

THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

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Turbulence models for viscoelastic fluids

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Summary

In many industrial processes we can find viscoelastic fluids under turbulent flows conditions and in other occasions it may be useful to have such fluids flowing under that conditions as for example the transport of fluids at long distances and in central district heating and cooling systems, because the corresponding drag reduction reduces significantly the cost of the process. For this reason it is necessary to develop numeric tools that can be used to solve engineering problems. At the present there are few viscoelastic turbulence models that can predict mean flow quantities and they are restricted to specific fluid and geometry sets. Recently, a more general viscoelastic turbulent model was developed by Pinho [1], Cruz et al. [2] and Resende et al. [3], which is not restricted to a single fluid or geometry. Although improvements were made in those works, for some of the viscoelastic fluids tested the predictions still fall short of the desired quality. In the first part of this thesis such models are precisely improved.

Specifically, a second order closure for predicting turbulent flows of viscoelastic fluids is proposed in this work and its performance is assessed by comparing its predictions with experimental data, for four different dilute polymeric solutions in fully-developed pipe turbulent flow. The main advantage of the present model is the capacity to capture well the drag reduction of the different viscoelastic fluids over a large range of Reynolds numbers. The model is an extension of an existing Reynolds stress closure for Newtonian fluids and includes low Reynolds number damping functions to properly deal with wall effects, which was modified to take into account viscoelasticity, especially in the pressure strain term. The new damping functions depend on rheological characteristics of the fluids, based on the theories of the previous developments of k - ε models for viscoelastic fluids by Cruz et al. [2]. This and the previous models are based on the use of a modified Generalized Newtonian fluid model to represent the rheology of the viscoelastic non-Newtonian fluids.

In the second part of this thesis, a different viscoelastic rheological model is adopted and a new low-Reynolds-number k - ε turbulence model is developed for turbulent flows of viscoelastic fluids. These are now described by the finitely extensible

nonlinear elastic rheological constitutive equation with Peterlin approximation (FENE-P model). This constitutive equation is truly viscoelastic and adequate to capture qualitative the main features of dilute polymeric solutions and the new turbulence model is valid at low and high drag reduction and was calibrated against direct numerical simulation data (DNS), thus extending and improving the performance of the earlier model of Pinho et al. [4], which was valid only at low drag reduction. In addition to extending the range of application to higher drag reduction, the new turbulence model relies on two main improvements, namely, extensions of the eddy viscosity closure, and of the transport equations of turbulent kinetic energy (k) and its rate of dissipation, to include direct contributions from viscoelasticity, and a new closure for the Reynolds averaged cross correlation between the fluctuating components of the polymer conformation and rate of strain tensors (NLT_{ij}). The NLT_{ij} quantity appears in the Reynolds averaged evolution equation for the conformation tensor (RACE), which is required to calculate the average polymer stress, and in the viscoelastic stress work in the transport equation of k . The predictions of mean velocity, turbulent kinetic energy, its rate of dissipation by the Newtonian solvent, conformation tensor and polymer and Reynolds shear stresses are improved compared to those obtained from the earlier model [4].

Finally, a low Reynolds number $k-\omega$ model for Newtonian fluids has been modified to predict drag reduction of viscoelastic fluids described by the FENE-P model. The predictions of the model are compared with DNS data and the predictions of the previous $k-\varepsilon$ model (developed in the second part of this thesis), for fully developed turbulent channel flow of FENE-P fluids. The viscoelastic closures in the $k-\omega$ model were developed for the low and high drag reduction regimes, respectively and the model compares similarly to the previous $k-\varepsilon$ closures in terms of both the flow and polymer characteristics, but is more stable and is a promising model for other types of flow to be tested in the near future. In this new model, the closures for the different viscoelastic terms were almost unchanged relative to those used in the context of $k-\varepsilon$ and in the case of the nonlinear term in the evolution equation of the polymer conformation tensor the numerical values of the parameters were kept unchanged, indicating that its main physics was captured by the closures.

Sumário

Os fluidos viscoelásticos estão presentes em muitos processos industriais e em escoamentos sob condições turbulentas. A vantagem da utilização de fluidos viscoelásticos em escoamentos turbulentos, pode ser observada no transporte de fluidos a longas distâncias e no aquecimento e refrigeração de sistemas, devido á sua redução do arrasto. Por isso é necessário desenvolver modelos de turbulência que possam ser utilizados em projectos de engenharia. Existem actualmente alguns modelos que são capazes de simular com precisão quantidades médias, mas infelizmente eles são restritos a um tipo de fluido e a condições restritas. Recentemente, um modelo turbulento do tipo $k-\varepsilon$ para baixos números de Reynolds, de carácter mais abrangente, e não sendo restrito a um determinado tipo de fluido ou geometria, foi proposto por Pinho [1], Cruz e tal. [2] e Resende et al. [3]. Apesar de vários melhoramentos não foi possível prever correctamente todos os fluidos testados, e nesse sentido foi desenvolvido, na primeira parte principal desta tese, um modelo que melhora as previsões.

Um modelo turbulento de segunda ordem é proposto nesta tese para prever fluidos viscoelásticos em escoamentos turbulentos, e a sua performance é analisada comparando as previsões com dados experimentais, para quatro diferentes soluções poliméricas diluídas em escoamentos turbulento desenvolvidos numa conduta. A principal vantagem do modelo presente é a sua capacidade de prever correctamente os diferentes comportamentos dos quatro fluidos viscoelásticos para uma larga gama de números de Reynolds. Este modelo é uma extensão de um fecho das tensões de Reynolds para fluidos Newtonianos e inclui funções de amortecimento para baixos números de Reynolds para lidar com os efeitos de parede, as quais foram modificadas para contabilizar a viscoelasticidade, especialmente no termo da pressão. As novas funções de amortecimento que dependem da reologia dos fluidos foram baseadas nos desenvolvimentos anteriores de modelos $k-\varepsilon$ para fluidos viscoelásticos de Cruz et al. [2].

Na segunda parte, é desenvolvido um novo modelo turbulento $k-\varepsilon$ de baixos números de Reynolds para escoamentos turbulentos com fluidos viscoelásticos, usando um modelo reológico diferente. O comportamento reológico é descrito pela equação constitutiva reológica elástica não linear com extensibilidade finita usando a aproximação de Peterlin, designada pelo o modelo FENE-P. Esta equação constitutiva é verdadeiramente viscoelástica e adequada para capturar qualitativamente as principais características de soluções poliméricas diluídas, sendo o novo modelo turbulento válido para baixos e altas reduções de arrasto. Este foi calibrado com base em dados de Simulação Numérica Directa (DNS), expandindo e melhorando a performance do modelo inicial de Pinho et al. [4], que era válido só para baixos regimes de redução do arrasto. Além da extensão do modelo para o alto regime de redução de arrasto, o novo modelo de turbulência consistiu em dois melhoramentos principais, nomeadamente, a extensão do fecho da viscosidade turbulenta e da inclusão directa de efeitos viscoelásticos nas equações da energia cinética de turbulência (k) e a sua dissipação, e um novo fecho para a média da correlação das flutuações do tensor conformação e do tensor da taxa de deformação (NLT_{ij}). O termo NLT_{ij} aparece da equação média da evolução de Reynolds para o tensor conformação (RACE), que é necessária para calcular a tensão polimérica média, e a dissipação viscoelástica da equação de transporte de k . As previsões da velocidade média, da energia cinética de turbulência e da sua dissipação da componente newtoniana, do tensor conformação e as tensões de corte de Reynolds são melhoradas quando comparadas com as previsões obtidas anteriormente pelo modelo inicial [4].

Finalmente, um modelo de turbulência $k-\omega$ para fluidos newtonianos e baixos números de Reynolds também foi alterado para prever fluidos viscoelásticos baseado no modelo FENE-P. As previsões de um escoamento turbulento desenvolvido em canal com um fluido FENE-P obtidas pelo o modelo são comparadas com os dados de DNS, e com as previsões do modelo anterior $k-\varepsilon$ (desenvolvido na segunda parte desta tese). Os fechos viscoelásticos foram baseados no modelo $k-\varepsilon$ para baixo e alto regime de redução do arrasto, obtendo previsões similares tanto nas características do escoamento e do polímero, com a vantagem de ser mais estável e também um modelo mais promissor em futuros testes em diferentes escoamentos. Neste novo fecho, os modelos para os

termos viscoelásticos são praticamente os mesmos relativamente aos que foram usados no contexto k - ε , e no caso do termo não linear da equação de evolução do tensor de conformação do polímero os parâmetros numéricos do modelo são exactamente os mesmos, indicando que a maior parte da física foi capturada pelo o fecho.

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Nomenclature

Latin symbols

A^+	Van Driest's parameter, $A^+=26.5$
A_ε	turbulence model parameter
B	constant parameter
C	turbulence model parameter in f_μ
C_0	parameter in anisotropic turbulence model
$\tilde{C}, C_\mu, C_{\varepsilon 1}, C_{\varepsilon 2}, C_{\varepsilon 4}$	isotropic turbulence model parameters
DR	drag reduction intensity
f	Darcy friction factor
f_t	damping function for turbulent diffusion of k and $\tilde{\varepsilon}$
f_v	damping function of molecular viscosity
f_μ	damping function of eddy viscosity
$f_{w,1}$	damping function in Reynolds stress model
H	half-height of a channel
k	turbulent kinetic energy
K_e	viscosity consistency index of Trouton ratio behavior
K_v	shear viscosity consistency index
L	extensibility parameter in FENE-P model
m	constant parameter
m_c	Cross model exponent
n	shear viscosity power index,
N_1	first normal stress difference
$\bar{p}$	mean pressure
p	viscosity power index of Trouton ratio behavior

r	radial coordinate
R	pipe radius
Re_g	generalized Reynolds number
Re	wall Reynolds number
Re_{ap}	Reynolds number based on apparent viscosity
R_T	turbulent Reynolds number
S	invariant of the rate of deformation tensor
s_{ij}	fluctuating rate of deformation tensor
S_{ij}	time-average rate of deformation tensor
t	time
u	local mean velocity
u_i	velocity vector component along coordinate
U	axial mean velocity
u_τ	friction velocity
u_R	characteristic turbulent scaling velocity
$-\overline{\rho uv}$	Reynolds shear stress
$-\overline{u_i u_j}$	Reynolds stress tensor
x	axial coordinate
y	distance measured from the wall
y^+	wall coordinate

Greek symbols

$\tilde{\alpha}_i$	parameter in anisotropic turbulence model
δ_{ij}	Kronecker symbol
ε	rate of dissipation of turbulent kinetic energy
$\tilde{\varepsilon}$	modified rate of dissipation of turbulent kinetic energy
$\dot{\varepsilon}$	invariant measurement of the strain rate (time average value)
$\dot{\varepsilon}'$	invariant measurement of the strain rate (fluctuating)

$\dot{\gamma}$	invariant measurement of the shear rate (time average value)
$\dot{\gamma}'$	invariant measurement of the shear rate (fluctuating)
η	parameter/ function in anisotropic model
η_e	extensional or elongational viscosity
η_s	solvent viscosity and parameter in turbulence model
η_p	polymer viscosity
η_v	shear (viscometric) viscosity
λ	parameter in Cross model and relaxation time of the polymer
ν_T	eddy viscosity
μ	molecular viscosity or viscosity in Cross model
$\bar{\mu}$	true time average molecular viscosity
$\bar{\mu}_h$	time average molecular viscosity for high Reynolds number turbulence
ρ	fluid density
σ_ε	turbulent Prandtl number for ε
σ_{ij}	stress tensor
σ_k	turbulent Prandtl number for k
τ	shear stress
$\bar{\tau}_{ij,p}$	Reynolds-averaged polymer stress

Subscripts

0	refers to zero shear rate
∞	refers to infinite shear rate
w	based on wall conditions

Superscript

+	designates quantities normalised with wall coordinates
'	designates fluctuation quantities

Chapter 1

Introduction

1.1 Introduction

The importance of the numerical simulations to solve engineering problems increased significantly in the last thirty years, especially for laminar and turbulent Newtonian flows.

The use of viscoelastic fluids, in particular the dilute polymeric solutions, instead of the Newtonian fluids, in turbulent flows generates drag reduction and improves the heat transfer. So, it becomes necessary to develop numerical tools to solve this type of engineering problems, for example, the transport of fluids at long distances and in district heating and cooling systems. A practical example is the injection of polymers in the Alaska pipeline to increase the volumetric flow rate in the petroleum transports.

The effect of the drag reduction is calculated by the deviation of the friction factor for the viscoelastic fluid in relation to a Newtonian fluid flowing at same Reynolds number, $(f^V - f^N)/f^N$, and researchers have identified three drag reduction regions: low ($DR < 30\%$), high ($30\% < DR < 60\%$) and maximum ($DR > 60\%$) drag reduction. If a viscoelastic turbulent model is able to predict correctly the drag reduction (DR) this means that the entire velocity field is also well captured, which is the main objective.

To develop the governing equations of a turbulence model it is necessary to choose initially a constitutive equation, governing the relation between the fluid properties and the flow characteristics. The simplest example is the Newton's law of viscosity used to represent the behaviour of very simple fluids, also known as Newtonian fluids. In the case of viscoelastic fluids the constitutive equations are more complex because it is necessary to capture such effects as fading memory, the enhanced extensional viscosity of elastic fluids, and the variable shear viscosity. All these features have a dramatic effect upon the flow characteristics, in particular when this flow takes place in the turbulent regime.

Using a simple constitutive equation, a modified form of the generalized Newtonian fluid model (GNF) Pinho and co-workers [1-3], developed a first order

turbulence model to predict the experimental behaviour of four different viscoelastic fluids in turbulent pipe flow. Such model was able to capture correctly the velocity field of two of the fluids, but showed deficiencies in the predictions for the remaining two fluids. In the first part of this thesis a new second order turbulence model is developed which improves significantly those predictions. It uses the same viscoelastic theories developed by Pinho and co-workers [1-3], and it was able to capture correctly the drag reduction of the all four tested fluids, for a wide range of Reynolds numbers, and consequently to predict well the velocity field. However the modified generalized Newtonian fluid model is not truly viscoelastic so it not contain memory effects, hence it can not predict the behaviour of the same fluids in laminar flows.

More recently, Pinho et al. [4] developed the first turbulence model for viscoelastic fluids represented by a better constitutive equation using kinetic molecular theory, the so-called FENE-P model (FENE-P stands for Finitely Extensible Nonlinear Elastic model, with Peterlin's closure). This model allows to capture more rheology phenomenon's when compared with the modified GNF model. The model of Pinho et al. [4] was tested only for low drag reduction, which limited their use. In the second part of this thesis Pinho et al.'s model is significantly improved and extended to predict in the low and high drag reduction regimes. The difficulties found in the viscoelastic modelling are due to the different fluid behaviour found in the different drag reduction regimes, which was analyzed in detail for low and high drag reductions.

At the end of this work, a second first order model for FENE-P fluids, a $k-\omega$ model, is proposed which is also able to describe the flow characteristics in the low and high drag reduction regimes without changes to the parameters and functions. This suggests that the essential physics used to model the various new Reynolds-average terms was captured, giving similar predictions to the previous model. The advantage of this model is the capacity to predict more complex flow with Newtonian fluids, something to be investigated in the future.

1.2 Main characteristics of viscoelastic turbulent flows

The main objective to be achieved with the viscoelastic turbulence models is to predict the mean quantities, for example the friction factor and the velocity profiles, of viscoelastic turbulent flows with different dilute polymeric solutions, for a wide range of Reynolds numbers and in many complex geometries. If a viscoelastic turbulent model is able to correctly predict different viscoelastic fluids this means that all the physics of the viscoelastic phenomenon is captured and the main objective is achieved.

The elastic contribution to the fluid rheology has a high impact in the friction factor and consequently in the velocity profile for viscoelastic fluids flowing in the turbulent flow regime. Hence, it is no surprise that by increasing fluid elasticity the flow characteristics change significantly. This phenomenon can be observed in **Fig. 1**, which presents experimental data of the Darcy friction factor in turbulent pipe flow with viscoelastic fluids, Escudier et al. [5]. It can be observed higher drag reduction (lower value of f), approaching the maximum drag reduction asymptotic of Virk defined by Eq. (1) with more elastic fluid, 0.125% PAA (polyacrylamide), when compared to less elastic fluid, the blend of 0.09% CMC (sodium carboxymethylcellulose) and 0.09% XG (xanthan gum). For a better understanding of the changes, we present in the same plot the friction factor for Newtonian fluids given by Eq. (2), which is used as a reference. The mean velocity profiles for the same of the flow conditions in **Fig. 1** can be visualized in **Fig. 2**. This plot shows that as the drag reduction increases there is a positive shift from the Newtonian log-law region approaching the maximum drag reduction asymptotic of Virk, given by Eq. (3).

$$1/\sqrt{f} = 9.5 \times \log(\text{Re}_w \sqrt{f}) - 19.06 \quad (1)$$

$$f = 0.316 \times \text{Re}^{-0.25} \quad (2)$$

$$u^+ = 11.7 \ln(y^+) - 17 \quad (3)$$

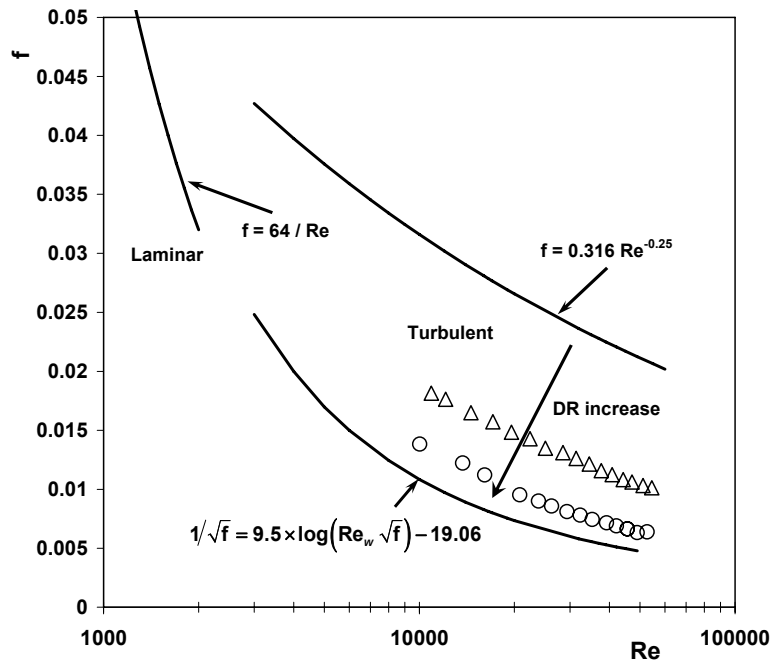


Fig. 1. Experiment data of the Darcy friction factor in turbulent pipe flow with viscoelastic fluids: Δ Blend 0.09% CMC / 0.09% XG; $\circ$ 0.125% PAA.

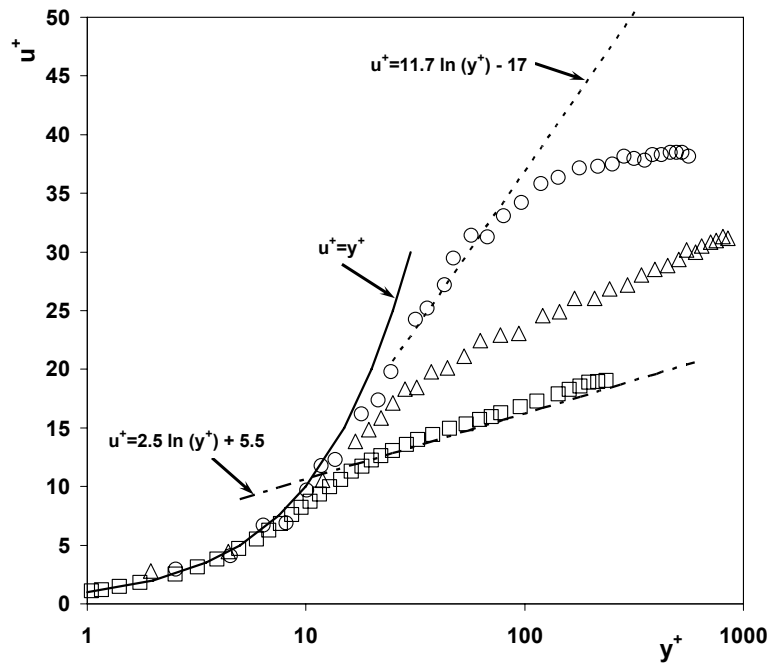


Fig. 2. Experiment data of the mean velocity profile in turbulent pipe flow with Newtonian and viscoelastic fluids: $\square$ Newtonian at $Re=7440$; Δ Blend 0.09% CMC / 0.09% XG at $Re=45300$; $\circ$ 0.125% PAA at $Re=42900$.

Note that the viscoelastic phenomenon does not affect only these two mean quantities; other mean and turbulent quantities are affected, with a higher intensity when the fluids are more elastic. Chapter 2 describes in more detail those other quantities that are also used to characterize the viscoelastic flows.

1.3 Governing equations development

The governing equations for turbulent flows of viscoelastic fluids are developed decomposing the instantaneous quantities into the sum of average and fluctuating quantities by the following relation $\hat{u} = \bar{u} + u'$ or $\hat{u} = U + u$, and Reynolds-averaging. The instantaneous momentum equation for a viscoelastic fluid is written as

$$\rho \frac{D\hat{u}_i}{Dt} = -\frac{\partial \hat{p}}{\partial x_i} + \frac{\partial \hat{\tau}_{ik}}{\partial x_k} \quad (4)$$

where the hat represents instantaneous values, u_i is the velocity vector, p is the pressure, ρ is the fluid density and τ_{ik} is the extra stress tensor, which includes two components: a solvent contribution of Newtonian behavior and a polymer contribution (the viscoelastic part).

Applying the Reynolds decomposition to the left hand-side of the momentum equation,

$$\begin{aligned} \rho \frac{\partial \hat{u}_i}{\partial t} + \rho \hat{U}_k \frac{\partial \hat{u}_i}{\partial x_k} &= \rho \frac{\partial (U_i + u_i)}{\partial t} + \rho (U_k + u_k) \frac{\partial (U_i + u_i)}{\partial x_k} = \\ &= \rho \frac{\partial U_i}{\partial t} + \rho \frac{\partial u_i}{\partial t} + \rho U_k \left(\frac{\partial U_i}{\partial x_k} + \frac{\partial u_i}{\partial x_k} \right) + \rho u_k \left(\frac{\partial U_i}{\partial x_k} + \frac{\partial u_i}{\partial x_k} \right) = \\ &= \rho \left\{ \frac{\partial U_i}{\partial t} + \frac{\partial u_i}{\partial t} + U_k \frac{\partial U_i}{\partial x_k} + U_k \frac{\partial u_i}{\partial x_k} + u_k \frac{\partial U_i}{\partial x_k} + \frac{\partial u_i u_k}{\partial x_k} \right\} \end{aligned} \quad (5)$$

and taking the time-average leads to Eq. (6)

$$\rho \left\{ \overline{\frac{\partial U_i}{\partial t} + \frac{\partial u_i}{\partial t} + U_k \frac{\partial U_i}{\partial x_k} + U_k \frac{\partial u_i}{\partial x_k} + u_k \frac{\partial U_i}{\partial x_k} + \frac{\partial u_i u_k}{\partial x_k}} \right\} = \rho \left\{ \frac{\partial U_i}{\partial t} + U_k \frac{\partial U_i}{\partial x_k} + \frac{\partial \overline{u_i u_k}}{\partial x_k} \right\} \quad (6)$$

Identically, for the right hand-side of the momentum equation

$$\begin{aligned}
-\frac{\partial \hat{p}}{\partial x_i} + \frac{\partial \hat{\tau}_{ik}}{\partial x_k} &= -\frac{\partial (p + p')}{\partial x_i} + \frac{\partial (\tau_{ik} + \tau'_{ik})}{\partial x_k} = \\
&= -\frac{\partial p}{\partial x_i} - \frac{\partial p'}{\partial x_i} + \frac{\partial \tau_{ik}}{\partial x_k} + \frac{\partial \tau'_{ik}}{\partial x_k}
\end{aligned} \tag{7}$$

and taking the time-average,

$$\overline{-\frac{\partial p}{\partial x_i} - \frac{\partial p'}{\partial x_i} + \frac{\partial \tau_{ik}}{\partial x_k} + \frac{\partial \tau'_{ik}}{\partial x_k}} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \tau_{ik}}{\partial x_k} + \frac{\partial \overline{\tau'_{ik}}}{\partial x_k}. \tag{8}$$

By definition, the time-average of a fluctuation is null so we set the time-average of the extra stress fluctuation equal to zero, $\overline{\tau'} = 0$. Assembling the time-average terms of the momentum equation, it becomes

$$\rho \frac{DU_i}{Dt} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_k} (\tau_{ik} - \rho \overline{u_i u_k}), \tag{9}$$

where the Reynolds stress tensor, $\overline{u_i u_k}$, was put on to the right hand-side as usual.

Applying the previous procedure to the continuity equation we will obtain the following equation

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{10}$$

In order to have a closed of equations it is necessary to developed a model for the Reynolds stress, but its is also necessary to adopt a specific constitutive rheological equation to determine the extra stress, τ_{ik} . This extra stress may also be influenced by the turbulence, so that additional terms may appear and may require adequate closure. There are different constitutive equations available which can be more or less complex depending on the required rheology characteristics. This will be described in chapter 3, where the constitutive equations to be used in the present work will be presented.

1.4 State of the art

1.4.1 Early turbulence models for viscoelastic fluids– first order models

The first turbulence models for viscoelastic fluid flows date from the 1970's with Mizushima et al. [6], Durst and Rastogi [7] and Poreh and Hassid [8] and were motivated and aimed at drag reduction by polymer solutions in turbulent pipe/channel flows. The scope of these earlier models was rather limited, because they depended on a large extent parameters that needed to be selected for each fluid in each flow situation and that were essentially modifications of turbulence models for Newtonian fluids, by an adequate modification of the von Kármán coefficient [7]. They had no obvious link to the non-Newtonian rheology, with the exception of Mizushima et al.'s model, which incorporated effects of relaxation time in the Van Driest damping function for the eddy viscosity, by introducing a coefficient related nonlinearly, and with a very large coefficient of the order of 10^8 , to the relaxation time of the linear viscoelastic Rouse model. In the 1980's and 1990's new turbulence models appeared (Politis [9], Malin [10], Cruz et al. [11]), this time attempting to link with the fluid rheology, describing the rheology by purely viscous rheological constitutive equations such as the power law or Bingham law for yield-stress fluids [10, 12], i.e., they were still limited to Generalized Newtonian fluids, where the material functions depended on the second invariant of the rate of deformation tensor. To extend the turbulence models to viscoelastic fluids one initial philosophy has been adopted in the works of Pinho and co-authors [1, 2, 13], which rely on the adoption of a generalized Newtonian constitutive equation, modified to incorporate elastic effects, that are known to be relevant in the context of turbulent flows of drag reducing fluids. This was accomplished by modifying the generalized Newtonian fluid constitutive equation, where the dependence of strain hardening of the fluid on the third invariant of the rate of deformation tensor was included. This set of models also included an anisotropic version to capture the

increased Reynolds stress anisotropy [3]. However, this constitutive equation is not truly elastic in nature, therefore it is unable to capture important features of elastic fluids, namely the memory effect and its spatiotemporal variation. In these works experimental data were used for both the fluid rheology and the flow dynamics, for the purpose of calibration and validation of the turbulence models.

The original first-order turbulence model developed following this approach is described in detail in [1, 13]. This was a low Reynolds k - ε model, which was developed on the basis of the Nagano and Hishida [14] closure for Newtonian fluids, and includes a closure for the Reynolds-averaged molecular viscosity, in order to properly account for the effect of fluctuating strain rates on the non-linear viscosity function, and a damping function for the eddy viscosity to account for wall proximity, shear-thinning of the shear viscosity and strain-thickening of the Trouton ration. However, this turbulence model neglected the new term of the momentum equation quantifying the cross-correlation between the fluctuating viscosity and rate of deformation tensor. Subsequently, a closure was developed for this specific stress term by Cruz et al. [2] and for the corresponding stress work appearing in the transport equation of turbulent kinetic energy leading to improvements in the prediction of maximum values of turbulent kinetic energy and in the prediction of friction factor at large Reynolds numbers.

Duct flows with drag reduction have enhanced anisotropy of the Reynolds stresses as shown in experimental work [3, 15, 16] and in DNS investigations with various differential viscoelastic models [17-19]. Turbulence anisotropy is not captured by linear forms of the k - ε turbulence model, but that can be achieved using higher order versions of the eddy viscosity closure as was done by Resende et al. [3] using a nonlinear k - ε model or higher-order turbulence models, which brings additional benefits to complex flow prediction.

In fact, first-order turbulence models have shortcomings when it comes to predicting Newtonian flows with separation or streamline curvature, amongst other things (see an early revision in Patel et al. [20]). The use of anisotropic first-order

models can offset some, but not all, of these disadvantages (Park et al. [21], Craft et al. [22]).

1.4.2 Second order models

The first second-order models for Newtonian fluids accounting for wall proximity, the so-called low Reynolds number Reynolds stress models, appeared in the 1970's like those of Launder et al. [23] and Hanjalić and Launder [24]. To extend their applicability to complex flows and better capture the anisotropic Reynolds stresses in the near-wall region, better near-wall closures were formulated by Launder and Reynolds [25], Prud'homme and Elghobashi [26] and So and Yoo [27]. However, some of the earlier [25] and improved [28] near-wall closures were not asymptotically consistent and to correct this deficiency Lai and So [28] analyzed in detail the anisotropic behaviour of the Reynolds stresses near the wall, and developed an asymptotically correct near-wall Reynolds-stress closure, by improving the closures for the pressure redistribution and viscous dissipation. Based on the earlier investigations of Shima [29], Lai and So [28] incorporated an extra contribution to the production of ε in the rate of dissipation equation, which impacted favourably in the budgets of $\overline{u_i u_j}$. This had been found originally by Hanjalić and Launder [24], but Shima realized that the model proposed by Hanjalić and Launder [24] was not asymptotically correct near the wall. The Lai and So [28] model captures well the Reynolds stress anisotropy in turbulent pipe flow of Newtonian fluids, as also confirmed by Thakre and Joshi [30], who compared its predictions with those of the Prud'homme and Elghobashi [26] model. It was chosen at this stage to adapt Lai and So's model to deal with viscoelastic fluids than other models, such as Craft's [31]. Craft's [31] model is an extension of the Craft and Launder [32] model and is also able to capture well the Reynolds stress anisotropy. It is particularly suitable to recirculating flows and flows near walls with curvature and its predictions are in reasonable agreement with experimental and DNS data. The advantage of Craft's model is its independence from wall-normal vectors and distances, thus allowing its easy use in complex geometries, at the expense of a rather complex

formulation, but its adoption would imply more severe modifications to deal with viscoelastic fluids. Note also that following a different approach, Shima [33] developed a simpler low-Reynolds-number second-moment closure, and tested it in thin shear layer flows. Its overall performance was good, but its predictions of the normal Reynolds stresses in Newtonian turbulent channel flow were less accurate than those of Craft's [31] model.

Based in a Newtonian second-order turbulence model, for the first time, in this first part of this thesis, a Reynolds stress model is developed for viscoelastic fluids described by the modified Generalized Newtonian model of Pinho [1] and applied to predict fully-developed turbulent channel flows of polymer solutions. The present Reynolds stress closure is a step forward in the hierarchy of models for viscoelastic fluids and is based on the model of Lai and So [28] for Newtonian fluids. This base model was selected because it combines simplicity with a low Reynolds number capability, which is an essential requirement to deal with viscoelastic fluids for which no universal law of the wall exists. The performance of the model is tested against the experimental data of Escudier et al. [5] and Resende et al. [3] for dilute polymeric aqueous solutions.

1.4.3 Recent developments in turbulence models for viscoelastic fluids

Another approach to turbulence modelling for viscoelastic fluid flows is more fundamental and has been adopted by a wider selection of research teams, such as Dubief et al. [34], Shaqfeh et al. [35] and Pinho et al. [36]). Here, the development of the turbulence closures and their calibration and validation rely on post-processed DNS data for viscoelastic constitutive equations, such as the Finitely Extensible Nonlinear Elastic model, with Peterlin's closure (FENE-P), and the existing discrepancies relative to experimental data [16] can be attributed to the inherent simplicity of the underlying dumbbell model, such as the lack of configurational degrees of freedom, the oversimplification of the Peterlin closure of the FENE equation and concentration and polymer degradation effects in experiments, amongst others. In spite of the different

rheological constitutive equations upon which the turbulence models are based on, they share common features and predictive capabilities, therefore they are somewhat complementary. As an example, the earlier k - ε model of Pinho et al. [1, 13] largely facilitated the development of the k - ε model for the FENE-P fluid of Pinho et al. [4].

Due to the limits of the GNF constitutive equation the adoption of a truly viscoelastic constitutive equation including memory effects, such as the finitely extensible nonlinear elastic model with Peterlin's modification (FENE-P), was the obvious choice given the availability of DNS data. The DNS predictions of viscoelastic turbulent flows by Dimitropoulos et al. [37], Housiadas et al. [38] and Li et al. [39], amongst others, give insight into the physics of drag reduction by polymer additives, while providing useful data for developing adequate turbulence models. We also note that the latter work includes a zero-order eddy viscosity closure. The FENE-P model was used to describe fluid rheology in the above studies although some research has also been carried out with the Oldroyd-B and Giesekus models [17, 40]. The use of DNS for engineering calculations is prohibitively expensive and hence, one must resort to such techniques as large eddy simulation (LES) or RANS methods.. The latter is implicitly adopted in this work and follows, with the necessary adaptations, the work developed by Pinho and co-workers [2, 3, 13] for a modified generalized Newtonian fluid model.

As mentioned, the constitutive equation used in [14-16] lacked memory effects and constitutive equations based on polymer kinetic theory, such as the FENE-P model, are physically more realistic in their description of the rheology of the dilute and semi-dilute polymer solutions. However, as pointed out by Ptasiński et al. [16] there is a quantitative discrepancy between the experimentally measured and numerically predicted (by DNS) amounts of drag reduction when using the FENE-P model with the relaxation time measured in shear rheology and there are several causes for it. As pointed out by Gupta et al. [41], part of the issue is related to the closure inherent to the FENE-P constitutive equation. Its predictions could be improved by suitably renormalizing the extensibility parameter in the model or by using a different FENE closure [42]. Another cause of discrepancy is the limitation of the underlying dumbbell model, namely the lack of configurational degrees of freedom. On the experimental

side, one also encounters concentration effects and polymer degradation is very intense especially when using low concentrations of polymers with a very high molecular weight [43, 44]. Nevertheless, the DNS predictions are qualitatively correct and they provide self consistent and physically meaningful depictions of the energy transfer mechanisms in turbulent polymer drag reduction [38, 45-47].

In addition to the zero-order eddy viscosity model of Li et al. [39], there have been some earlier attempts at developing RANS/RACE turbulence closures for the FENE-P fluid (RACE stands for Reynolds-Averaged Conformation Equation), but unfortunately they have not appeared in the archival literature. Leighton et al. [48] derived a second order Reynolds stress model, where the main modifications were in the corresponding transport equation, namely in the pressure strain term and in the new terms containing the interactions between fluctuations of the polymer stress and kinematic quantities, for which closures were proposed.

Shaqfeh et al. [35] and Iaccarino et al. [49] modified the v^2 - f model of Durbin [50] relating the time-average polymer stress as a function of the conformation, as is obvious from its evolution equation, but in a simplified manner by invoking exclusively the relevance of extensional flow. As a consequence, instead of working with the full conformation tensor only an equation for its trace is required. They also introduced changes to the transport equation of k and especially to the transport equation of v^2 , where the term corresponding to the pressure strain is modified to depend on viscoelastic quantities. Instead of calculating the Reynolds average polymer stress from its definition and the Reynolds averaged conformation equation, which contains nonlinear terms that need to be closed as by [4], Iaccarino et al. [49] modelled directly the Reynolds-averaged polymer stress leading to a turbulence model with a smaller number of coefficient and functions. In the v^2 - f approach the eddy viscosity is made to depend on the transverse normal Reynolds stress rather than on the turbulent kinetic energy, but there is the extra cost of solving two additional differential equations, one of which is of elliptic nature. Their predictions were generally good in both low and high drag reduction, but regarding the turbulent kinetic energy the k - ε - v^2 - f model showed again deficiencies. At low drag reduction it underpredicted the peak turbulence and matched the turbulence in the log-law region as in Pinho et al. [4], but at high drag

reduction the good prediction of peak turbulence comes together with a significant over-prediction in the log law region.

Recently, in their development of a first order k - ε model for FENE-P fluids, Pinho et al. [4] relied on the Reynolds averaged form of the conformation tensor equation (C_{ij}) to determine the average polymer stress, as can be seen in Eq. (11), and they came up with a simple closure for the nonlinear tensor term, that quantifies the *cross-correlation between the fluctuating conformation and velocity gradient tensors arising from the distortion term of Oldroyd's upper convective derivative, hereafter referred to as NLT_{ij}* .

$$\frac{\partial C_{ij}}{\partial t} + U_k \frac{\partial C_{ij}}{\partial x_k} - \underbrace{\left(C_{jk} \frac{\partial U_i}{\partial x_k} + C_{ik} \frac{\partial U_j}{\partial x_k} \right)}_{M_{ij}} + \underbrace{u_k \frac{\partial c_{ij}}{\partial x_k}}_{CT_{ij}} - \underbrace{\left(c_{kj} \frac{\partial u_i}{\partial x_k} + c_{ik} \frac{\partial u_j}{\partial x_k} \right)}_{NLT_{ij}} = - \frac{\bar{\tau}_{ij,p}}{\eta_p} \quad (11)$$

Further they developed accurate closures for the viscoelastic stress work and for the viscoelastic - turbulent diffusion appearing in the transport equation of the turbulent kinetic energy (k). Since this set of closures was calibrated only with low drag reduction DNS data, their model was unable to predict higher drag reductions. The model also had deficiencies in predicting accurately secondary quantities such as the rate of dissipation of turbulent kinetic energy, but to our best knowledge is still the only existing first-order closure for a FENE-P fluid which is extensively documented in the archival literature.

