in the Fourier space can be re-written as:

$$\frac{d\hat{u}_i}{dt} + \nu \left( \hat{k}_i k^2 \hat{u}_i \right) = - \left( \delta_{ij} - \frac{k_j k_i}{k^2} \right) \hat{N}_j + \frac{\partial \hat{n}[\hat{n}_i^*]}{\partial x_j} + \hat{f}, \quad (3.39)$$

where the forcing $\hat{f}$ is defined as:

$$\hat{f}(k, t) = A_{\text{rand}}(k, t)e_1(k) + B_{\text{rand}}(k, t)e_2(k) \quad (3.40)$$

with $A_{\text{rand}}$ and $B_{\text{rand}}$ random complex numbers and $e_1$, $e_2$ are unit vectors. The random force is built to be divergent free, i.e. $u(x, t).f(x, t) = 0$, so that the force is projected in the same plane as the velocity field, which implies that $e_1$ and $e_2$ are orthogonal to each other and to the wavenumber vector. The numbers $A_{\text{rand}}$ and $B_{\text{rand}}$ are given by:

$$A_{\text{rand}} = \left( \frac{f(k)}{2\pi |k|^2} \right)^{1/2} e^{ia_1} g_A(c) \quad (3.41)$$

$$B_{\text{rand}} = \left( \frac{f(k)}{2\pi |k|^2} \right)^{1/2} e^{ia_2} g_B(c) \quad (3.42)$$

where $f(k)$ is the a priori prescribed forcing spectrum, $g_A$ and $g_B$ are two real-valued functions whose sum is the unity, $g_A + g_B = 1$, $a_1$ and $a_2 \in [0, 2\pi]$ and $c \in [0, \pi]$ are random numbers generated at each wavenumber. In order to produce an isotropic forcing the functions $g_A$ and $g_B$ are defined as:

$$g_A = \sin 2c \quad (3.43)$$

$$g_B = \cos 2c \quad (3.44)$$
The shape of the forcing spectrum is imposed as:

\[ f(\|k\|) = A \exp \left[ -\frac{(\|k\| - k_0)^2}{c_f} \right] \] (3.45)

which peaks at \( k_0 \), and is restricted to a range of small wavenumbers limited between, \( \|k\| \in [k_a, k_b] \).

The degree of concentration determined by \( c_f \), and the constant \( A \) is defined to satisfy the required input power \( P \)

\[ P = \Delta t \int_{k_a}^{k_b} f(\|k\|) dk \] (3.46)

hence:

\[ A = \frac{P}{\Delta t} \left( \int_{k_a}^{k_b} \exp \left[ -\frac{(\|k\| - k_0)^2}{c_f} \right] dk \right)^{-1} \] (3.47)

Since the turbulence is maintained by a forcing that is independent of the velocity field, assuming that the random numbers generator is uncorrelated with the velocity field and is not periodic in time, the same procedure can be used to generate the initial vorticity field.

### 3.5 Stability

The time step used in the numerical computation of momentum and conformation tensor transport equations is bounded by stability restrictions. In problems where convection is the dominant term (such as those analysed here), the key parameter governing the numerical method stability is the Courant number [81], expressed by:

\[ C = \frac{|u| \Delta t}{\Delta x} \] (3.48)

In this case, the limiting Courant number is found by making an assessment of Eq. 3.48 for each of the flow directions. For viscoelastic fluids, the limit value of \( C < 1/6 \approx 0.1667 \) was found, comparing to the limit value of Newtonian fluid \( C < 0.6 \) [63].
Chapter 4

Results

4.1 Direct numerical simulations of isotropic turbulence: physical and computational parameters

4.1.1 Newtonian Fluid

Table 4.1 lists the physical and computational parameters of the reference Newtonian DNS. The simulation uses $N = 384^3$ collocation points, kinematic viscosity equal to $\nu = 0.003 \, \text{m}^2\text{s}^{-1}$, and the forcing $\hat{f}(k, t)$ is concentrated in the first 4 wavenumbers, with a gaussian profile centred in wavenumber $k = 3$ with a total power input equal to $P = 3.3 \, \text{m}^2\text{s}^{-3}$. All the integral flow quantities are computed directly from the kinetic energy spectrum defined by,

$$E(k) = 4\pi k^2 \left\langle \frac{1}{2} \hat{u}_i(k, t) \hat{u}^*_i(k, t) \right\rangle_{|k|},$$

(4.1)

where \( \ast \) represents a complex conjugate and \( \left\langle \hat{\phi} \right\rangle_{|k|} \) denotes the spherical-shell average of the quantity \( \hat{\phi} \) i.e.,

$$\left\langle \hat{\phi}(k, t) \right\rangle_{|k|} = \frac{1}{N_k} \sum_k \hat{\phi}(k, t),$$

(4.2)

where the summation is carried over all the $N_k$ modes within a shell, of thickness $\Delta k = 1$, centred at $k = |k|$. The turbulent kinetic energy and viscous (solvent) dissipation rate are computed as,

$$K = \sum_{k_{\text{min}}}^{k_{\text{max}}} E(k)$$

(4.3)

and

$$\varepsilon^{[s]} = 2\nu^{[s]} \sum_{k_{\text{min}}}^{k_{\text{max}}} k^2 E(k),$$

(4.4)

respectively, while the integral, Taylor and Kolmogorov micro-scales are given by,
\[ \ell = \left(\frac{\pi}{2K}\right) \sum_{k_{\text{min}}}^{k_{\text{max}}} \frac{E(k)}{k}, \] (4.5)

\[ \lambda = \sqrt{\frac{10\nu[s]K}{\varepsilon[s]}}, \] (4.6)

and

\[ \eta = \left(\frac{\nu[s]^3}{\varepsilon[s]}\right)^{1/4}, \] (4.7)

respectively. Notice that due to stationarity the power of the input forcing balances the viscous dissipation rate \( P = \varepsilon[s] \). Finally, the Reynolds number based in the Taylor micro-scale is defined by,

\[ Re_\lambda = \sqrt{\frac{2K}{3} \frac{\lambda}{\nu[s]}}. \] (4.8)

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 Table 4.2).

Table 4.1: Physical and computational parameters of the reference (Newtonian) DNS: Taylor based Reynolds number \( Re_\lambda \); turbulent kinetic energy \( K \); solvent dissipation \( \varepsilon[s] \); Taylor micro-scale \( \lambda \); integral scale \( \ell \); maximum effective wavenumber \( k_{\text{max}} \) normalised by the Kolmogorov micro-scale. SI units have been used for all dimensional quantities.

| \( \nu[s] \) \( m^2 s^{-1} \) | \( Re_\lambda \) | \( K \) \( m^2 s^{-2} \) | \( \varepsilon[s] \) \( m^2 s^{-3} \) | \( \ell \) \( m \) | \( \lambda \) \( m \) | \( k_{\text{max}} \eta \) |  \\
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<td>4.00</td>
<td>3.27</td>
<td>0.45</td>
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Fig. 4.1 shows the show the Kinetic energy spectra \( E(k) \) for the (reference) Newtonian DNS. Since the \( Re_\lambda > 100 \), the inertial range with slope of \( k^{-5/3} \) is clearly seen.
The scale-by-scale power budget in wavenumber space which is the wavenumber counterpart of the von Kármán-Howarth-Monin equation in the physical space [32], also know as Lin equation [83] is presented:

$$\frac{\partial E(k, t)}{\partial t} = T(k, t) - 2\nu|s|k^2 E(k, t) + f(k, t), \quad (4.9)$$

where $E(k, t)$ is the kinetic energy spectrum and $2\nu|s|k^2 E(k)$ is the viscous dissipation within the solvent at wavenumber $k$, respectively, while $f(k, t)$ is the spherical-shell averaged input forcing function,

$$f(k, t) = 4\pi k^2 \left\langle \frac{1}{2} \hat{f}(k, t) \hat{f}^*(k, t) \right\rangle_{|k|}, \quad (4.10)$$

$T(k, t)$ represent transfers of kinetic energy across wavenumber $k$ within the solvent with positive/negative values of $T(k, t)$ representing kinetic energy transfers within the solvent from wavenumbers smaller than $k$ into/from wavenumbers larger than $k$. The non-linear kinetic energy transfer within the solvent at wavenumber $k = |k|$ is given by the kinetic energy transfer function $T(k, t)$,

$$T(k, t) = 4\pi k^2 \left\langle \hat{T}(k, t) \right\rangle_{|k|}, \quad (4.11)$$

obtained by spherical shell-averaging the non-linear kinetic energy transfer at wavenumber $k$, which is given by,

$$\hat{T}(k, t) = \Re \left\{ \hat{u}^*_i(k, t) \hat{N}_i(k, t) \right\}, \quad (4.12)$$

where $\Re$ denotes the real part of the term inside brackets. Due to the statistically stationarity of the flow equation (4.9) becomes,

$$f(k) = -T(k) + 2\nu|s|k^2 E(k), \quad (4.13)$$

and after integrating each term in Eq. (4.13) (from 0 to $k$) one gets,

$$F(k) = \Pi(k) + D(k), \quad (4.14)$$

where each term represents the same physical mechanism as in Eq. (4.13), integrated up to wavenumber $k$. Note, the sign swap of the term $\Pi(k) = -\int_0^k T(k)dk$, so that it is a positive quantity. This definitions can be used to compute the total solvent dissipation,

$$\varepsilon^{[s]} = D(k_{max}), \quad (4.15)$$

so that statistically stationarity implies that the total power input from the forcing is equal to the the solvent dissipation,

$$P = \varepsilon^{[s]}, \quad (4.16)$$
Figure 4.2 shows the Spectral energy budget for the (reference) Newtonian DNS.

Figure 4.2: Spectral energy budget showing the spectral forcing function $F(k)$, non-linear energy transfer within the solvent $\Pi(k)$, normalised by the dissipation $\varepsilon$ for the Newtonian DNS.

Iso-surfaces of the second invariant of the velocity gradient tensor $Q = 1/2 (\omega_i \omega_i - 2S_{ij}^2)$, where $\omega_i$ is the vorticity vector, for the Newtonian DNS, are shown in figure 4.3. The iso-surfaces of $Q > 0$, associated with a predominance of enstrophy over strain show a typical ‘worm’ or tube-like structures.

Figure 4.3: Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{rms}$) corresponding to a threshold equal to $Q/Q_{rms} = 7$ for the Newtonian DNS.

4.1.2 Viscoelastic Fluids

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 ($\varepsilon = 0.003 \text{ m}^2\text{s}^{-1}$) and the same input forcing characteristics (e.g. $P = 3.3 \text{ m}^2\text{s}^{-3}$). Table 4.2 lists the physical and computational parameters of these 6 simulations, which differ mainly in the maximum relaxation time of the polymer molecules, taking the values $\tau_p = [0.025, 0.05, 0.1, 0.2, 0.4, 0.6]$, which is accounted for in the Deborah and Weissenberg (non-dimensional) numbers,
De = \frac{\tau_p \sqrt{K}}{t},
\tag{4.17}

and

Wi = \frac{\tau_p}{\tau_\eta},
\tag{4.18}

that represent the ratio between the relaxation time of the polymer molecules with an eddy turnover and Kolmogorov time scales, respectively (\(\tau_\eta = (\nu^{[i]} / \varepsilon^{[i]})^{1/2}\)). Finally, Lumley's length scale \([7]\), \(r_L = \sqrt{\varepsilon^{[i]} \tau_p^3}\), defined as the scale below which the turbulent eddies within the solvent are affected by the polymer, together with its corresponding wavenumber \(k_L = r_L^{-1}\) \([20]\) is also computed.

Table 4.2: Physical and computational parameters of the reference DNS: non-dimensional viscosity ratio (\(\beta\)); Polymer relaxation time normalised by the Kolmogorov time-scale (\(Wi^{[3]}\)); Weissenberg number (\(Wi\)); Deborah number (\(De\)); Taylor based Reynolds number (\(Re_\lambda\)); turbulent kinetic energy (\(K\)); solvent dissipation (\(\varepsilon^{[s]}\)); polymer dissipation (\(\varepsilon^{[p]}\)); Taylor micro-scale (\(\lambda\)); integral scale (\(\ell\)); maximum effective wavenumber normalised by the Kolmogorov micro-scale (\(k_{max}\)); fraction of maximum polymer extension (\(\langle C^{[2]}_{ii} \rangle / L^2\)). All the simulations use \(N = 384^3\) collocation points, kinematic viscosity of the solvent \(\nu^{[s]} = 0.003\) m\(^2\)/s\(^-1\), and \(\beta = 0.8\). The input power forcing has the same characteristics as the Newtonian reference simulation, e.g. \(P = 3.3\) m\(^3\)/s\(^-2\). SI units have been used for all dimensional quantities.

<table>
<thead>
<tr>
<th>(De)</th>
<th>(Wi)</th>
<th>(Re_\lambda)</th>
<th>(K)</th>
<th>(\varepsilon^{[s]})</th>
<th>(\varepsilon^{[p]})</th>
<th>(\ell)</th>
<th>(\lambda)</th>
<th>(k_{max})</th>
<th>(\langle C^{[2]}_{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>2.12</td>
<td>2.00</td>
<td>0.51</td>
<td>0.30</td>
<td>1.5</td>
<td>0.6</td>
</tr>
<tr>
<td>0.62</td>
<td>2.9</td>
<td>182</td>
<td>3.03</td>
<td>0.61</td>
<td>2.73</td>
<td>0.56</td>
<td>0.38</td>
<td>1.9</td>
<td>2.7</td>
</tr>
<tr>
<td>0.91</td>
<td>4.4</td>
<td>159</td>
<td>2.04</td>
<td>0.36</td>
<td>2.94</td>
<td>0.63</td>
<td>0.41</td>
<td>2.1</td>
<td>8.9</td>
</tr>
<tr>
<td>1.23</td>
<td>6.7</td>
<td>126</td>
<td>1.65</td>
<td>0.38</td>
<td>2.93</td>
<td>0.62</td>
<td>0.36</td>
<td>2.1</td>
<td>15.9</td>
</tr>
</tbody>
</table>

Arguably, the most important role of any subgrid-scale model is the accurate modelling of the kinetic energy flux between the grid-scale and the subgrid-scales of motion. This mechanism already was been studied in great detail in the Fourier space \([21]\), by using the scale-by-scale kinetic energy budget in wavenumber space, analysed through a Lin-type equation \([75, 83]\) which has been modified to include the kinetic energy transfer between the solvent and the polymers,

\[
\frac{\partial E(k, t)}{\partial t} = T(k, t) - T^{[p]}(k, t) - 2\nu^{[s]}k^2 E(k, t) + f(k, t),
\tag{4.19}
\]