In the context of single point closures, such as the k - ε , k - ω or Reynolds stress transport models, the Reynolds-averaged evolution equation for the conformation tensor contains the new term NLT_{ij} that requires closure so that the average polymer stress contribution to the turbulent momentum balance can be calculated. However, the relevance of NLT_{ij} is not limited to the evolution equation of the conformation tensor. As shown by Pinho et al. [4], NLT_{ij} and its trace also appear in closures developed for the viscoelastic stress work term of the transport equations of the Reynolds stresses and of the turbulent kinetic energy for viscoelastic fluids, respectively. The closure for the viscoelastic stress work developed in [4] was tested against DNS data for low drag reduction. An essential step in devising more generally applicable single point turbulence models for viscoelastic fluids described by the FENE-P rheological equation

of state is the development of a more accurate closure for NLT_{ij} , which is one of the aims of the second part of this thesis.

In their previous investigation, Pinho et al. [4] devised a simple model for NLT_{ij} based on a functional single-point relationship between this tensor and the set of parameters on which it depends. This functional relationship was reduced through the application of the principles of symmetry, invariance, permutation and realizability as inspired by Younis et al. [51, 52], but there could be still some problems of invariance due to the use of the vorticity tensor, which we address in the present development, amongst others. Besides, the model derived in [4] was limited to low drag reduction ($DR < 30\%$) and was unable to capture some of the features of the NLT_{ij} tensor, such as the negative peak of NLT_{11} at the buffer layer, and it underestimated NLT_{33} . The new closure for NLT_{ij} presented here is derived from its exact equation using physical insight from post-processed DNS data, order of magnitude analysis of terms and arguments from homogeneous isotropic turbulence. Here, the closures are extended to the high drag reduction regime. Specifically, additional modifications to the original model of Pinho et al. [4] include the direct incorporation of viscoelastic properties into the eddy viscosity model for the Reynolds stresses and the transport equation for the rate of dissipation of turbulence by the Newtonian solvent, which must necessarily be affected by the presence of polymer additives. Some of the closures developed by Pinho et al. [4] were also revisited, because on going from low to high drag reduction there were also changes in the relative magnitudes of the double and triple correlations that contributed to them.

More than one closure is developed for the NLT_{ij} tensor. Two are intended to be used in the context of first order turbulence models, and a third one is to be used within a second order turbulence model, even though here only a complete first order turbulence model, a $k-\varepsilon$ model, is proposed completing the second part of this thesis. Appropriate DNS data is used to justify some of the simplifying options and to calibrate the model coefficients. The DNS data pertain to the low and high drag reduction regimes and are part of the large sets of data produced by Li et al. [39] and Kim et al. [53, 54] for FENE-P fluids in fully-developed turbulent channel flow.

It is known that there are problems with the k - ε turbulence model associated to the lack of natural boundary condition of ε , and the appearance of higher-order correlations in the balance of the dissipation rate at the wall, which force the use of higher-order derivatives of the turbulent kinetic energy, leading to a not asymptotic behaviour and consequently to numerical stiffness. A possible solution to this problem is the use of a different turbulent length scale for the eddy viscosity closure which does not rely on ε . In this context Wilcox [55] developed the k - ω model, where the exact viscous terms next to the wall do not require modelling, thus leading to better predictions without the use of damping functions as is typical in k - ε closures. In addition, the k - ω model leads to more robust computations [56]. Nevertheless the behaviour of the original Wilcox model was asymptotically incorrect, because the contribution of the viscous cross-diffusion term was neglected. According to Menter [57], although the k - ω model predicts better wall-bounded flows than the standard k - ε model, in free shear layers the k - ω model is overly sensitive to free stream conditions. This deficiency was cured with the development of a combined k - ω and k - ε closure, called the SST (shear stress transport) model ([58, 59]), since the k - ε is robust where the k - ω has weaknesses and vice-versa. Other improvements to the original k - ω model involve the inclusion of the exact term of viscous cross-diffusion and of damping functions to obtain the correct asymptotic behaviour, as done by Speziale et al. [58] and Menter [59]. Their models improve the predictions in turbulent boundary layers especially under adverse pressure gradients. Further developments improved the performance in complex flows with recirculation, as done by Peng et al. [60] and Bredberg et al. [61], who also eliminated the dependence on a wall-function, while predicting the correct asymptotic behavior near walls.

In the third and final part of this thesis we investigate the improvements that a k - ω turbulence model can bring to the prediction of viscoelastic turbulent channel flow related to the k - ε framework and propose a k - ω turbulence model is developed for FENE-P fluids valid for both the low and high drag reduction regimes. The model is a modified form of the k - ω model of Wilcox [56], as presented by Bredberg et al. [61], incorporating new terms associated with fluid elasticity. The model is calibrated using

DNS data for fully-developed channel flow provided by Li et al. [19, 39] and Kim et al. [53] for the low and high drag reduction regimes ($DR < 30\%$ and $30\% < DR < 70\%$, respectively).

1.5 Contribution of this thesis

In the first part of this work a second order turbulence closure is developed, which is a contribution to the first group of turbulence models developed by Pinho and co-workers [2, 3, 13], i.e., it adopts as a constitutive equation the modified Generalized Newtonian fluid mimicking viscoelastic effects of relevance to turbulent flow. The advantage of the present Reynolds stress model, when compared to the previous $k-\varepsilon$ model, is the capacity to predict correctly the velocity profiles for all viscoelastic fluids tested. Thus, this second order model finishes a series of works where the adopted philosophy was to start from experiments and theory from some physical insight in to the causes of drag reduction.

In the second part, we developed models based on a different philosophy. Here, a proper viscoelastic constitutive equation that is adequate to model some of the most relevant physics of the dilute polymer solutions is adopted *ab initio*. Then, the turbulence models are developed. First, a $k-\varepsilon$ turbulence model is developed to predict low and high drag reductions building on the original model of Pinho et al. [4] and this, involves the development of a new closure for the non linear term, designated by NLT_{ij} , appearing in the tensor conformation equation (C_{ij}), which is necessary to solve the polymeric stress. A new closure for the eddy viscosity is also developed where the fluid viscoelasticity is directly incorporated. Finally, there are also other improvements to the model originally developed by Pinho et al. [4] for low drag reduction.

Then a second turbulence model for FENE-P fluids is developed, this time a new $k-\omega$ turbulence model for which most of the individual closures developed in the context of the $k-\varepsilon$ model apply. The advantages of the $k-\omega$ model are well know documented for Newtonian fluids, namely its capability to better predict turbulent flows in complex geometries, when compared to the previous model. The viscoelastic closures

developed in the context of the $k\text{-}\varepsilon$ model were implemented without any change in the $k\text{-}\omega$ model, meaning that the main viscoelastic physics was captured.

1.6 Organization of this thesis

This thesis is organized as follows: The next chapter presents flow characteristics and rheology of dilute polymeric solutions that exhibit drag reduction, and specifically the fluid properties used in the simulations and calibrations of the models. The constitutive equations used to represent the rheology of the elastic fluids are defined in chapter 3. In chapter 4 the first turbulence model is developed, namely the second order Reynolds stress turbulence model developed on the basis of the GNF constitutive equation and its performance is assessed in comparing with experimental data. For the FENE-P constitutive equation fluids the $k\text{-}\varepsilon$ and a $k\text{-}\omega$ first order turbulence models are developed in chapters 5 and 6, respectively. For these two models, the assessment of performance is carried out in comparison with DNS data. The paper closes with a summary of the main conclusions and suggestions of future work.

Chapter 2

Flow characteristics and rheology of dilute polymeric solutions

2.1 Flow characteristics

2.1.1 Experiments results

For the first time, in 1949, Toms reported the phenomenon of the drag reduction when using viscoelastic fluids in turbulent flows. In his work he measured the relation between the pressure drop and the volumetric flow rate in pipe turbulent flow, using dilute solutions at a high molecular weight polymer, in a Newtonian solvent. Since then, this phenomenon has attracted the attention of many researchers, which dedicated their time to understand the behaviour of viscoelastic fluids under turbulent flow conditions, due to the potential in engineering applications, such as in district heating and cooling systems or long distances fluid transportation.

It was also demonstrated extensively over the last fifty years [62-65] that the addition of small amounts of additives that impart viscoelastic properties to fluids is an effective way to reduce drag and heat transfer. These works and those referred to within were aimed at gathering information about the relationship between fluid rheology, polymer molecular weight and concentration on one side and drag reduction, Reynolds stresses and velocity profiles on the other. These investigations contributed to a significant increase in our phenomenological understanding of drag reduction and was carried out both experimentally and numerically, the latter via Direct Numerical Simulations (DNS).

Several researchers characterized the phenomenon of the non-Newtonian turbulent flow. For example: Dodge and Metzner [66] developed one correlation to predict the mean velocity profile and the pressure drop for shear thinning purely viscous fluids; Metzner and Park [67] studied viscoelastic fluids and measured a more intense drag reduction when comparing with inelastic fluids, observing also turbulence suppression in this type of flows; Virk [68] demonstrated that the drag reduction of the polymeric solutions leads to a positive shift of the mean velocity profile (in wall coordinates) from the Newtonian logarithm region. Also developed in 1967 were the

maximum drag reduction asymptotes, for the Darcy friction factor and for the mean velocity profile in wall coordinates (asymptote of Virk [68]). Other efforts were made in years 60 and 70 from the XX century, allowing a complete description of the drag reduction (DR) phenomenon and the proposal of several theories to explain the phenomenon. The first extensive bibliography reviews about the DR are from that period of time, (Hoyt [69] and Virk [70]), being updated later by Gyr and Bewersdorff [71].

Studies that contributed to a deeper understanding of the physics of wall flows, due to development of the optic diagnostic techniques, were the recently experiments of Pinho and Whitelaw [72], Pereira and Pinho [73], Escudier et al. [5] e Warholic et al. [74], among others. An important contribution of Escudier et al. [5] consisted in the measurements of the extensional rheology properties of the polymeric solutions for several concentrations, together with the measurements of the mean quantities of the turbulent flow, such as the friction factor and the corresponding mean velocity profiles.

Also using shear thinning viscoelastic polymeric solutions, Pinho and Whitelaw [72] measured the mean velocity profiles and the normal Reynolds stresses in turbulent pipe flows and verified the existence of an increase of turbulence anisotropy, corresponding to an increase of the axial turbulence and a reduction of the other two normal components of the Reynolds stress tensor. They also quantified a delay in the transition from laminar to turbulent flow, due to the suppression of turbulence (especially in the tangential and radial components), caused by the presence of the polymer molecules. Besides, they showed for the first time that the use of the wall viscosity with these shear-thinning solutions instead of the solvent viscosity was more appropriate to represent the similarity of the flow dynamics, due to the polymer effect near the wall. The behaviour of the normal Reynolds stresses for viscoelastic fluids can be observed in **Fig. 3**, namely the increase of the axial normal Reynolds stress component and the reduction of the other two normal components for pipe turbulent flow with 0.125% PAA at $Re=42900$, Resende et al. [3].

The subsequent studies of Pereira and Pinho [73], with low molecular weight polymer solutions confirmed the difficulty in finding shear-thinning fluids based in polymeric

additives that did not show viscoelastic drag reduction, confirming the experimental results obtained before by Pinho and Whitelaw [72], but to a smaller degree.

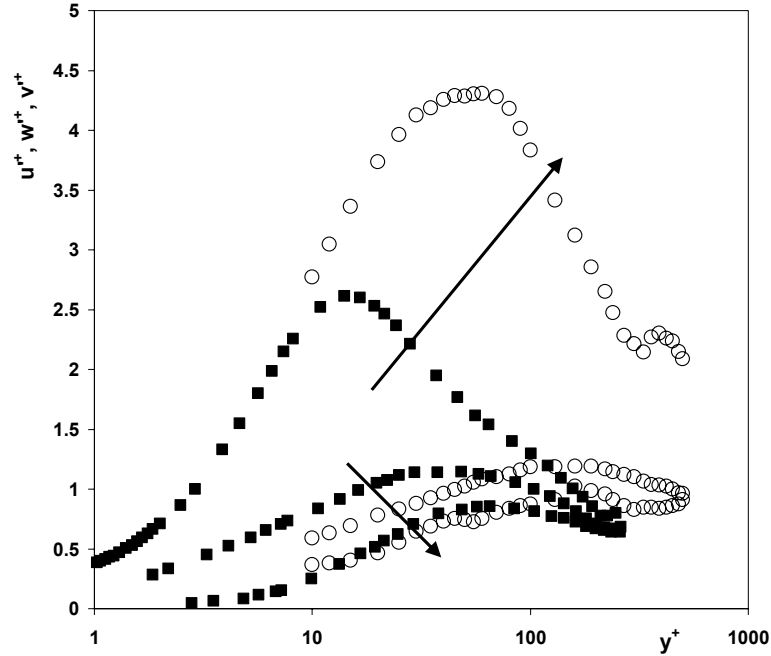


Fig. 3. Experiment data of the normal Reynolds stresses in turbulent pipe flow with Newtonian and viscoelastic fluids: ■ Newtonian at $Re=7440$; ○ 0.125% PAA at $Re=42900$. From Resende et al. [3].

Another characteristic behaviour, found in experimental investigations of channel flows, was the drastic reduction of the Reynolds shear stress. The deficit observed in the shear Reynolds stress must be considered by the appearance of an extra shear stress of elastic origin that, at the present date, has not yet been directly measured. This finding suggests a new turbulence dynamics involving, among others, the connection between the elastic stress fluctuations and the velocity gradients. It was confirmed by the experiments of Ptasiński et al. [15, 16], which found that the polymer stress fluctuations interact with the turbulence and the mean flow. In certain conditions the effect is similar to an increase of the dissipation, having also similarities with the anisotropic effect in the stresses. In fact, when decoupling the shear stress into viscous, inertial and polymer components, the latter can assume both positive and negative values, i.e. it can act as a source or as a sink of turbulent kinetic energy. The behaviour

of the shear Reynolds stress reduction with drag reduction increase can be observed in **Fig. 4**, based in experimental data of Ptasiński et al. [15] in turbulent pipe flow with partially hydrolyzed polyacrylamide fluids for different concentrations, 20 wppm (weight parts per million) and 103 wppm, which corresponds a drag reduction of 23% and 63%, respectively.

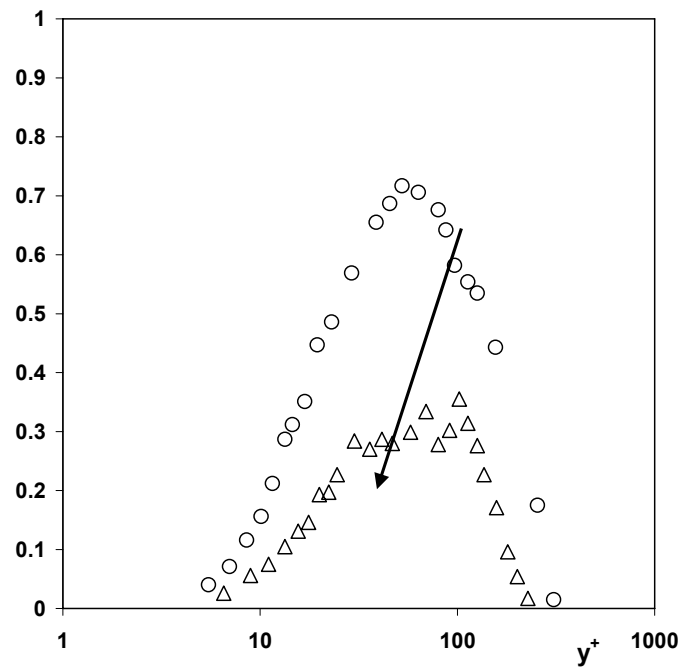


Fig. 4. Experimental data of the shear Reynolds stress in turbulent pipe flow with different concentrations of partially hydrolyzed polyacrylamide fluids: ○ 20 wppm (weight parts per million), DR=23%; Δ 103 wppm, DR=63%.

The theory initially formulated by Lumley [75] to explain the drag reduction, is still seen as physically relevant. The mechanism proposed was based on an increase of the extensional viscosity near to the wall, caused by the extensional deformation of the molecules by turbulence. As the molecules are stretched, their resistance to extension increases, and consequently increasing the viscosity. Higher resistance to the extensional deformation interferes with the vortex stretching mechanisms and consequently with the energy cascade, interfering deeply with the physical mechanisms of turbulence. In steady laminar shear flows, the stretching and rotation of the molecules occurs simultaneously, therefore the molecules do not stand on the deformation field too

long, and their total deformation is limited; still, under turbulence conditions, there are molecules stretching without rotation and in this case the molecules can be drastically stretched if flow conditions are such that the molecules go beyond the coil-stretch transition. Note that the theory developed before is speculative because the extensional viscosity of the polymeric solutions was not measured in the same conditions that occurs in the turbulent flow.

The theory described before gained support as the experimental results demonstrated the appearance of normal deformation rates in the flows, next to the wall, with polymeric solutions, like the studies of Luchik and Tiederman [76], among others. According to these authors, the resistance of fluid molecules to the normal deformation increases exponentially with the deformation rate and not linearly; this increase of the resistance to the normal deformations interferes with the turbulence production specially with the dissipation mechanisms, thus increasing the dimensions of the vortices and the correspondingly reducing its frequency. Summarizing, this picture suggests that is the entanglement of the polymeric chains, in a presence of turbulent flows with polymeric solutions that provoke an increase of the fluid extensional viscosity interfering with the turbulence dynamics and reduction the friction, due to the extension and contraction of the polymeric molecules. The appearance of the DNS simulations helped to better understand the interplay between polymer chain dynamics, i.e., extensional viscosity, relaxation time and polymer stress, and flow dynamics, i.e., turbulent fluctuations and coherent structures.

2.1.2 DNS simulations

The availability of increased computer power has offered an important research alternative by providing the means for direct numerical simulations (DNS). Starting with Massah et al. [77] the DNS have provided useful information on the molecular conformation of polymeric solutions and on the corresponding rheological properties, confirming the relevance of the extensional effects on the turbulence. Note that the initial DNS investigations were not self-consistent as they only solved the constitutive

equation, usually the FENE-P model, for fixed Newtonian kinematics. This strategy, adopted Hanratty and co-workers [77] e [78] was not able to predict drag reduction, as happened with the Newtonian DNS, but gave insight into the evolution of the molecular configurations and the corresponding fluid properties, with the turbulence dynamics. One of their main findings was the large molecular extensions in the viscous sublayer but not significant molecular extensions in the buffer layer. For viscoelastic fluids there is, however, an important difficulty when comparing to Newtonian DNS; *a priori* we do not know for sure what is the correct rheological constitutive equation for a specific fluid. Even so, the DNS techniques are supplying useful information that allows researchers a better choice in terms of constitutive equation, and more importantly, to develop closures more accurately for classics models or for new turbulence models.

Others initial DNS investigations had exploratory objectives concentrated in a purely viscous constitutive model to analyze the different characteristics and potential of the models and physics properties. Den Toonder et al. [79] and [64], and Orlandi [80] showed only small magnitudes of drag reduction when using purely viscous isotropic constitutive equations, but demonstrated a strong effect associated to the use of anisotropy viscous and elastic constitutive models. In contrast, the DNS simulations of turbulent channel flows of Sureshkumar et al. [81] using FENE-P and Giesekus fluids, achieved significant amounts of drag reduction and showed that the results were qualitatively in agreement with experiments. They also emphasized a possible strong relationship between the drag reduction intensity and the extensional viscosity of the polymeric solutions, due to the extensions of the polymeric chains which was later confirmed in more advanced DNS studies. In conclusion the DNS simulations clearly demonstrated that purely viscous constitutive equations can not predict the high drag reductions observed and that elasticity is an essential ingredient for such phenomenon.

DNS investigations allowed more conclusions to be drawn and one of the findings was the change in the turbulence kinetic energy distribution by the polymer, for example by Dubief et al. [82] studied the turbulence-enhancing behaviour of polymers in wall flows and verified that polymers were responsible for dampening near-wall vortices and enhance streamwise kinetic energy in near-wall streaks, leading to a self-sustained drag-reduced turbulent flow. This modification of the turbulent cascade by

polymeric additives was also confirmed by De Angelis et al. [83] who verified two situations: a pure damping of the entire range of scales, for small Deborah numbers; and a depletion of the small scales accompanied by increased fluctuations at large scales at larger values of De . They also observed an increase of turbulence intensity when the crossover scale becomes larger than the Taylor microscale, where the flow, from being inertia-dominated, becomes controlled by viscoelasticity. Results from Tesauro et al. [84] of the elastic energy budget showed that the interactions between polymers and turbulence appeared to be small in an average balance, but reaching very large values instantaneously and intermittently, which implied a strong local interaction between turbulence and polymers. This also demonstrated that the amount of interaction between polymers and turbulence depends largely on the extensibility parameter b , which is an important parameter for polymer drag reduction.

Dimitropoulos et al. [37] have also provided budgets of turbulence kinetic energy, Reynolds stresses and vorticity and consequently it is a major reference for the development of single-point turbulence closures. But even with an increased availability of computational power, our predictive capability of non-Newtonian viscoelastic turbulent flows remains very limited. This has motivated the use of DNS of viscoelastic turbulent flow in a simple geometry such as the plane channel [38, 64, 81] to help differentiate among low order turbulence closures, which could be employed in the modelling of complicated flows encountered in industrial applications [4, 39, 85]. These models are developed within the framework of Reynolds-Averaged Navier-Stokes (RANS) equations.

2.2 Rheology of viscoelastic fluids

2.2.1 Basic principles of rheology

The most important rheological property of dilute polymeric solutions is the viscosity, which often shows shear-thinning, i.e., a decrease as the shear rate increases.

This can be seen in the Fig. 5, where two different shear viscosity behaviours are presented.

Note that for very dilute polymer solutions the amount of shear-thinning can be very small, even non-existing. Elastic fluids of constant viscosity are called Boger fluids [86] and these are important fluids as they allow the separation of elastic and shear-thinning effects.

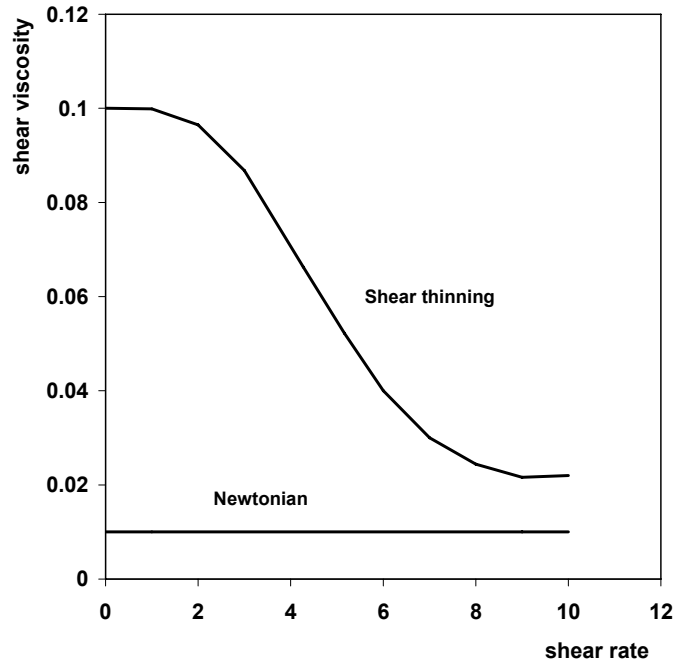


Fig. 5. Example of the shear viscosity behaviour of a Newtonian and a dilute polymeric solution fluids.

The viscoelastic fluids present simultaneously viscous and elastic effects, with a main characteristic of storing energy under elastic form. One of the effects that viscoelastic fluids demonstrate in steady shear flow are non-zero normal stress differences, N_1 and N_2 . In this type of flows the first normal stress difference, $N_1 = \sigma_{11} - \sigma_{22}$, takes positive values, meanwhile the second normal stress difference, $N_2 = \sigma_{22} - \sigma_{33}$, take negative values, obeying the relation $|N_1| \geq |N_2|$. Both are null for Newtonian fluids.

Extensional flows of non-Newtonian elastic fluids exhibit different characteristics when compared to Newtonian fluids, so it constitutes another fundamental rheological flow. Here, the relevant fluid propriety is the extensional viscosity.

In a uniaxial extensional flow the velocity field is defined by:

$$v_1 = \dot{\epsilon}x, \quad v_2 = -\dot{\epsilon}/2 y \quad \text{and} \quad v_3 = -\dot{\epsilon}/2 z \quad (12)$$

where $\dot{\epsilon}$ is the constant extensional strain rate. This means that a positive extensional strain exists in the xx (or 11) direction, $\dot{\epsilon}_{11} = \dot{\epsilon}$, and by continuity the yy (or 22) and zz (or 33) components are $\dot{\epsilon}_{22} = -\dot{\epsilon}/2$ and $\dot{\epsilon}_{33} = -\dot{\epsilon}/2$. The correlated stress distributions are

$$\begin{aligned} \sigma_{11} - \sigma_{22} = \sigma_{11} - \sigma_{33} &= \eta_e(\dot{\epsilon}) \cdot \dot{\epsilon}, \\ \sigma_{12} = \sigma_{13} = \sigma_{23} &= 0, \end{aligned} \quad (13)$$

where η_e is the uniaxial extensional viscosity, which is a function of the extensional strain rate, as the shear viscosity is a function of shear rate $\dot{\gamma}$. Parameters $\dot{\epsilon}$ and $\dot{\gamma}$ have a direct physical interpretation: in simple shear flows, $\dot{\gamma}$ reduces to shear rate and $\dot{\epsilon}$ becomes null; in uniaxial extensional flows, $\dot{\epsilon}$ reduces to strain rate and $\dot{\gamma} = 0$. For a Newtonian fluid the extensional viscosity obeys the relationship $\eta_e = 3\eta$.

We can conclude that the extensional viscosity is related to the difference of the normal stresses by the following equation,

$$\eta_e = \frac{\sigma_{11} - \sigma_{22}}{\dot{\epsilon}} = \frac{N_1}{\dot{\epsilon}} \quad (14)$$

Thus, it is possible to determine the elasticity of the viscoelastic fluid through N_1 e N_2 in shear and in extensional flows, but it is important to understand that there are others fundamental flows that provide a measure of the elastic behaviour of non-Newtonian fluids, such as oscillatory shear flow under small amplitude (SAOS-small amplitude oscillatory shear).

In a oscillatory shear flow we impose a sinusoidal periodic strain of low amplitude (γ_0),

$$\gamma(t) = \gamma_0 \cos(\omega t) \quad (15)$$

and measure the corresponding stress

$$\tau(t) = \tau_0 \cos(\omega t - \delta) \quad (16)$$

This equation gives two distinct limits behaviours: the pure elastic solids behaviour, where the stress is proportional to the strain amplitude (Hooke law), and the pure viscous fluids behaviour, where the stress is proportional to the shear rate (Newton law). For viscoelastic fluids there is a phase difference, δ , between the stress and the imposed strain, so the fluid response can be divided in two components: one with a phase equals to the strain and the other with a phase shift to of 90° , corresponding to the elastic and viscous parts, respectively.

The fluid properties are defined by these two components, elastic and viscous, through (i) the ratio between the stress and the strain, (ii) and the ratio between the stress and shear rate. The total resistance to the strain is given by the complex shear modulus,

$$G^* = G' + iG'', \quad (17)$$

defined by the elasticity modulus, G' ,

$$G' = \frac{\tau_0}{\gamma_0} \cos \delta \quad (18)$$

that represents a measurement of the reversible storage strain energy (elastic component) and by the dissipation modulus, G'' ,

$$G'' = \frac{\tau_0}{\gamma_0} \sin \delta \quad (19)$$

that represents a measurement of the irreversible energy loss by the fluid (viscous component). The two moduli give a measurement of the material viscoelasticity degree, i.e., if the material approaches to an elastic solid or a viscous liquid.

The oscillatory shear test only presents characteristics independent of this kinematics if the test is carried out at low strain conditions, i.e., only under these conditions the fluid behaves in the linear regime where the fluid moduli are independent of the amplitude of the applied stress or strain.

Another parameter that the rheology researchers introduced was the Trouton ratio, Tr , which is defined by the ratio between the extensional and the shear viscosities,

$$Tr = \frac{\eta_e(\dot{\epsilon})}{\eta(\dot{\gamma})} \quad (20)$$

Elastic fluids are characterized by high Trouton ratios. In the case of inelastic fluids, the shear viscosity is evaluated by $\dot{\epsilon}$ through the relation $\dot{\gamma} = \sqrt{3}\dot{\epsilon}$ and the Trouton ratio in uniaxial extension becomes constant at a value 3, for all range of $\dot{\epsilon}$.

The viscoelastic fluids of polymeric solutions analyzed in the present work, are shear-thinning in terms of shear viscosity, but they are strain-thickening of the Trouton ratio. This means that we can have different combinations of shear and extensional viscosities.

2.2.2 Fluid properties

After the development of the turbulence models, it is required to calibrate and validate them based on experimental data or DNS data. So is essential to have for the same fluids the rheological properties as well as the flow measurements, such as the global mean quantities of the flow (for example, the friction factor and volumetric flow) and the local mean quantities, which characterize the mean and turbulent flow (mean velocity profiles, normal Reynolds stresses). In the case of the turbulence models

developed for FENE-P fluids and based in the DNS data, the flow characteristics are analyzed by changing the rheological parameters, and not in experimental fluid rheology. In this chapter, the rheology proprieties of the experimental fluids used to calibrate and validate the Reynolds stress turbulence model is presented.

The experimental data used to validate the Reynolds stress turbulence model developed of the modified GNF fluids is that of Escudier et al. [5]. The rheology and the fluid dynamics properties measurements use the following polymer solutions:

- Semi-rigid molecule chain, but flexible (CMC - sodium carboxymethylcellulose), with a concentration of 0.25% by weight;
- Rigid tubular molecule form (XG – xanthan gum), with a concentration of 0.2% by weight;
- Very flexible expanded molecule chain (PAA - polyacrylamide), with a concentration of 0.125% by weight.

A blend of 0.09% CMC with 0.09% XG was also used.

The 0.125% PAA and the 0.2% XG were selected to calibrate the turbulence model, and the remaining fluids were used in the validation process. Note that the calibration and validation was only possible because Escudier et al. [5] measured both kinematic flow quantities and the fluid rheology of the viscoelastic fluids.

Each of these polymer solutions has already extensively used in previous investigations of non-Newtonian flows (for example, Pereira and Pinho [87] and Escudier et al. [5]).

The shear viscosity of those polymer solutions plotted in **Fig. 6**, where the shear-thinning effect of each fluid is well captured by the Cross model, Eq. (21).

$$\frac{\mu_0 - \mu}{\mu - \mu_\infty} = (\lambda \dot{\gamma})^{m_c} \quad (21)$$

The values of the parameters of Eq. (21) for each fluid, are listed in Table 1. Although these rheological data are shown for a temperature of 20 °C, similar measurements were made over a range of temperatures so that the viscosity values used to evaluate the Reynolds numbers correspond to the measured liquid temperature during the flow experiments. In a plot of the shear viscosity versus shear rate in log–log

coordinates, a Newtonian plateau at low shear rates is evident for the CMC solution. Otherwise, all fluids were found to exhibit almost power-law behaviour except at the highest shear rates ($>1000/s$) for PAA where the data were adversely affected by the onset of secondary flow, according Escudier et al. [5].

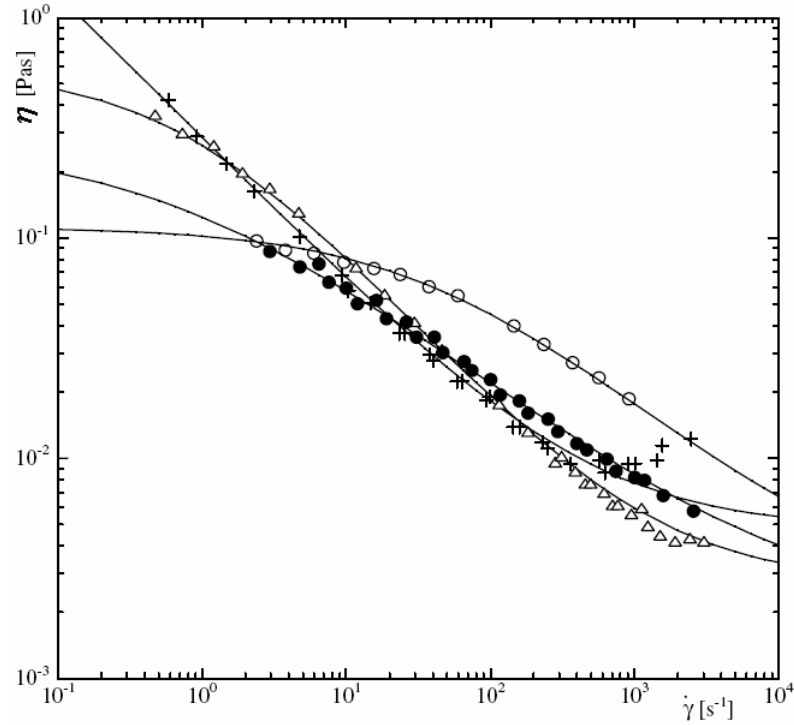


Fig. 6. Shear viscosity against shear rate measurements for polymeric solutions, Escudier et al. [5]: o 0.25% CMC, • 0.09% CMC / 0.09% XG, Δ 0.2% XG, + 0.125% PAA. Solid lines curves represent the Cross-model.

Table 1. Cross-model parameters at 20 °C, Escudier et al. [5].

Fluid	$\mu_0(Pas)$	$\mu_\infty(Pas)$	$\lambda(s)$	m
0.25% CMC	0.112	0.00239	0.0214	0.595
0.09% CMC / 0.09% XG	0.267	0.00200	1.34	0.512
0.2 % XG	0.578	0.00276	1.30	0.724
0.125 % PAA	29.6	0.00481	1090	0.664

At the concentrations used here, the first normal-stress differences for CMC, XG and CMC/XG were below the sensitivity of the rheometer even at the highest shear rates. However, as suggested by Barnes et al. (1989), at higher concentrations it was found that $N_1(\tau)$ followed a power law master curve for each fluid, almost independent of concentration, from which it was possible to extrapolate to lower concentrations. This procedure, also used by Escudier et al. [5], is not ideal but has to suffice in the absence of either a direct measurement or a more sophisticated extrapolation algorithm. The data result that are showed in Fig. 7, result from the following empirical expressions

$$N_1 = 0.85\tau^{1.25} \quad 0.6\text{-}1.5\% \text{ CMC}, \quad (22)$$

$$N_1 = 0.97\tau^{1.47} \quad 1.0\text{-}1.5\% \text{ XG}, \quad (23)$$

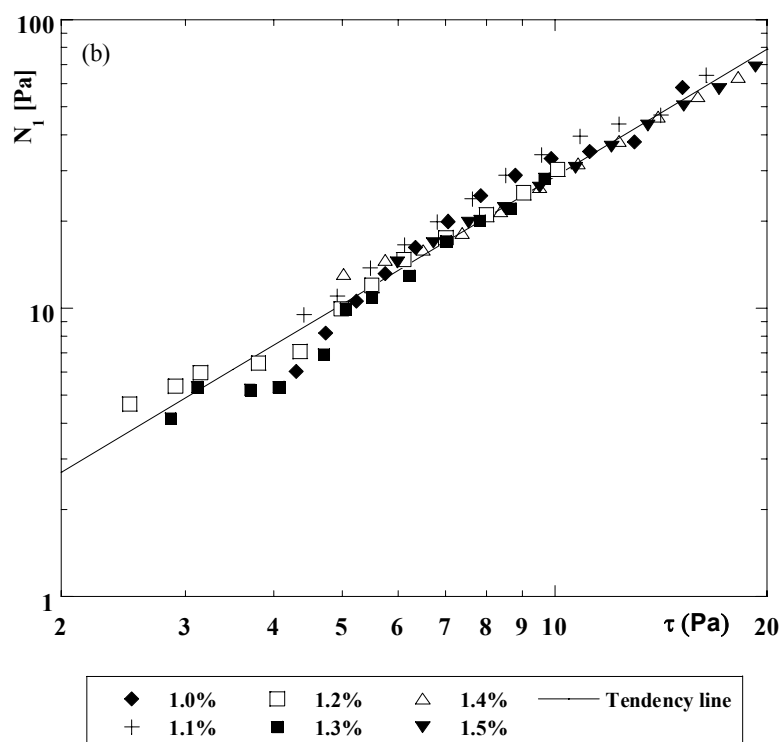
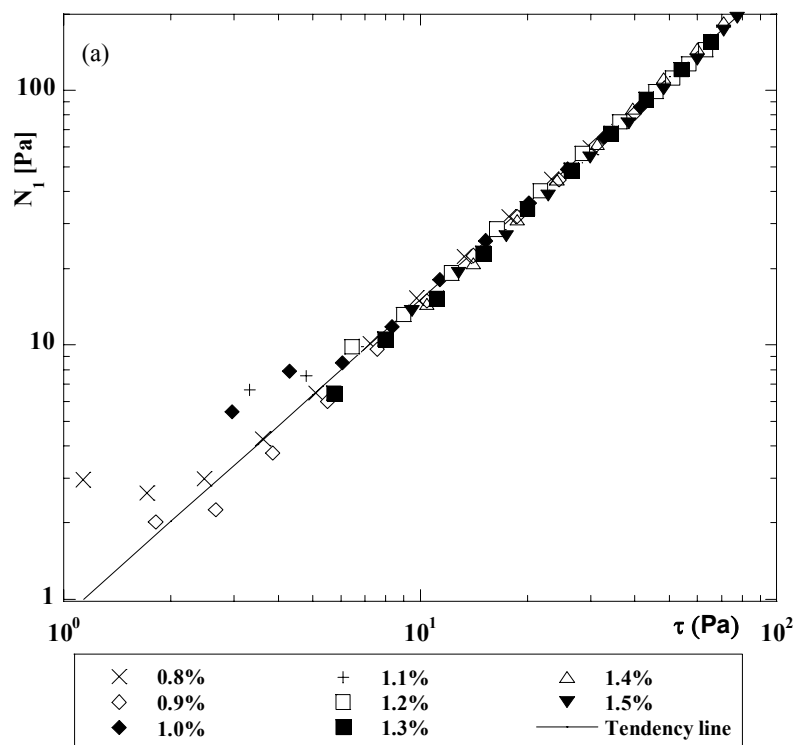
$$N_1 = 1.35\tau^{1.18} \quad 0.4/0.4\text{-}1.5/1.5\% \text{ CMC/XG}. \quad (24)$$

According to Barnes et al., a recoverable shear (i.e., $N_1/2\tau$) greater than 0.5 indicates a highly elastic state. For the three polymer solutions considered here, this condition corresponds to shear stresses in excess of 1.9 Pa (CMC), 1.1 Pa (XG) and 0.2 Pa (CMC/XG), i.e., they are highly elastic according to the plots. Note that for PAA the N_1 values were above the sensitivity limit of our rheometer and it was possible to obtain (N_1 versus $\dot{\gamma}$) data directly and these are well represented by

$$N_1 = 16.3\tau^{1.48} \quad 125\% \text{ PAA} \quad (25)$$

so that 0.125% PAA can be said to be highly elastic for $\tau > 0.003$ Pa.

The normal stress characteristics $N_1(\dot{\gamma})$ for all the fluids tested are shown together in **Fig. 8**. Observing the figure, we can conclude that the fluid viscoelasticity at low shear rates is by the following order: CMC, CMC/XG, XG e PAA, meanwhile for high shear it becomes: XG, CMC/XG, CMC e PAA.



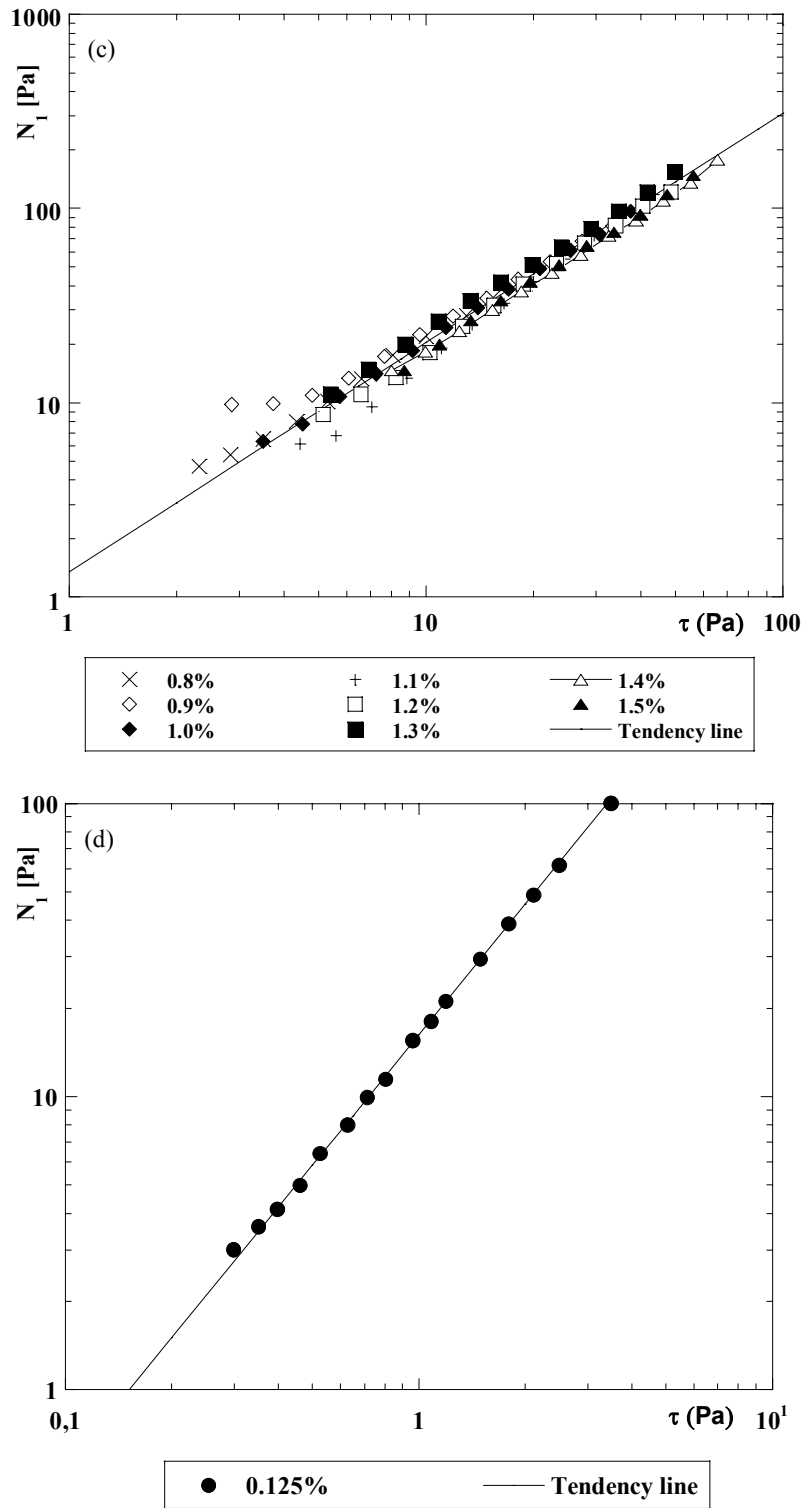


Fig. 7. Viscoelastic characteristics of the polymeric solutions concentrations, Escudier et al. [5]: (a) CMC; (b) XG; (c) CMC/XG; (d) 0.125% PAA.

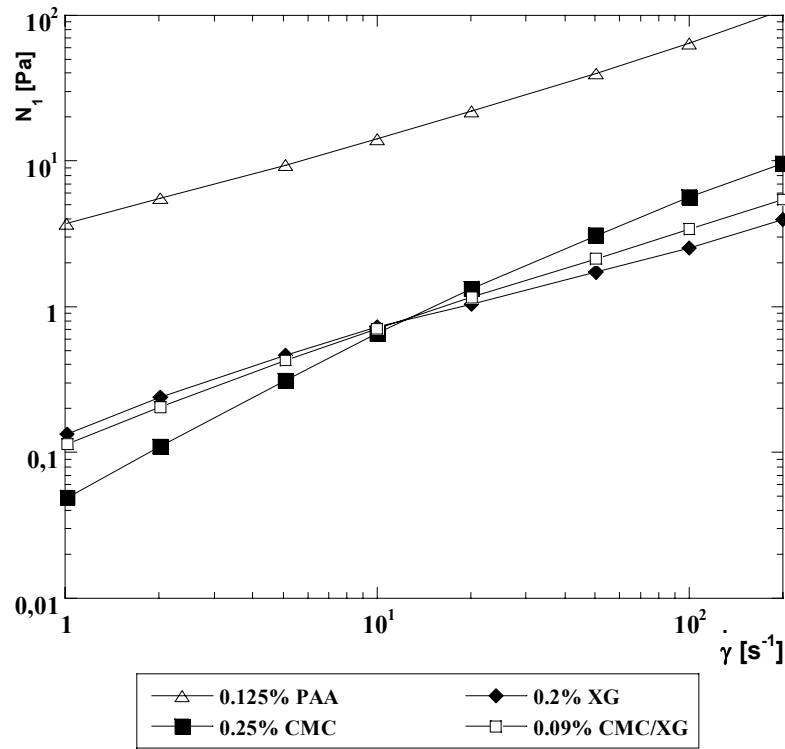


Fig. 8. First normal stress difference for the different polymeric solutions used, Escudier et al. [5].

Fig. 9 presents the extensional viscosity versus strain rate measured directly by the RFX opposed-nozzle rheometer, data obtained by Escudier et al. [5]. The anomalous behaviour detected was that XG appeared to be more elastic than PAA at very low strain rates. This trend is not totally unexpected since the solution of XG behaves as a gel at low rates of deformation and its structure breaks down in strong shear and/or extension.

It is important to note that the RFX does not provide the exact extensional viscosity, but an apparent extensional viscosity, i.e., the data must be regarded with some caution.

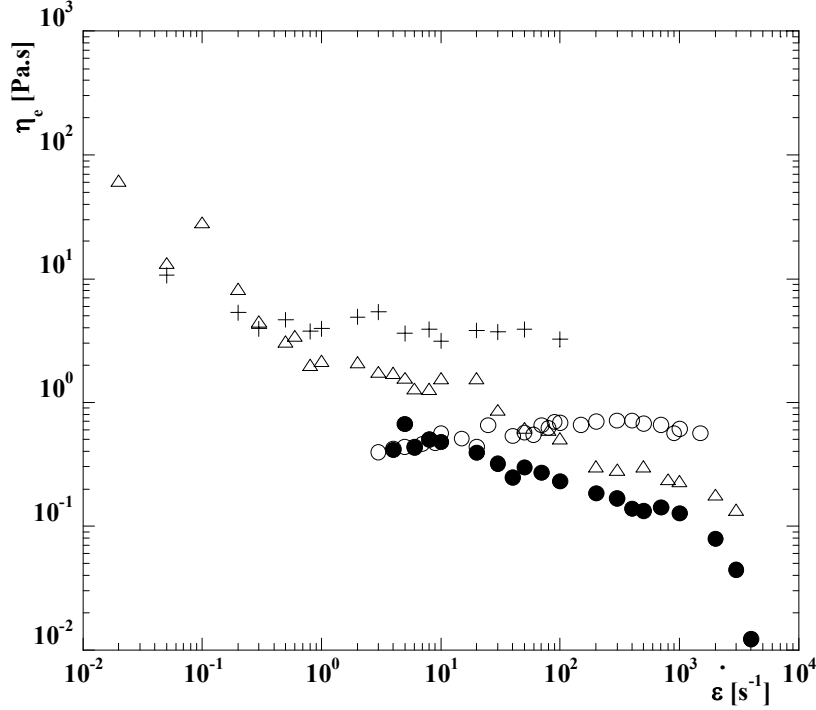


Fig. 9. Extensional viscosity variations versus strain rate for polymeric solutions, Escudier et al. [5]: o 0.25% CMC, • 0.09% CMC / 0.09% XG, Δ 0.2% XG, + 0.125% PAA.

2.3 Closure

The rheology characteristics measured for the viscoelastic fluids allowed to adjust the rheological parameters of the fluids used in the numeric simulations. The main objective is to capture the kinematics of the flow for each viscoelastic fluid, because for the same geometry and initial flow conditions, we will obtain different flow behaviour, as the elastic contribution of the fluid increases. And the rheological parameters give the elastic degree of the fluid, essential to the turbulence model to capture the correct viscoelastic phenomenon, predicting correctly the mean and local quantities of the flow.

To capture the rheological phenomenons described before of the polymeric dilute solutions: the shear-thinning viscosity effect and the strain-thickening of the Trouton ratio; it is necessary to choose the constitutive equation creating the link to the kinematic of the flow through the turbulence model. In the next chapter will be defined the constitutive equations used in this thesis.

Chapter 3

Constitutive equations

3.1 Basic principles

Constitutive equations are relations that describe the complex rheological behaviour of fluids relating the stress tensor with the kinematic quantities. Depending on the mathematical relationship, the equation can be linear, quasi-linear or non-linear, but mostly are non-linear. This classification applies to viscoelastic fluids and the linear rheological constitutive equation is based on a simple principle where the response at any time is directly proportional to the value of the input signal, i.e., for example, for a fixed stress we obtain a directly proportional strain rate. The differential equations, in the linear viscoelasticity theory, are linear and the coefficients of the time differentials are defined by the material parameters. These material parameters such as, for example, the viscosity coefficient and the rigidity modulus, are constant not depending on variables such as strain or strain rate.

The simplest constitutive equations used for viscoelastic fluids were based in the generalized Newtonian fluids constitutive equation, defined by Eq. (26), where the viscosity is not constant and depends on the shear rate $\mu(\dot{\gamma})$, capturing only the shear thinning effect of the polymeric solutions. This type of model is not viscoelastic because it is not able to predict the elastic contribution, i.e., it neither has memory effect nor normal stress effects.

$$\tau = \mu\dot{\gamma} \quad (26)$$

One of the first linear viscoelastic constitutive equation, was the Maxwell model, which combines viscous with elastic behaviour by the following equation,

$$\tau + \frac{\eta}{G} \frac{\partial \tau}{\partial t} = \eta\dot{\gamma} \quad (27)$$

For steady flows this equation reduces to a Newtonian fluid, with constant viscosity, η . For rapid stress variations, the time derivative term dominates (left side of the equation), and when integrated in time it simplifies to a Hooke solid with elastic modulus G . Another form to present the Maxwell model, Eq. (27), is

$$\tau + \lambda \dot{\tau} = \eta \dot{\gamma} \quad (28)$$

with $\lambda = \eta/G$. If a particular strain rate $\dot{\gamma}$ is suddenly applied at $t = 0$ and held at that value for subsequent times, the stress evolution over time (for $t > 0$) becomes

$$\tau = \eta \dot{\gamma} [1 - \exp(-t/\lambda)], \quad (29)$$

i.e., the stress relaxes exponentially from its equilibrium value to zero.

Another similar model to the Maxwell is the Kelvin model, which is defined by the following equation

$$\tau = G\gamma + \eta \dot{\gamma} \quad (30)$$

In this case, if a stress $\hat{\tau}$ is applied in the instant $t=0$ and kept constant, the strain, using the Kelvin model, becomes

$$\gamma = (\hat{\tau}/G) [1 - \exp(-t/\lambda)] \quad (31)$$

This means that the strain is retarded and not obtained "instantaneously" the final value of strain, typically in a Hooke elastic solid.

The linear constitutive models like the Maxwell and Kelvin models, among others, can only be used as theoretical models due to their limitations. They can only be applied to flows with small infinitesimal strain gradients. These models can not: (i) predict normal stresses (non-linear effect); and (ii) describe variable viscosity.

3.2 Quasi-linear constitutive models

A more severe limitation of the linear constitutive models is that they do not obey the principle of Oldroyd's material objectivity where they had to be formulated for general validity. The quasi-linear constitutive models solved this problem by replacing the material derivatives with Oldroyd's convected derivatives. For example, both the Upper Convected Maxwell (UCM) and the Oldroyd-B models result from a substitution of the material derivatives by the contravariant convected derivative, and have the capacity to

predict the first normal stress coefficient and are invariant to coordinate system changes. The Oldroyd-B model is defined by the following equation

$$\tau + \lambda_1 \dot{\tau}_{(1)} = -\eta_0 \left(\dot{\gamma}_{(1)} + \lambda_2 \dot{\gamma}_{(2)} \right) \quad (32)$$

with

$$\begin{aligned} \dot{\gamma}_{(1)} &= \dot{\gamma} \\ \dot{\gamma}_{(2)} &= \frac{D}{Dt} \dot{\gamma}_{(1)} - \left\{ (\nabla v)^\dagger \cdot \dot{\gamma}_{(1)} + \dot{\gamma}_{(1)} \cdot (\nabla v) \right\} \end{aligned} \quad (33)$$

and

$$\dot{\tau}_{(1)} = \frac{D}{Dt} \dot{\tau} - \left\{ (\nabla v)^\dagger \cdot \dot{\tau} + \dot{\tau} \cdot (\nabla v) \right\} \quad (34)$$

This constitutive equation contains three parameters: η_0 , the zero-shear-rate viscosity; λ_1 , the relaxation time and λ_2 , the retardation time. The model contains, as special cases the following models: if $\lambda_2 = 0$ the model reduces to the Upper Convected Maxwell model; if $\lambda_1 = 0$ the model simplifies to a second-order fluid with a vanishing second normal stress coefficient; and if $\lambda_1 = \lambda_2$, the models reduces to a Newtonian fluid with viscosity η_0 , more details can be found in Bird et al. [88].

The quasi-linear models are capable of describing time-dependent flows, however, these models are not able to portray well the rheological proprieties of the polymeric solutions. For example, the deficiencies of constant viscosity and normal stress coefficients in steady shear flow and the infinitive elongational viscosity at finite elongation rates.

3.3 Non-linear constitutive models

To correct the limitations of the previous models, non-linear differential models have been formulated which include, among others invariant properties by the

dependence on $\dot{\gamma} = \sqrt{(\dot{\gamma}_{(1)} : \dot{\gamma}_{(1)})}/2$; quadratic terms in velocity gradient; and nonlinear terms in stress, associated to the polymeric contribution. These models are designated by the non-linear constitutive models, like for example the Giesekus model, given by the Eq. (35).

$$\tau_p + \lambda_1 \dot{\tau}_{p(1)} - \alpha \frac{\lambda_1}{\eta_p} \{\tau_p \bullet \tau_p\} = -\eta_p \dot{\gamma} \quad (35)$$

The Giesekus model contains four parameters: a relaxation time λ_1 ; the solvent and polymeric viscosities, η_s and η_p , contributions to the zero-shear-rate viscosity, η_0 ; and the dimensionless mobility factor α . The origin of the term involving α can be traced back to the anisotropic Brownian motion and/or anisotropic hydrodynamics drag on the constituent polymer molecules.

The inclusion of the $\{\tau_p \bullet \tau_p\}$ term in Eq. (35) gives material functions that are more realistic than those obtained with the Oldroyd-B model. For example, capturing shear-thinning of the viscosity and of the normal stress difference coefficients, and bounding the extensional viscosity.

Besides the Giesekus model, there are more complex models, where the stress coefficients are variable quantities depending on stress invariants. Some very well known models are based on molecular kinetic theories such as the FENE-dumbbell (“finitely extensive, non-linear elastic”), developed to represent dilute or semi-dilute polymeric solutions, which is capable to predict the shear-thinning effect of the viscosity and of normal stress difference coefficient.

The FENE dumbbell is an elementary non-linear kinetic model in which the polymeric part is described by two identical Brownian beads connected through an entropic spring. The beads experience the action of Brownian forces and the Stokes drag exerted by the solvent, while the entropic spring models intramolecular interactions, Lielens et al. [89]. The configuration of the polymer is given by the length and orientation of the vector $\underline{Q}$ that connects the two beads, as can be observed in Fig. 10.

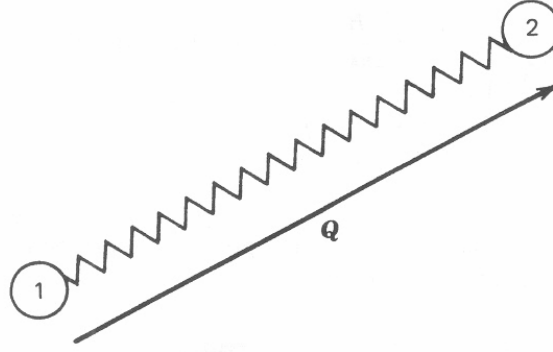


Fig. 10. Elastic dumbbell with configuration given by vector Q .

For a single FENE dumbbell, the spring force F^c is defined as

$$F^c(Q) = \frac{H}{1 - Q^2/Q_0^2} Q \quad (36)$$

where H is a spring constant and Q_0 the maximum spring length. The polymer contribution τ_p , to the stress tensor, is given by

$$\tau_p = n \langle Q F^c(Q) \rangle - nkTI \quad (37)$$

where n is the dumbbell number density, k the Boltzmann constant, T the absolute temperature, and the angular brackets denote the configuration space average. Normally the equations are presented in a dimensional form, for this reason the connector vector Q , the time t , the velocity gradient κ and the polymer stress τ_p are made dimensionless with $(kTH)^{1/2}$, λ , λ^{-1} and nkT , respectively. The relaxation time, λ , is defined by $\lambda = \xi/4H$, where ξ is the beads friction coefficient. In dimensionless form, the equations presented before become,

$$F^c(Q) = \frac{Q}{1 - Q^2/b} \quad (38)$$

$$\tau_p = \langle Q F^c(Q) \rangle - I \quad (39)$$

with $b = HQ_0^2/(kT)$ designated by dimensionless finite extensibility parameter.

It is not possible to solve directly Eq. (39) due to the high computation effort and for this reason simplifications were made, a well known approximation is the FENE-P model, which consists in pre-averaging the non-linear spring law,

$$F^c(Q) = \frac{Q}{1 - \langle Q^2 \rangle / b} \quad (40)$$

But the difficulty presented by the FENE model is the configuration space average calculation, which is necessary to solve an extra equation designated by the evolution equation, Eq. (41), derivate from diffusion equation and based in a distribution function, more details can be found in Bird et al. [88].

$$\frac{DC}{Dt} = I + \kappa \cdot C + C \cdot \kappa^T - \underbrace{\langle Q F^c(Q) \rangle}_{A^c} \quad (41)$$

where $C = \langle QQ \rangle$. Using the typical function distribution of the FENE-P closure,

$$A^c \approx \frac{1}{1 - Tr(C)/b} C, \quad (42)$$

the final equations to solve are

$$\tau_p = \frac{1}{1 - Tr(C)/b} C - I \quad (43)$$

and

$$\frac{DC}{Dt} = I + \kappa \cdot C + C \cdot \kappa^T - \frac{1}{1 - Tr(C)/b} C \quad (44)$$

Also, using the molecular kinetic theory it is possible to capture more realistic rheological properties with the Oldroyd-B model, given by Eq. (45) and Eq. (46). The first DNS simulations used the Oldroyd-B model, but the appearance of instabilities at high drag reduction regime due to the unbounded elongational viscosity at finite elongation, limited the use of this model to the fluids with small elongational viscosities.

$$\tau_p = C - I \quad (45)$$

and

$$\frac{DC}{Dt} = I + \kappa \cdot C + C \cdot \kappa^T - C \quad (46)$$

Another closure of the FENE dumbbell model is the FENE-LS, a simplification of the FENE-L. Both FENE-L and FENE-LS use a second order closure to the function distribution instead of the first order like the FENE-P model. So the FENE-LS is more accurate in correcting the limitations of the FENE-P model to reproduce hysteretic behaviour in strong flows involving stress growth and subsequent relaxation, as point out by Lielens et al. [89], but the equations necessary to solve this model are numerical more complex, as can be observed below. The stress tensor is given by

$$\tau_p = \frac{C}{Tr(C)} \underbrace{\int_0^{\sqrt{b}} \frac{Q^2}{1-Q^2/b} \rho^c(Q) dQ}_{A^c} - I \quad (47)$$

and

$$\frac{DC}{Dt} = I + \kappa \cdot C + C \cdot \kappa^T - \frac{C}{Tr(C)} \underbrace{\int_0^{\sqrt{b}} \frac{Q^2}{1-Q^2/b} \rho^c(Q) dQ}_{A^c} \quad (48)$$

where

$$A^c = \left(C \frac{1-K}{f-K} \right) \left[\frac{f-2K}{1-2K} \left(1 - \frac{C}{b} \frac{1-K}{f-K} \right)^{-1} + \frac{1-f}{R^2(1-2K)} \right] \quad (49)$$

with $K = (R^2 + 1)^{-1}$, $f = C^2/B$ and $R^2 = 5$. The tensor B is given by the following equation,

$$\frac{DB}{Dt} = 10Tr(C) + 4 \frac{B}{Tr(C)} \kappa : C - \frac{C}{Tr(C)} 2 \underbrace{\int_0^{\sqrt{b}} \frac{Q^4}{1-Q^2/b} \rho^c(Q) dQ}_{B^c}, \quad (50)$$

where

$$B^c = \left(C \frac{1-K}{f-K} \right)^2 \left[\frac{f-2K}{1-2K} \left(1 - \frac{C}{b} \frac{1-K}{f-K} \right)^{-1} + \frac{1-f}{R^4(1-2K)} \right]. \quad (51)$$

The issue of whether a FENE-P is an adequate representation of the FENE model in the context of turbulent flow, and in particular turbulent channel flow, as also been investigated by Zhou and Akhavan [42], who concluded that the FENE-P dumbbell was accurate only in the steady state, incurring large errors at all phases of transient elongational flows. Contrasting to the FENE model where demonstrated a good approximation in transient elongational flows.

So, it is clear that an important step is the correct choice of the constitutive equation and as demonstrated they can be more or less complex, capturing more or less rheological properties. Sometimes a complex model is not the best choice, for example in channel turbulent flow without hysteretic behaviour, both FENE-P and FENE-LS models predict with the same accuracy, but the numerical complexity of the FENE-LS model increase significantly, and so the FENE-P model should be preferred instead of the FENE-LS model, at least at this initial stage of turbulence modelling of viscoelastic fluids.

Note that the non-linear viscoelastic models do not resume the models described before.

3.4 Constitutive models used

The present work is divided essentially in two main parts. In the first part a Reynolds stress second order turbulence model is developed, for viscoelastic fluids which are described by a modified form of the generalized Newtonian fluid (GNF) constitutive equation. This constitutive model is not genuinely viscoelastic and has to be

understood only in the context of turbulence modelling. In fact, the adopted constitutive equation behaves as an inelastic model in laminar flow. For this reason the present GNF constitutive equation was modified to include elastic effect, introducing an elongational parameter into the viscosity to simulate the extensional viscosity effect in turbulent flows but this feature only works in turbulent flows. The Reynolds stress closure is complex, due to the appearance of new viscoelastic terms in the transport equations, for which there is not *a priori* information. This effort came as a follow up to the previous investigations of Resende et al. [3], Cruz et al. [2] and Cruz and Pinho [13], in developing first order models. One advantage of the GNF constitutive equation is its numerical simplicity when compared to a truly viscoelastic constitutive equation, like for example the FENE-P or FENE-LS. This choice allows us to reduce the number of viscoelastic terms to be modelled, and the assumptions made, capturing correctly the viscoelastic phenomenon. Other advantage is the capacity to predict accurately the shear-thinning effect of the viscous fluids. Simultaneously the predictions and the fluid rheology are assessed on the basis of experimental data from real fluids and the corresponding flow dynamics in fully-developed pipe flow. The disadvantage is that the constitutive equation is not valid for laminar flow and in other turbulent flows it may be necessary to further develop turbulence models. This seems to show that turbulence still has to be properly investigated.

The limitations of the GNF model forced us to choose a real elastic rheological constitutive equation for polymeric solutions that can be use in any laminar as well as in turbulent flow. On the second part of this work a viscoelastic turbulence model was developed using a FENE-P constitutive equation, where the elastic part is naturally captured by the model even in laminar flow. An important advantage of this constitutive equation is the availability of DNS data for drag reduction flows, thus allowing us to assess the behaviours of various turbulent viscoelastic correlations. The developed turbulence model benefits from previous first order turbulence models of FENE-P fluids of Pinho et al. [4] and expands it to high DR, presenting also new viscoelastic closures, based in FENE-P constitutive equation.

3.4.1 GNF constitutive equation

The stress tensor, σ , is defined by using as basic principle, a power series of the rate of deformation tensor, S ,

$$\sigma = f(S) = \sum a_n (S)^n \quad (52)$$

Applying the Cayley-Hamilton theorem to equation (52) we can truncate the power series into just two terms

$$\sigma = a_1 (I_S, II_S, III_S) S + a_2 (I_S, II_S, III_S) S^2, \quad (53)$$

where the coefficients a_1 and a_2 depend on the first, second and third invariants of the deformation rate tensor. If the second term, related to normal stress effects, is not considered, the constitutive equation of a generalized Newtonian fluid becomes

$$\sigma = a_1 (I_S, II_S, III_S) \cdot 2S. \quad (54)$$

This simple model for non-Newtonian viscous fluids, where the stress tensor is directly proportional to the rate of deformation tensor, has the capacity to predict with accuracy the viscous effects, provided the a_1 function is adequate. The usual form is

$$\sigma = 2\mu S \quad (55)$$

with $S = \frac{(\nabla U + \nabla U^T)}{2} = \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)$ and a variable viscosity function μ which is,

in general, a function of the three principal invariants of the tensor deformation rate

$$\mu(I_S, II_S, III_S) \quad (56)$$

Since non-Newtonian liquids behave as incompressible fluids, $I_S = \text{tr } S = 0$, and in the laminar two-dimensional case the third invariant also vanishes ($III_S = \det S = 0$),

which leaves the viscosity to depend only on the second invariant $\mu = \mu(\dot{\gamma})$ with $\dot{\gamma} = \sqrt{-4II_S} = \sqrt{2S_{ij}S_{ij}}$.

However, turbulent flows are always locally three-dimensional, even when the flow is two-dimensional on the average, and if the normal rates of deformation play an important role in the mechanisms of turbulence generation, then the third invariant of the rate of deformation tensor should certainly be taken into consideration. For this reason, an explicit dependence of viscosity on both the second and the third invariants of S was kept as in

$$\mu = \mu(\dot{\gamma}, \dot{\varepsilon}), \quad (57)$$

where the shear parameter $\dot{\gamma}$ was defined above and the elongational parameter $\dot{\varepsilon}$ is given by

$$\dot{\varepsilon} = \frac{6 \det S}{\text{tr} S^2}. \quad (58)$$

Using the following expression from tensorial algebra

$$\det S = \frac{1}{6} \left[(\text{tr} S)^3 - 3(\text{tr} S)(\text{tr} S^2) + 2(\text{tr} S^3) \right] \quad (59)$$

and the incompressibility condition, we can simplify the definition of $\dot{\varepsilon}$ to

$$\dot{\varepsilon} = \frac{2 \text{tr} S^3}{\text{tr} S^2} \quad (60)$$

So, the variable viscosity become equal to Eq. (61), a function of invariants ($\dot{\gamma}$, $\dot{\varepsilon}$) of the rate of deformation tensor, S , which combine the shear and extensional viscosities,

$$\mu = \underbrace{K_v [\dot{\gamma}^2]^{(n-1)/2}}_{\eta_v} \underbrace{K_e [\dot{\varepsilon}^2]^{(p-1)/2}}_{\eta_e}. \quad (61)$$

The strain-thickening dependence of μ is quantified by the ratio of the extensional (η_e) to the shear (η_v) viscosities as

$$K_e \left[\dot{\epsilon}^2 \right]^{(p-1)/2} = \frac{1}{3} \frac{\eta_e(\dot{\epsilon})}{\eta_v(\dot{\gamma})}. \quad (62)$$

with $\dot{\gamma} = \sqrt{3}\dot{\epsilon}$ and K_e and p representing fitting parameters to the Trouton ratio. The procedures and concepts described in this section were presented before by Pinho [1].

3.4.2 FENE-P constitutive equation

The FENE-P model is used to calculate an extra stress due to the polymeric presence, and so the total stress is a combination of a solvent stress and polymeric stress, given by the following Eq. (63),

$$\tau = \tau_s + \tau_p \quad (63)$$

with

$$\tau_s = 2\eta_s S \quad (64)$$

where the τ_s is solvent stress, S is the rate of deformation tensor, $S_{ij} = \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)$

and η_s is the constant shear viscosity of the solvent.

The polymeric stress of the Eq. (63) (τ_p) is based on the FENE-P model and given by Eq. (65), equal to Eq. (43) but presented now in dimensionless form

$$\tau_{ij,p} = \frac{\eta_p}{\lambda} \left[f(C_{kk}) C_{ij} - f(L) \delta_{ij} \right], \quad (65)$$

where η_p is the polymeric viscosity and C_{ij} is conformation tensor which is determined by an evolution equation using Oldroyd's upper convective derivate of C_{ij} to keep the material objectivity, i.e.

$$\left(\frac{\partial C_{ij}}{\partial t} + U_k \frac{\partial C_{ij}}{\partial x_k} - C_{jk} \frac{\partial U_i}{\partial x_k} - C_{ik} \frac{\partial U_j}{\partial x_k} \right) = -\frac{\tau_{ij,p}}{\eta_p}. \quad (66)$$

The functions appearing in the polymer stress are

$$f(C_{kk}) = \frac{L^2 - 3}{L^2 - C_{kk}} \text{ and } f(L) = \frac{L^2 - 3}{L^2 - 3} \quad (67)$$

where L^2 is the maximum extensibility of the dumbbell model.

3.5 Closure

To better understand the difference between the modified GNF model and FENE-P model described above, **Fig. 11 (a)-(b)** compares the shear and extensional viscosities for both models, where the extensional viscosity is related to the Trouton ratio by $Tr = \eta_e(\dot{\epsilon})/\eta(\dot{\gamma})$. According to Purnode and Crochet [90] the equations that describe shear and extensional viscosities with the FENE-P model are Eq. (68) and (71), respectively. The shear and extensional viscosity behaviour for the modified GNF model are both described in Eq. (61), as seen in the figures. The main difference occurs in the extensional viscosity demonstrating the necessity to upgrade to a better rheological model, but in terms of the shear viscosity both models are quite similar, as expected.

$$\eta = \eta_s + \eta_{p0} \left(\frac{L^6}{4\lambda^2 \dot{\gamma}^2 (L^2 - 3)^2} \right)^{1/3} \left(\Delta_1^{1/3} + \Delta_2^{1/3} \right) \quad (68)$$

with

$$\Delta_1 = 1 + \sqrt{1 + \frac{2L^6}{27\lambda^2 \dot{\gamma}^2 (L^2 - 3)^2}} \quad (69)$$

$$\Delta_2 = 1 - \sqrt{1 + \frac{2L^6}{27\lambda^2 \dot{\gamma}^2 (L^2 - 3)^2}} \quad (70)$$

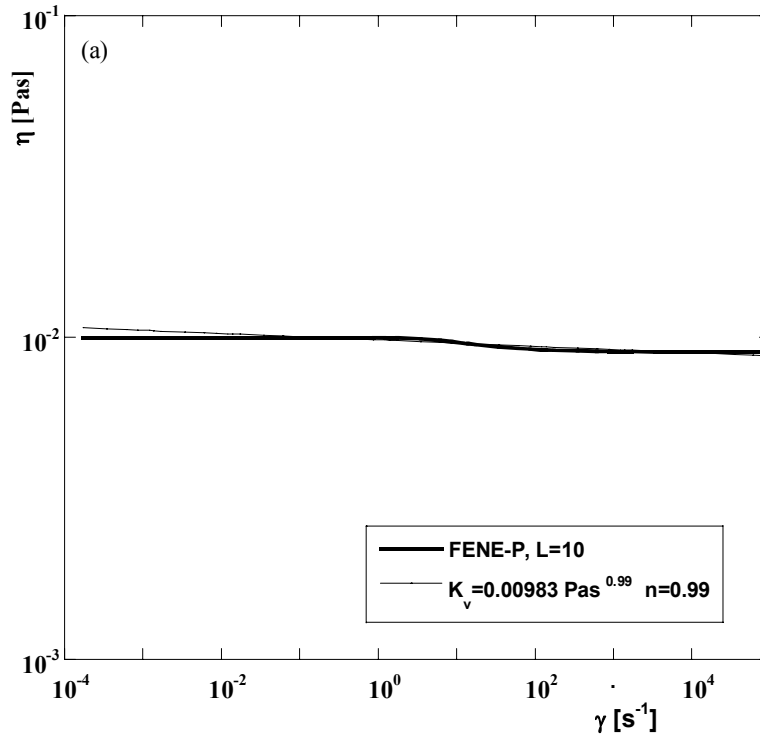
$$\eta_e = 3 \left[\eta_s + \frac{\eta_{p0} L^2}{(L^2 - 3)} \frac{\alpha}{\lambda \dot{\epsilon} (1 - \alpha - 2\alpha^2)} \right] \quad (71)$$

The α parameter obeys the following cubic equation

$$2\alpha^3 - \left[2\lambda\dot{\varepsilon} - L^2/(L^2 - 3)\right]\alpha^2 - \left[\lambda\dot{\varepsilon} + L^2/(L^2 - 3)\right]\alpha + \lambda\dot{\varepsilon} = 0, \quad (72)$$

for which there is a solution.

To conclude, this chapter described the formulations of constitutive equations for polymer solutions and in particular introduced those used here to represent the rheological properties of the viscoelastic fluids for which the two sets of turbulence models will be developed. This refers to the modified GNF constitutive equation for a second order Reynolds stress turbulence model, developed in chapter 4, and the FENE-P model for the two first order turbulence model, a $k-\varepsilon$ and $k-\omega$ turbulence models, developed in chapters 5 and 6, respectively.



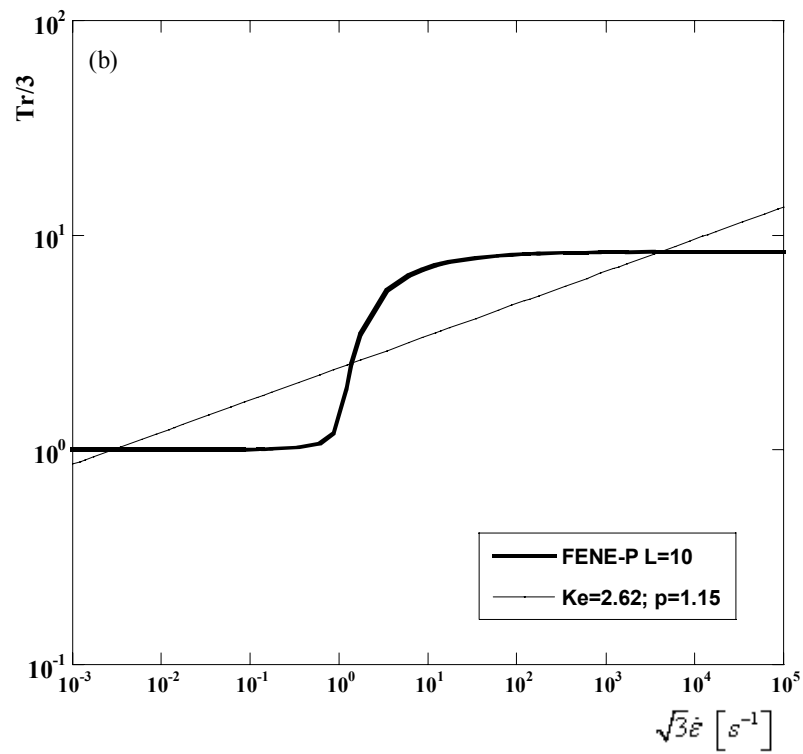


Fig. 11. Comparison between the viscosities of FENE-P model for the case of Dimitropoulos et al. [17] with $L=10$ and the modified GNF model: (a) shear viscosity; (b) extensional viscosity by the Trouton ratio parameter.

Chapter 4

Reynolds stress model for the modified GNF fluid model

This chapter is based on the manuscript *Development of a Reynolds stress model to predict turbulent flows with viscoelastic fluids* , which is about to be submitted to an archival journal

A Reynolds stress model is developed based on a modified Generalized Newtonian Fluid constitutive equation. First, we present the governing equations and the viscoelastic closures. Then we analyze the performance of the model by comparing its predictions with the experimental data for four viscoelastic fluids in turbulent pipe flow.

4.1 Governing equations

In what follows overbars or upper-case letters are used to denote Reynolds-average quantities and lower case letters are used for fluctuating quantities. The indicial notation of Einstein is used throughout the chapter.