\(T^{[p]}(k, t)\) represent transfers of kinetic energy across wavenumber \(k\) between the solvent and polymer molecules, with positive/negative values of \(T^{[p]}(k, t)\) representing transfers of kinetic energy into/from the polymer molecules at wavenumber \(k = |k|\), and is given by \([56, 84]\),

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

\[
= 8\pi k^2 \left\langle R \left\{ \hat{S}_{ij}^{[s]}(k, t) \hat{\sigma}_{ij}^{[p]}(k, t) \right\} \right\}_{|k|}
\tag{4.20}
\]
obtained by spherical shell-averaging the non-linear kinetic energy transfer at wavenumber $k$. Due to the statistically stationarity of the flow equation (4.19) becomes,

$$f(k) = -T(k) + T^p(k) + 2\nu k^2 E(k), \quad (4.21)$$

and after integrating each term in Eq. (4.21) (from 0 to $k$) one gets,

$$F(k) = \Pi(k) + \Pi^p(k) + D(k), \quad (4.22)$$

where each term represents the same physical mechanism as in Eq. (4.21), integrated up to wavenumber $k$, and these definitions can be used to compute the total solvent and polymer dissipations,

$$\varepsilon^{[s]} = D(k_{\text{max}}), \quad (4.23)$$

and,

$$\varepsilon^{[p]} = \left\langle \sigma_{ij}^p S_{ij} \right\rangle = \sum_{k_{\text{min}}}^{k_{\text{max}}} T^p(k), \quad (4.24)$$

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

$$P = \varepsilon^{[s]} + \varepsilon^{[p]}. \quad (4.25)$$

To characterise the new simulations and to illustrate the challenges behind subgrid-scale modelling in the context of viscoelastic flows, figures 4.4 (a-f) show the Kinetic energy spectra $E(k)$ for the all the viscoelastic simulations together with Lumley’s length scale $k_L$, and with the filter sizes used in the subsequent analysis with $\Delta / \Delta x = 4$, and 16. In all the six curves one can clearly discern the effect of the forcing in low wavenumber range $k < 4$, followed by an inertial range region, which deviates from the classical $-5/3$ slope for intermediate $De$ numbers [21], followed again by a dissipative range region. While Lumley’s scale is below the maximum wavenumber and the Kolmogorov micro-scale for $De = 0.11$, it is well within the inertial range region for $De = 0.62$, where the subgrid-scale closures are supposed to be active. Recall that an accurate modelling of the kinetic energy transfer between resolved/unresolved scales is crucial in LES. It is therefore likely that in this 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 new additional difficulties for LES of these cases, since modelling of the non-linear cascade has to take into account possible effects from (smaller scale and thus unavailable) polymer effects. Worse still is the situation corresponding to $De = 1.23$, where Lumley’s scale is right at the forcing range implying that the polymer effects will be felt on the entire range of scales of motion i.e. the non-linear energy cascade flux will be affected by the polymer dynamics in its entire region.

Figures 4.5 (a-f) show the spectral energy budgets with the spectral forcing function $F(k)$, the non-
linear energy transfer within the solvent $\Pi(k)$, and kinetic/elastic energy transfers between the solvent and the polymer molecules $\Pi^p[k]$, respectively, for all the viscoelastic DNS. These budgets have been extensively studied in Ref. [21] and will be analysed below in the context of subgrid-scale modelling of viscoelastic turbulence. The six figures detail a different energy cascade picture for different $De$ numbers, as anticipated above which underscores the challenge behind subgrid-scale closures for viscoelastic flows. While in Newtonian turbulence the total energy input from the forcing equals to the non-linear energy transfer and the total viscous dissipation,

$$ P = F(k_{max}) = max\left\{\Pi(k)\right\} = D(k_{max}), \quad (4.26) $$

(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.,

$$ P = F(k_{max}) = D(k_{max}) + \Pi^p[k_{max}], \quad (4.27) $$

so that $P = \varepsilon^s + \varepsilon^p$. Notice that $\Pi^p[k]$ describes all the energy cascade dynamics within the solvent caused by its interaction with the polymer molecules, comprising i) the energy dissipation and (additional)

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**Figure 4.4:** Kinetic energy spectral $E(k)$ for all viscoelastic DNS with two filter sizes $\Delta/\Delta x = 4$ and 16. (the vertical dashed line represents the wavenumber corresponding to the Lumley scale).
ii) energy input caused by the polymer molecules.

In contrast to the case with $De = 0.11$, where most of the dissipation is assured by the solvent ($\epsilon^{[s]} < \epsilon^{[p]}$), in $De = 0.62$ the dissipation is largely caused by the polymer molecules $\epsilon^{[p]} > \epsilon^{[s]}$. Moreover, for $De = 0.62$ the Lumley scale is at wavenumbers smaller than the wavenumbers associated with the dissipation, where $D(k) \approx D(k_{max})$ is approximately constant, thus interfering with these scales of motion. The case with $De = 1.23$ shows a 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 affected by the presence of the polymers.

![Figure 4.5: Spectral energy budget (Eq. 4.22) for all viscoelastic DNS, showing the spectral forcing function $F(k)$, non-linear energy transfer within the solvent $\Pi(k)$, and kinetic/elastic energy transfers between the solvent and the polymer molecules $\Pi^{[p]}(k)$, normalised by the total power input $P$. The filter sizes $\Delta/\Delta x = 4$ and $16$ are also shown. (the dashed vertical line represents the wavenumber corresponding to the Lumley scale).](image)

It is well known that the flow structures from viscoelastic flows are markedly different from Newtonian turbulence [85]. Since it will be interesting also to analyse the role of subgrid-scale models in these structures, figures 4.6 (a-f), show iso-surfaces of the second invariant of the velocity gradient tensor $Q$ for the six viscoelastic simulations. For $De = 0.11$ the iso-surfaces of $Q > 0$, associated with a predominance of enstrophy over strain show a typical tube-like structures which are very similar to the reference Newtonian DNS, while for $De = 0.62$ and $De = 1.23$ $Q > 0$ displays both tube and sheet like structures, or only sheet-like regions structures, respectively. An accurate subgrid-scale model
for viscoelastic flows will need to capture the different flow topologies for different $De$ numbers, as these structures are strongly linked with the solvent/polymer interactions, as with the drag reduction mechanism [54].

Figure 4.6: Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{rms}$) corresponding to a threshold equal to $Q/Q_{rms} = 7$ for all DNS.