The Reynolds-average governing equations are the continuity and momentum equations and the Reynolds stress is calculated by its transport equation, which contains several terms requiring adequate closures. The constitutive equation used is based on a modification of the Generalized Newtonian Fluid (GNF), Eq. (73), developed by Pinho [1]. This incorporates non-Newtonian characteristics which are relevant for turbulent flow of viscoelastic fluids, such as a non-dimensional strain-hardening extensional viscosity, η_e^* , and a shear-thinning shear viscosity, η_v , via a variable molecular viscosity, Eq. (74). Note that in a pure shear flow the equation reduces to the shear viscosity contribution, but in the presence of turbulent fluctuations it contains a non-unitary contribution from the extensional viscosity.

$$\sigma = \mu S_{ij} \quad (73)$$

$$\mu = \underbrace{K_v [\dot{\gamma}^2]^{(n-1)/2}}_{\eta_v} \underbrace{K_e [\dot{\epsilon}^2]^{(p-1)/2}}_{\eta_e^*} \quad (74)$$

In Eq. (74) $\dot{\gamma} = \sqrt{2S_{ij}S_{ij}}$ and $\dot{\epsilon} = \dot{\gamma}/\sqrt{3}$ are invariants of the rate of strain tensor [1] The remaining parameters K_v and n are the consistency and exponent of the power law fit to the shear viscosity, and K_e and p represent fitting parameters to the non-dimensional

Trouton ratio. These parameters depend of the viscoelastic fluid rheology measurements; more details of this model and on the definition of K_e and p can be found in Pinho [1] and Cruz and Pinho [13].

The momentum equation, Eq. (75), contains the divergent of the average molecular stress, of the Reynolds stresses, and of a new non-Newtonian stress,

$$\rho \frac{\partial U_i}{\partial t} + \rho U_k \frac{\partial U_i}{\partial x_k} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_k} \left(2\bar{\mu} S_{ik} - \rho \overline{u_i u_k} + 2\overline{\mu' s_{ik}} \right) \quad (75)$$

where p is the pressure, $\bar{\mu}$ is the average molecular viscosity, u_i is the i - component of the velocity vector and S_{ij} is the rate of deformation tensor defined as

$$S_{ij} \equiv \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) / 2.$$

To determine the extra stress of the fluid, $2\overline{\mu' s_{ik}}$, also called pseudo-elastic stress, a model needs to be developed, the subject of the next section. The average molecular viscosity ($\bar{\mu}$) is also affected by turbulence, so an appropriate closure is needed. Here we use the closure of Pinho [1] given by Eq. (76), which combines the pure viscometric viscosity contribution, η_v , defined in Eq. (74), for a Reynolds-averaged shear rate ($\bar{\dot{\gamma}}$), with the high Reynolds number Reynolds-average molecular viscosity contribution ($\bar{\mu}_h$) of eq. (77).

$$\bar{\mu} = f_v \bar{\mu}_h + (1 - f_v) \eta_v, \quad (76)$$

$$\begin{aligned} \bar{\mu}_h = & \left(C_\mu \rho \right)^{3m(m-1)A_2 / (8+3m(m-1)A_2)} \times 2^{4m(m-1)A_2 / (8+3m(m-1)A_2)} \\ & \times k^{6m(m-1)A_2 / (8+3m(m-1)A_2)} \times \varepsilon^{([8-3(m-1)A_2]m) / (8+3m(m-1)A_2)} \times B^{8 / (8+3m(m-1)A_2)} \end{aligned} \quad (77)$$

In Eq. (77)

$$m = \frac{n+p-2}{n+p} \text{ and } B = \left[\frac{K_v K_e}{A_e^{p-1}} \right]^{1-m} 2^{[(n-1)-m(n+1)]/2} \rho^m \quad (78)$$

and f_v , defined by Eq. (79), is a damping function equal to f_μ and developed in the context of a k - ε model [2, 13]. k and ε represent the turbulent kinetic energy and its rate

of dissipation, respectively, $A_\varepsilon = 10$ and $A_2 = 0.45$. More details regarding this model of $\bar{\mu}$ can be found in Pinho [1].

$$f_v = \left\{ 1 - \left[1 + \left| \frac{1-n}{1+n} \right| y^+ \right]^{-1+n/1-n/A^+} \right\} \times \left\{ 1 - \left[1 + \left| \frac{p-1}{3-p} \right| y^+ C^{\frac{1-p}{2-p}} \right]^{-3-p/p-1/A^+} \right\} \quad (79)$$

The Reynolds stress tensor ($\overline{\rho u_i u_k}$) is determined via its transport equation (80), which contains various terms that are modeled in Section 4.2.2.

$$\begin{aligned} \rho \frac{D \overline{u_i u_j}}{Dt} + \overline{\rho u_j u_k} \frac{\partial U_i}{\partial x_k} + \overline{\rho u_i u_k} \frac{\partial U_j}{\partial x_k} = & -\rho \frac{\partial}{\partial x_k} \overline{u_i u_j u_k} - \left(\frac{\partial}{\partial x_i} \overline{p' u_j} + \frac{\partial}{\partial x_j} \overline{p' u_i} \right) + \\ & + p' \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) + \bar{\mu} \frac{\partial^2 \overline{u_i u_j}}{\partial x_k \partial x_k} - 2 \bar{\mu} \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} + \frac{\partial \bar{\mu}}{\partial x_k} \frac{\partial u_i u_j}{\partial x_k} \\ & + \frac{\partial \bar{\mu}}{\partial x_k} \left(\frac{\partial \overline{u_k u_j}}{\partial x_i} + \frac{\partial \overline{u_k u_i}}{\partial x_j} - 2 \overline{u_k s_{ij}} \right) + \mu' \frac{\partial^2 \overline{u_i u_j}}{\partial x_k \partial x_k} - 2 \mu' \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} \\ & + \frac{\partial \mu'}{\partial x_k} \frac{\partial \overline{u_i u_j}}{\partial x_k} + \frac{\partial \mu'}{\partial x_k} \left(u_j \frac{\partial u_k}{\partial x_i} + u_i \frac{\partial u_k}{\partial x_j} \right) + \overline{\mu' u_j} \frac{\partial^2 U_i}{\partial x_k \partial x_k} \\ & + \overline{\mu' u_i} \frac{\partial^2 U_j}{\partial x_k \partial x_k} + u_j \frac{\partial \mu'}{\partial x_k} \left(\frac{\partial U_i}{\partial x_k} + \frac{\partial U_k}{\partial x_i} \right) + u_i \frac{\partial \mu'}{\partial x_k} \left(\frac{\partial U_j}{\partial x_k} + \frac{\partial U_k}{\partial x_j} \right) \end{aligned} \quad (80)$$

The Reynolds stress transport equation contains the rate of dissipation of turbulent kinetic energy, ε , a quantity that is determined by its own transport equation. The exact form of this transport equation is rather complex so it is used in the modelled form of Eq. (81), which was adopted by Lai and So [28], without any modification.

$$\begin{aligned} \frac{D\varepsilon}{Dt} = & \frac{\partial}{\partial x_k} \left(\nu \frac{\partial \varepsilon}{\partial x_k} \right) + \frac{\partial}{\partial x_k} \left(C_s \frac{k}{\varepsilon} \overline{u_k u_i} \frac{\partial \varepsilon}{\partial x_i} \right) + C_{\varepsilon_1} (1 + \sigma f_{w,2}) \frac{\varepsilon}{k} \tilde{P} - \\ & - C_{\varepsilon_2} f_\varepsilon \frac{\varepsilon \tilde{\varepsilon}}{k} + f_{w,2} \left[\left(\frac{7}{9} C_{\varepsilon_2} - 2 \right) \frac{\varepsilon \tilde{\varepsilon}}{k} - \frac{1}{2k} \left(\varepsilon - \frac{2\nu k}{y^2} \right)^2 \right] \end{aligned} \quad (81)$$

In Eq. (81), the pseudo dissipation is given by

$$\tilde{\varepsilon} = \varepsilon - 2\nu \left(\frac{\partial k^{1/2}}{\partial x_y} \right)^2. \quad (82)$$

4.2 Closures for non-Newtonian terms

4.2.1 Momentum equation

The momentum equation contains two stress terms related to the variable viscosity, which require modelling. The closure for the Reynolds-average molecular viscosity ($\bar{\mu}$) was presented in the previous section, so the stress $2\bar{\mu}S_{ik}$ can be determined. Next we discuss the closure for the pseudo-elastic stress, $2\overline{\mu'}s_{ik}$. Cruz et al. [2] proposed a closure for this term in the context of their low Reynolds number k - ε model. Inspired by their derivation, we propose here an extended version consistent with the use of the full Reynolds stress model. Therefore, the expression for the pseudo-elastic stress used here is developed without invoking the eddy viscosity concept. Following Cruz et al. [2], the fluctuating viscosity is proportional to

$$\mu' \propto K_v K_e (\dot{\varepsilon}')^{p-1} (\dot{\gamma}')^{n-1} \quad (83)$$

with

$$\dot{\gamma}' \sim \sqrt{s_{ij}s_{ij}} \quad \text{e} \quad \dot{\varepsilon}' \sim \frac{\sqrt{s_{ij}s_{ij}}}{A_\varepsilon} \quad (84)$$

where $\dot{\gamma}'$ and $\dot{\varepsilon}'$ are fluctuating invariants, and A_ε is an empirical parameter used to quantify the relation between shear rates and strain rates within the flow [2]. Denoting $S \equiv \sqrt{s_{ij}s_{ij}}$ and back-substituting

$$\mu' \propto \frac{K_v K_e}{A_\varepsilon^{p-1}} S^{p+n-2}. \quad (85)$$

Combining this with the fluctuating rate of strain tensor, one gets

$$\mu' s_{ij} \propto \frac{K_v K_e}{A_\varepsilon^{p-1}} S^{p+n-2} s_{ij}. \quad (86)$$

To arrive at closures for S and s_{ij} concepts of near-wall turbulence are invoked, specifically: (1) that we are in the equilibrium region, where production of turbulence is

balanced by its rate of dissipation and (2) that this balance is not affected significantly by the new pseudo-elastic stress. We further assume that $\rho\varepsilon$ is essentially equal to $2\bar{\mu}S^2$, i.e., for channel flow one gets

$$P_k = -\overline{\rho uv} \frac{\partial U}{\partial y} \approx \rho\varepsilon \equiv 2\overline{\mu s_{ij}^2} \sim 2\bar{\mu}S^2 \Rightarrow S^2 = \frac{-\overline{\rho uv} \frac{\partial U}{\partial y}}{2\bar{\mu}}. \quad (87)$$

We now make the generalization of the result in Eq. (87), which must be positive by definition, to become

$$S^2 = \left| \frac{-\overline{\rho u_i u_j}}{4\bar{\mu}} S_{ij} \right|. \quad (88)$$

Within the boundary layer $s_{ij} \approx \partial u_i / \partial x_j$ and $u_i \sim \sqrt{u_i u_j}$, thus we can estimate s_{ij} by

$$s_{ij} \sim \frac{\partial u_i}{\partial x_j} \sim \frac{u_i}{L_c}, \quad (89)$$

where L_c is an estimate of the spatial scales of turbulence developed by Cruz et al. [2]. This length scale is given by

$$\frac{1}{L_c} = \frac{\varepsilon}{u_R^3}, \quad (90)$$

where u_R is a velocity scale defined by

$$u_R^2 = \frac{k}{\left| \exp\left(-\left(k/u_\tau^2\right)^\alpha\right) - 1 \right|^{1/\alpha}} \text{ with } \alpha = 2. \quad (91)$$

To conclude, the final expression for the pseudo-elastic stress in the context of a second order turbulence closure is

$$2\overline{\mu' s_{ij}} = \tilde{C} \frac{K_v K_e}{A_e^{p-1}} \left[\left| \frac{\overline{\rho u_i u_j}}{4\bar{\mu}} S_{ij} \right| \right]^{\frac{(p+n-2)}{2}} \times \frac{1}{L_c} \times \frac{\overline{u_i u_j}}{\sqrt{|\overline{u_i u_j}|}} \quad (92)$$

with

$$\tilde{C} = (1 + C_0)^{p+n-2} - 1. \quad (93)$$

The pseudo-elastic stress vanishes in the Newtonian limit ($n=1$ and $p=1$), an effect properly accounted for by parameter $\tilde{C}$, which depends on parameter C_0 . This parameter C_0 takes on a new numerical value different from that in Cruz et al. [2], $C_0 = -0.95$.

4.2.2 Reynolds stress transport equation

The Reynolds stress transport equation contains terms identical to those for Newtonian fluids and new non-Newtonian terms associated with the Reynolds-averaged viscosity and the fluctuating viscosity. Even though the Reynolds-averaged viscosity depends on turbulence, its terms play a similar role to the corresponding viscous terms for Newtonian fluids.

Pinho [1] made an order of magnitude analysis of all terms of this transport equation to assess the relevance of the new terms in comparison to the terms found in the corresponding equation for Newtonian fluids. In that analysis the following scales were used: U was the velocity scale for the mean flow, $u \approx \sqrt{k}$ was the velocity scale for velocity fluctuations, L represented the large length scale for the mean flow and the energy containing eddies and l was the length scale associated with small fluctuations and its gradients. This small length scale is related to the Kolmogorov length scale, $\eta = (\bar{\nu}^3/\varepsilon)^{1/4}$, therefore the ratio of small to large length scales is $l/L \sim (uL/\bar{\nu})^{-3/4}$, where use was made of the inviscid estimative of the rate of dissipation, $\varepsilon = u^3/L$.

Since the viscosity is not constant it was also necessary to estimate the magnitude of the viscosity fluctuations and Pinho [1] arrived at

$$\frac{\nu'}{\bar{\nu}} \sim \left(\frac{uL}{\bar{\nu}} \right)^{3a/4} - 1 \quad (94)$$

where $a = 0.225m(m-1)$ and $m = (n+p-2)/(n+p)$.

Table 2, reproduced from Table 1 in Pinho [1], presents the numerical values of the order of magnitude of the non-Newtonian terms relative to the Newtonian dissipative term $(2\bar{\mu}(\partial u_i/\partial x_k)(\partial u_j/\partial x_k))$.

Table 2. Order of magnitude relative to the dissipative term (adapted from Pinho [1])

Term	Order	Estimate
$\frac{\partial \bar{\mu}}{\partial x_k} \frac{\partial \overline{u_i u_j}}{\partial x_k} + \frac{\partial \bar{\mu}}{\partial x_k} \left(\frac{\partial \overline{u_k u_j}}{\partial x_i} + \frac{\partial \overline{u_k u_i}}{\partial x_j} - 2\overline{u_k s_{ij}} \right)$	$\left(\frac{uL}{\bar{\nu}} \right)^{-3/2}$	1×10^{-6}
$-\frac{\partial \bar{\mu}}{\partial x_k} \overline{2u_k s_{ij}}$	$\left(\frac{uL}{\bar{\nu}} \right)^{-3/4}$	1×10^{-3}
$\overline{\mu' \frac{\partial^2 u_i u_j}{\partial x_k \partial x_k}} - 2\overline{\mu' s_{ij}}$	$\left(\frac{uL}{\bar{\nu}} \right)^{3a/4} - 1$	1
$\frac{\partial \mu'}{\partial x_k} \frac{\partial \overline{u_i u_j}}{\partial x_k} + \frac{\partial \mu'}{\partial x_k} \left(u_j \frac{\partial u_k}{\partial x_i} + u_i \frac{\partial u_k}{\partial x_j} \right)$	$\left(\frac{uL}{\bar{\nu}} \right)^{3a/4} - 1$	1
$\overline{\mu' u_j} \frac{\partial^2 U_i}{\partial x_k \partial x_k} + \overline{\mu' u_i} \frac{\partial^2 U_j}{\partial x_k \partial x_k}$	$\left[\left(\frac{uL}{\bar{\nu}} \right)^{3a/4} - 1 \right] \frac{U}{u} \left(\frac{uL}{\bar{\nu}} \right)^{-3/2}$	1×10^{-5}
$\overline{u_j \frac{\partial \mu'}{\partial x_k} \left(\frac{\partial U_i}{\partial x_k} + \frac{\partial U_k}{\partial x_i} \right)} + \overline{u_i \frac{\partial \mu'}{\partial x_k} \left(\frac{\partial U_j}{\partial x_k} + \frac{\partial U_k}{\partial x_j} \right)}$	$\left[\left(\frac{uL}{\bar{\nu}} \right)^{3a/4} - 1 \right] \frac{U}{u} \left(\frac{uL}{\bar{\nu}} \right)^{-3/4}$	1×10^{-3}

Hence, it is necessary to model the terms on the left-hand-side of Eqs. (95), (96), (97) and the term in Eq. (98) involving the fluctuating viscosity. There is lack of information in the literature regarding the triple correlations of Eqs. (95) and (96) involving gradients of fluctuating viscosity and their impact on the Reynolds stress equation, so here we model those terms as follows:

$$\frac{\partial \bar{\mu}}{\partial x_k} \frac{\partial \overline{u_i u_j}}{\partial x_k} + \frac{\partial \mu'}{\partial x_k} \frac{\partial \overline{u_i u_j}}{\partial x_k} \sim C_{v1} \times \frac{\partial \bar{\mu}}{\partial x_k} \frac{\partial \overline{u_i u_j}}{\partial x_k}, \quad (95)$$

$$\frac{\partial \bar{\mu}}{\partial x_k} \left(\frac{\partial \overline{u_k u_j}}{\partial x_i} + \frac{\partial \overline{u_k u_i}}{\partial x_j} - 2 \overline{u_k s_{ij}} \right) + \frac{\partial \mu'}{\partial x_k} \left(u_j \frac{\partial u_k}{\partial x_i} + u_i \frac{\partial u_k}{\partial x_j} \right) \sim C_{V2} \times \frac{\partial \bar{\mu}}{\partial x_k} \left(\frac{\partial \overline{u_k u_j}}{\partial x_i} + \frac{\partial \overline{u_k u_i}}{\partial x_j} \right), \quad (96)$$

where C_{V1} and C_{V2} are parameters to be quantified later. In both terms, there is no need for any special near-wall treatment.

There is also one diffusion-like triple correlation involving the fluctuating viscosity, for which there is again lack of information, so that the two contributions to the molecular diffusion of Reynolds stresses (D_{ij}^v) are modelled as in equation (97).

$$\bar{\mu} \frac{\partial^2 \overline{u_i u_j}}{\partial x_k \partial x_k} + \mu' \frac{\partial^2 \overline{u_i u_j}}{\partial x_k \partial x_k} \approx \bar{\mu} \frac{\partial^2 \overline{u_i u_j}}{\partial x_k \partial x_k}, \quad (97)$$

Finally, it is also necessary to model the second term in the third line of Table 2. This is a triple correlation related to the rate of dissipation tensor of the Reynolds stresses, ε_{ij} , which is defined as (cf. Pinho [1])

$$-2\bar{\mu} \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} - 2\mu' \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} = \rho \varepsilon_{ij}. \quad (98)$$

This tensor needs to be modelled considering turbulence anisotropy and near wall effects related to the fluid rheology, which are quantified through the damping function $f_{w,1}$. The adopted model of ε_{ij} is that of Lai and So [28], developed by Shima [29], and is given in Eq. (99).

$$\varepsilon_{ij} = \frac{2}{3} \varepsilon (1 - f_{w,1}) \delta_{ij} + \frac{f_{w,1} (\varepsilon/k) \left[\overline{u_i u_j} + \overline{u_i u_k} n_k n_j + \overline{u_j u_k} n_k n_i + n_i n_j \overline{u_k u_l} n_l \right]}{1 + 3 \overline{u_k u_l} n_l n_k / 2k} \quad (99)$$

All other terms of the transport equation are similar to those used in the context of Newtonian turbulence, i.e., they do not contain any molecular viscosity and they are modelled as in Lai and So [28], assuming high Reynolds number turbulent flow, as discussed next.

It is known from DNS data for polymer solutions (cf. Dimitropoulos et al [37]) that the turbulent diffusion terms, the triple correlation of the velocity fluctuations, and in particular the pressure fluctuation correlations, are affected by drag reduction. The

triple correlation, denoted as turbulent diffusion, D_{ij}^T , is modelled as originally by Lai and So in Eq. (100)

$$-\rho \frac{\partial}{\partial x_k} \overline{u_i u_j u_k} = \rho \frac{\partial}{\partial x_k} \left\{ C_s \frac{k}{\varepsilon} \left[\overline{u_i u_l} \frac{\partial \overline{u_j u_k}}{\partial x_l} + \overline{u_j u_l} \frac{\partial \overline{u_k u_i}}{\partial x_l} + \overline{u_k u_l} \frac{\partial \overline{u_i u_j}}{\partial x_l} \right] \right\} \quad (100)$$

The two pressure fluctuation correlations, ϕ_{ij}^* , are the pressure diffusion, ϕ_{ij}^p , and the pressure strain, ϕ_{ij} , the first and second terms on the right-hand-side of Eq. (101), respectively.

$$\phi_{ij}^* = - \underbrace{\left(\frac{\partial}{\partial x_i} \overline{p' u_j} + \frac{\partial}{\partial x_j} \overline{p' u_i} \right)}_{\phi_{ij}^p} + \underbrace{p' \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right)}_{\phi_{ij}} \quad (101)$$

Normally ϕ_{ij}^p is neglected in Reynolds stress closures, because of its small impact in comparison to D_{ij}^T for high Reynolds number flows, Laufer [91]. The pressure strain ϕ_{ij} is responsible for the distribution of turbulent kinetic energy among its three normal components, therefore it plays an important role since non-Newtonian fluids exhibit a different distribution of normal Reynolds stresses than Newtonian fluids. Its adequate modelling requires a sub-model to capture correctly the behaviour of the Reynolds stresses next to the wall. Therefore, the pressure strain is modelled as in Eq. (102), where $\phi_{ij,w} f_{w,1}$ compensates for the shortcomings of $\phi_{ij,1}$ next to the wall, in particular introducing the different behaviour of the Reynolds stress according to the orientation of the flow and wall (for instance, the Reynolds stress normal to the wall is subject to a stronger attenuation than the other two normal stress components).

$$\phi_{ij}^* = \phi_{ij} = \phi_{ij,1} + \phi_{ij,w} f_{w,1}, \quad (102)$$

This closure allows the turbulence model to handle successfully a wide variety of complex flows and includes other turbulence models, for example, for Newtonian fluids the model developed by Launder et al. [23], used also by Lai and So [28]. The closures

for $\phi_{ij,1}$ and $\phi_{ij,w}$ used are those of Lai and So [28], and presented in Eqs. (103) and (104).

$$\phi_{ij,1} = -C_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) - \alpha \left(P_{ij} - \frac{2}{3} \tilde{P} \delta_{ij} \right) - \beta \left(D_{ij} - \frac{2}{3} \tilde{P} \delta_{ij} \right) - \gamma k \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right), \quad (103)$$

$$\phi_{ij,w} = C_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) - \frac{\varepsilon}{k} \left(\overline{u_i u_k n_k n_j} + \overline{u_j u_k n_k n_i} \right) - \alpha^* \left(P_{ij} - \frac{2}{3} \tilde{P} \delta_{ij} \right), \quad (104)$$

Where

$$P_{ij} = \overline{u_j u_k} \frac{\partial U_i}{\partial x_k} + \overline{u_i u_k} \frac{\partial U_j}{\partial x_k}; D_{ij} = \left[\overline{u_i u_k} \frac{\partial U_k}{\partial x_j} + \overline{u_j u_k} \frac{\partial U_k}{\partial x_i} \right],$$

$$\tilde{P} = \frac{1}{2} P_{ii}, \alpha = \frac{(8 + C_2)}{11}, \beta = \frac{(8C_2 - 2)}{11}, \gamma = \frac{(30C_2 - 2)}{55}. \quad (105)$$

The damping function used by Lai and So [28] ($f_{w,1}^{LS}$) is

$$f_{w,1}^{LS} = \exp \left[- \left(\frac{R_T}{150} \right)^2 \right], \quad (106)$$

where the local turbulent Reynolds number, R_T , is defined in Eq. (107) and depends also on the local Reynolds-average kinematic viscosity.

$$R_T = \bar{\nu} k^2 / \varepsilon \quad (107)$$

To properly capture the effect of the wall during drag reduction the damping function $f_{w,1}$ was modified as in Eq. (108).

$$f_{w,1} = \exp \left[- \left(2.5 \left\{ 1 - \left[1 + \left| \frac{1-n}{1+n} \right| y^+ \right]^{\frac{1+n}{1-n} / A^+} \right\} \times \left\{ 1 - \left[1 + \left| \frac{p-1}{3-p} \right| y^+ C^{\frac{1-p}{2-p}} \right]^{\frac{3-p}{p-1} / A^+} \right\} \right)^{1.1} \right], \quad (108)$$

The numerical values of the coefficients in Eq. (108) are $C=25$ and $A^+=35$.

Instead of R_T function $f_{w,1}$ it depends on another local Reynolds number containing the distance to the wall ($y^+ = u_\tau y / \nu_w$), in addition to the two power indices of the constitutive equation as in Cruz and Pinho [13] (shear-thinning of the viscometric

viscosity for $n < 1$ and Trouton ratio thickening of the extensional viscosity for $p > 1$). This is a consequence of the different definition of wall coordinate for power law fluids (cf. Dodge and Metzner [66]). The damping function $f_{w,1}$ is a Van Driest type of function (see [13] for a demonstration). For Newtonian fluids ($n = 1$) it behaves adequately and gives similar predictions to those of Lai and So's model for turbulent channel flow. However, since it is now based on y^+ rather than R_T , this model is not identical to the model of Lai and So, but is a variation.

Finally, Table 3 summarizes the remaining parameters and damping functions used by the model.

Table 3. Constants and damping functions used by the Reynolds stress model (identical to those of Lai and So's [28] model)

Constants				
$C_1 = 1.5$	$C_2 = 0.4$	$C_{\epsilon_1} = 1.35$	$C_{\epsilon_2} = 1.8$	$C_s = 0.11$
$\alpha^* = 0.45$	$C_\epsilon = 0.15$	$C_{\nu_1} = -1.7$	$C_{\nu_2} = 0.2$	$C_0 = -0.95$
Damping functions				
$f_{w,2} = \exp\left[-\left(\frac{R_T}{64}\right)^2\right]$		$f_\epsilon = 1 - \left(\frac{2}{9}\right) \exp\left[-\left(\frac{R_T}{6}\right)^2\right]$		

4.3 Results and discussion

The program used to carry out the numerical simulations for fully-developed pipe flow is based on a finite-volume discretization with staggered meshes and the TDMA solver is used to calculate the solution of the discretized algebraic governing equations. The mesh is non-uniform with 199 cells across the pipe, giving mesh-independent results for Newtonian and non-Newtonian fluids within 0.1%. The full domain is mapped in the transverse direction, hence only the following wall boundary conditions need to be imposed:

$$U_i = 0; \overline{u_i u_j} = 0 \text{ and } \varepsilon = 2\bar{\nu} \left(\frac{\partial k^{1/2}}{\partial y} \right)^2 \text{ at } r = R$$

Following the philosophy of earlier works [1,2,6], the turbulence model was calibrated using the experimental data from one single fluid, an aqueous solution of PAA at 0.125% by weight concentration taken from Escudier et al. [5]. Then, the performance of the model was assessed for the remaining three viscoelastic flows, which were aqueous solutions of 0.2% XG, 0.25% CMC and 0.09% / 0.09% XG / CMC without changing the turbulence model. The viscosity parameters used in the average molecular viscosity, defined by Eq. (74), (76) and (77), are presented in Table 4. These are the same as used previously by Cruz and Pinho [13] and Cruz et al. [2], and were obtained from the experimental shear and extensional viscosity data of Escudier et al. [5].

Table 4. Parameters of viscosity law used to fit the viscosity data by Cruz et al. [2].

Fluid	K_V (Pas ⁿ)	n	K_e	p
0.25% CMC	0.2639	0.6174	2.0760	1.2678
0.09% CMC / 0.09% XG	0.15178	0.5783	2.1833	1.1638
0.2% XG	0.2701	0.4409	3.8519	1.2592
0.125% PAA	0.2491	0.425	8.25	1.4796

4.3.1 Newtonian fluids

For Newtonian fluids, the present model differs from the model of Lai and So, because of the change in the damping function $f_{w,1}$, so here we assess the effect of this modification for fully-developed turbulent pipe flow. The modification of $f_{w,1}$ was carried out to bring into the model the capability to predict flows of viscoelastic fluids, but in this test flow the differences relative to the Newtonian predictions by the original formulation of Lai and So [28] are small. For the Darcy friction coefficient they are of the order of 2% relative to the predictions by the original model of Lai and So [28].

Relative to the Blasius equation, the differences are larger, but that is a consequence of the Lai and So model itself, as shown in Table 5. The small difference between the predictions of our model and those of Lai and So's model are also clear in the comparison between the mean velocity profiles in wall coordinates shown in **Fig. 12**. At larger Reynolds numbers our model approaches Lai and So's model predictions even better, with differences in the velocity profiles becoming negligible.

Table 5. Darcy friction factor for Newtonian flow. Comparison between the present model, Lai and So's [28] and the Blasius equation (109).

Re	7430	13450	21490	33530
f_{Bl} - Blasius equation	0.03404	0.02934	0.02610	0.02335
f_{LS} - Lai and So [39]	0.03755	0.03066	0.02622	0.02323
f - present model	0.03673	0.03006	0.02578	0.02279
$(f_{LS} - f_{Bl})/f_{Bl}$	10.2%	4.5%	0.46%	-0.52%
$(f - f_{Bl})/f_{Bl}$	7.9%	2.4%	-1.2%	-2.4%
$(f - f_{LS})/f_{LS}$	-2.2%	-2%	-1.7%	-1.9%

$$f = 0.316 \times \text{Re}^{-0.25} \quad (109)$$

The corresponding profiles of the normalized turbulent kinetic energy and Reynolds normal stresses are compared in **Fig. 13**, which includes experimental data from Durst et al. [92]. Actually, our predictions are closer to the experimental data than those of the original model of Lai and So [28], specifically for the peaks in u^{+} , and consequently in k^{+} . These turbulent quantities are normalised using the friction velocity (u_τ) as in Eq. (110).

$$u^{+} = \sqrt{u^2}/u_\tau; v^{+} = \sqrt{v^2}/u_\tau; w^{+} = \sqrt{w^2}/u_\tau \quad (110)$$

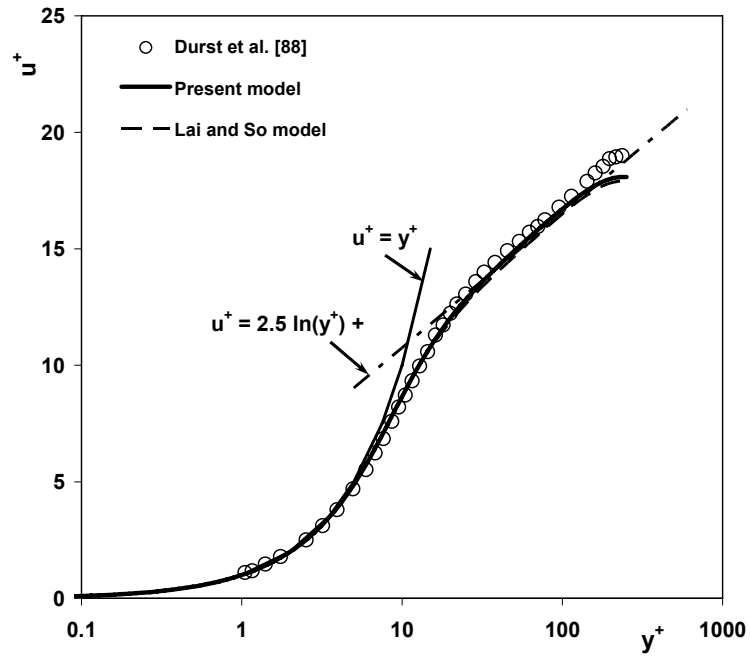


Fig. 12. Comparison between the predicted and the measured mean velocity profile for fully-developed turbulent pipe flow of Newtonian fluid at $Re=7430$ in wall coordinates.

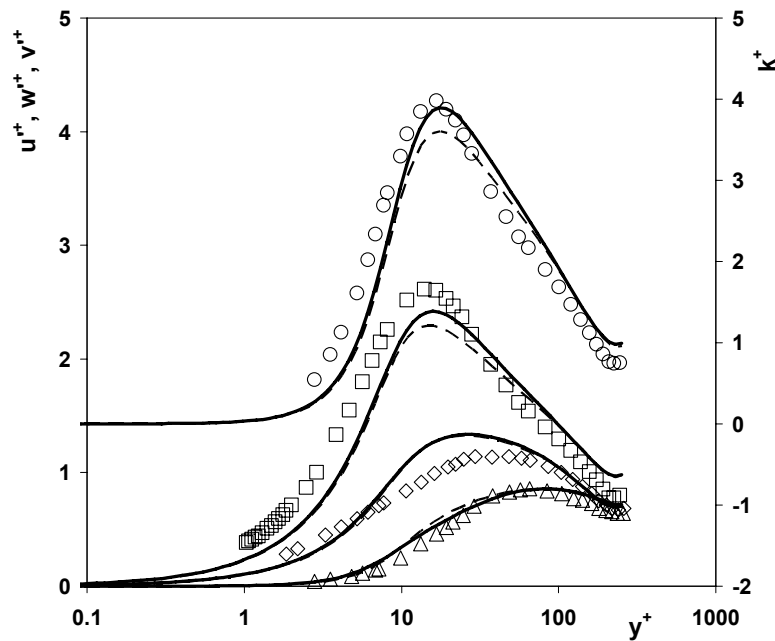


Fig. 13. Comparison between the predicted and the measured profiles of normalized turbulent kinetic energy and Reynolds normal stresses for fully-developed turbulent pipe flow of Newtonian fluid at $Re=7430$ in wall coordinates: $\circ$ k^+ , $\square$ u^+ , $\diamond$ w^+ , Δ v^+ data of Durst et al. [92]; — Present model; - - Lai and So model [28].

4.3.2 Non-Newtonian fluids

First we compare predictions with the experimental data of Escudier et al. [5] and Resende et al. [3] for fully-developed turbulent pipe flow of the polymer solutions in Table 4. Subsequently we will analyze and discuss the evolution of the different viscoelastic stresses in the context of the modified constitutive equation for GNF fluids.

4.3.2.1. Measured polymer solutions

The variation of the Darcy friction factor with Reynolds number for the 0.125% PAA solution can be observed in **Fig. 14**, and the corresponding mean velocity profile in wall coordinates for $Re=42900$ in **Fig. 15**. The predictions of both quantities compare well with the experimental data, except at low Reynolds number, where there is a difference of about 16 % at $Re=10000$. The variation of f versus Re is similar to that seen with the previous model of Cruz et al. [2]. According to Resende et al. [3], the 0.125% PAA solution is a highly elastic fluid with a large drag reduction approaching the maximum given by Virk's maximum drag reduction asymptotic (MDRA) [68] of Eq. (111).

$$1/\sqrt{f} = 9.5 \times \log(Re_w \sqrt{f}) - 19.06 \quad (111)$$

Fig. 14 includes the Blasius Eq. (109) describing the friction factor for Newtonian fluids. The corresponding MDRA for the velocity profile is given by Eq. (112) and plotted in **Fig. 15**. The velocity profile for this 0.125% PAA solution is close to this MDRA, corresponding to a drag reduction of 60 to 70%, a result consistent with the friction factor data.

$$u^+ = 11.7 \ln(y^+) - 17 \quad (112)$$

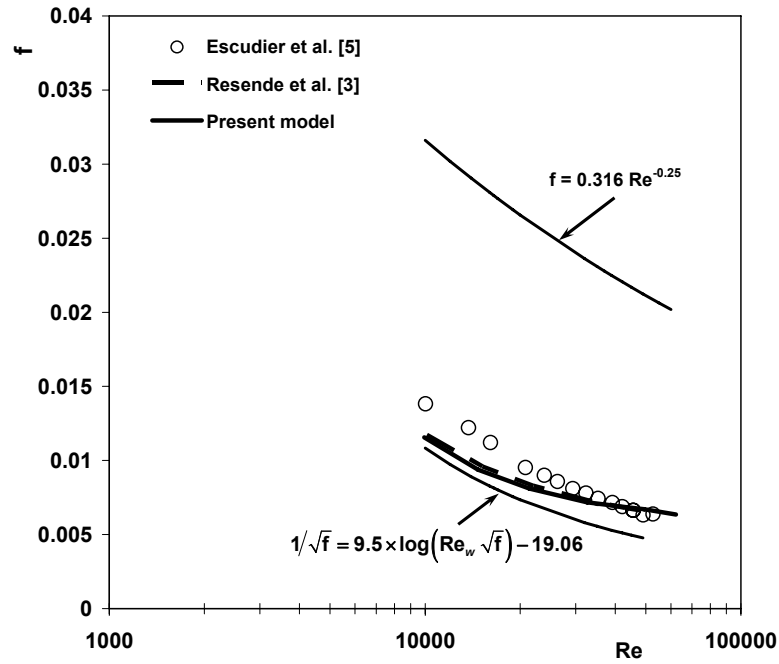


Fig. 14. Comparison between predictions and measurements of Darcy friction factor in wall coordinates for fully-developed pipe turbulent flow with 0.125% PAA fluid.

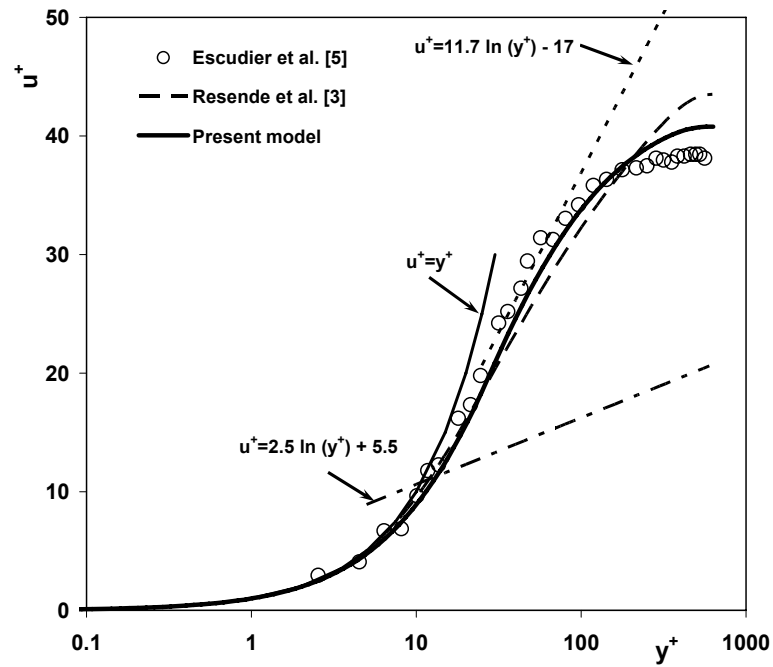


Fig. 15. Comparison between the predicted and measured mean velocity profile for fully-developed pipe turbulent flow with the 0.125% PAA solution at $Re=42900$ in wall coordinates.

The corresponding profiles of turbulent kinetic energy and normal Reynolds stresses are shown in **Fig. 16**. The experimental data of Resende et al. [3] demonstrates the increased turbulence anisotropy in drag reducing flows by polymer additives via an increased $\overline{u^2}$ and lower $\overline{v^2}$ and $\overline{w^2}$. As we can see, the present model under-predicts k and $\overline{u^2}$ near the wall, especially in the region of the peak stress. The prediction of $\overline{w^2}$ is good, but there is also an under-prediction of $\overline{v^2}$, near and away from the wall. So, the variations of the Reynolds stress with the polymer additive are captured by the present Reynolds stress turbulence model, but not so well as by the k - ε non-linear model of Resende et al. [3].

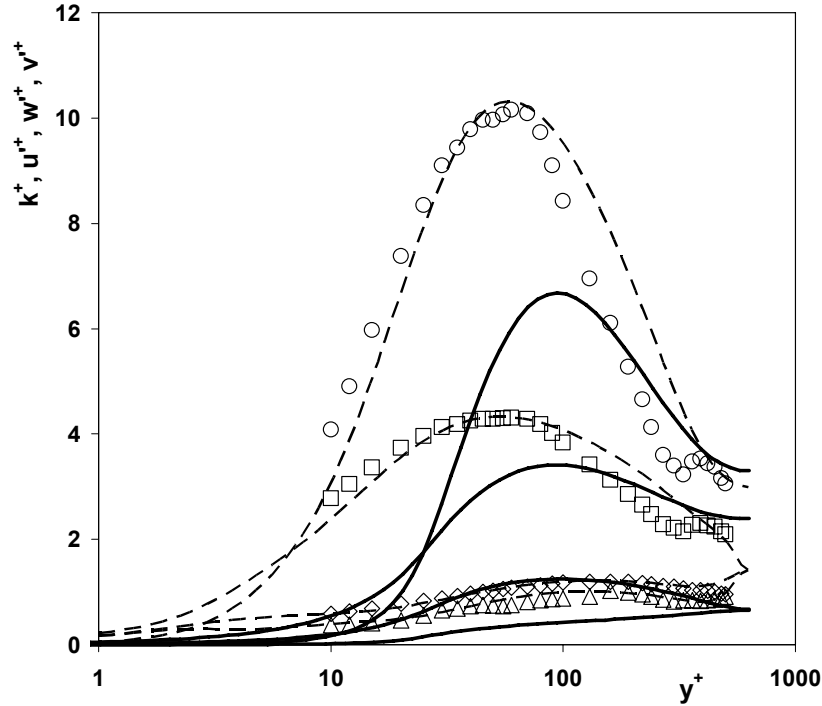


Fig. 16. Comparison between the predicted and the measured profiles of normalized turbulent kinetic energy and Reynolds normal stresses for fully-developed turbulent pipe flow of 0.125% PAA fluid at $Re=42900$ in wall coordinates: $\circ$ k^+ data of Escudier et al. [5]; $\square$ u^+ , $\diamond$ w^+ , Δ v^+ data of Resende et al. [3]; — Present model; - - Resende et al. [3].

This is so because in developing this Reynolds stress model we kept the modifications of the Lai and So model to a minimum and essentially only one damping function was changed. In contrast, in the previous anisotropic k - ε model of Resende et al. [3] several

damping functions were used and the authors were thus able to match more closely the experimental and numerical data. Nevertheless, and in spite of the minimal number of changes made in the present model, the shift of the location of peak turbulence away from the wall is captured, but this came at the expense of an increased dissipation of the turbulence leading to a reduction of the peak value of k .

For the 0.25% CMC fluid the predictions of f as a function of the Reynolds number, and of the mean and turbulent velocities at $Re=16600$ are presented in **Fig. 17**, **Fig. 18** and **Fig. 19**, respectively. The slope of the predicted $f-Re$ curve is lower than that of the experiments by a small amount and the mean velocity profile shows also a good agreement with the experiments. In terms of the turbulent quantities, these are well predicted in terms of magnitude, but the locations of the peak axial normal stress and k are shifted to higher values of y^+ .

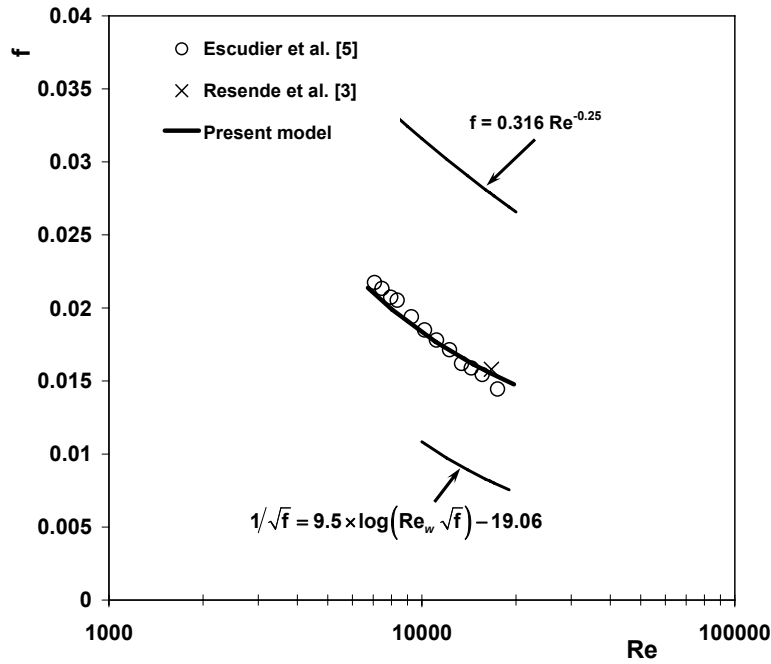


Fig. 17. Comparison between predictions and measurements of Darcy friction factor in wall coordinates for fully-developed pipe turbulent flow with 0.25% CMC fluid.

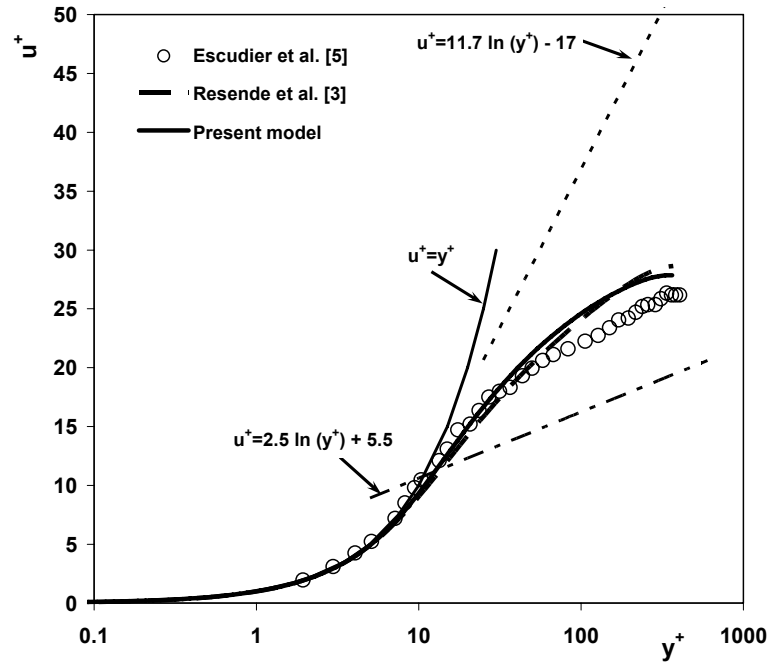


Fig. 18. Comparison between the predicted and measured mean velocity profile for fully-developed pipe turbulent flow with the 0.25% CMC solution at $Re=16600$ in wall coordinates.

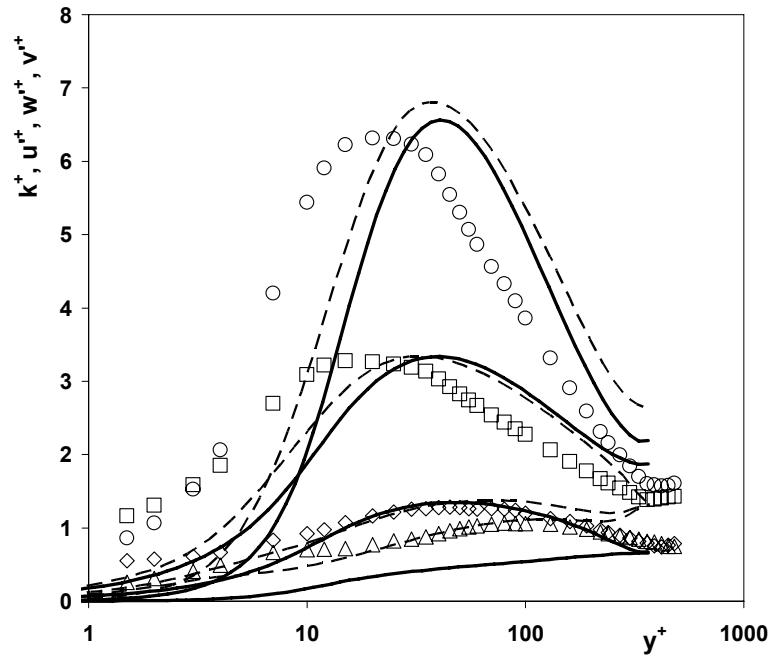


Fig. 19. Comparison between the predicted and the measured profiles of normalized turbulent kinetic energy and Reynolds normal stresses for fully-developed turbulent pipe flow of 0.25% CMC fluid at $Re=16600$ in wall coordinates: $\circ$ k^+ data of Escudier et al. [5]; $\square$ u^+ , $\diamond$ w^+ , Δ v^+ data of Resende et al. [3]; — Present model; - - Resende et al. [3].

The predictions of the Darcy friction factor for the two aqueous polymer solutions based on xantham gum (XG), the blend of 0.09% CMC with 0.09% XG and the 0.2% XG solution, match very well the experimental data as shown in **Fig. 20** and **Fig. 21**. For the blend, there is a 16% difference in the value of f at $Re=52400$, which decreases at lower Reynolds numbers. The opposite variation is observed to occur with the 0.2% XG fluid: now there is a 9% difference between the predicted and the experimental f at $Re=15000$, which decreases with increasing Reynolds numbers.

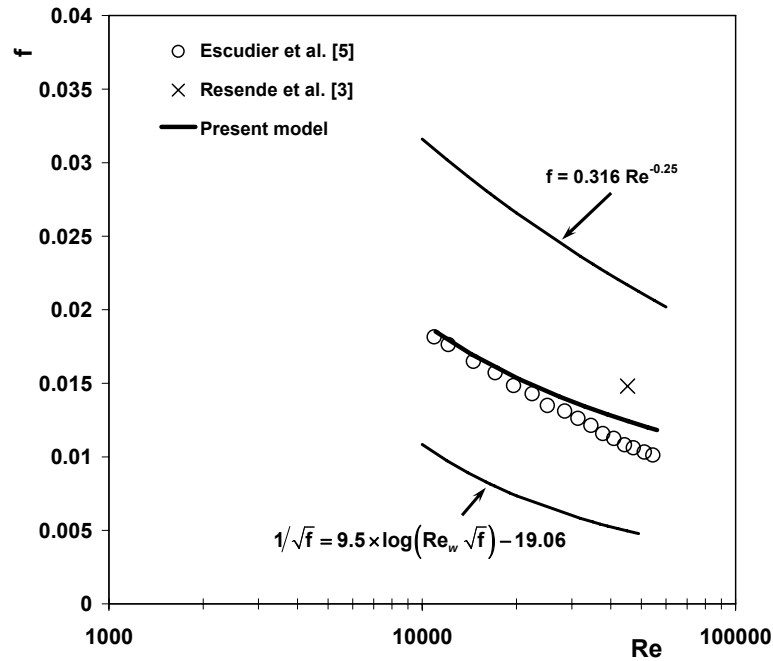


Fig. 20. Comparison between predictions and measurements of Darcy friction factor in wall coordinates for fully-developed pipe turbulent flow with 0.09% / 0.09% CMC / XG fluid.

It must be emphasised at this stage that the predictions for these two fluids, and in particular for the 0.2% XG solution, are significantly better than was previously achieved by any of the first-order closures developed in the past for viscoelastic fluids [2, 3, 13] and in particular by the anisotropic $k-\varepsilon$ model [3]. This is an important achievement of the current Reynolds stress model as is clear from the previous and subsequent plots, which include the predictions by the nonlinear $k-\varepsilon$ model.

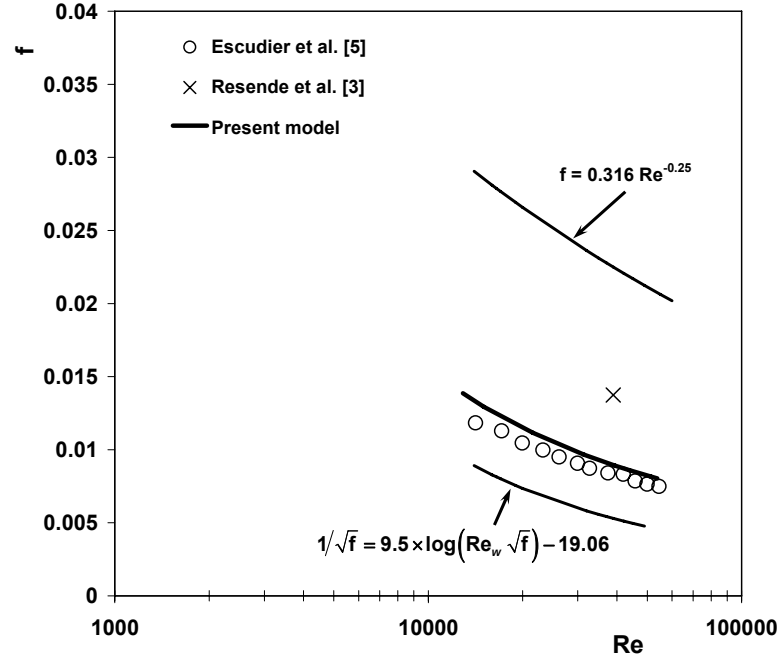


Fig. 21. Comparison between predictions and measurements of Darcy friction factor in wall coordinates for fully-developed pipe turbulent flow with 0.2% XG fluid.

The corresponding predictions of the mean velocity and of the normal Reynolds stresses for the blend (0.09% / 0.09% CMC / XG) and the 0.2% XG solutions, at $Re=45200$ and $Re=39000$, respectively match the experimental data. This is shown in **Fig. 22** and **Fig. 23** for the blend and in **Fig. 24** and **Fig. 25** for the 0.2% XG solution. The predictions are better than those by the previous model [3] with significant improvements, especially for the 0.2% XG solution. As for the previous two non-Newtonian fluids, the axial and radial Reynolds normal stresses and k are underpredicted near the wall. For the 0.2% XG solution the tangential Reynolds normal stress is slightly over-predicted. All these results show that although the model was calibrated with the velocity profile data from two fluids, the 0.125% PAA and the 0.2% XG, it does not predict so well in the 0.125% PAA solution, but in contrast it does a much better job with the remaining three solutions. In addition, there is almost always an under-prediction in k , $\overline{u^2}$ and $\overline{v^2}$ near the wall, whereas $\overline{w^2}$ is usually well predicted.

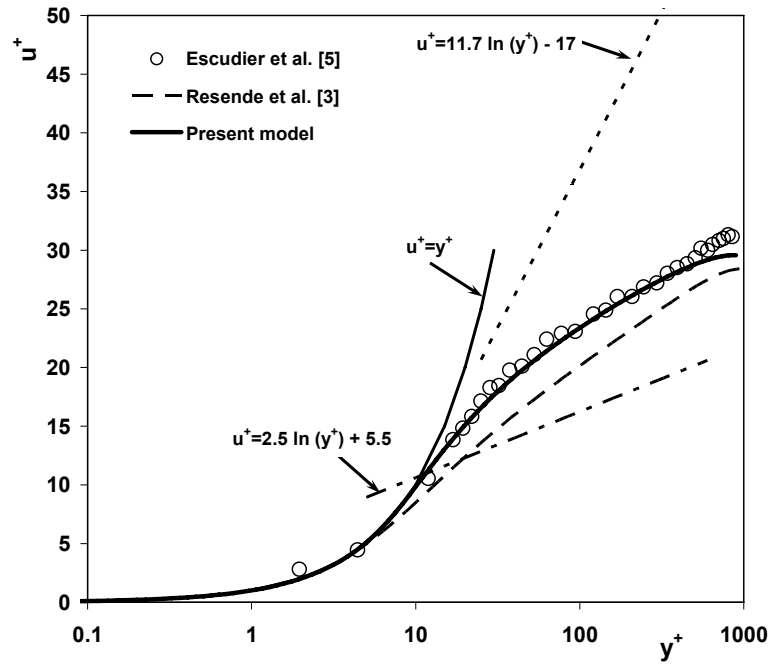


Fig. 22. Comparison between the predicted and measured mean velocity profile for fully-developed pipe turbulent flow with the 0.09% / 0.09% CMC / XG solution at $Re=45300$ in wall coordinates.

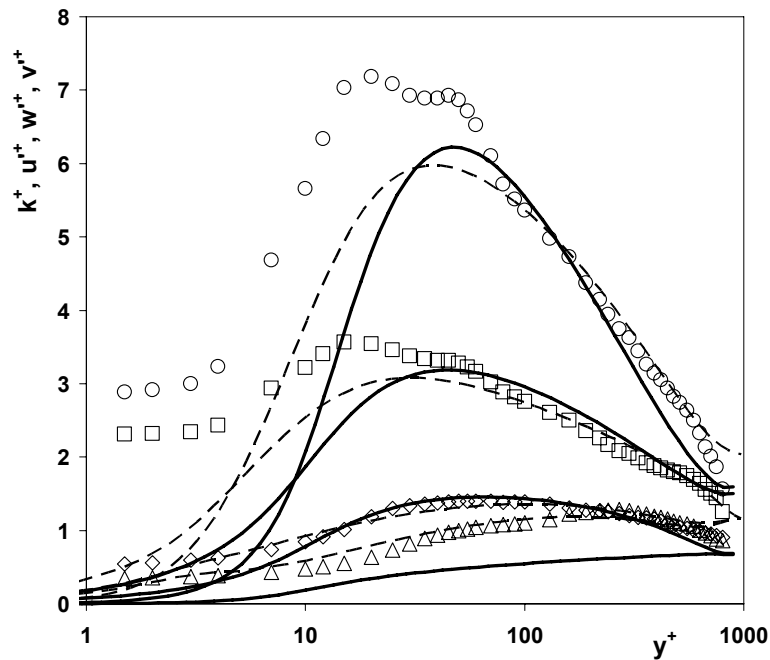


Fig. 23. Comparison between the predicted and the measured profiles of normalized turbulent kinetic energy and Reynolds normal stresses for fully-developed turbulent pipe flow of 0.09% / 0.09% CMC / XG fluid at $Re=45300$ in wall coordinates: $\circ$ k^+ data of Escudier et al. [5]; $\square$ u'^+ , $\diamond$ w'^+ , Δ v'^+ data of Resende et al. [3]; — Present model; - - Resende et al. [3].

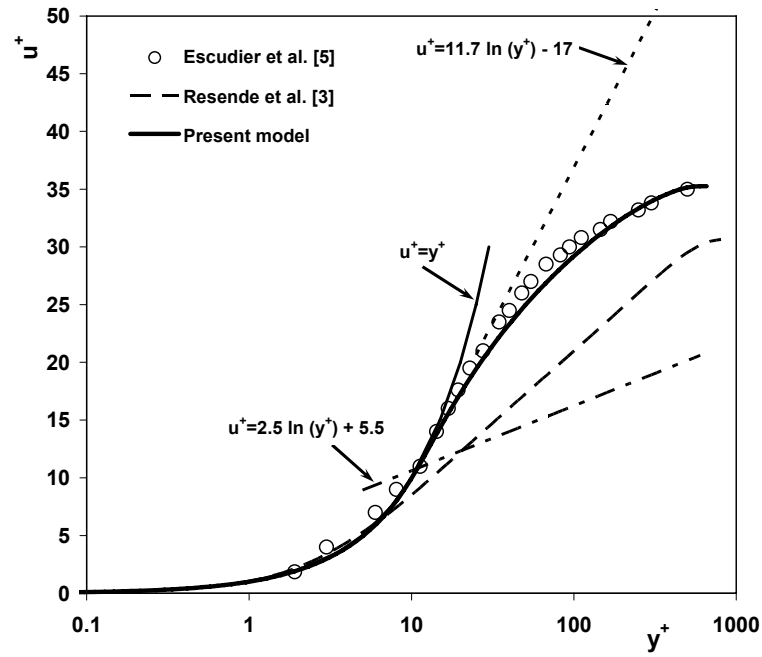


Fig. 24. Comparison between the predicted and measured mean velocity profile for fully-developed pipe turbulent flow with the 0.2% XG solution at $Re=39000$ in wall coordinates.

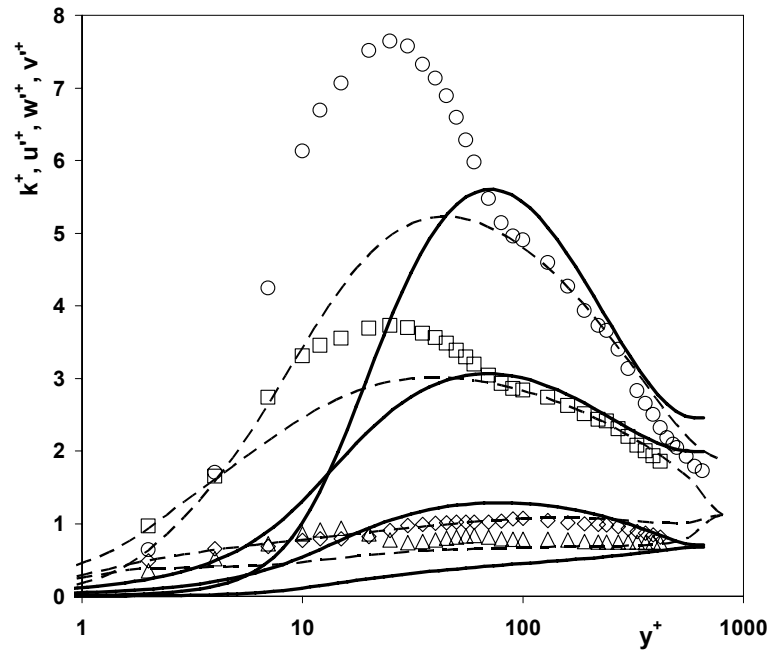
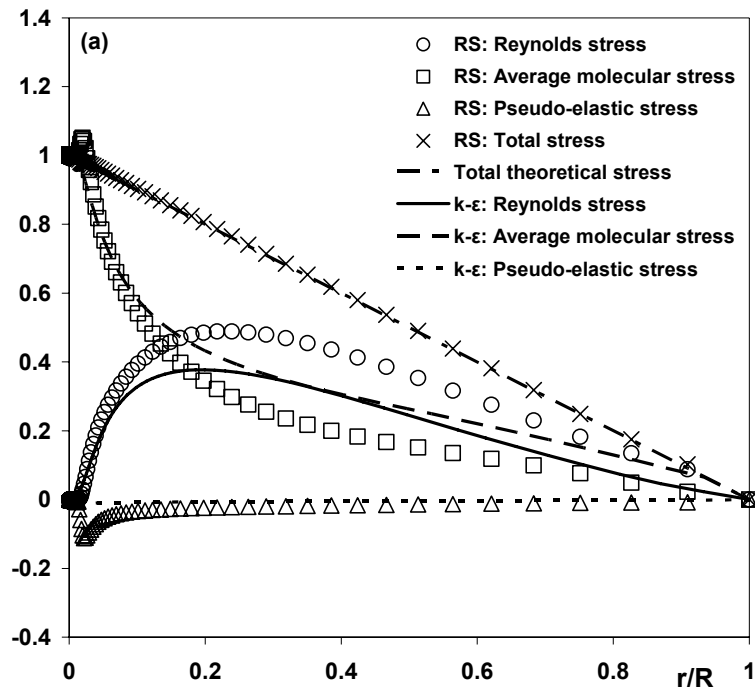


Fig. 25. Comparison between the predicted and the measured profiles of normalized turbulent kinetic energy and Reynolds normal stresses for fully-developed turbulent pipe flow of 0.20% XG fluid at $Re=39000$ in wall coordinates: $\circ$ k^+ data of Escudier et al. [5]; $\square$ u^+ , $\diamond$ w^+ , Δ v^+ data of Resende et al. [3]; — Present model; - - Resende et al. [3].

In **Fig. 26 (a) and (b)** the various shear stress distributions for the 0.125% PAA and 02% XG fluids are plotted, showing in particular their impact on the buffer layer. For the 0.125% PAA the predictions of all these shear stresses are similar to those of the $k-\epsilon$ model of [3], as expected, since the performance of the two turbulence models is similar as this solution is the one used for calibration. However, the two turbulence models behave differently for the solution of 0.2% XG. In particular, the pseudo-elastic stress is larger with the 0.2% XG solution than with the 0.125% PAA leading to an increase in the average molecular stress in the buffer layer to compensate and improving significantly the performance of the present turbulence model relative to the previous $k-\epsilon$ models.



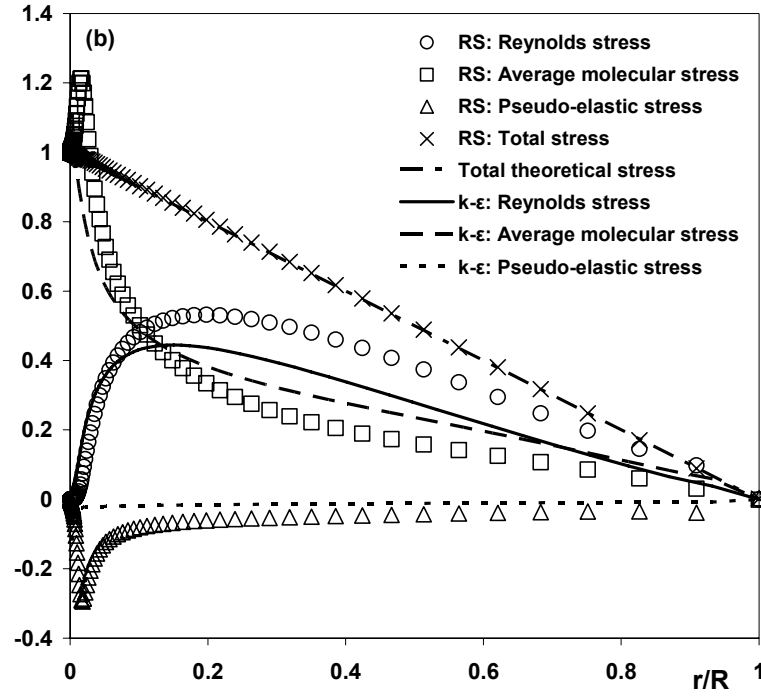


Fig. 26. Comparison between the Reynolds stress and $k-\epsilon$ turbulence models of the various shear stresses across the pipe flow: (a) 0.125% PAA at $Re=42900$; (b) 0.2% XG at $Re=39000$.

In this Reynolds stress model, the pseudo-elastic stresses are larger than in the model of Cruz et al. [2], but they are still negative. This negative sign is not a deficiency of the model because the polymer contribution to the total extra stress equals the sum of the pseudo-elastic stress with part of the molecular shear stress, i.e.

$$\tau_p = 2\bar{\mu}S_{xy} + 2\overline{\mu'}s_{xy} - 2\mu_s S_{xy}, \quad (113)$$

where μ_s is the solvent viscosity (here taken as η_∞ in the fittings of the Cross model to the experimental viscosity data for each fluid - cf. equation 1 of Escudier et al. [5]). The transverse variation of τ_p , $-\rho u'v'$ and τ_s are plotted in **Fig. 27** for the same cases of **Fig. 26**, also for 0.125% PAA and 0.2% XG. Both flows belong to the maximum drag reduction regime ($60\% < DR < 70\%$) with $DR = 60.3\%$ for 0.2% XG at $Re=3900$ and $DR=69\%$ for 0.125% PAA at $Re=42900$, and the variation of those stresses is qualitatively similar to those seen by Ptasiński et al. [15] in their turbulent pipe flow experiments with other viscoelastic fluids.

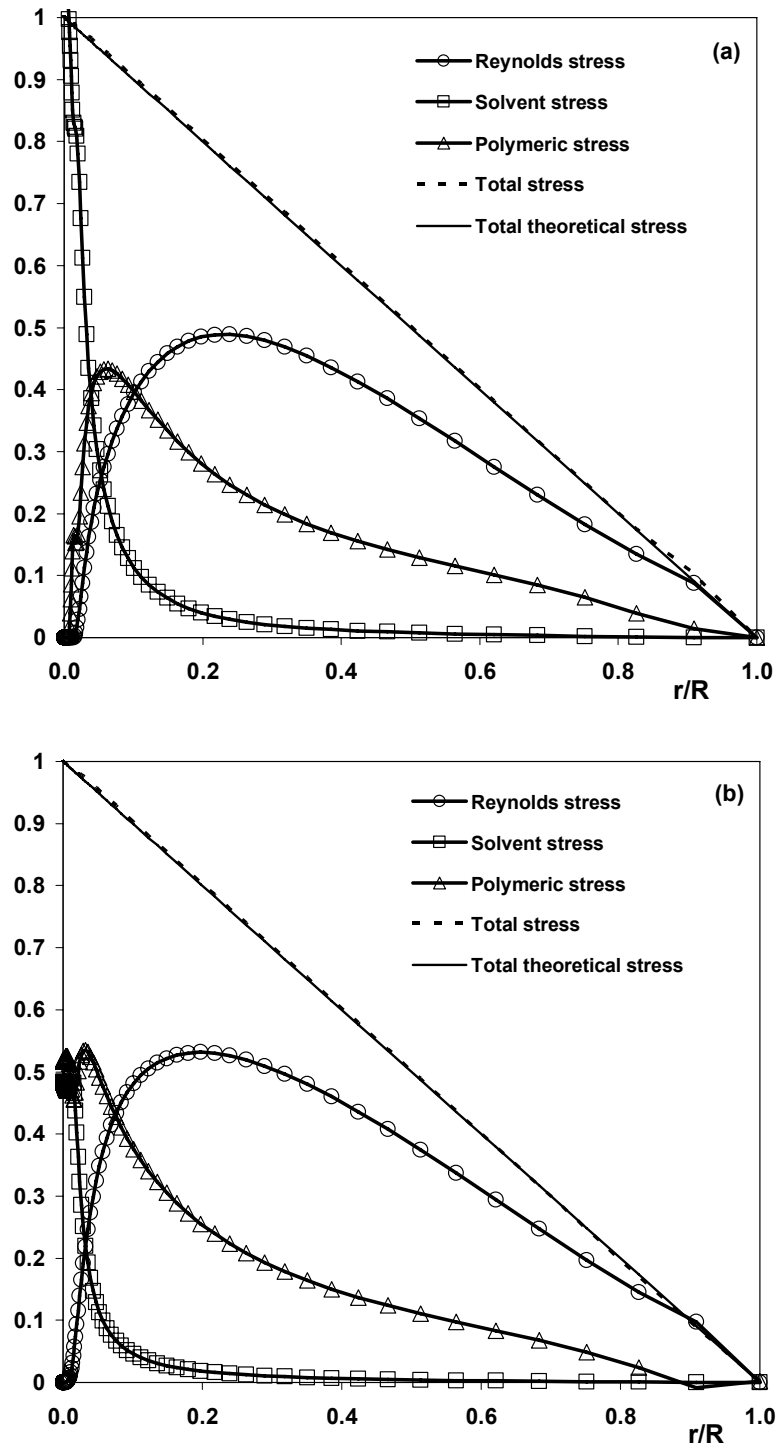


Fig. 27. Distribution of the various shear stresses predictions of the Reynolds stress model, across the pipe flow: (a) 0.125% PAA at $Re=42900$; (b) 0.2% XG at $Re=39000$.

With this definition, the polymer shear stress (τ_p) remains positive and increases with drag reduction as it should. When added to the positive solvent shear stress and to the positive Reynolds shear stress, which decreases with DR, the total stress now varies linearly across the pipe flow as it must from the momentum equation balance and regardless of the assumptions used to model it.

The various non-Newtonian terms of the momentum and Reynolds stress equations affect different flow regions. The pseudo-elastic stress directly affects the buffer layer, but this is sufficient to change the flow across the whole pipe and is especially important to create drag reduction. Indeed, and in contrast to the earlier $k - \varepsilon$ model of Cruz et al. [2], where the drag reduction was basically achieved by a reduction of the eddy viscosity, and the pseudo-elastic stress played a small role, this Reynolds stress model has a more correct behaviour because the drag reduction is achieved by the increasing importance of the polymer stress (τ_p) and not just by a reduction of the Reynolds stress, in agreement with experimental and DNS investigations for viscoelastic fluids, like for example Ptasinski et al. [15] and Li et al. [19]. In the context of the rheological model used here, this is achieved also via the pseudo-elastic stress (cf. Eq. (113)) and not exclusively by $2\bar{\mu}S_{ij}$. Additionally, the Reynolds stress turbulence model captures the increased turbulence anisotropy, and in particular the reduction in the transverse normal Reynolds stress which is usually associated with drag reduction. As the pseudo-elastic stress increases with drag reduction there is also an increase of k^+ , which represents an additional improvement over the $k - \varepsilon$ closure of Cruz et al. [2].

4.4 Conclusions

The Reynolds stress model is a modified version of the Lai and So [28] low Reynolds number turbulence model which includes several new non-Newtonian terms. Closures for all these new terms were developed as well as for the pseudo-elastic stress term appearing in the momentum equation. In the development of the new model modifications to the base model of Lai and So were kept to a minimum in order to facilitate its use over a wide range of flows.

The predictions of this model are very good for all fluids tested, in particular for the friction factor and the mean velocity profiles. In particular, this turbulence model was able to successfully predict the flows involving polymer solutions containing the semi-rigid xanthan gum molecule, for which the linear and nonlinear $k - \varepsilon$ models of Cruz et al. [2] and Resende et al. [3] systematically under-predicted the measured levels of drag reduction. Regarding turbulence quantities, the model was able to capture the enhanced turbulence anisotropy with drag reduction and the shift away from the wall of the peak values of k typical of increasing drag reduction levels. However, the streamwise Reynolds normal stress ($\overline{u^2}$) was in general under-predicted especially near the wall. The azimuthal Reynolds stress ($\overline{w^2}$) was always well predicted and in all cases $\overline{v^2}$ was always under-predicted, near and away from the wall. Note that these predictions of the normal stresses are as good as those obtained by the anisotropic $k-\varepsilon$ model by Resende et al. [3], except for the 0.125% PAA solution where the present model underpredicts turbulence.

Even though the present model represents a significant improvement over the previous turbulence models for viscoelastic solutions, all of which are of first-order, it will be necessary to extend the analysis to more complex geometries in order to assess whether the Reynolds stress model is able to behave effectively. Since the changes to the original model of Lai and So were kept to a minimum, it is our belief that this model will perform better than the earlier first-order closures [2, 3].

Chapter 5

***k-ε* model for the FENE-P constitutive equation**

This chapter is an extended version of the paper *A FENE-P $k-\epsilon$ turbulence model for low and high drag reductions*, submitted to the Journal of Non-Newtonian Fluid Mechanics.

A k - ε turbulence model is developed using the FENE-P model, to represent the viscoelastic fluids in turbulent flows. The governing equations and the viscoelastic closures will be presented in the next sections. The results section compares the model predictions to the DNS data for turbulent channel flow. Note that for a better understanding of this work, we will maintain the structure of the previous chapter so that, for example, the description of the governing equations, will be repeated, with the modifications inherit to the constitutive equation.