4.2 A priori tests: DNS of isotropic viscoelastic turbulence

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

4.2.1 Modification of the Smagorinsky model constant $C_S$ in viscoelastic flows

As described above the proposed subgrid-scale model for viscoelastic flows relies in the classical Smagorinsky model to model the subgrid-scale stresses from the momentum equation $\tau_{ij}$. In order to appreciate the influence of the Deborah number and filter sizes in the Smagorinsky model constant $C_S$, the DNS data banks were used to compute this constant using classical a priori tests. $C_S$ is computed as [80].
\[ C_S^2 = \frac{\langle -\tau_{ij} S_{ij} \rangle}{2\sqrt{2} \Delta^2 \langle S_{ij} S_{ij} \rangle^{3/2}}, \]  

(4.28)

where the brackets represent time and volume averages for each simulation, for all the simulations used in this work and for filter sizes \( \Delta/\Delta x = 2, 4, 8 \) and 16, and the results are displayed in figure 4.7. The Newtonian case is also shown for comparison and it is interesting to see that in this case \( C_S \) increases with the filter size in the range \( 0.14 \leq C_S \leq 0.17 \), which is due to finite Reynolds number effects. Recall that for Newtonian isotropic turbulence and by assuming an inertial range energy spectrum \( E(k) = C_K \left( e^{[n]} \right)^{2/3} k^{-5/3} \), where \( C_K \) is the Kolmogorov constant, the Smagorinsky constant is \( C_S = 0.16 \) for \( C_K = 1.6 \). Therefore the present value of \( 0.14 \leq C_S \leq 0.17 \) are quite close to the ‘exact’ value of \( C_S = 0.16 \). In the viscoelastic simulations the constant exhibits the same trend of decreasing \( C_S \) for the higher \( De \) numbers. This reflects the depletion of kinetic energy flux into the subgrid-scales of motion described above. In particular for \( De = 1.23 \) the constant is \( C_S \approx 0.10 \), which is already quite small than the classical value suggests that corrections to this constant need to be made for viscolelastic flows. However, no such study was pursued here for the reasons indicated below.

Figure 4.7: Smagorinsky constant \((C_S)\) computed with Eq. (4.28) for filter sizes \( \Delta/\Delta x = 2, 4, 8 \) and 16 and all the reference simulations used in this work.

4.2.2 Peterlin term of the filtered conformation tensor transport equation: H1

The first hypothesis used in the present model is described in equation (2.44). Figures 4.8 (a-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 of the correlation is observed for higher Deborah numbers. The same result was observed for the other simulations and filter sizes. Given the soundness of assumption H1 this hypothesis was used in the remaining of this work.
4.2.3 Subgrid-scale advection conformation tensor term: H2

Now, the modelling the subgrid-scale advection conformation tensor $\psi_{ij}$ defined in Eq. (2.41) is discussed. In the present model this term is essentially neglected in assumption H2 described in Eq. (2.45). In order to assess the accuracy of this assumption we analyse the transport equation for the filtered trace of the conformation equation (4.29) written as,

$$\frac{\partial C_{ii}}{\partial t} + \frac{u_k}{\partial x_k} = 2C_{ik}\frac{\partial u_i}{\partial x_k} - \frac{1}{\tau_p} \left[ f(C_{kk})C_{ii} - \delta_{ii} \right] - \psi_{ii} + \gamma_{ii}, \quad (4.29)$$

where the approximation H1 (Eq. 2.44) has been used. The terms in the left-hand side of equation (4.29) are the temporal variation ($C_i$), convective transport ($C_a$) of $C_{ii}$, respectively, while the terms on the right-hand side represent the production ($C_p$) and dissipation ($C_d$). These terms are followed by the unknown subgrid-scale terms associated with the advection $\psi_{ii}$, and polymer stretching $\gamma_{ii}$, respectively.

Since due to isotropy the mean value of the subgrid-scale advection is zero $\langle \psi_{ii} \rangle = 0$, the only way to assess the relevance of this term by comparing its local/instantaneous value in comparison with the other terms. For this purpose figures 4.9 (a-c) and 4.10 (a-c) show the probability density function of $\gamma_{ii}$ and $\psi_{ii}$ for the DNS with $De = 0.11, 0.38$ and $0.91$, and for filter sizes $\Delta/\Delta x = 4$ and $16$ respectively.

Figure 4.9: Probability density function (PDF) of the subgrid-scale trace of the conformation tensor and polymer stretching terms normalised by their root-mean-square, for the DNS with $De = 0.11, 0.38$ and $0.91$ and filter size $\Delta/\Delta x = 4$. 
Figure 4.10: Probability density function (PDF) of the subgrid-scale trace of the conformation tensor and polymer stretching terms normalised by their root-mean-square, for the DNS with $De = 0.11$, $0.38$ and $0.91$ and filter size $\Delta/\Delta x = 16$.

Clearly the skewness of $\psi_{ii}$ is much higher than of $\psi_{ij}$ (notice that $\langle \gamma_{ii} \rangle \neq 0$), with a very low probability associated to events with $\psi_{ii} \gg \gamma_{jj}$. Similar results were observed for the other simulations and filter sizes. Assumption H2 is therefore strongly supported by the available DNS data.

4.2.4 Scale-similarity of the subgrid-scale polymer stretching: H3

The scale-similarity for the subgrid-scale polymer stretching term used by the present model is described by Eq. (2.47). In order to assess this approximation figures 4.11 (a-c) and 4.12 (a-c) show joint probability density functions (JPDF) between $\gamma_{ii}$ and $G_{ii}$ for filter sizes $\Delta/\Delta x = 4$ and $16$, and for the simulations with $De = 0.11$, $0.38$ and $0.91$. The definition of correlation coefficient is also introduced and is given by $C_\rho = \langle X'Y' \rangle / [(\langle X'^2 \rangle \langle Y'^2 \rangle)]^{1/2}$ where $X$ and $Y$ are two random variables. 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 $16$. These JPDFs are a first indication that this assumption may be a good starting point for a model of the subgrid-scale polymer stretching term in Eq. (2.40). The Table 4.3 shows in detail the correlation coefficients for all simulations and several filter sizes.

Table 4.3: Correlation coefficients between the trace of the subgrid-scale polymer stretching terms at filter sizes $\Delta$ and $2\Delta$, $\gamma_{ii}$ and $G_{ii}$, respectively, for all the reference DNS used in the present work and for filter sizes $\Delta/\Delta x = 2, 4, 8,$ and $16$.

<table>
<thead>
<tr>
<th>$De$</th>
<th>$\Delta/\Delta x = 2$</th>
<th>$\Delta/\Delta x = 4$</th>
<th>$\Delta/\Delta x = 8$</th>
<th>$\Delta/\Delta x = 16$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.11</td>
<td>0.93</td>
<td>0.84</td>
<td>0.75</td>
<td>0.62</td>
</tr>
<tr>
<td>0.22</td>
<td>0.87</td>
<td>0.81</td>
<td>0.75</td>
<td>0.70</td>
</tr>
<tr>
<td>0.38</td>
<td>0.83</td>
<td>0.67</td>
<td>0.66</td>
<td>0.65</td>
</tr>
<tr>
<td>0.62</td>
<td>0.87</td>
<td>0.67</td>
<td>0.48</td>
<td>0.57</td>
</tr>
<tr>
<td>0.91</td>
<td>0.89</td>
<td>0.76</td>
<td>0.55</td>
<td>0.43</td>
</tr>
<tr>
<td>1.23</td>
<td>0.60</td>
<td>0.43</td>
<td>0.52</td>
<td>0.43</td>
</tr>
</tbody>
</table>
Next, it is shown that $\gamma_{ii}$ and $G_{ii}$ exhibit closely similar statistical characteristics, in terms of the range of existing magnitudes and their distribution. The figures 4.13 (a-c) and 4.14 (a-c) show the probability density functions of $\gamma_{ii}$ and $G_{ii}$ for $\Delta/\Delta x = 4$ and 16 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.

Figure 4.11: Joint probability density functions between the real (exact) traces of polymer stretching terms $\gamma_{ii}$ and $G_{ii}$ normalised by their root-mean-square), at filter size $\Delta/\Delta x = 4$ for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$.

Figure 4.12: 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 with $De = 0.11$, $De = 0.38$ and $De = 0.91$.