5.1 Governing equations and non-dimensional numbers

In what follows uppercase letters and overbars denote Reynolds-averaged quantities, whereas lowercase letters and primes denote fluctuations. A caret is used to identify instantaneous quantities. The equations are written in the indicial notation of Einstein, with $\delta_{ij} = 0$ when $i \neq j$ and $\delta_{ij} = 1$ for $i = j$. The exact instantaneous equations for turbulent flow of incompressible FENE-P fluids are the continuity equation (114), momentum equation (115), where the total stress is a sum of solvent and polymeric contributions, Eq. (116). The polymeric stress is defined by Eq. (117), the evolution equation of the conformation tensor, $\hat{c}_{ij}$, is Eq (118) and the Peterlin function is given in equation (119), where L^2 denotes the maximum molecular extensibility and $\hat{c}_{kk}$ is the trace of the instantaneous conformation tensor.

$$\frac{\partial \hat{u}_k}{\partial x_k} = 0 \quad (114)$$

$$\rho \left(\frac{\partial \hat{u}_i}{\partial t} + \hat{u}_k \frac{\partial \hat{u}_i}{\partial x_k} \right) = - \frac{\partial \hat{p}}{\partial x_i} + \frac{\partial \hat{\tau}_{ik}}{\partial x_k} \quad (115)$$

$$\hat{\tau}_{ik} = \hat{\tau}_{ik}^s + \hat{\tau}_{ik}^p \quad (116)$$

$$\hat{\tau}_{ij}^p = \frac{\eta_p}{\lambda} \left(f(\hat{c}_{kk}) \hat{c}_{ij} - f(L) \delta_{ij} \right) \quad (117)$$

$$\frac{\partial \hat{c}_{ij}}{\partial t} + \hat{u}_k \frac{\partial \hat{c}_{ij}}{\partial x_k} - \left(\hat{c}_{kj} \frac{\partial \hat{u}_i}{\partial x_k} + \hat{c}_{ik} \frac{\partial \hat{u}_j}{\partial x_k} \right) = \hat{c}_{ij}^\nabla = - \frac{\hat{\tau}_{ij}^p}{\eta_p} \quad (118)$$

$$f(\hat{c}_{kk}) = \frac{L^2 - 3}{L^2 - \hat{c}_{kk}} \text{ and } f(L) = 1, \quad (119)$$

In the context of Reynolds averaged calculations of turbulent flow, they become the so-called Reynolds-averaged Navier-Stokes (RANS)/ Reynolds averaged conformation evolution (RACE) equations after performing the Reynolds decomposition [93] (see also [4]), hence being generally called (RANS/RACE) models. Note that, strictly speaking, the momentum equations for a non-Newtonian fluid are no longer called as Navier-Stokes equations [94]. The RANS/RACE equations are the continuity equation (120), the momentum equation (121) and a constitutive equation, here equations (122) and (123).

$$\frac{\partial U_i}{\partial x_i} = 0 \quad (120)$$

$$\rho \frac{\partial U_i}{\partial t} + \rho U_k \frac{\partial U_i}{\partial x_k} = - \frac{\partial \bar{p}}{\partial x_i} + \eta_s \frac{\partial^2 U_i}{\partial x_k \partial x_k} - \frac{\partial}{\partial x_k} (\rho \overline{u_i u_k}) + \frac{\partial \bar{\tau}_{ik}^p}{\partial x_k} \quad (121)$$

In equations (120) and (121) $\bar{p}$ is the mean pressure, U_i is the mean velocity, ρ is the fluid density, $-\rho \overline{u_i u_k}$ is the Reynolds stress tensor and $\bar{\tau}_{ik}^p$ is the Reynolds-averaged polymer stress. In the FENE-P model the time-averaged extra stress is the sum of a Newtonian solvent contribution of viscosity coefficient η_s with a polymeric contribution, as in equation (122). This total extra stress has already been incorporated into the momentum equation (121).

$$\bar{\tau}_{ij} = \eta_s \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + \bar{\tau}_{ij,p} \quad (122)$$

The Reynolds-averaged polymer stress $\bar{\tau}_{ij,p}$ results from Reynolds-averaging the instantaneous FENE-P stress equation [4], relating the instantaneous stress and conformation tensors, and is given by equation (123). Then, the average conformation tensor (C_{ij}) is given by the Reynolds average conformation evolution equation (124-a),

where the first-term inside the brackets on the left-hand-side is Oldroyd's upper convective derivative of C_{ij} .

$$\bar{\tau}_{ij,p} = \frac{\eta_p}{\lambda} \left[f(C_{kk}) C_{ij} - f(L) \delta_{ij} \right] + \frac{\eta_p}{\lambda} \overline{f(C_{kk} + c_{kk}) c_{ij}} \quad (123)$$

$$\left(\frac{\partial C_{ij}}{\partial t} + U_k \frac{\partial C_{ij}}{\partial x_k} - C_{jk} \frac{\partial U_i}{\partial x_k} - C_{ik} \frac{\partial U_j}{\partial x_k} \right) + u_k \frac{\partial c_{ij}}{\partial x_k} - \left(c_{kj} \frac{\partial u_i}{\partial x_k} + c_{ik} \frac{\partial u_j}{\partial x_k} \right) = -\frac{\bar{\tau}_{ij,p}}{\eta_p} \quad (124-a)$$

For compactness and later understanding it is advantageous to rewrite equation (124-a) as equation (122-b),

$$\frac{DC_{ij}}{Dt} - M_{ij} + CT_{ij} - NLT_{ij} = \frac{S_{ij}}{\eta_p} \quad (122-b)$$

thus introducing the following definitions:

$$M_{ij} = C_{jk} \frac{\partial U_i}{\partial x_k} + C_{ik} \frac{\partial U_j}{\partial x_k}; CT_{ij} = u_k \frac{\partial c_{ij}}{\partial x_k}; NLT_{ij} = c_{kj} \frac{\partial u_i}{\partial x_k} + c_{ik} \frac{\partial u_j}{\partial x_k} \text{ and } T_{ij} = -\bar{\tau}_{ij,p}$$

Note that in Eq. (122-b) use was made of the material derivative ($D/Dt = \partial/\partial t + U_k \partial/\partial x_k$).

The functions appearing in equation (123) are those in equation (119) and here and henceforth it is very important to realize that

$$\overline{f(\hat{c}_{kk})} = \frac{\overline{L^2 - 3}}{L^2 - \hat{c}_{kk}} \neq f(\hat{c}_{kk}) = f(C_{kk}) = \frac{L^2 - 3}{L^2 - C_{kk}} \quad (125)$$

The other parameters of the model are the relaxation time of the polymer λ and its viscosity coefficient η_p . To calculate the molecular conformation and the corresponding polymer stress, it is necessary to quantify the three terms with overbars in equations (123) and (124-a) using adequate closures.

Housiadas et al. [38] and Li et al. [39] have shown that all terms of $CT_{ij} = -u_k \frac{\partial c_{ij}}{\partial x_k}$ are negligible in comparison with the other terms of equation (5) at both low and high drag reduction. Pinho et al. [4] have demonstrated that it is also adequate to neglect $\overline{f(\hat{c}_{kk}) c_{ij}}$ in equation (123), at least for low drag reduction. To

assess whether that remains valid in the high drag reduction regime, **Fig. 28** compares the magnitudes of $\overline{f(\hat{c}_{kk})c_{ij}}$ and $f(C_{kk})C_{ij}$ for the shear component for the two sets of DNS data. The two sets are characterized by the following parameters: a Reynolds number of $Re_{\tau_0} = 395$, a ratio of solvent to total zero-shear-rate viscosities (β) of 0.9 and a maximum extension $L^2 = 900$.

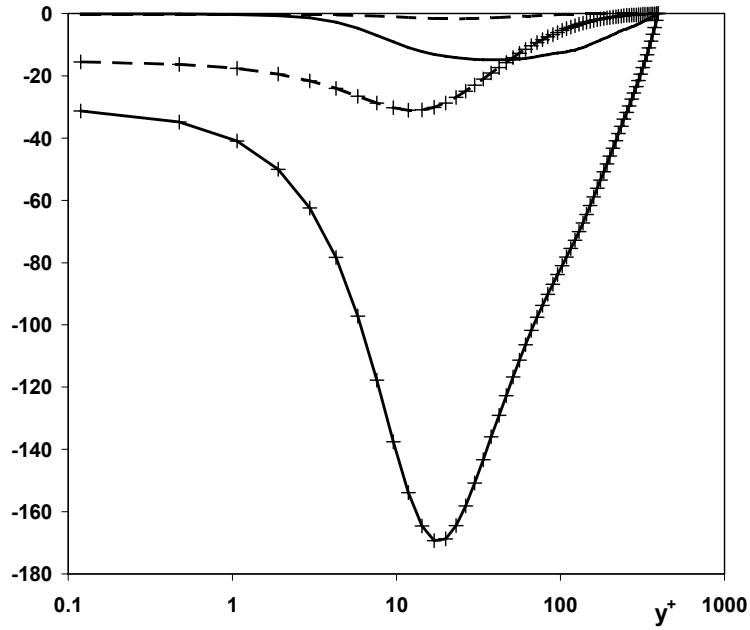


Fig. 28. Comparison between DNS data of $\overline{f(C_{kk} + c_{kk})c_{12}}$ and $f(C_{kk})C_{12}$ for the channel flow of a FENE-P with $Re_{\tau} = 395$, $L^2 = 900$ and $\beta = 0.9$: (---) $\overline{f(C_{kk} + c_{kk})c_{12}}$ and (-+-) $f(C_{kk})C_{12}$ for $We_{\tau} = 25$, DR=18%; (—) $\overline{f(C_{kk} + c_{kk})c_{12}}$ and (+) $f(C_{kk})C_{12}$ for $We_{\tau} = 100$, DR=37%.

The Weissenberg numbers are $We_{\tau_0} = 25$ and $We_{\tau_0} = 100$, corresponding to drag reductions of 18% and 37%, respectively. At the peak of $\overline{f(\hat{c}_{kk})c_{ij}}$, the ratio $\overline{f(\hat{c}_{kk}c_{ij})}/f(C_{kk})C_{ij}$ varies from around 5% at low drag reduction to 20% at high drag reduction. Hence, as a first approximation this double correlation can still be neglected, but it could be necessary to develop a closure for $\overline{f(\hat{c}_{kk})c_{ij}}$ as drag reduction increases

and approaches the maximum drag reduction. As a consequence, to close equation (5) it is only necessary to develop a closure for the NLT_{ij} term, which accounts for the interactions between the fluctuating components of the conformation and velocity gradient tensors that originate from Oldroyd's upper convected derivative.

The Reynolds stress tensor is modelled by invoking the Boussinesq turbulent stress-strain relationship (126)

$$-\overline{\rho u_i u_j} = 2\rho \nu_T S_{ij} - \frac{2}{3} \rho k \delta_{ij} \quad (126)$$

where k is the turbulent kinetic energy and S_{ij} is the rate of deformation tensor defined in equation (127)

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \quad (127)$$

In equation (126) ν_T is the eddy viscosity, here modelled by a modified form of the Prandtl- Kolmogorov closure, to be explained later. Now, it suffices to say that ν_T is a function of k and ε^N , the rate of dissipation of k by the Newtonian solvent. These two quantities are obtained from their transport equations.

The transport equation for the turbulent kinetic energy is given by Eq. (128), a contraction of the Reynolds stress equation developed by Dimitropoulos et al. [37],

$$\rho \frac{Dk}{Dt} + \overline{\rho u_i u_k} \frac{\partial U_i}{\partial x_k} = -\overline{\rho u_k} \frac{\partial k}{\partial x_k} - \frac{\partial \overline{p' u_i}}{\partial x_i} + \eta_s \frac{\partial^2 k}{\partial x_k^2} - \eta_s \frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_k} + \frac{\partial}{\partial x_k} \left(\overline{\tau_{ik}^{vp} u_i} \right) - \left(\overline{\tau_{ik}^{vp} \frac{\partial u_i}{\partial x_k}} \right) \quad (128)$$

Introducing the polymeric stress fluctuations into Eq. (128), we obtain the following transport equation for k

$$\begin{aligned} \rho \frac{Dk}{Dt} = & -\overline{\rho u_i u_k} \frac{\partial U_i}{\partial x_k} - \overline{\rho u_k} \frac{\partial k}{\partial x_k} - \frac{\partial \overline{p' u_i}}{\partial x_i} + \eta_s \frac{\partial^2 k}{\partial x_k^2} - \eta_s \frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_k} + \\ & + \frac{\eta_p}{\lambda} \frac{\partial}{\partial x_k} \left[C_{ik} \overline{f(C_{mm} + c_{mm}) u_i} + \overline{c_{ik} f(C_{mm} + c_{mm}) u_i} \right] - \\ & - \frac{\eta_p}{\lambda} \left[\overline{C_{ik} f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}} + \overline{c_{ik} f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}} \right] \end{aligned} \quad (129)$$

The various terms in equation (129) have the following meaning, according to the notation of Dimitropoulos et al. [37]. The term on the left-hand-side is the advection of k and the remaining terms are designated by

$$P_k = -\overline{\rho u_i u_j} \frac{\partial U_i}{\partial x_j}, \text{ the rate of production of } k;$$

$$Q_k = -\frac{\partial}{\partial x_i} \left(\overline{\rho u_i u_k u_k} + \overline{p' u_i} \right), \text{ the turbulent transport of } k \text{ by velocity and pressure}$$

fluctuations;

$$D_k^N = \eta_s \frac{\partial^2 k}{\partial x_k \partial x_k}, \text{ the molecular diffusion of } k \text{ associated with the Newtonian solvent};$$

$$\varepsilon^N = \nu_s \overline{\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}}, \text{ the viscous dissipation of } k \text{ by the Newtonian solvent};$$

$$Q^V \equiv \frac{\partial \overline{\tau'_{ik,p} u_i}}{\partial x_k} = \frac{\eta_p}{\lambda} \frac{\partial}{\partial x_k} \left[C_{ik} \overline{f(C_{mm} + c_{mm}) u_i} + c_{ik} \overline{f(C_{mm} + c_{mm}) u_i} \right], \quad \text{the viscoelastic}$$

turbulent transport;

$$\varepsilon^V \equiv \frac{1}{\rho} \overline{\tau'_{ik,p} \frac{\partial u_i}{\partial x_k}} = \frac{\eta_p}{\rho \lambda} \left[C_{ik} \overline{f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}} + c_{ik} \overline{f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}} \right], \quad \text{the viscoelastic}$$

stress work, which can be positive or negative, acting as a dissipative or productive mechanism, respectively.

The transport equation for the rate of dissipation of turbulent kinetic energy by the Newtonian solvent was derived by Pinho et al. [4] and is given by Eq. (130),

$$\begin{aligned} \rho \frac{\partial \varepsilon^N}{\partial t} + \rho U_k \frac{\partial \varepsilon^N}{\partial x_k} = & -2\eta_s \left[\frac{\partial U_i}{\partial x_m} \overline{\frac{\partial u_i}{\partial x_m} \frac{\partial u_i}{\partial x_k}} + \frac{\partial U_i}{\partial x_k} \overline{\frac{\partial u_i}{\partial x_m} \frac{\partial u_k}{\partial x_m}} \right] - 2\eta_s \frac{\partial^2 U_i}{\partial x_m \partial x_k} \overline{u_k \frac{\partial u_i}{\partial x_m}} \\ & - 2\eta_s \overline{\frac{\partial u_i}{\partial x_m} \frac{\partial u_i}{\partial x_k} \frac{\partial u_k}{\partial x_m}} - \frac{\partial}{\partial x_k} \left[\overline{\rho u_k \varepsilon^{N'}} + 2\nu_s \overline{\frac{\partial p'}{\partial x_m} \frac{\partial u_k}{\partial x_m}} \right] + \eta_s \frac{\partial^2 \varepsilon^N}{\partial x_k \partial x_k} - 2\eta_s \nu_s \overline{\frac{\partial^2 u_i}{\partial x_m \partial x_k} \frac{\partial^2 u_i}{\partial x_m \partial x_k}} \\ & + 2\nu_s \frac{\eta_p}{\lambda(L^2 - 3)} \overline{\frac{\partial u_i}{\partial x_m} \frac{\partial}{\partial x_k} \left\{ \frac{\partial}{\partial x_m} \left[f(C_{nn}) f(\hat{c}_{pp}) \hat{c}'_{qq} C_{ik} \right] \right\}} \end{aligned} \quad (130)$$

Except for the last term, the viscoelastic contribution to the transport equation of ε^N , all other terms are identical to those for a Newtonian fluid.

The non-dimensional numbers appearing throughout the paper are defined as follows: the Reynolds number $Re_{\tau_0} \equiv hu_\tau/\nu_0$ is based on the friction velocity (u_τ), the channel half-height (h) and the zero shear-rate kinematic viscosity of the solution, which is the sum of the kinematic viscosities of the solvent and polymer ($\nu_0 = \nu_s + \nu_p$). The Weissenberg number is given by $We_{\tau_0} \equiv \lambda u_\tau^2/\nu_0$ and the ratio between the solvent viscosity and the solution viscosity at zero shear rate is β ($\beta \equiv \nu_s/\nu_0$).

The quantities plotted in all figures are non-dimensional using the normalization of the original DNS data [39], as follows: the velocity scale is always the friction velocity, leading to the use of superscript $+$ as in $u_i = u_i^+ u_\tau$, but for the spatial coordinates either the channel half-height ($x_i = x_i^* h$) or the viscous length are used ($x_i = x_i^+ \nu_0/u_\tau$), leading to superscripts $*$ and $+$, respectively. Both normalizations are used in the original DNS data. When mixing the two types of normalization, i.e. wall/viscous and physical velocity and length scales, the superscript used is $*$, as in $NLT_{ij} = NLT_{ij}^* u_\tau/h$.

In the following sections we will develop the new turbulence model in the following sequence: first we develop and assess a closure for NLT_{ij} , followed by a new eddy viscosity model for viscoelastic fluids and then the other required closures in the transport equations of k and ε^N .

5.2 Closure of the Reynolds Average Conformation Equation

As explained in Pinho et al. [4], an order of magnitude analysis of DNS data for the RACE equation (also performed by Li et al. [39]) shows the need to model the NLT_{ij} term. Here, we present a new closure for NLT_{ij} , following a different approach from that of Pinho et al. [4], and based on the exact form of the equation for NLT_{ij} .

5.2.1 Exact and approximate equations for NLT_{ij}

Denoting by operator L ($\hat{c}_{kj}$) the instantaneous evolution equation of $\hat{c}_{kj}$, an exact expression for NLT_{ij} can be derived as $\overline{L(\hat{c}_{kj}) \frac{\partial u_i}{\partial x_k} \frac{1}{f(\hat{c}_{mm})}} + \overline{L(\hat{c}_{ik}) \frac{\partial u_j}{\partial x_k} \frac{1}{f(\hat{c}_{mm})}}$, which is given as equation (131).

$$\begin{aligned}
& \overline{c_{kj} \frac{\partial u_i}{\partial x_k} + c_{ik} \frac{\partial u_j}{\partial x_k}} + \frac{\lambda}{L^2} \left\{ -\frac{\partial C_{ik}}{\partial t} \overline{c_{mm} \frac{\partial u_j}{\partial x_k}} - \frac{\partial C_{kj}}{\partial t} \overline{c_{mm} \frac{\partial u_i}{\partial x_k}} + (L^2 - C_{mm}) \left[\overline{\frac{\partial u_j}{\partial x_k} \frac{\partial c_{ik}}{\partial t}} + \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial c_{kj}}{\partial t}} \right] \right\} \\
& - \frac{\lambda}{L^2} \left\{ \overline{c_{mm} \frac{\partial c_{ik}}{\partial t} \frac{\partial u_j}{\partial x_k}} + \overline{c_{mm} \frac{\partial c_{kj}}{\partial t} \frac{\partial u_i}{\partial x_k}} + U_n \left[\overline{\frac{\partial C_{kj}}{\partial x_n} c_{mm} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial C_{ik}}{\partial x_n} c_{mm} \frac{\partial u_j}{\partial x_k}} \right] \right\} \\
& + \frac{\lambda}{L^2} \left\{ (L^2 - C_{mm}) \left[\overline{\frac{\partial C_{kj}}{\partial x_n} u_n \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial C_{ik}}{\partial x_n} u_n \frac{\partial u_j}{\partial x_k}} \right] - \overline{\frac{\partial C_{kj}}{\partial x_n} c_{mm} u_n \frac{\partial u_i}{\partial x_k}} - \overline{\frac{\partial C_{ik}}{\partial x_n} c_{mm} u_n \frac{\partial u_j}{\partial x_k}} \right\} \\
& + \frac{\lambda}{L^2} \left\{ (L^2 - C_{mm}) U_n \left[\overline{\frac{\partial u_j}{\partial x_k} \frac{\partial c_{ik}}{\partial x_n}} + \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial c_{kj}}{\partial x_n}} \right] - U_n \left[\overline{c_{mm} \frac{\partial u_i}{\partial x_k} \frac{\partial c_{kj}}{\partial x_n}} + \overline{c_{mm} \frac{\partial u_j}{\partial x_k} \frac{\partial c_{ik}}{\partial x_n}} \right] \right\} \\
& + \frac{\lambda}{L^2} \left\{ (L^2 - C_{mm}) \left[\overline{u_n \frac{\partial u_j}{\partial x_k} \frac{\partial c_{ik}}{\partial x_n}} + \overline{u_n \frac{\partial u_i}{\partial x_k} \frac{\partial c_{kj}}{\partial x_n}} \right] - \overline{u_n c_{mm} \frac{\partial u_i}{\partial x_k} \frac{\partial c_{kj}}{\partial x_n}} + \overline{u_n c_{mm} \frac{\partial u_j}{\partial x_k} \frac{\partial c_{ik}}{\partial x_n}} \right\} \\
& + \frac{\lambda}{L^2} \left\{ C_{jn} \overline{\frac{\partial U_k}{\partial x_n} c_{mm} \frac{\partial u_i}{\partial x_k}} + C_{kn} \overline{\frac{\partial U_i}{\partial x_n} c_{mm} \frac{\partial u_j}{\partial x_k}} - (L^2 - C_{mm}) \left[\overline{\frac{\partial U_k}{\partial x_n} c_{jn} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial U_i}{\partial x_n} c_{kn} \frac{\partial u_j}{\partial x_k}} \right] \right\} \\
& + \frac{\lambda}{L^2} \left\{ \overline{\frac{\partial U_k}{\partial x_n} c_{mm} c_{jn} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial U_i}{\partial x_n} c_{mm} c_{kn} \frac{\partial u_j}{\partial x_k}} - (L^2 - C_{mm}) \left[\overline{C_{jn} \frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{C_{kn} \frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right] \right\} \\
& + \frac{\lambda}{L^2} \left\{ \overline{C_{jn} c_{mm} \frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{C_{kn} c_{mm} \frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} - (L^2 - C_{mm}) \left[\overline{c_{jn} \frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{kn} \frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right] \right\}
\end{aligned}$$

$$\begin{aligned}
& + \frac{\lambda}{L^2} \left\{ \overline{c_{jn} c_{mm} \frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{kn} c_{mm} \frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} + C_{kn} \frac{\partial U_j}{\partial x_n} \overline{c_{mm} \frac{\partial u_i}{\partial x_k}} + C_{in} \frac{\partial U_k}{\partial x_n} \overline{c_{mm} \frac{\partial u_j}{\partial x_k}} \right\} \\
& + \frac{\lambda}{L^2} \left\{ - (L^2 - C_{mm}) \left[\frac{\partial U_j}{\partial x_n} \overline{c_{kn} \frac{\partial u_i}{\partial x_k}} + \frac{\partial U_k}{\partial x_n} \overline{c_{in} \frac{\partial u_j}{\partial x_k}} \right] + \frac{\partial U_j}{\partial x_n} \overline{c_{mm} c_{kn} \frac{\partial u_i}{\partial x_k}} + \frac{\partial U_k}{\partial x_n} \overline{c_{mm} c_{in} \frac{\partial u_j}{\partial x_k}} \right\} \\
& + \frac{\lambda}{L^2} \left\{ - (L^2 - C_{mm}) \left[C_{kn} \overline{\frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + C_{in} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right] + \overline{C_{kn} c_{mm} \frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{C_{in} c_{mm} \frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right\} \\
& + \frac{\lambda}{L^2} \left\{ - (L^2 - C_{mm}) \left[\overline{c_{kn} \frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{in} \frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right] + \overline{c_{kn} c_{mm} \frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{in} c_{mm} \frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right\} \\
& = - \frac{f(L)}{L^2} \left[\overline{c_{mm} \frac{\partial u_i}{\partial x_k} \delta_{kj}} + \overline{c_{mm} \frac{\partial u_j}{\partial x_k} \delta_{ik}} \right] \tag{131}
\end{aligned}$$

An alternative much shorter equation was also derived by Pinho [95] as

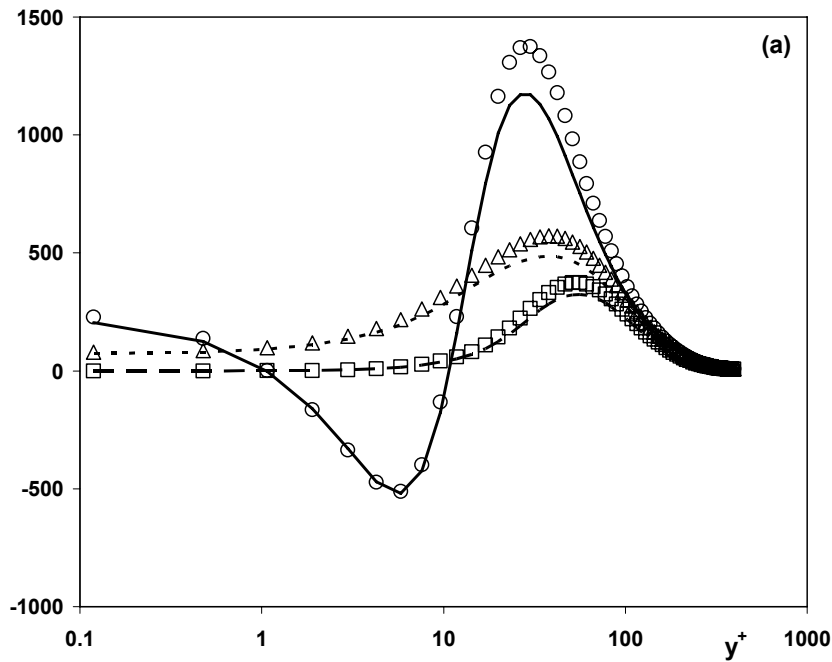
$L \left(\hat{c}_{kj} \right) \frac{\partial u_i}{\partial x_k} + L \left(\hat{c}_{ik} \right) \frac{\partial u_j}{\partial x_k}$ given here as equation (132).

$$\begin{aligned}
& \overline{f(\hat{c}_{mm}) c_{kj} \frac{\partial u_i}{\partial x_k}} + \overline{f(\hat{c}_{mm}) c_{ik} \frac{\partial u_j}{\partial x_k}} = -\lambda \left[\frac{\partial u_i}{\partial x_k} \frac{\partial c_{kj}}{\partial t} + \frac{\partial u_j}{\partial x_k} \frac{\partial c_{ik}}{\partial t} \right] - \left(C_{kj} f(\hat{c}_{mm}) \frac{\partial u_i}{\partial x_k} + C_{ik} f(\hat{c}_{mm}) \frac{\partial u_j}{\partial x_k} \right) \\
& - \lambda \left[\frac{\partial C_{kj}}{\partial x_n} \overline{u_n \frac{\partial u_i}{\partial x_k}} + \frac{\partial C_{ik}}{\partial x_n} \overline{u_n \frac{\partial u_j}{\partial x_k}} + \frac{\partial (U_n c_{kj})}{\partial x_n} \overline{\frac{\partial u_i}{\partial x_k}} + \frac{\partial (U_n c_{ik})}{\partial x_n} \overline{\frac{\partial u_j}{\partial x_k}} + u_n \frac{\partial c_{kj}}{\partial x_n} \overline{\frac{\partial u_i}{\partial x_k}} + u_n \frac{\partial c_{ik}}{\partial x_n} \overline{\frac{\partial u_j}{\partial x_k}} \right] \\
& + \lambda \left[\frac{\partial U_k}{\partial x_n} \left(\overline{c_{jn} \frac{\partial u_i}{\partial x_k}} + \overline{c_{in} \frac{\partial u_j}{\partial x_k}} \right) + \frac{\partial U_j}{\partial x_n} \overline{c_{kn} \frac{\partial u_i}{\partial x_k}} + \frac{\partial U_i}{\partial x_n} \overline{c_{kn} \frac{\partial u_j}{\partial x_k}} + C_{kn} \left(\overline{\frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right) \right] \\
& + \lambda \left[C_{jn} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + C_{in} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} + \overline{c_{jn} \frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{in} \frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} + \overline{c_{kn} \frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{kn} \frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right] \tag{132}
\end{aligned}$$

Note that equation (132) is an exact expression for its left-hand-side, and the link between equation (133) and NLT_{ij} comes from the validity of approximation in equation (133), which needs to be verified.

$$\overline{f(\hat{c}_{mm})c_{kj}\frac{\partial u_i}{\partial x_k}} + \overline{f(\hat{c}_{mm})c_{ik}\frac{\partial u_j}{\partial x_k}} \approx f(C_{mm})\left(\overline{c_{kj}\frac{\partial u_i}{\partial x_k}} + \overline{c_{ik}\frac{\partial u_j}{\partial x_k}}\right) = f(C_{mm})NLT_{ij} \quad (133)$$

To assess the validity of this approximation **Fig. 29** compares the exact term on the left-hand-side of equation (133) with the corresponding approximation on the right-hand-side, using DNS data. The comparisons are for several components of the tensors with data for low drag reduction in **Fig. 29 - (a)** and for high drag reduction in **Fig. 29 - (b)**. In all cases the triple correlation and the corresponding approximation have the same form, an indication that the latter captures the features of the former and that only a coefficient of proportionality is required, which varies with the distance to the wall and the Weissenberg number. Near the wall there is always a good match between the triple correlation and $f(C_{mm})NLT_{ij}$ and a difference is shown essentially to occur in region of the positive peak, which increases with Weissenberg number. As will be seen the essential feature is to capture this Weissenberg number dependence away from the wall, because the modelled term (NLT_{ij}) will not be that important close to the wall, i.e. a discrepancy between the exact term and its approximation/closure in the near wall region will be of little consequence to the turbulence model predictions.



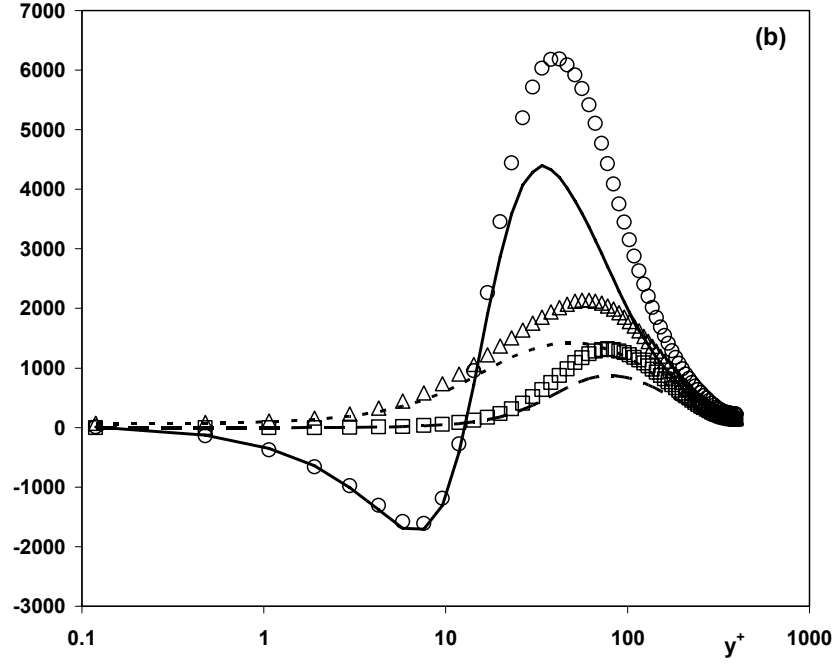
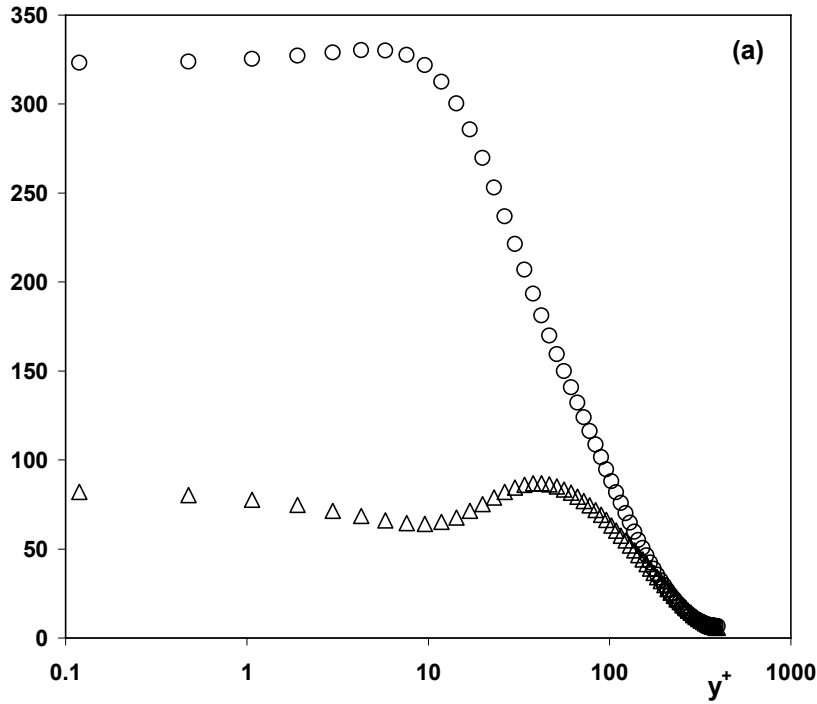


Fig. 29. Comparison between components of $f(\hat{C}_{mm})c_{kj}\frac{\partial u_i^*}{\partial x_k} + f(\hat{C}_{mm})c_{ik}\frac{\partial u_j^*}{\partial x_k}$ (symbols) and of $f(C_{mm})NLT_{ij}^*$ (lines) for channel flow of FENE-P fluids at $Re_\tau = 395$, $L^2 = 900$ and $\beta = 0.9$:
 (a) $We_\tau = 25$, DR=18%; b) $We_\tau = 100$, DR=37%: $\circ 2\overline{fc'_{1k}\partial u_1'/\partial x_k^*}$; $\Delta 2\overline{fc'_{3k}\partial u_3'/\partial x_k^*}$; $\square 2\overline{fc'_{2k}\partial u_2'/\partial x_k^*}$; — $f(C_{kk})NLT_{11}^*$ - - $f(C_{kk})NLT_{22}^*$ --- $f(C_{kk})NLT_{33}^*$.

In **Fig. 30** the time-averaged trace of the conformation tensor (C_{kk}) is compared with its r.m.s. value ($\sqrt{c_{kk}^2}$) for DR= 18% and 37%. Near the walls, where the molecules are more stretched and consequently traces of the conformation tensor are larger, $f(\hat{c}_{kk})$ is different from its equilibrium value of 1 (not shown for conciseness) and $\sqrt{c_{kk}^2} \ll C_{kk}$, $\sqrt{c_{kk}^2}/C_{kk}$ decreases with drag reduction varying from 23% at DR= 18% to 10% for DR=37%. Thus, in this region it is justifiable to neglect the r.m.s. in comparison with the time-averaged value with all its implications regarding function $f(\hat{c}_{kk})$. On the channel centreline region $\sqrt{c_{kk}^2}$ approaches C_{kk} , but both quantities decrease to small values and consequently $f(\hat{c}_{kk}) \approx f(C_{kk}) \approx 1$ (for $C_{kk} = 50$ and 100,

$f(C_{kk}) = 1.06$ and 1.12 , respectively). This justifies neglecting $\sqrt{c_{kk}^2}$ in comparison with C_{kk} when calculating $f(C_{kk})$, as found previously by Pinho et al. [4] for low drag reduction. At high drag reduction the molecules are more stretched (cf. **Fig. 30**), the difference in magnitudes of these two quantities actually increases and on the centreline region $\sqrt{c_{kk}^2}$ is now lower than C_{kk} . Given the form of function $f(\hat{c}_{kk})$ the fluctuations c_{kk} have a small influence on the triple correlation in equation (133) and the function $f(\hat{c}_{kk})$ can come out of the time-average. A second implication of $\sqrt{c_{kk}^2} \ll C_{kk}$ is that it is also justifiable to consider $\overline{f(\hat{c}_{kk})} \approx f(C_{kk})$, which will be used extensively to derive the closure for NLT_{ij} .

To conclude, instead of using the exact equation, to construct a closure for NLT_{ij} we rely on equation (132) together with the approximation of equation (133).



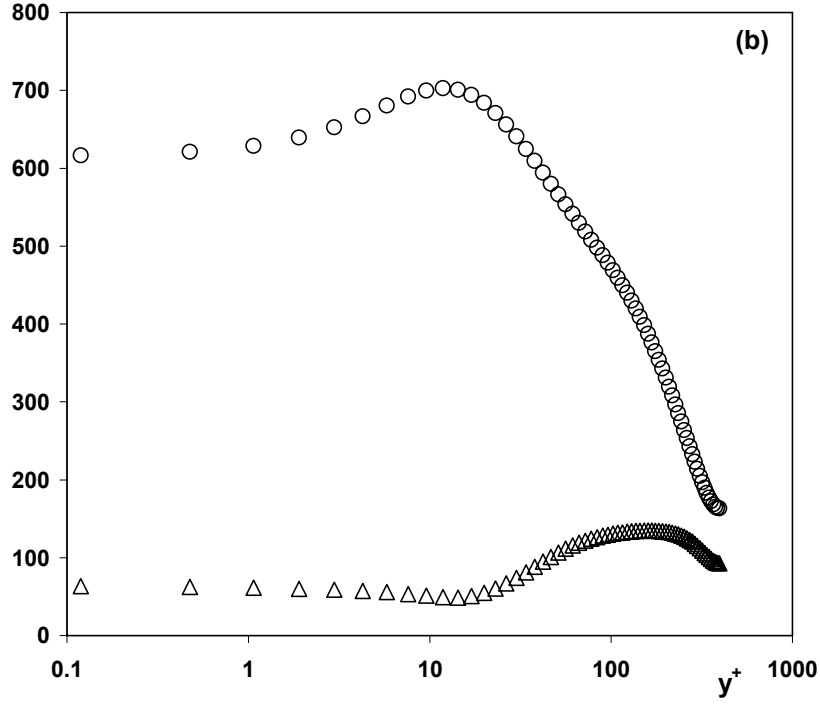


Fig. 30. Transverse profiles of C_{kk} ($\circ$) and $\sqrt{c_{kk}^2}$ (Δ) for channel flow of FENE-P fluids with $Re_\tau = 395$, $L^2 = 900$ and $\beta = 0.9$: (a) $We_\tau = 25$, DR=18%; b) $We_\tau = 100$, DR=37%.