Figure 4.13: 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 with $De = 0.11$, $De = 0.38$ and $De = 0.91$.
Figure 4.14: Probability density functions of traces of subgrid-scale polymer stretching terms $\gamma_{ii}$ and $G_{ii}$ at filter size $\Delta/\Delta x = 16$ for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$.

To emphasise this aspect table 4.4 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 are 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 $\gamma_{ii}$.

Table 4.4: Root-mean-square (Rms) of $\gamma_{ii}$ and $G_{ii}$ using the reference DNS with $De = 0.11$, $0.38$, and $0.91$ with filter sizes $\Delta/\Delta x = 4$ and $16$.

<table>
<thead>
<tr>
<th>Rms</th>
<th>$De = 0.11$</th>
<th>$De = 0.38$</th>
<th>$De = 0.91$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta/\Delta x$</td>
<td>4</td>
<td>16</td>
<td>4</td>
</tr>
<tr>
<td>$\gamma_{ii}$</td>
<td>11.8</td>
<td>21.2</td>
<td>44.4</td>
</tr>
<tr>
<td>$G_{ii}$</td>
<td>11.8</td>
<td>2.7</td>
<td>51.8</td>
</tr>
</tbody>
</table>

A question that arises when facing the model definition in Eq. (2.47) is whether the model constant $C_{\gamma}$ is ‘isotropic’ i.e. given the well known anisotropy of the polymer stresses one might be tempted to extend the present model by using an anisotropic version of the model constant $C_{\gamma_{ij}}$, defined in by,

$$\gamma_{ij} = C_{\gamma_{ij}}G_{ij} \text{ (no summation).} \quad (4.30)$$

To clarify this issue figures 4.15 (a-c) and 4.16 (a-c) show several joint probability density functions (JPDFs) involving the quantities $C_{\gamma_{11}}$, $C_{\gamma_{22}}$, and $C_{\gamma_{12}}$ for filter size $\Delta/\Delta = 4$, and for the reference DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$, defined by,

$$C_{\gamma_{11}} = \frac{\gamma_{11}}{G_{11}}, \quad (4.31)$$

$$C_{\gamma_{22}} = \frac{\gamma_{22}}{G_{22}}, \quad (4.32)$$

and,
Clearly the quantities $C_{\gamma_{11}}, C_{\gamma_{22}}$, and $C_{\gamma_{12}}$, are statistically independent, and similar observations were made for filter size $\Delta/\Delta = 16$. This supports the use of an 'isotropic' constant $C_{\gamma}$ in the present model and finalises the assessment of the hypothesis H3.

\[ C_{\gamma_{12}} = \frac{\gamma_{12}}{\eta_{12}}. \]  

(4.33)

4.2.5 Global equilibrium of the polymeric elastic energy: H41

The present model uses the assumption of global equilibrium of the polymers elastic energy described in equation (2.48). It was checked that indeed the two sides of equation (2.48) are equal to within numerical uncertainty, in all the reference DNS and for all the Deborah numbers and filter sizes used in the present work. Notice that the present DNS data bank consists of statistically stationary and homogeneous turbulence, where the averaged temporal variation, and averaged convective terms are zero. Therefore this hypothesis does not need any additional discussion. It is however interesting to discuss the possibility of using a local equilibrium approximation, with the aim of extending the present model to other flows where statistical stationarity and/or homogeneity are generally not present.
4.2.6 Local equilibrium of the polymeric elastic energy: H42

The local equilibrium assumption defined by equation (2.49) is not used in the present model but is discussed here because of its usefulness in possible 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 'local' equilibrium of the elastic energy (which is proportional to the trace of the conformation tensor) is in some ways similar. The local equilibrium of the subgrid-scale stresses however is a flawed hypothesis [86] 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 (see Tables A.1, A.2 and A.3 in the Appendix).

This can be appreciated in figures 4.17 (a-c) and 4.18 (a-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 (2.43) for several Deborah numbers and filter sizes \( \Delta/\Delta x = 4 \) and 16. The correlation between \( C_p \) and \( C_d \) is 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, which is described quantitatively in the table 4.5.

![Figure 4.17](image-url)

Figure 4.17: Joint probability density functions between polymer stretching \( C_p \) and dissipation \( C_d \) terms from the trace of the conformation tensor transport equation (2.43), for DNS with \( De = 0.11 \), \( De = 0.38 \) and \( De = 0.91 \) and for filter size \( \Delta/\Delta x = 4 \).

The assessment of the assumption H42 is not complete however without showing that the other terms in Eq. (2.49), terms \( C_t \) and \( C_a \), are not 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 4.19 (a-c) and 4.20 (a-c) show the probability density functions of all the terms in Eq. (2.43) \( (C_t, C_a, C_p \text{ and } C_d) \) for \( \Delta/\Delta x = 4 \) and 16 and \( De = 0.11, 0.38 \), and 0.91. In some cases \( C_t \) and \( C_a \) attain much smaller magnitudes than the terms \( C_p \) and \( C_d \) e.g. for \( De = 0.11 \), however in other situations the reverse is observed e.g. for \( De = 0.38 \), but all instances one sees that the probability density functions of \( C_t \) and \( C_a \) are very similar. The same is true of the other simulations and filter sizes (not shown).
strongly supported by the DNS data banks which suggests that it can probably be used in viscoelastic

Figure 4.18: Joint probability density functions between polymer stretching $C_p$ and dissipation $C_d$ terms from the trace of the conformation tensor transport equation (2.43), for DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$ and for filter size $\Delta/\Delta x = 16$.

Table 4.5: Correlation coefficients between the polymer stretching and dissipation terms, $C_p$ and $C_d$, respectively, for all the reference DNS used in the present work and for filter sizes $\Delta/\Delta x = 2, 4, 8$, and $16$.

<table>
<thead>
<tr>
<th>$De$</th>
<th>$\Delta/\Delta x = 2$</th>
<th>$\Delta/\Delta x = 4$</th>
<th>$\Delta/\Delta x = 8$</th>
<th>$\Delta/\Delta x = 16$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.11</td>
<td>0.92</td>
<td>0.93</td>
<td>0.96</td>
<td>0.98</td>
</tr>
<tr>
<td>0.22</td>
<td>0.87</td>
<td>0.88</td>
<td>0.91</td>
<td>0.95</td>
</tr>
<tr>
<td>0.38</td>
<td>0.85</td>
<td>0.85</td>
<td>0.86</td>
<td>0.89</td>
</tr>
<tr>
<td>0.62</td>
<td>0.83</td>
<td>0.84</td>
<td>0.84</td>
<td>0.85</td>
</tr>
<tr>
<td>0.91</td>
<td>0.77</td>
<td>0.78</td>
<td>0.79</td>
<td>0.80</td>
</tr>
<tr>
<td>1.23</td>
<td>0.68</td>
<td>0.69</td>
<td>0.71</td>
<td>0.74</td>
</tr>
</tbody>
</table>

Figure 4.19: Probability density function of the trace of the polymer temporal variation ($C_t$), convective transport and ($C_a$), production due to polymer stretching/distortion by the flow ($C_p$), and dissipation into potential elastic energy ($C_d$) for $\Delta/\Delta x = 4$ and for the DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$.

Therefore the only possibility for the local equilibrium assumption to hold is when $C_t$ and $C_a$ are strongly anti-correlated, so that their joint effect is cancelled and Eq. (2.43) is well approximated by the remaining terms $C_p$ and $C_d$. This is indeed what happens as can be seen in figures 4.21 (a-c) and 4.22 (a-c) showing the joint probability density functions between $C_t$ and $C_a$ for $De = 0.11$, $0.38$ and $0.91$ and for $\Delta/\Delta x = 4$ and $16$, respectively. Thus, the present results convincingly show that assumption H42 is strongly supported by the DNS data banks which suggests that it can probably be used in viscoelastic
Figure 4.20: Probability density function of the trace of the polymer temporal variation \( (C_t) \), convective transport and \( (C_a) \), production due to polymer stretching/distortion by the flow \( (C_p) \), and dissipation into potential elastic energy \( (C_d) \) for \( \Delta/\Delta x = 16 \) and for the DNS with \( D_e = 0.11 \), \( D_e = 0.38 \) and \( D_e = 0.91 \).

inhomogeneous turbulent flows, where the global (Eq. 2.48) does not necessarily hold.

Figure 4.21: Joint probability density functions between the trace of the polymer temporal variation \( (C_t) \) and convective transport and \( (C_a) \) (normalised by their root-mean-square), at filter size \( \Delta/\Delta x = 4 \) for the DNS with \( D_e = 0.11 \), \( D_e = 0.38 \) and \( D_e = 0.91 \).

Figure 4.22: Joint probability density functions between the trace of the polymer temporal variation \( (C_t) \) and convective transport and \( (C_a) \) (normalised by their root-mean-square), at filter size \( \Delta/\Delta x = 16 \) for the DNS with \( D_e = 0.11 \), \( D_e = 0.38 \) and \( D_e = 0.91 \).
4.2.7 Influence of the Deborah number and filter size on $C_\gamma$

Next, the sensitivity of the model constant $C_\gamma$ is analysed to the filter size and Deborah number. Two procedures are employed. In the first, one of the constants is computed using globally averaged quantities,

$$C_\gamma = \left\langle \frac{\gamma_{ii}}{\mathcal{G}_{jj}} \right\rangle,$$  \hspace{1cm} (4.34)

where the brackets represent a volume average which is computed for each time step of the simulations (see figure 4.23 a). In the second procedure the constant is computed locally,

$$C_\gamma = \left\langle \frac{\gamma_{ii}}{\mathcal{G}_{jj}} \right\rangle,$$  \hspace{1cm} (4.35)

i.e. using the definition of the constant at each point of the flow domain and for each time step, and averaging the constant $C_\gamma$ thus obtained in the whole domain (see figure 4.23 b). Equations (4.34) and (4.35) thus use a "local" and a "global" equilibrium assumptions, respectively.

![Figure 4.23: Mean value of the model constant $C_\gamma$ defined by Eq. (2.47) and computed using Eq. (2.50) i.e. a global or box averaging defined by the brackets in this equation, or averaging the locally obtained $C_\gamma$, 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.](image)

The two figures are remarkably similar which again confirms that the local and global equilibrium assumptions H41 and H42 are equally valid and lead essentially to the same results. The model constant is, as expected $O(C_\gamma) = 1$ and remains bounded by $0 \leq C_\gamma \leq 5$, with a tendency of increasing with the Deborah number and the filter size. The cases corresponding to $De \approx 1$ are interesting in that $C_\gamma$ approaches $\approx 0$, which is connected with a depletion of the non-linear energy cascade [21], where almost all the energy input is dissipated by the elastic stresses from the polymers.

Finally, figures 4.24 (a-c) show the probability density functions of the local constant $C_\gamma$ i.e. again
computed through Eq. (2.50) without the averaging operation, for all the filter sizes considered in this work and filter sizes $\Delta/\Delta x = 2, 4, 8,$ and $16$. The figures show that the events corresponding to large deviations from the mean values obtained before are very rare, particularly for the higher filter sizes, again suggesting that the local approximation is also 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 a priori tests are concerned the results indicate that the present model can be used for simulating viscoelastic inhomogeneous flows away from solid boundaries.

![Graphs showing probability density functions for different filter sizes.](image)

Figure 4.24: Probability density functions of the 'local' constant $C_\gamma$ defined by Eq. (2.47) without the volume (brackets) average for filter sizes $\Delta/\Delta x = 2, 4, 8$ and $16$, and the reference DNS with $De = 0.11$, $De = 0.38$ and $De = 0.91$.

### 4.3 A posteriori tests: LES of isotropic viscoelastic turbulence

In this section, the results from LES obtained with the present model are discussed. A total of 6 LES were carried out using the same physical parameters described in table 4.2, but using a grid with $N = 48^3$ collocation points instead. This corresponds to an implicit LES filter with $\Delta/\Delta x = 8$ which is located in the inertial range region of the energy spectra. In order to compare the LES results with the results obtained from the reference DNS the reference 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.

#### 4.3.1 Final set of governing equations for LES of viscoelastic isotropic turbulence

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

$$\frac{\partial \mathbf{u}}{\partial x_i} = 0,$$

momentum transport,
\[
\frac{\partial \tau_{ij}}{\partial t} + \frac{u_k \partial \tau_{ij}}{\partial x_k} = \frac{\partial p}{\partial x_i} + 2 \frac{\partial}{\partial x_j} \left[ (\nu_s + \nu_t) S_{ij} \right] + \frac{\partial}{\partial x_j} \left\{ \frac{\nu_p}{\tau_p} [f(C_{kk})C_{ij} - \delta_{ij}] \right\},
\]
(4.37)

and conformation tensor
\[
\frac{\partial C_{ij}}{\partial t} + \frac{u_k \partial C_{ij}}{\partial x_k} = \frac{\partial u_i}{\partial x_k} C_{jk} - \frac{\partial u_j}{\partial x_k} C_{ik} - \frac{1}{\tau_p} f(C_{kk})C_{ij} - \delta_{ij} + C_{ij} G_{ij},
\]
(4.38)

respectively. The subgrid-scale stresses tensor \(\tau_{ij}\) is computed by using the Smagorinsky model [22]:
\[
\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = 2\left\{ (CS\Delta)^2 |\mathbf{S}| \right\} S_{ij}
\]
(4.39)

and using a model constant equal to \(CS = 0.16\). As discussed above, the \textit{a priori} tests suggest that a smaller \(CS\) 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 \(CS = 0.16\) value \textit{i.e.} it is hoped that and 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 \(CS\). The subgrid-scale polymer stretching term is computed directly from its definition (Eq. 2.46),
\[
G_{ij} = \left[ \frac{\partial u_i}{\partial x_k} C_{jk} - \frac{\partial u_j}{\partial x_k} C_{ik} \right] + \left[ \frac{\partial u_j}{\partial x_k} C_{ik} - \frac{\partial u_j}{\partial x_k} C_{ik} \right]
\]
Finally, the model constant for the conformation tensor transport equations \(C_{ij}\), is calculated by the following formula,
\[
C_{ij} = \frac{\epsilon_p}{\rho \nu_s} \left\langle \frac{1}{f(C_{kk})} \right\rangle - \left\langle \frac{\partial u_i}{\partial x_k} C_{jk} \right\rangle - \left\langle \frac{\partial u_j}{\partial x_k} C_{ik} \right\rangle,
\]
(4.40)

which has shown to be computationally more stable than its direct definition through Eq. (2.50). The polymer dissipation \(\epsilon[p] = P - \epsilon[s]\) is computed from the energy balance equation (4.25) since the total power input \(P\) is imposed and the solvent dissipation \(\epsilon[s]\) can be computed from its definition (Eq. 4.4), and the following equality has been used [21],
\[
\epsilon[p] = \frac{f(C_{kk}) \sigma_{kk}}{2\tau_p}.
\]
(4.41)

For consistency, each new modelling term has been computed using the same numerical method used in its corresponding (DNS) term \textit{e.g.} \(G_{ij}\) has been computed using 2\textsuperscript{nd} order central finite differences. There is one requirement to use successfully this model: it can only be activated after the enstrophy peak during the initial stage of the simulation, \textit{i.e.}, in the case of this work after 6 − 7 turnover times, when the simulations enters in a semi-stationary state.
### 4.3.2 Drag reduction and coherent structures obtained from the LES

Table 4.6 lists the values of the drag-reduction (DR), defined as

\[
DR = \frac{\varepsilon[p]}{\varepsilon[s] + \varepsilon[p]},
\]

that has been used before to characterise simulations of isotropic turbulence with polymer additives [56] 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 from the LES as outlines above).