5.2.2 Development of a model for NLT_{ij}

Invoking the approximation of equation (133), the equation for NLT_{ij} that will be modelled is equation (134).

$$\begin{aligned}
 NLT_{ij} \approx & -\frac{\lambda}{f(C_{mm})} \left[\frac{\partial u_i}{\partial x_k} \frac{\partial c_{kj}}{\partial t} + \frac{\partial u_j}{\partial x_k} \frac{\partial c_{ik}}{\partial t} \right] - \frac{1}{f(C_{mm})} \left(C_{kj} f(\hat{C}_{mm}) \frac{\partial u_i}{\partial x_k} + C_{ik} f(\hat{C}_{mm}) \frac{\partial u_j}{\partial x_k} \right) \\
 & - \frac{\lambda}{f(C_{mm})} \left[\frac{\partial C_{kj}}{\partial x_n} u_n \frac{\partial u_i}{\partial x_k} + \frac{\partial C_{ik}}{\partial x_n} u_n \frac{\partial u_j}{\partial x_k} + \frac{\partial (U_n c_{kj})}{\partial x_n} \frac{\partial u_i}{\partial x_k} + \frac{\partial (U_n c_{ik})}{\partial x_n} \frac{\partial u_j}{\partial x_k} + u_n \frac{\partial c_{kj}}{\partial x_n} \frac{\partial u_i}{\partial x_k} + u_n \frac{\partial c_{ik}}{\partial x_n} \frac{\partial u_j}{\partial x_k} \right] \\
 & + \frac{\lambda}{f(C_{mm})} \left[\frac{\partial U_k}{\partial x_n} \left(c_{jn} \frac{\partial u_i}{\partial x_k} + c_{in} \frac{\partial u_j}{\partial x_k} \right) + \frac{\partial U_j}{\partial x_n} c_{kn} \frac{\partial u_i}{\partial x_k} + \frac{\partial U_i}{\partial x_n} c_{kn} \frac{\partial u_j}{\partial x_k} + C_{kn} \left(\frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k} + \frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k} \right) \right]
 \end{aligned}$$

$$+ \frac{\lambda}{f(C_{mm})} \left[C_{jn} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + C_{in} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} + c_{jn} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + c_{in} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} + c_{kn} \overline{\frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + c_{kn} \overline{\frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right] \quad (134)$$

On the basis of DNS data analysis some terms in equation (134) will be neglected with physical insight and theoretical considerations providing the arguments for the closure of the remaining terms. This will require assumptions, some of which will need to be confirmed in the future from DNS data for higher and maximum drag reductions. Nevertheless, these assumptions are adopted here as a first approximation and discussed in more detail below. The assumptions are:

(1) All cross-correlations between velocity fluctuations and gradients of the fluctuating conformation tensor ($\overline{u_n (\partial c_{ij} / \partial x_k)}$) are negligible, regardless of the indices. This is correct for CT_{ij} [38, 81], but needs to be demonstrated for other index combinations;

(2) Turbulence is homogeneous away from walls leading to the neglect of contributions having similarities with turbulent diffusion of turbulent kinetic energy. This requires confirmation for polymer flows, at least for some combinations of indices. For Newtonian fluids it is a reasonable assumption except near walls. This assumption implies that

$$\overline{u_n \frac{\partial u_j}{\partial x_k}} = 0; \quad (135)$$

(3) Invariance laws require that convective terms are null except as part of a material derivative which is not the case here. Hence,

$$U_n \left(\overline{\frac{\partial c_{kj}}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial c_{ik}}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right) + u_n \overline{\frac{\partial c_{kj}}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + u_n \overline{\frac{\partial c_{ik}}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \approx 0 \quad (136)$$

Based on these three assumptions, equation (134) simplifies to equation (137), which still contains terms that need to be modelled.

$$NLT_{ij} \approx - \frac{1}{f(C_{mm})} \left(C_{kj} \overline{f(\hat{C}_{mm}) \frac{\partial u_i}{\partial x_k}} + C_{ik} \overline{f(\hat{C}_{mm}) \frac{\partial u_j}{\partial x_k}} \right)$$

$$\begin{aligned}
& + \frac{\lambda}{f(C_{mm})} \left[\frac{\partial U_k}{\partial x_n} \left(\overline{c_{jn} \frac{\partial u_i}{\partial x_k}} + \overline{c_{in} \frac{\partial u_j}{\partial x_k}} \right) + \frac{\partial U_j}{\partial x_n} \overline{c_{kn} \frac{\partial u_i}{\partial x_k}} + \frac{\partial U_i}{\partial x_n} \overline{c_{kn} \frac{\partial u_j}{\partial x_k}} + C_{kn} \left(\overline{\frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right) \right] \\
& + \frac{\lambda}{f(C_{mm})} \left[C_{jn} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + C_{in} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} + \overline{c_{jn} \frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{in} \frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} + \overline{c_{kn} \frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{kn} \frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right] \quad (137)
\end{aligned}$$

5.2.2.1. Closure for the double correlations between fluctuating strain rates

To model equation (137) we start with the four terms on its right-hand-side (r.h.s), those involving the cross-correlations between two fluctuating rates of strain, which are singled out as (138).

$$C_{kn} \left(\overline{\frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right) + C_{jn} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + C_{in} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \quad (138)$$

The relation between the double correlation of fluctuating strain rates and the turbulence kinetic energy in homogeneous isotropic turbulence is given by equation (139) [96], where λ_f is Taylor's longitudinal micro-scale. This length scale is associated with streamwise gradients of fluctuating streamwise quantities, whereas for the gradients of cross-stream quantities Taylor's transversal length scale (λ_g) is used, but both are related by $\lambda_g^2 = \lambda_f^2/2$.

$$\overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_l}} = \frac{8}{3} \frac{k}{\lambda_f^2} \left[\delta_{ij} \delta_{kl} - \frac{1}{4} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \right] \quad (139)$$

In homogeneous isotropic turbulence Eq. (139) has the following four possible outcomes:

$$(1) \text{ when } i=j=k=l, \quad \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_l}} = \frac{4}{3} \frac{k}{\lambda_f^2} \quad (140-a)$$

$$(2) \text{ when } i=j \text{ and } k=l, \text{ with } i \neq k, \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_l}} = \frac{8}{3} \frac{k}{\lambda_f^2} \quad (25-b)$$

$$(3) \text{ when } i=l \text{ and } k=j, \text{ with } i \neq k, \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_l}} = -\frac{2}{3} \frac{k}{\lambda_f^2} \quad (25-c)$$

$$(4) \text{ zero otherwise} \quad (25-d)$$

At high Reynolds number homogeneous isotropic turbulence, Taylor's longitudinal microscale is related to the dissipation of turbulent kinetic energy via equation (141). Here, we consider that this dissipation is that by the Newtonian solvent (ε^N).

$$\varepsilon^N = 20 \frac{\nu_s k}{\lambda_f^2} \quad (141)$$

Hence, those four terms are modelled as

$$C_{kn} \left(\overline{\frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right) + C_{jn} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + C_{in} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \approx \frac{4}{15} \times \frac{\varepsilon^N}{\nu_s} \times C_{mm} \times \delta_{ij} \quad (142)$$

which brings the rate of dissipation of k by the Newtonian solvent to contribute to NLT_{ij} .

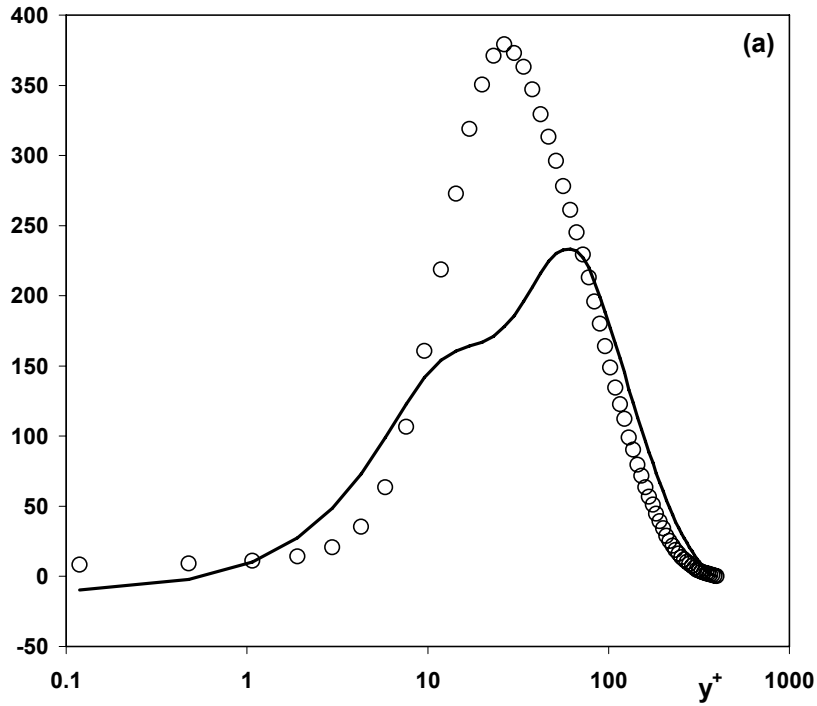
Without further modification, the model of equation (142) is isotropic, whereas DNS shows NLT_{ij} to be an anisotropic quantity. Of course, the model of NLT_{ij} is a sum of several closures for the various terms in equation (137) and the assessment of the performance of the full model, which is being built along this text, required improvements in several of its components. Accordingly, the closure in equation (142) also required modifications for the improvement of the performance of the overall NLT_{ij} model. Essentially, the main contribution of equation (142) to the full NLT_{ij} model is in the prediction of its yy and zz components. Tensor NLT_{ij} is anisotropic and behaves very much like the Newtonian rate of dissipation tensor, ε^N_{ij} , and this has implications. If the model for NLT_{ij} is to be used in the context of a second order turbulence closure, the Newtonian rate of dissipation tensor is available and can be used, instead of its first invariant, to provide the anisotropy. This leads to an alternative proposal for the closure

of term (142) given as below, where we invoke an argument of isotropy in reverse, i.e.,

that $\varepsilon_{ij}^N = \frac{2}{3} \varepsilon^N \delta_{ij} \rightarrow \varepsilon^N \delta_{ij} = \frac{3}{2} \varepsilon_{ij}^N$ turning the model of equation (142) into

$$C_{kn} \left(\overline{\frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right) + C_{jn} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + C_{in} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \approx \frac{2}{5} \times \frac{\varepsilon_{ij}^N}{\nu_s} \times C_{mm} \quad (143)$$

The advantage of using the anisotropic distribution of the dissipation tensor in equation (143) is that it captures the significant anisotropy in the normal components of NLT_{ij} . However, as shown in **Fig. 31**, this results in a deficit of predictions of NLT_{12} , which increases with drag reduction. This figure compares the DNS for NLT_{12} with the prediction of this quantity by the full closure using the contribution of equation (143) for the cross correlation between fluctuating strain rates. Obviously, the closure in equation (143) only makes sense in the context of second order turbulence models, where the rate of dissipation of the Reynolds stresses (ε_{ij}^N) is calculated without necessarily invoking isotropy arguments.



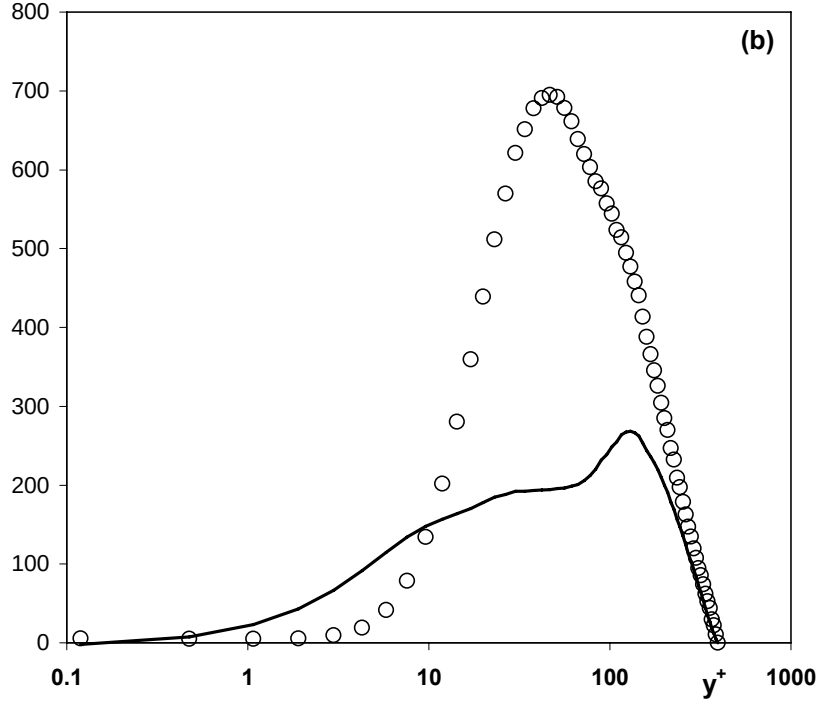
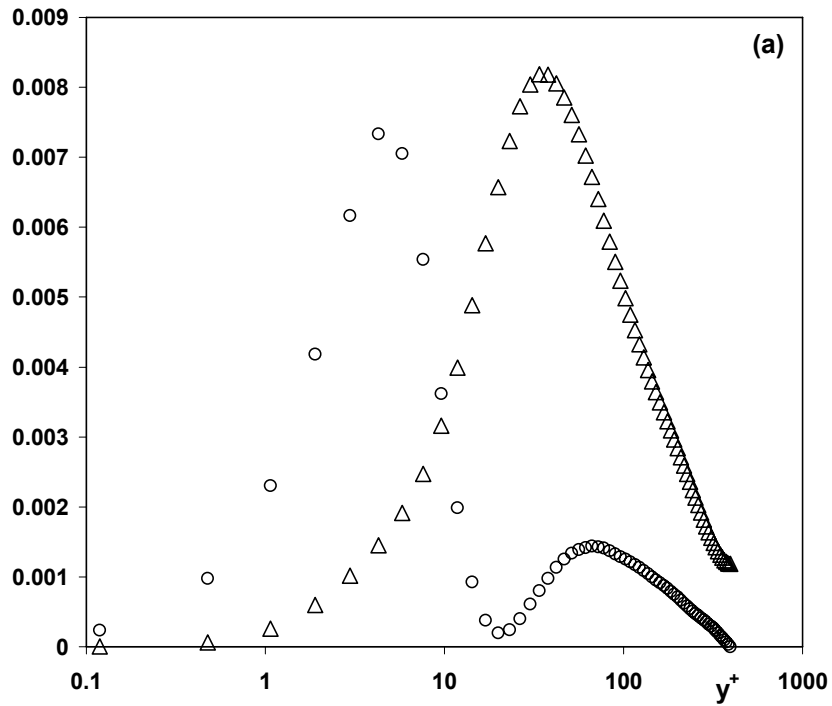


Fig. 31. Transverse profiles of DNS data for NLT_{12}^* ($\circ$); and the (—) NLT_{12}^* general model with anisotropic effect through the dissipation tensor, ε_{ij}^N , in channel flow of FENE-P fluids with $Re_\tau = 395$, $L^2 = 900$, $\beta = 0.9$: (a) $We_{\tau_0} = 25$, DR=18% and (b) $We_{\tau_0} = 100$, DR=37%.

If the model for NLT_{ij} is to be used in the context of first order turbulence closures, like k - ε or k - ω , ε_{ij}^N is calculated assuming that $\varepsilon_{ij}^N = \frac{2}{3} \varepsilon^N \delta_{ij}$, hence equation (143) becomes equation (141) and to introduce anisotropy to the full closure of NLT_{ij} via this contribution a different approach is used, as described next.

This contribution was calibrated essentially considering its contribution to the NLT_{22} component, this implying that we are approaching the ε^N profile with the DNS profile of ε_{22}^N . This component of NLT_{ij} was chosen, because it is the most important to predict a correct evolution of the conformation tensor close to the wall, very much as with the corresponding component of the Reynolds stress tensor in second order turbulence models. This procedure generates a deficit in the predictions of NLT_{33} and especially in the NLT_{12} component, because the isotropy hypothesis inherent in equation

(142) leads a null contribution to the shear component, whereas that is not true as observed in the DNS plots of **Fig. 31** and **Fig. 32**. **Fig. 31** shows that NLT_{12} is non-zero and as will be shown later, its peak value is of the order of the peak value of NLT_{22} . Similarly, at both low and high drag reductions ε_{12}^N is of same order as ε_{22}^N although the peaks are found at different locations. Inspecting **Fig. 32** one observes for DR=18% that $14\% \varepsilon_{22}^N < \varepsilon_{12}^N < 25\% \varepsilon_{22}^N$ in the region $42 < y^+ < 100$, whereas for DR=37% the two components are qualitatively different with ε_{12} being negative at $17 < y^+ < 100$, whereas at $y^+ > 100$ it has the same behaviour as at LDR. Since it is necessary for the closure to bring this difference in behaviour, and in particular to improve the predictions for the shear component of NLT_{ij} , the term below was introduced into the model of equation (21) to capture this shear effect.



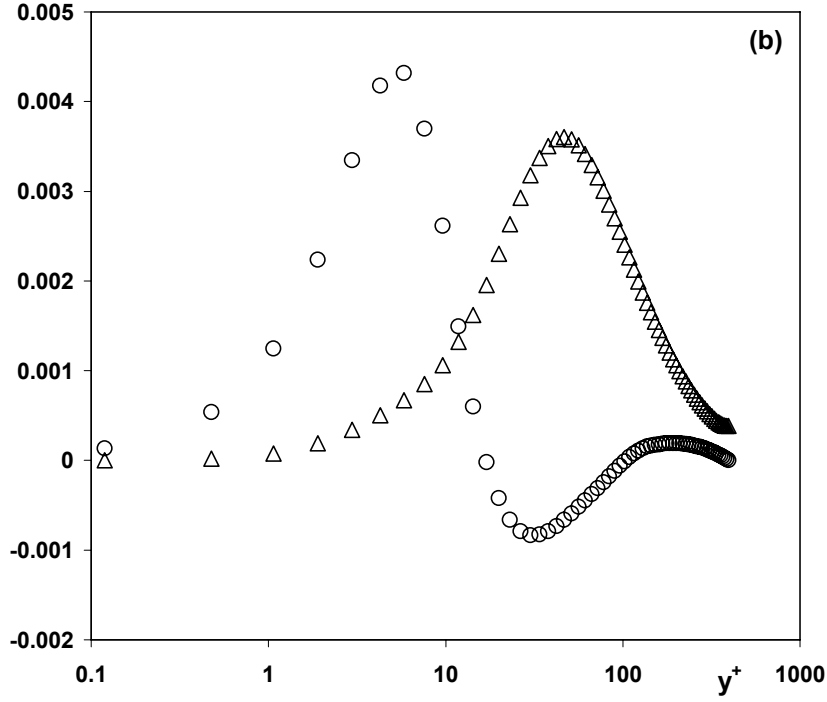


Fig. 32. Transverse profiles of DNS data for ε_{12}^+ ($\circ$) and ε_{22}^+ (Δ) in channel flow of FENE-P fluids with $Re_\tau = 395$, $L^2 = 900$, $\beta = 0.9$: (a) $We_{\tau_0} = 25$, DR=18% and (b) $We_{\tau_0} = 100$, DR=37%.

The impact of this modification is clear in **Fig. 33**, where the predictions of NLT_{ij} with and without this correction are compared.

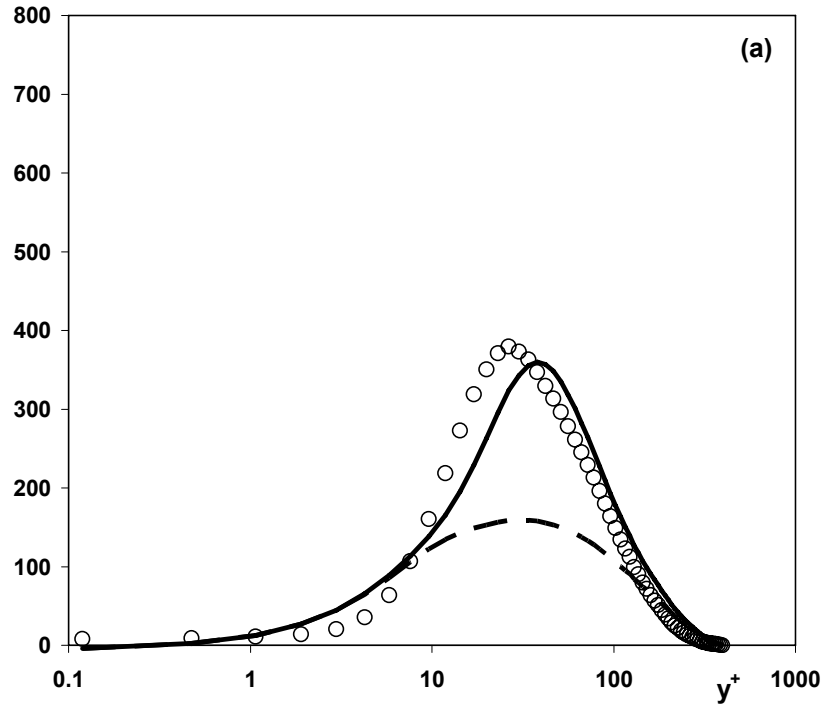
$$\frac{S_{ij}}{\sqrt{2S_{pq}S_{pq}}} \quad (144)$$

The final form of the closure of the terms in (138) is given by equation (145)

$$\begin{aligned} & C_{kn} \left(\overline{\frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{\frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \right) + C_{jn} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + C_{in} \overline{\frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} \\ & \approx \left(\frac{25}{We_{\tau_0}} \right)^{0.883} \left[C_{\varepsilon_F} \frac{4}{15} \times \frac{\varepsilon^N}{\nu_s \times \beta} C_{mm} \times f_{F2} \times \left(\delta_{ij} + \frac{S_{ij}}{\sqrt{2S_{pq}S_{pq}}} \right) \right], \end{aligned} \quad (145)$$

where parameter C_{ε_F} was introduced to account for modelling simplifications, the damping function f_{F2} takes care of low Reynolds number effects near the wall and the

corrective Weissenberg number ratio $\left(\frac{25}{We_{\tau 0}}\right)^{0.883}$ corrects for the faster increase in the triple correlation than of NLT_{ij} (cf. equation (133)) seen above in **Fig. 29**. The quantification of parameter C_{ε_F} and the specific form of function f_{F2} were obtained using DNS data at the same time as for the other coefficients and functions in order to construct the best possible model for NLT_{ij} . Those functions and the numerical values of all coefficients are listed in Table 6.



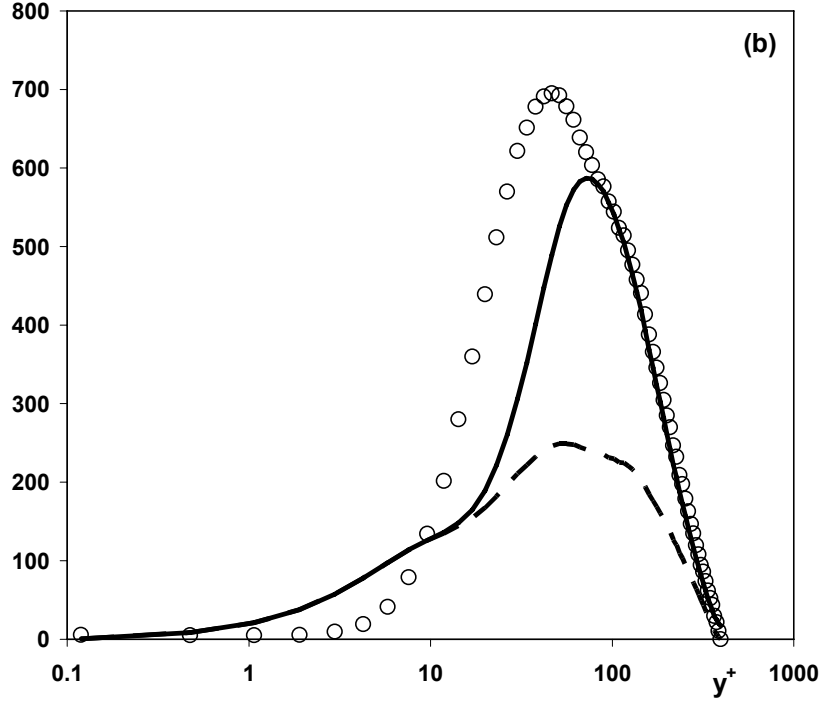


Fig. 33. Transverse profiles of DNS data for NLT_{12}^* ($\circ$); and the NLT_{12}^* model without (--) and with (—) anisotropic effect (S_{ij} extra term in Eq. (145)) in channel flow of FENE-P fluids with $Re_\tau = 395$, $L^2 = 900$, $\beta = 0.9$: (a) $We_{\tau 0} = 25$, DR=18% and (b) $We_{\tau 0} = 100$, DR=37%.

5.2.2.2. Closure for the double correlation with $f(\hat{c}_{mm})$

Invoking the previously adopted assumptions, the model for the terms containing

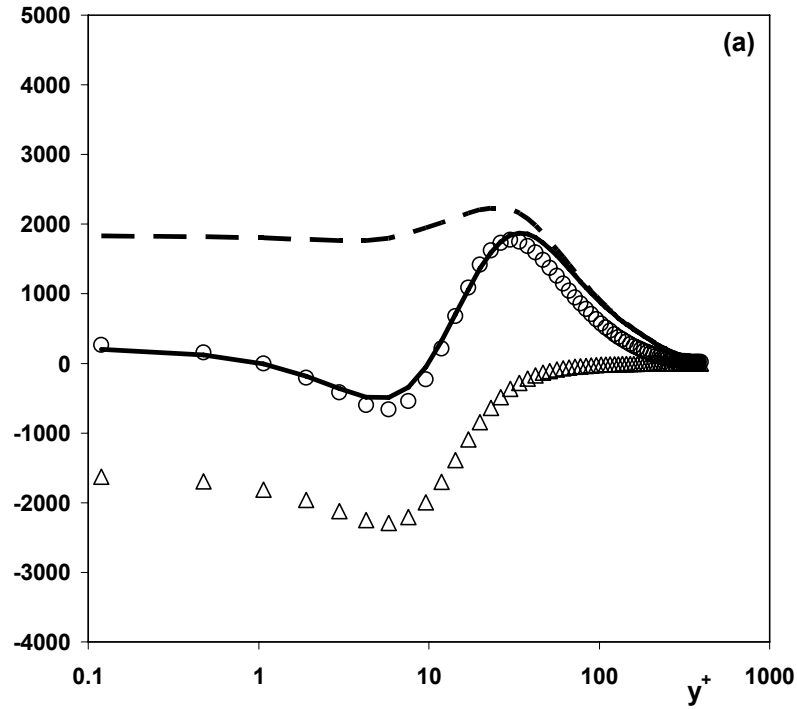
$\overline{f(\hat{c}_{mm}) \frac{\partial u_i}{\partial x_k}}$ and $\overline{f(\hat{c}_{mm}) \frac{\partial u_j}{\partial x_k}}$ in equation (16) should be zero, see equation (146).

$$\overline{C_{kj} f(\hat{c}_{mm}) \frac{\partial u_i}{\partial x_k}} \approx \overline{C_{kj} f(C_{mm}) \frac{\partial u_i}{\partial x_k}} = 0 \quad (146)$$

However, there are advantages in modelling this term as in equation (147), where the fluctuating quantities are simply substituted by the corresponding time-averaged quantities (a decoupling of the double correlation into the corresponding individual time-average terms). This is equivalent to a near wall region model, where velocity fluctuations are of the order of the mean velocity ($O(u) \sim O(U)$). Not surprisingly, it is

also here that the mean velocity gradient, mean conformation tensor and function $f(C_{mm})$ reach their maxima and where this modelled term is important. We designate the closure in equation (147) as the C_{F2} term and its contribution to the NLT_{ij} model is assessed in **Fig. 34**. Here, the C_{F2} term contribution is plotted as well as the NLT_{ij} model with and without this contribution. Note that in fully-developed channel flow this term only contributes to the NLT_{11} component.

$$\overline{C_{kj} f(\hat{c}_{mm}) \frac{\partial u_i}{\partial x_k}} + \overline{C_{ik} f(\hat{c}_{mm}) \frac{\partial u_j}{\partial x_k}} \approx C_{F2} \left[C_{kj} f(C_{mm}) \frac{\partial U_i}{\partial x_k} + C_{ik} f(C_{mm}) \frac{\partial U_j}{\partial x_k} \right] \quad (147)$$



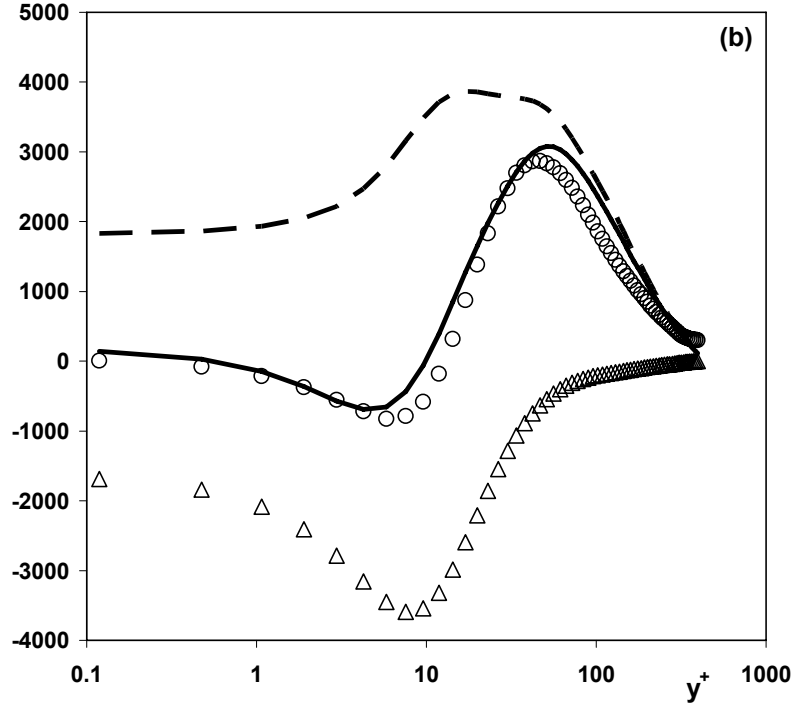


Fig. 34. Transverse profiles of DNS data for NLT_{11}^* ($\circ$), C_{F2} term (Δ), and NLT_{11}^* model without (--) and with (—) the C_{F2} contribution for channel flow of FENE-P fluids with $Re_\tau = 395$, $L^2 = 900$, $\beta = 0.9$: (a) $We_{\tau 0} = 25$, DR=18% and (b) $We_{\tau 0} = 100$, DR=37%.

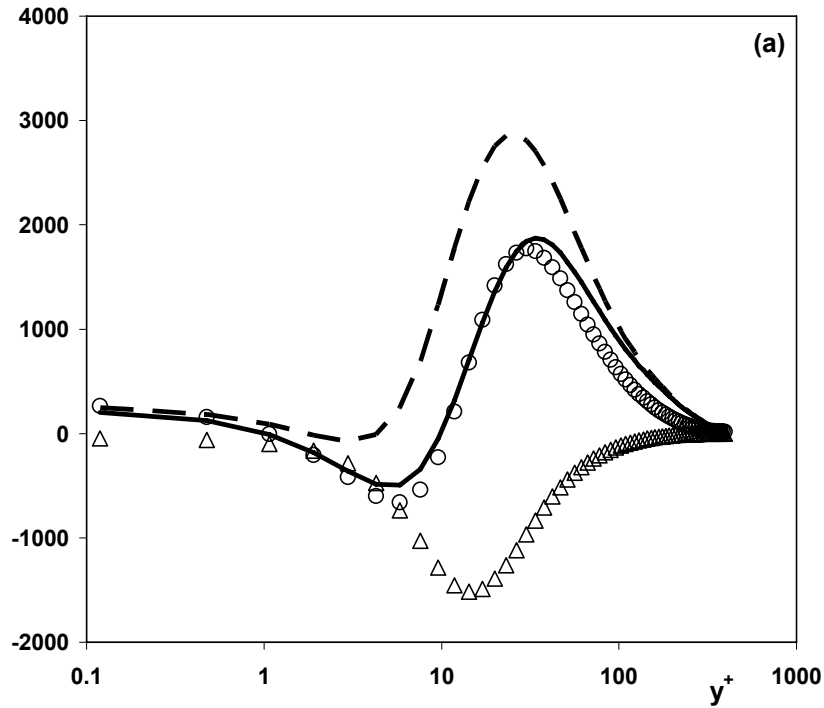
5.2.2.3. Closure for the triple correlations

To deal with the four triple correlations of equation (134) we followed on the steps of classical turbulence modelling and constitutive equation modelling, where to a first approximation an n^{th} -order correlation can be decoupled into the product of lower order correlations (this was already invoked regarding the term of equation (145) together with near-wall region arguments, as explained above). In the case of equation (148), there was a direct transformation of all fluctuating quantities into their corresponding time-averaged quantities and there was also the need to account for low Reynolds number effects via a second damping function f_{F1} .

$$\overline{c_{jn} \frac{\partial u_k}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{in} \frac{\partial u_k}{\partial x_n} \frac{\partial u_j}{\partial x_k}} + \overline{c_{kn} \frac{\partial u_j}{\partial x_n} \frac{\partial u_i}{\partial x_k}} + \overline{c_{kn} \frac{\partial u_i}{\partial x_n} \frac{\partial u_j}{\partial x_k}}$$

$$\approx -f_{F1} \times \frac{C_{F4}}{We_{\tau 0}} \times \left[C_{jn} \frac{\partial U_k}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{in} \frac{\partial U_k}{\partial x_n} \frac{\partial U_j}{\partial x_k} + C_{kn} \frac{\partial U_j}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{kn} \frac{\partial U_i}{\partial x_n} \frac{\partial U_j}{\partial x_k} \right] \quad (148)$$

An alternative closure for this term, based on a decoupling of the third order correlation into the product of the time-averaged conformation tensor with the double correlation of the fluctuating rates of deformation, would lead to a contribution identical to that of equation (138) thus adding nothing to the NLT_{ij} closure. Consequently, the model of equation (148), designated as the C_{F4} term, was adopted instead. This contribution corrects the behavior of NLT_{ij} in the buffer layer and inner log-layer and its impact is higher in the low drag reduction regime as shown in **Fig. 35**, where the DNS data is compared with the NLT_{ij} closure without and with this contribution.



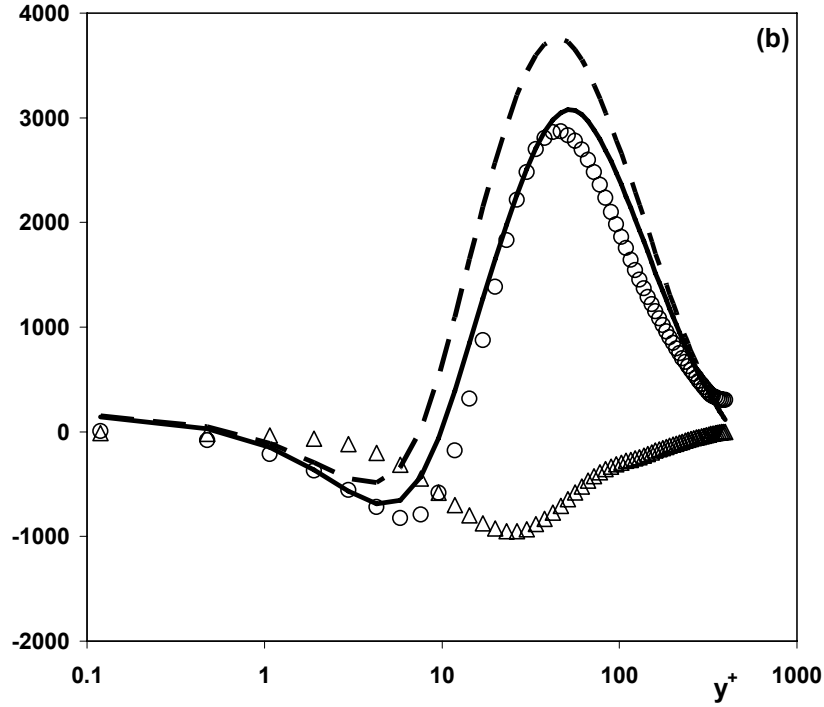


Fig. 35. Transverse profiles of DNS data for NLT_{11}^* ($\circ$), C_{F4} term (Δ), and NLT_{11}^* model without (--) and with (—) the C_{F4} term in channel flow of FENE-P fluids with $Re_\tau = 395$, $L^2 = 900$, $\beta = 0.9$: (a) $We_{\tau 0} = 25$, DR=18% and (b) $We_{\tau 0} = 100$, DR=37%.

5.2.2.4. Closure for the double cross- correlation between fluctuating strain rate and conformation tensors

Modelling of the term in equation (149) was found to be the most difficult and in the end an *ad-hoc* approach was adopted as a first approximation, but still based on some physical arguments. On the one hand the cross correlation between the fluctuating conformation and strain rate tensors was decoupled as in equation (150), which introduced a mixed viscous and turbulent length scale, $l \approx \nu_0 / \sqrt{u'_t u'_m}$, based on the Reynolds stress tensor, in order to capture anisotropy effects near the wall. We also found convenient to use the Reynolds shear stress when modelling normal components of NLT_{ij} , so in the end the approximation of equation (150) transformed a second order tensor into the product of two second order tensors, thus requiring the inclusion of

further quantities for tensorial consistency. The final expression of the model must comply with symmetry and invariance properties of the original exact term and the outcome is the model on the r.h.s of equation (151). Other physical arguments used to model this term were the need to account for the increased anisotropy of the Reynolds stress and conformation tensors with drag reduction. However, the degree of anisotropy introduced by the Reynolds stress tensor was too strong near the wall and it had to be somewhat reduced by the introduction of the trace of the conformation tensor in the denominator instead of the use of a damping function. Parameter C_{F3} takes the numerical value listed in Table 6.

$$\frac{\partial U_k}{\partial x_n} \left(\overline{c_{jn} \frac{\partial u_i}{\partial x_k}} + \overline{c_{in} \frac{\partial u_j}{\partial x_k}} \right) + \frac{\partial U_j}{\partial x_n} \overline{c_{kn} \frac{\partial u_i}{\partial x_k}} + \frac{\partial U_i}{\partial x_n} \overline{c_{kn} \frac{\partial u_j}{\partial x_k}} \quad (149)$$

$$\frac{\partial U_j}{\partial x_n} \overline{c_{kn} \frac{\partial u_i}{\partial x_k}} \sim \frac{\partial U_j}{\partial x_n} C_{kn} \frac{\sqrt{u_i u_m}}{L} \quad (150)$$

$$\begin{aligned} & \frac{\partial U_k}{\partial x_n} \left(\overline{c_{jn} \frac{\partial u_i}{\partial x_k}} + \overline{c_{in} \frac{\partial u_j}{\partial x_k}} \right) + \frac{\partial U_j}{\partial x_n} \overline{c_{kn} \frac{\partial u_i}{\partial x_k}} + \frac{\partial U_i}{\partial x_n} \overline{c_{kn} \frac{\partial u_j}{\partial x_k}} \\ & \approx \frac{C_{F3}}{C_{mm}} \times \left[\frac{\partial U_j}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + \frac{\partial U_i}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + \right. \\ & \quad \left. \frac{\partial U_k}{\partial x_n} \frac{\partial U_m}{\partial x_k} \left(C_{jn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + C_{in} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} \right) \right] \quad (151) \end{aligned}$$

5.2.2.5. *Extra contribution and full NLT_{ij} model for second order turbulence closures*

Finally, to ensure a well - behaved closure for NLT_{ij} , there was the need to add an extra term. As can be seen in **Fig. 36**, without the inclusion of such a corrective term there is a deficit in the prediction of NLT_{11} in the viscous sublayer and in the buffer layer. This situation is frequent in turbulence modelling, where the invoked assumptions

can over-simplify the physics. The added term is given in equation (152) and is denoted as the C_{F1} term.

$$C_{F1} \times \frac{C_{ij} \times f(C_{mm})}{\lambda} \quad (152)$$

Putting together all terms, the final form of the full model for NLT_{ij} is

$$\begin{aligned} NLT_{ij} \equiv \overline{c_{kj} \frac{\partial u_i}{\partial x_k}} + \overline{c_{ik} \frac{\partial u_j}{\partial x_k}} &\approx C_{F1} \times \frac{C_{ij} \times f(C_{mm})}{\lambda} - C_{F2} \left[C_{kj} \frac{\partial U_i}{\partial x_k} + C_{ik} \frac{\partial U_j}{\partial x_k} \right] \\ &+ \frac{\lambda}{f(C_{mm})} \left[\frac{C_{F3}}{C_{mm}} \times \left(\frac{\partial U_j}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + \frac{\partial U_i}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} \right. \right. \\ &\quad \left. \left. + \frac{\partial U_k}{\partial x_n} \frac{\partial U_m}{\partial x_k} \left(C_{jn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + C_{in} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} \right) \right) \right] \\ &- \frac{\lambda}{f(C_{mm})} \times f_{F1} \times \frac{C_{F4}}{We_{\tau 0}} \times \left[C_{jn} \frac{\partial U_k}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{in} \frac{\partial U_k}{\partial x_n} \frac{\partial U_j}{\partial x_k} + C_{kn} \frac{\partial U_j}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{kn} \frac{\partial U_i}{\partial x_n} \frac{\partial U_j}{\partial x_k} \right] \\ &+ \frac{\lambda}{f(C_{mm})} \left(\frac{25}{We_{\tau 0}} \right)^{0.883} \left[C_{\varepsilon_F} \frac{4}{15} \times \frac{\varepsilon^N}{\nu_s \times \beta} C_{mm} \times f_{F2} \times \left(\delta_{ij} + \frac{S_{ij}}{\sqrt{2S_{pq} S_{pq}}} \right) \right] \end{aligned} \quad (153)$$

where the numerical values of the coefficients obtained during the calibration are listed in Table 6. With the exception of C_{ε_F} all other parameters are of order 1, an indication of the goodness of the used approaches.