<table>
<thead>
<tr>
<th>DR:</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>

For small \( De \) numbers, the absence of a model for the subgrid-scale polymer stretching term leads to \( DR \) values that significantly underpredict the correct values. In contrast, the addition of the present model clearly allows the recovery of the \( DR \) from the simulations, which is a strong indication that the model is indeed performing well its role. For high values of \( De (De \geq 0.91) \) the differences between the \( DR \) obtained with DNS, with and without model are not very important. As it is seen, 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. Figures 4.25, 4.26 and 4.27 shows iso-surfaces of the second invariant of the velocity gradient tensor obtained for the LES with \( De = 0.11, De = 0.38 \) and \( De = 0.91 \), respectively, compared with the filtered DNS, using the same threshold. The flow structures seem to be very well captured by the present model, as the size and shape of the flow vortices see to be virtually equivalent in the two simulations. The same is true of the other simulations which again indicates that the new model is able to capture the large-scale feature of the simulations.
Figure 4.25: Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{\text{rms}}$) corresponding to a threshold equal to $Q/Q_{\text{rms}} = 4$ for the filtered reference DNS with $De = 0.11$ with $\Delta/\Delta x = 8$ and LES with $N = 48^3$ collocation points.

Figure 4.26: Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{\text{rms}}$) corresponding to a threshold equal to $Q/Q_{\text{rms}} = 4$ for the filtered reference DNS with $De = 0.38$ with $\Delta/\Delta x = 8$ and LES with $N = 48^3$ collocation points.

Figure 4.27: Iso-surfaces of the second invariant of the velocity gradient tensor $Q$ (normalised by their root-mean-square $Q_{\text{rms}}$) corresponding to a threshold equal to $Q/Q_{\text{rms}} = 4$ for the filtered reference DNS with $De = 0.91$ with $\Delta/\Delta x = 8$ and LES with $N = 48^3$ collocation points.
4.3.3 Kinetic energy spectra and spectral budgets

In order to assess the detailed spectral behavior of the present model figures 4.28 (a-f) and 4.29 (a-f) show the kinetic energy spectra $E(k)$, and the spectral energy budgets, respectively, from all the viscoelastic LES, compared with the reference (filtered) DNS and also with simulations without polymer subgrid-scale model. In all cases the subgrid-scale stresses in the momentum equations are closed with the classical Smagorinsky model with a constant equal to $C_S = 0.16$.

![Figure 4.28: Kinetic energy spectra $E(k)$ for all the viscoelastic LES in a grid with $N = 48^3$ collocation points. The results for filtered DNS (DNS) and without polymer subgrid-scale model ((−)) are also shown.](image)

For the lower Deborah numbers $De = 0.38$ and 0.62 (figures 4.28 c,d) the energy spectra obtained from LES closely follows the filtered DNS spectra, until a given high wavenumber $k_{cLES}$. The simulations without polymer subgrid-scale model also display the same feature, however until at a much lower wavenumber $k_{c}^{(-)} < k_{cLES}$, after which the two simulations (with and without model for each $De$ number) start to deviate from the filtered DNS data, even if no particular accumulation of kinetic energy at high wavenumbers can be observed. The comparison between the results with and without polymer model for intermediate $De$ numbers already indicates that the present model does achieve an improvement over the simulations without model for these cases, even though one must keep in mind that the kinetic energy dynamics is being largely handled by the Smagorinsky model.

The situation is slightly different for high $De$ numbers as shown in figure 4.28 (f) corresponding to
the case with $De = 1.23$. Here both the LES with and without polymer subgrid-scale model show very similar energy spectra, which also follow closely the filtered DNS spectra until a given (approximately similar) wavenumber $k_{(\nu)}^c \approx k_{c,LES}^c$, above which the spectra display less energy, than the filtered DNS spectra. 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 production, such is the power of the polymer dissipation 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 used here $C_S = 0.16$ is much higher than the value suggested by the a priori tests in the form of figure 4.7, where one sees that a constant of the order of $C_S \approx 0.1$ should have been used instead. However, since these cases i.e. $De \geq 1$ are not particularly challenging, and the drag-reduction (see table 4.6) and flow structures are well captured, no investigations were made further.

The spectral budgets for the same cases, (figures 4.29 (a-f)) 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. (4.43) is,

$$F(k) = \Pi(k) + \Pi[p](k) + D(k),$$

where the bar "−" represents data available in the LES grid, however, for clarity the figures use the same notation as before i.e. without the bar over each term of the spectral budget.

Before analysing these results it is important to stress 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 exact (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 and thus allows us to gain further insight into the results from the present model.

From the outset it is important to stress that as expected for all $De$ numbers the filtered DNS, LES and 'no-model' simulations lead exactly the same result since these term is imposed in the, moreover, fully resolved wavenumber range, $F^{LES}(k) = F^{DNS}(k) = F^{(-)}(k)$. In the simulations with $De = 0.38$ (figure 4.29 c) the non-linear energy transfer function $\Pi(k)$ is very well captured by the new subgrid-scale model, $\Pi^{LES}(k) = \Pi^{DNS}(k)$, while the 'no-model' simulation significantly over-predicts this quantity. The resolved solvent dissipation is well captured by both simulations, LES and 'no-model', $D^{LES}(k) = D^{DNS}(k) = D^{(-)}(k)$ although the LES displays a nearly perfect agreement, in contrast with the 'no-model' simulation at high wavenumbers. Finally, the solvent-elastic energy transfer is very well predicted by the LES model simulation for the first wavenumbers $\Pi[p]^{LES}(k) = \Pi[p]^{DNS}(k)$ for $k \leq 4$, and under-predicts $\Pi[p]^{DNS}(k)$ for the remaining wavenumbers $5 < k < 24$, while the 'no-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 4.6), since for these range of $De$ numbers the leading term in the spectral energy budget is $\Pi^{DNS}(k)$ 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.

For 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 (see figure 4.43 b). Again the leading term is well captured by the LES using the present model i.e. $\Pi^{p|LES}(k) \approx \Pi^{p|DNS}(k)$. As in figure 4.29 (d) the solvent dissipation is well captured both in the LES and 'no-model' simulations, the LES performing slightly better. The main difference between the LES and 'no-model' cases compared to the previous case concerns the slightly better agreement of the 'no-model' case with $\Pi^{DNS}(k)$, however only for $k < 5$, but this term is much less important than $\Pi^{p|DNS}(k)$ for this value of $De$, which explains the overall better agreement of the LES, as translated in the results of $E(k)$ (figure 4.28 d) as well as in the $DR$ (see table 4.6).

Finally, we discuss what is probably the least interesting case, corresponding to the simulation with
As described before in subsection 4.1.2 in this case the polymer dissipation term \( \Pi_p \) largely dominates the other transfer terms and is largely dominated by the fully resolved large scale motions, thus, the role of the subgrid-scale models are less critical here than in the other cases, even considering that according to the \textit{a priori} tests, the Smagorinsky model constant used here \( C_S = 0.16 \) is higher than the optimal value, which is probably reflected in the slightly smaller value of \( \Pi_{p,LES} \) for this case. This is attested by the accuracy of the simulations without subgrid-scale polymer model. This fact 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.

This concludes the analysis of the results from the LES using the present model. In any cases, the curves from the simulations using the new subgrid-scale model for viscoelastic fluids display excellent agreement with the corresponding (filtered) DNS results, and are superior to the results obtained without subgrid-scale model for the conformation tensor transport equation.

### 4.4 Energy Spectrum Equation for Elasto-Inertial Range

In recent experimental works in grid turbulence with polymer additives, a region in the energy spectrum below the inertial sub-range, where the slope is \( k^{-3} \), was observed [58]. This region can be interpreted as the elasto-inertial range. An approximate formula for the energy spectrum on this subrange can be obtained using dimensional analysis. The time-scale \( \tau_L \) is defined such that the energy flux is the available energy of wavenumber \( k \) defined by [24]:

\[
\tau_L(k) \sim (k^3 E(k))^{-1/2}
\]  
(4.44)

If the characteristic time-scale \( \tau_L \) of the largest eddies is equal to the Zimm relaxation time of the polymer \( \tau_p \), the following expression is obtained:

\[
E(k) \sim \tau_p^{-2} k^{-3}
\]  
(4.45)

Since the polymers only affect the flow when \( Wi > 1 \), then the equation has to be restricted for these cases and it will be:

\[
E(k) = C_{EI} \tau_p^{-2} k^{-3} \log(Wi)
\]  
(4.46)

where \( C_{EI} \sim 1.5 \) is a constant of this region of the order of \( C_K \). This equation was tested for the reference viscoelastic DNS, and as can be seen in figure 4.30 for \( De = 0.38, De = 0.62 \) and \( De = 0.91 \), the elasto-inertial region equation shows an excellent agreement for these cases where \( k^{-3} \) slope of the energy spectrum is easily seen. More DNS with different Reynolds and Deborah numbers are need to test the universality of this new equation.
Figure 4.30: Kinetic energy spectra (ES) $E(k)$ for the reference viscoelastic DNS corresponding to $De = 0.38, 0.62$ and $0.91$ and the elasto-inertial equation (EIR) $E(k) = C_{EI} \tau_\nu^{-2} k^{-3} \log(Wi)$, with $C_{EI} = 1.5$. The dashed vertical line represents the wavenumber corresponding to the Lumley scale.
Chapter 5

Conclusions

5.1 Achievements

In this work a new subgrid-scale model is developed for large-eddy simulations (LES) of Newtonian solvents carrying small amounts of long chain polymer molecules, simulated by the Finitely Extensible Nonlinear Elastic continuous model closed with the Peterlin approximation (FENE-P).

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

The analysis of the filtered momentum and conformation tensor transport equations showed that the only term that requires an additional model, compared to a Newtonian simulation, is the subgrid-scale polymer stretching term $\gamma_{ij}$, while all the other terms arising from the filtering procedure can be neglected e.g. the subgrid-scale conformation tensor advection $\psi_{ij}$.

It is shown that the Smagorinsky constant associated with the dissipation of kinetic energy within the solvent should be decreased for viscoelastic LES for higher Deborah numbers, due to a observed decrease of the non-linear kinetic energy transfer from the resolved into the unresolved scales of motion.

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

Finally, the new model is tested in LES of viscoelastic turbulence covering the same physical parameters of the reference DNSs, but using a grid with (only) $N = 48^3$ collocation points. The LESs consistently show that the new model is able to reproduce the global flow quantities, such as the $DR$, the flow structures, the kinetic energy spectra, and the detailed spectral budgets, thus proving that the present model presents a major progress in the numerical simulation of turbulent Newtonian flows with diluted polymer molecules.
Additionally to the objectives defined in the beginning of this work, an energy spectrum equation for the elasto-inertial range was deduced recurring to dimensional algebra and physical arguments. Although, the new equation shows an excellent agreement with the DNS data bank, more cases with different Reynolds and Deborah numbers are need to ensure the universality of this equation.

5.2 Future Work

For future work, the natural sequence of the present work is the extension and testing of the new subgrid-scale model into inhomogeneous viscoelastic flows, starting with free-shear flows and proceeding after into wall-bounded flows. The procedure would involve the same steps used here into the creation of DNS data banks for turbulent planar jets of FENE-P fluid for several Reynolds numbers, Deborah numbers and polymer extensibility; *a priori* data analysis to quantify the grid/subgrid scales/rheology interactions in the governing equations for turbulent planar jets for several Reynolds numbers, Deborah numbers and polymer extensibility values; *a priori* analysis of the unresolved terms of the governing equations for the turbulent channel flow of FENE-P fluids to quantify the grid/subgrid scales/rheology interactions as a function of Reynolds and Deborah numbers and polymer extensibility; and development of LES closures for the non-negligible unresolved (SGS) terms of the governing equations for FENE-P.
Bibliography


Appendix A

Appendix: *A priori tests*

A.1 Tables for the local equilibrium of the polymeric elastic energy assumption: H42

Table A.1: Mean and Root-mean-square (Rms) of terms from the *a priori* analysis using the reference DNS with $De = 0.11$, with four filter sizes ($\Delta/\Delta x = 2, 4, 8, 16$). Terms from the trace of the conformation tensor $C_{ii}$ governing equation: temporal variation ($C_t$), convection ($C_a$), polymer stretching ($C_p$), and dissipation ($C_d$). $\gamma_{ii}$ and $\mathcal{G}_{ii}$ are the (exact) traces of the subgrid-scale stretching terms at scales $\Delta$ and $2\Delta$, respectively.

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Table A.2: Mean and Root-mean-square (Rms) of terms from the *a priori* analysis using the reference DNS with $De = 0.38$, with four filter sizes ($\Delta/\Delta x = 2, 4, 8, 16$). Terms from the trace of the conformation tensor $C_{ii}$ governing equation: temporal variation ($C_t$), convection ($C_a$), polymer stretching ($C_p$), and dissipation ($C_d$). $\gamma_{ii}$ and $\mathcal{G}_{ii}$ are the (exact) traces of the subgrid-scale stretching terms at scales $\Delta$ and $2\Delta$, respectively.

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Table A.3: Mean and Root-mean-square (Rms) of terms from the \textit{a priori} analysis using the reference DNS with $De = 0.91$, with four filter sizes ($\Delta/\Delta x = 2, 4, 8, 16$). Terms from the trace of the conformation tensor $C_{ii}$ governing equation: temporal variation ($C_t$), convection ($C_a$), polymer stretching ($C_p$), and dissipation ($C_d$). $\gamma_{ii}$ and $G_{ii}$ are the (exact) traces of the subgrid-scale stretching terms at scales $\Delta$ and $2\Delta$, respectively.

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