The two damping functions required to fix the near wall behaviour vary, as usual for Newtonian fluids, from zero at the wall to one far from the wall and are given by equations (154) and (155).

$$f_{F1} = \left(1 - 0.67 \exp \left(-\frac{y^+}{17} \right) \right)^4 \quad (154)$$

$$f_{F2} = \left(1 - \exp \left(-\frac{y^+}{25} \right) \right)^4 \quad (155)$$

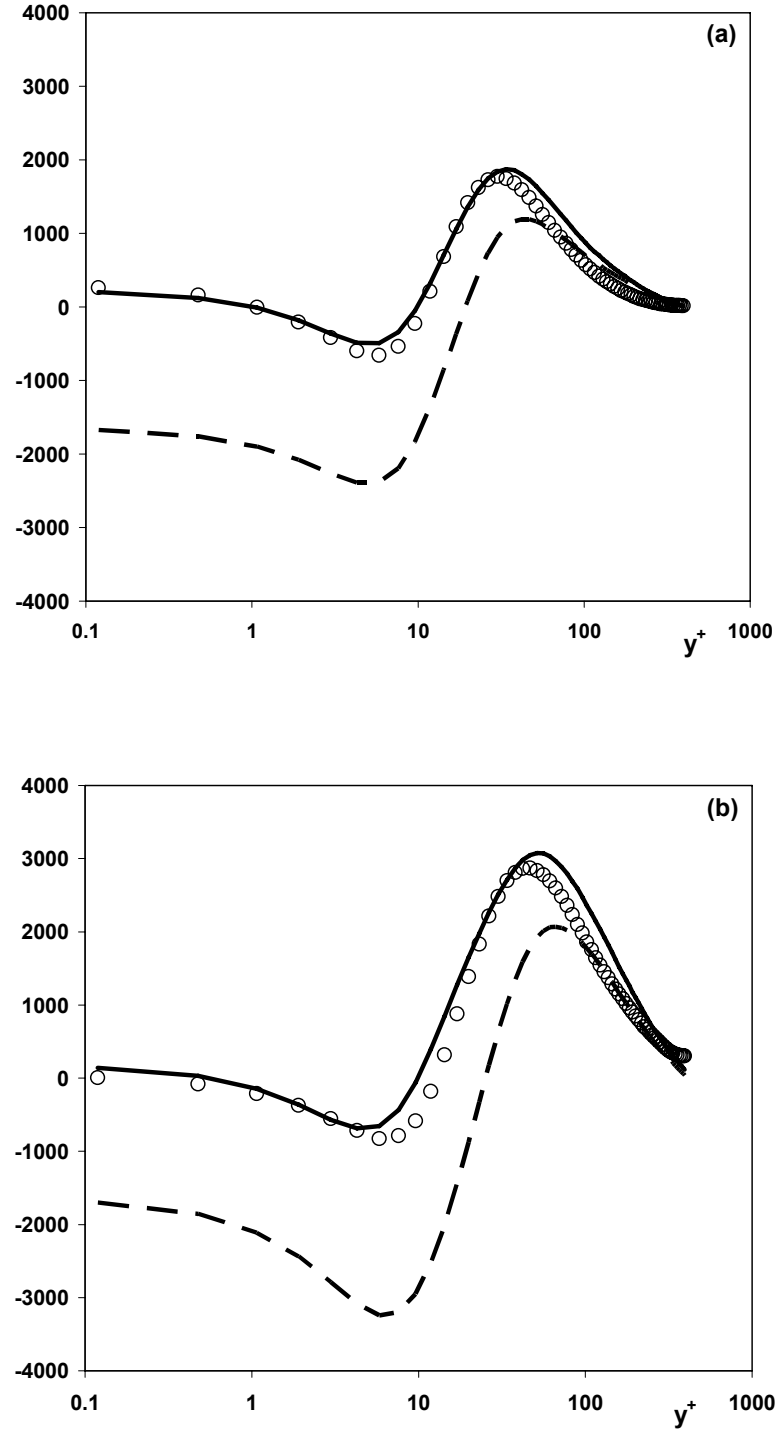


Fig. 36. Axial profile of DNS data for NLT_{11}^* ($\circ$) and NLT_{11}^* model without (--) and with (—) the C_{F1} term for the channel flow of FENE-P fluids with $Re_{\tau} = 395$, $L^2 = 900$, $\beta = 0.9$: (a) $We_{\tau_0} = 25$, $DR=18\%$ and (b) $We_{\tau_0} = 100$, $DR=37\%$.

Table 6. Values of the model parameters and damping functions for the second order model for NLT_{ij} .

C_{F1}	C_{F2}	C_{F3}	C_{F4}	C_{ε_F}
0.24	0.2	2	10	0.049

It is worth mentioning here that the model was initially developed and calibrated only against DNS data for 18% drag reduction. Subsequently it was corrected to 37% drag reduction with minor adjustments in the numerical values of the coefficients C_{F4} and C_{ε_F} , which is a good sign regarding the robustness of the model. These two sets of data pertain to the low and high drag reduction regimes and it remains to be seen whether the model works well at higher drag reductions including maximum drag reduction conditions. This also should involve an increase in parameter L^2 and the correct quantification of its effect on the closure. Finally, note that this model is actually to be used in the context of second order closures, whereas for first order closures slight modifications in the numerical values of the coefficients are required, as will be explained next.

5.2.2.6. Full NLT_{ij} model for first order turbulence closures

The model of equation (153) relies on the rate of dissipation of turbulent kinetic energy by the solvent, but also on the Reynolds stress tensor. Hence, it can be used for both first and second order closures, but there is an implication that must be accounted for when relying on isotropic first order turbulence models, such as the k - ε or the k - ω models. As a consequence of using the Boussinesq model of equation (126), the normal Reynolds stresses are calculated with equation (156), where k is the turbulent kinetic energy, so the anisotropy on which the model of equation (153) was developed is no longer present. Consequently, the NLT_{ij} closure needs to be modified for such cases. Its overall form is still the same as in equations (153), but the isotropy of the normal Reynolds stresses requires an adjustment of the numerical value of the coefficients.

$$\overline{u_1 u_1} = \overline{u_2 u_2} = \overline{u_3 u_3} = \frac{2}{3} k \quad (156)$$

To calibrate the "isotropic" NLT_{ij} model, which is presented in equation (157), the same two sets of DNS data were used and the same strategy followed: the closure was initially developed on the basis of data for DR= 18% and its extension to DR= 37% only required minor adjustments in the coefficients, which are listed in Table 7. Except for coefficient C_{F3} all other coefficients are of order 1. Regarding the damping functions, f_{F2} remains the same whereas function f_{F1} is slightly modified to that of equation (157).

$$\begin{aligned} NLT_{ij} \equiv \overline{c_{kj} \frac{\partial u_i}{\partial x_k}} + \overline{c_{ik} \frac{\partial u_j}{\partial x_k}} \approx C_{F1} \times \frac{C_{ij} \times f(C_{mm})}{\lambda} - \frac{C_{F2}}{We_{\tau 0}} \left[C_{kj} \frac{\partial U_i}{\partial x_k} + C_{ik} \frac{\partial U_j}{\partial x_k} \right] \\ + \frac{\lambda}{f(C_{mm})} \left[C_{F3} \times \left(\frac{\partial U_j}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + \frac{\partial U_i}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + \frac{\partial U_k}{\partial x_n} \frac{\partial U_m}{\partial x_k} \left(C_{jn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + C_{in} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} \right) \right) \right] \\ - \frac{\lambda}{f(C_{mm})} \times f_{F1} \times C_{F4} \times \left(\frac{We_{\tau 0}}{25} \right)^{0.228} \times \left[C_{jn} \frac{\partial U_k}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{in} \frac{\partial U_k}{\partial x_n} \frac{\partial U_j}{\partial x_k} + C_{kn} \frac{\partial U_j}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{kn} \frac{\partial U_i}{\partial x_n} \frac{\partial U_j}{\partial x_k} \right] \\ + \frac{\lambda}{f(C_{mm})} \left[\frac{C_{\varepsilon_F}}{We_{\tau 0}} \frac{4}{15} \times \frac{\varepsilon^N}{\nu_s \times \beta} C_{mm} \times f_{F2} \times \delta_{ij} \right] \end{aligned} \quad (157)$$

$$f_{F1} = \left(1 - 0.8 \exp \left(-\frac{y^+}{30} \right) \right)^2 \quad (158)$$

To appreciate the difference between the "isotropic" NLT_{ij} model of Eq. (157) and the "second order" NLT_{ij} model of Eq. (153) we must recall that the C_{F3} term in Eq. (153) was aimed at introducing anisotropy as well as some shear effect to the NLT_{ij} closure. The substitution of the anisotropic Reynolds stress tensor by equation (7) partially reduced the former effect and for compensation the trace C_{kk} was removed from the denominator and coefficient C_{F3} modified. The former value of $C_{F3}/C_{kk} = 2/(\approx 300) \approx 0.0067$ (cf. value of C_{F3} in Table 1) is substituted by 0.017 (the new $C_{F3} = 0.026$, cf. Table 7 since $2/3 C_{F3}^{isotropic} = 2/3 \times 0.026 = 0.017$), which is essentially twice as large as before. Consequently, this raised excessively the shear contribution of the

C_{F3} term to the closure of NLT_{12} and this could only be corrected by removing the shear correction of equation (144).

Table 7. Values of the model parameters and damping functions for the isotropic NLT_{ij} model.

C_{F1}	C_{F2}	C_{F3}	C_{F4}	C_{ε_F}
0.32	5	0.026	0.806	1.4275

5.2.2.7. NLT_{ij} closure with isotropic turbulence for first order turbulence closures

The NLT_{ij} models presented above, Eq. (153) and Eq. (157), were developed on the basis of the DNS data, but they are to be used in the context of turbulence closures which themselves are based on simplifying assumptions. For instance, if using the NLT_{ij} closure within the scope of a k - ε model the assumption of turbulence isotropy in the latter will naturally affect the performance of the former, since the turbulence is not isotropic. For this reason minor modifications to the above NLT_{ij} closures are necessary for it to work properly when integrated in the k - ε model. These are just modifications in the numerical values of the parameters and the introduction of the polymeric viscosity in the lat term of the closure, everything else remaining unchanged. Hence, the final form of the NLT_{ij} closure implemented in the present viscoelastic k - ε turbulent model is given by equation (159).

$$\begin{aligned}
 NLT_{ij} \equiv \overline{c_{kj} \frac{\partial u_i}{\partial x_k}} + \overline{c_{ik} \frac{\partial u_j}{\partial x_k}} \approx C_{F1} \left(0.0552 \frac{We_{\tau 0}}{25} + 0.116 \right) \times \frac{C_{ij} \times f(C_{mm})}{\lambda} - C_{F2} We_{\tau 0}^{0.743} \left[C_{kj} \frac{\partial U_i}{\partial x_k} + C_{ik} \frac{\partial U_j}{\partial x_k} \right] \\
 + \frac{\lambda}{f(C_{mm})} \left[C_{F3} \times \left(\frac{25}{We_{\tau 0}} \right)^{0.718} \times \left(\frac{\partial U_j}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + \frac{\partial U_i}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} \right. \right. \\
 \left. \left. + \frac{\partial U_k}{\partial x_n} \frac{\partial U_m}{\partial x_k} \left(C_{jn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + C_{in} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} \right) \right) \right]
 \end{aligned}$$

$$\begin{aligned}
& -\frac{\lambda}{f(C_{mm})} \times f_{F1} \times C_{F4} \times \left(\frac{25}{We_{\tau_0}} \right)^{0.7} \times \left[C_{jn} \frac{\partial U_k}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{in} \frac{\partial U_k}{\partial x_n} \frac{\partial U_j}{\partial x_k} + C_{kn} \frac{\partial U_j}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{kn} \frac{\partial U_i}{\partial x_n} \frac{\partial U_j}{\partial x_k} \right] \\
& + \frac{\lambda}{f(C_{mm})} \left[\frac{C_{\varepsilon_F}}{We_{\tau_0}} \frac{4}{15} \times \frac{\varepsilon^N}{(\nu_s + \nu_{\tau_p})^\times \beta} C_{mm} \times f_{F2} \times \delta_{ij} \right]
\end{aligned} \tag{159}$$

The numerical values of the coefficients of this NLT_{ij} closure are: $C_{F1}=1$, $C_{F2}=0.0105$, $C_{F3}=0.046$, $C_{F4}=1.05$ and $C_{\varepsilon_F}=2$, whereas the damping functions remain unchanged.

5.2.3 Assessment of the performance of the NLT_{ij} model against DNS data

The performance of the two models of NLT_{ij} , designated by second-order and isotropic models, developed above are discussed separately through comparisons with the DNS data, but the data are plotted together for better comparison. We discuss first the general closure for second order model (Eqs. (153) to (155)) followed by the "isotropic" NLT_{ij} closure of Eqs. ((157)to (158)).

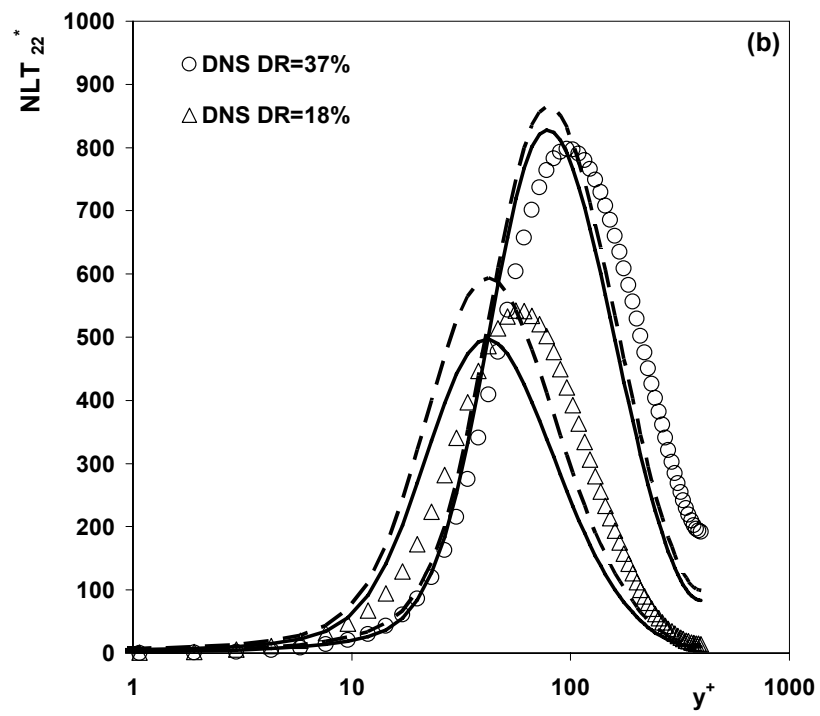
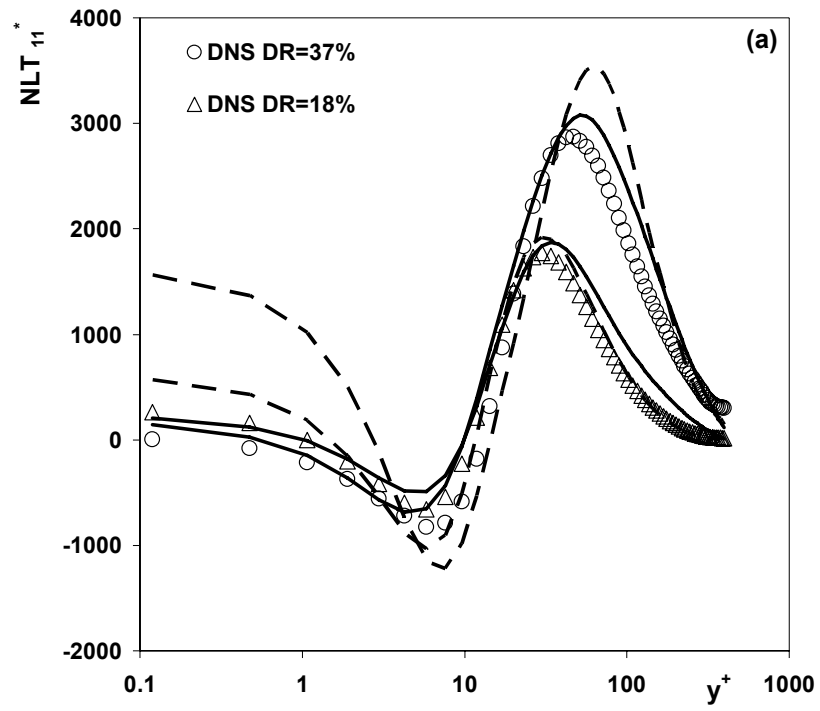
Fig. 37 - (a) to (d) compares the DNS data for the non-zero components of the NLT_{ij} tensor with the model predictions as full lines. Note that the quantities appearing in the model equations are also from DNS, so only the closure for NLT_{ij} is really being assessed here.

Careful inspection of **Fig. 37** shows that the model in general predicts well both the low and high drag reduction regimes. In assessing the model performance we must distinguish between the viscous sublayer region and the buffer and log-law regions. NLT_{ij} in the viscous sublayer is not so important, because the exact terms in the governing equations are much larger than this contribution, as shown by Li et al. [39] and Pinho et al. [4]. Therefore, the discrepancies in the wall region seen in **Fig. 37** are essentially of no consequence. The buffer and log-law regions are those that matter and here **Fig. 37** shows that the model performs well. It slightly overpredicts NLT_{11} and it predicts well the magnitude of NLT_{22} , but with a slight shift in the location of its peak

value towards the wall. For NLT_{33} both sets are underpredicted and for NLT_{12} the model behaves very well in the outer region but underpredicts in the inner region.

The performance of the "isotropic" NLT_{ij} model is also plotted in **Fig. 37** as dashed line. In general the "isotropic" model is as good as the general model with deviations in some components being compensated by improvements in other components. NLT_{11} is not so well predicted as by the previous model especially at HDR. For NLT_{22} and NLT_{33} the "isotropic" model compares with DNS as the general model with minor improvements at some locations. Regarding the shear component the "isotropic" model is definitely better than the general model in the log-law region. It is worse in the inner region, but this is of no consequence as mentioned. The two models for NLT_{ij} are similar at low drag reductions, but differ more at high drag reduction, with the "isotropic" model deviating more from the DNS data and performing less well. This can be justified by the increase of anisotropic effects with drag reduction, something that is not totally captured by the "isotropic" NLT_{ij} model.

As drag reduction increases, both models capture well the shift away from the wall of the peak of the various components of NLT_{ij} . In the context of a two-equation turbulence model, such as the k - ε model, the most important component of NLT_{ij} is actually NLT_{22} , which strongly affects C_{22} since the other terms in the evolution equation of C_{22} are null. Then, this affects the polymer shear stress $\tau_{12,p}$ and the momentum equation. In the governing equations of the other stresses, such as $\tau_{11,p}$ the other exact terms of $\tau_{11,p}$ far outweigh NLT_{11} , even though NLT_{11} is the largest component of NLT_{ij} . The capacity of this turbulence model to predict the negative peak of NLT_{11} in the near wall region contributes to a correct prediction of C_{kk} , and more specifically to the increase of its near wall peak with drag reduction, cf. **Fig. 30**.



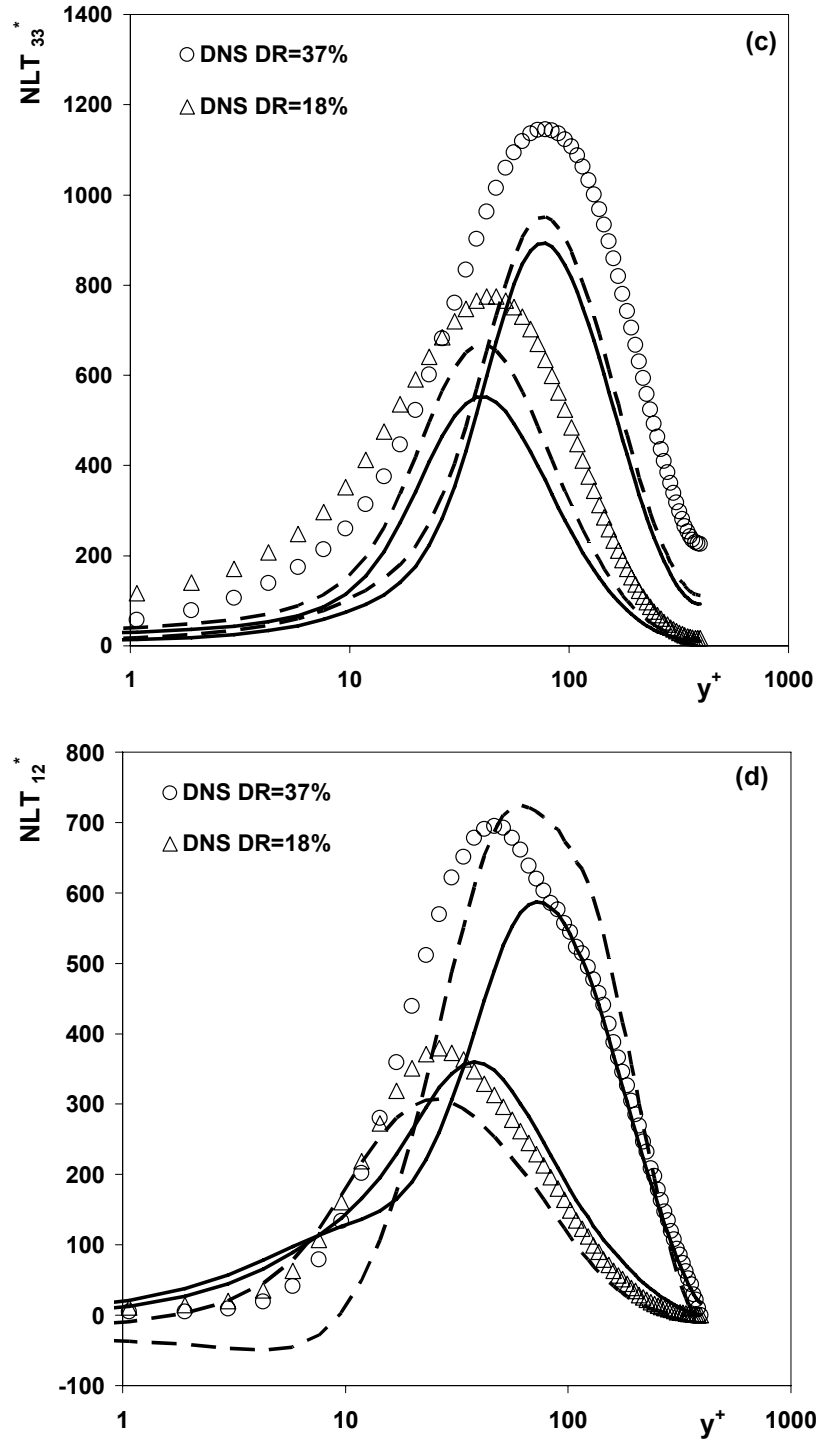


Fig. 37. Comparison between DNS data (symbols), the second-order model (—) and the isotropic model (---) of NLT_{ij}^* and for $Re_{\tau_0} = 395$, $L^2 = 900$, $\beta = 0.9$ with $We_{\tau_0} = 25$ (DR=18%) and $We_{\tau_0} = 100$ (DR= 37%): (a) NLT_{11}^* ; (b) NLT_{22}^* ; (c) NLT_{33}^* ; (d) NLT_{12}^* .

5.3 Eddy viscosity model

Experiments on drag reduction [16] as well as DNS data of Sureshkumar et al [81] and Li et al [39], amongst others, show a reduction in the normalised Reynolds shear stress as DR is increased, which implies a reduction in the eddy viscosity. The model used by Pinho et al [4] for the eddy viscosity is that of Jones and Launder [97], which required an increase in ε^N in order to predict the correct behavior of the Reynolds stress with drag reduction. However, this is in contradiction with the literature regarding the behavior of ε^N and the implication is that polymers affect directly the distribution of the eddy viscosity and consequently quantifiers of viscoelasticity should appear in a model for ν_T . In this work we propose a new closure for the eddy viscosity of the polymer solution, which corrects the deficiencies of the previous model used by Pinho et al. [4], which was essentially identical to that for a Newtonian fluid. This new closure is given by Eq. (160). As will be shown, the polymer contribution to the eddy viscosity (ν_T^P) is proportional to such quantities as the trace of the conformation tensor, the Weissenberg number and the viscoelastic stress work, in addition to the classical quantities (k and ε^N).

$$\nu_T = \nu_T^N - \nu_T^P = \nu_T^N \left(1 - \frac{\nu_T^P}{\nu_T^N} \right) \quad (160)$$

with

$$\nu_T^N = C_\mu \times f_\mu \times \frac{k^2}{\varepsilon} \quad \text{and} \quad \frac{\nu_T^P}{\nu_T^N} = C_\mu^P \times f_\mu^P \times f_{DR}^P \times C_{mm} \quad (161)$$

Here f_μ^P accounts for the different damping of the wall acting on the polymer contribution to ν_T and f_{DR}^P introduces a Weissenberg number effect. Both functions take the forms in Eq. (1), which include also the classical Van Driest damping function f_μ and they were developed using the two DNS data sets. Here, and elsewhere in the turbulence model, we adopt the model of Nagano and Hishida [14] for the terms common to the corresponding turbulence model for a Newtonian fluid, such as for f_μ

and other damping functions in the transport equations of k and ε^N , with modifications to the turbulent Prandtl numbers as will be explained below. Hence, coefficients $C_\mu = 0.09$ and $C_\mu^P = 0.00045$.

$$\begin{aligned} f_\mu^P &= \left[1 + 2.55 \times \exp\left(-\frac{y^+}{44}\right) \right]; \\ f_{DR}^P &= \left[1 - \exp\left(-\frac{We_{\tau 0}}{6.25}\right) \right]^4 \times \left[\frac{25}{We_{\tau 0}} \right]^{0.8}; \\ f_\mu &= \left[1 - \exp\left(-\frac{y^+}{26.5}\right) \right]^2 \end{aligned} \quad (162)$$

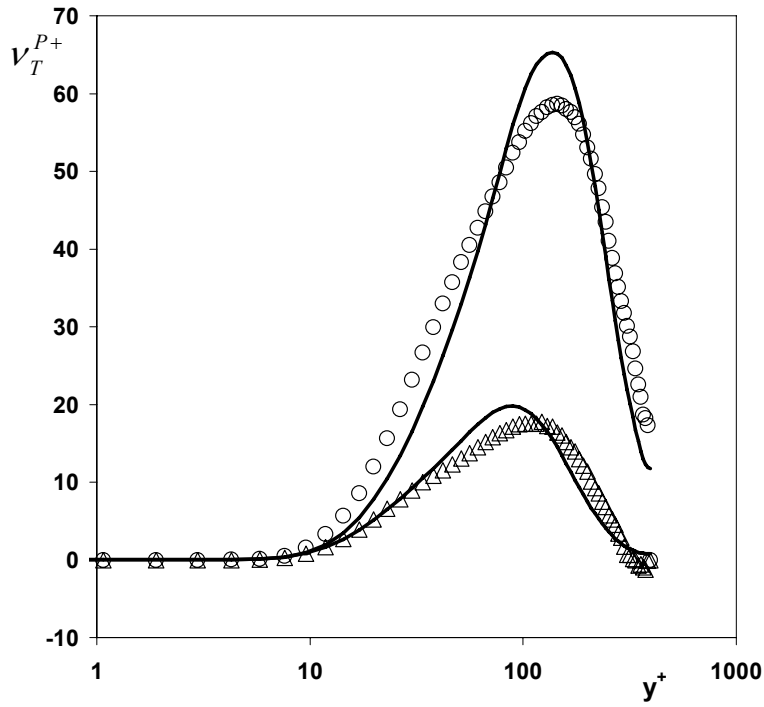


Fig. 38. Comparison between DNS data (symbols) and the model predictions (lines) of the polymeric turbulent viscosity, v_T^P , normalized by zero shear viscosity, v_0 , defined by Eq. (161) for turbulent channel flow with $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$: Δ 18% DR and $\circ$ 37% DR.

The evolution of the polymeric turbulent viscosity is compared with the model of Eq. (161) in **Fig. 38**, whereas the total eddy viscosity, including the Newtonian and the

polymeric contributions are compared in **Fig. 39**, where the model data corresponds to the predictions by the k - ε model. The new turbulent viscosity model has a direct impact in the buffer layer, and it has an important role to correctly predict the shear stresses and the rate of dissipation as will be shown in section 5.5.

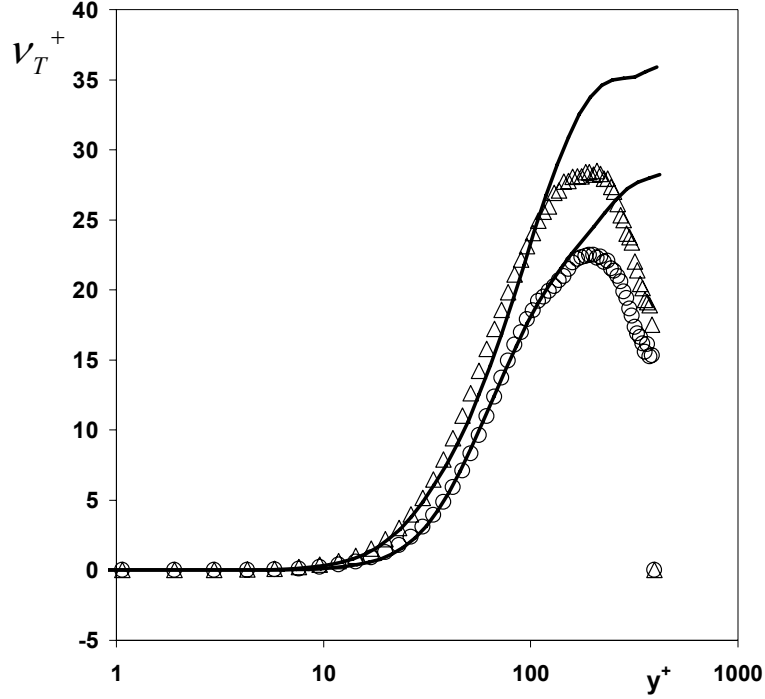


Fig. 39. Comparison between DNS data (symbols) and the turbulence model predictions (lines) of the turbulent viscosity ν_T normalized by zero shear viscosity, ν_0 , for DR= 18% (Δ) and 37% ($\circ$) in a turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$.

5.4 Closures in the transport equations of k and ε^N

The Reynolds stress in the momentum equation is calculated by equation (126) which requires a model for the eddy viscosity and the knowledge of the turbulent kinetic energy (k). The eddy viscosity itself also depends on k . The turbulent kinetic energy is given by its transport equation, which also contains terms that need to be modelled in addition to existing terms modelled in the context of Newtonian fluid mechanics that may need to be modified. As explained, one of terms is the rate of

dissipation of turbulent kinetic energy by the Newtonian solvent ($\tilde{\varepsilon}^N$), which is also given by a transport equation, the exact form of which is equation (129) derived by Pinho et al. [4]. In this work we adopt classical Newtonian closures as much as possible and describe the closures of terms containing viscoelastic contributions, or on classical terms that are modified by the presence of the polymer additives. As a consequence the transport equations for k and $\tilde{\varepsilon}^N$ that we actually solve are equations (163) and (164), respectively, which are discussed next. In equation (163) use was made of the relation between the rate of dissipation (ε^N) and its modified form ($\mathcal{E}^N$), given by $\varepsilon^N = \mathcal{E}^N + D$.

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho U_i k}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\left(\eta_s + \frac{\rho f_i v_T}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] - \rho u_i u_k \frac{\partial U_i}{\partial x_k} + \eta_s \frac{\partial^2 k}{\partial x_i \partial x_i} - \rho (\mathcal{E}^N + D) + Q^V - \rho \varepsilon^V \quad (163)$$

$$\begin{aligned} \frac{\partial \rho \tilde{\varepsilon}^N}{\partial t} + \frac{\partial \rho U_i \tilde{\varepsilon}^N}{\partial x_i} = & \frac{\partial}{\partial x_i} \left[\left(\eta_s + \frac{\rho f_i v_T}{\sigma_\varepsilon} \right) \frac{\partial \tilde{\varepsilon}^N}{\partial x_i} \right] + f_1 C_{\varepsilon_1} \frac{\tilde{\varepsilon}^N}{k} P_k \\ & - f_2 C_{\varepsilon_2} \rho \frac{\tilde{\varepsilon}^{N^2}}{k} + \eta_s v_T (1 - f_\mu) \left(\frac{\partial^2 U_i}{\partial y \partial y} \right)^2 + E_{\tau_p} \end{aligned} \quad (164)$$

$$D = 2(\nu_s + \nu_{\tau_p}) \left(\frac{d\sqrt{k}}{dy} \right)^2 \quad (165)$$

The LHS of both Eqs. (163) and (164) concern the advection of the transported quantities. The first term on the RHS of both equations account for turbulent diffusion of the transported quantities and are here modeled as for Newtonian fluids following Nagano and Hishida [14], but modified by a variable turbulent Prandtl number via function f_i as suggested by Nagano and Shimada [98] and Park and Sung [99]. Note also that we follow the standard approach of working with a modified Newtonian rate of dissipation of k ($\tilde{\varepsilon}^N$), related to the true dissipation (ε^N) by $\varepsilon^N = \tilde{\varepsilon}^N + D$, where D is given in Eq. (165). Regarding D , it was necessary to account for the shear-thinning inherent to the FENE-P model so the viscosities appearing in its definition are the solvent kinematic viscosity (ν_s) and the local polymer kinematic viscosity given by $\nu_{\tau_p} = \bar{\tau}_{xy,p} / (\rho \dot{\gamma})$, where $\dot{\gamma}$ is the local shear rate.

The final terms on the RHS of Eqs. (163) and (164) introduce the polymer effect, in particular the two last terms in Eq. (163) are the viscoelastic turbulent transport (Q^V) and the viscoelastic stress work (ε^V), whereas the last term in Eq. (164) (E_{τ_p}) is the viscoelastic contribution to the equation of $\tilde{\varepsilon}_N$. The remaining terms are those of the base Newtonian turbulence model, as mentioned above, and the corresponding damping functions taking account of the low Reynolds number behaviour are $f_\mu = [1 - \exp(-y^+/26.5)]^2$, with $y^+ = u_\tau y / \nu_{wall}$ based on the wall kinematic viscosity of the solution, $f_1 = 1.0$ and $f_2 = 1 - 0.3 \exp(-R_t^2)$ with $R_t = k^2 / (\nu_s \tilde{\varepsilon}_N)$. To correct the turbulent diffusion near to the wall we use the damping function $f_t = 1 + 3.5 \exp[-(R_t/150)^2]$ (c.f. [98, 99]). The numerical values of the remaining coefficients are: $\sigma_k = 1.1$, $\sigma_\varepsilon = 1.3$, $C_{\varepsilon_1} = 1.45$ and $C_{\varepsilon_2} = 1.90$.

To finalize the turbulence model we specifically present in the next section the closures developed for the three viscoelastic terms appearing in the transport equations of k and $\tilde{\varepsilon}_N$.

5.4.1 Closures for the viscoelastic terms in k and $\tilde{\varepsilon}_N$ equations

The closures developed by Pinho et al. [4] for low drag reduction (LDR) were modified to deal also with the high drag reduction (HDR) regime. In addition it was also necessary to take into account that the order of magnitude of some of the terms changed on going from LDR to HDR. Finally, in order to improve the performance of the closures it was necessary to develop/include extra contributions in many/one case(s).

5.4.1.1. *Viscoelastic stress work model for the turbulent kinetic energy transport equation*

Pinho et al. [4] have shown that another role of NLT_{ij} is in modelling the viscoelastic stress work appearing in the transport equations of turbulence kinetic

energy and of the Reynolds stresses, as will be discussed below. The former relies exclusively on the trace of NLT_{ij} , whereas for the latter all its components are required. Hence, in the context of first-order turbulence closures, such as a k - ε turbulence closure, it is extremely important for the closure developed for NLT_{ij} to be able to predict accurately its trace, NLT_{kk} . The comparison between DNS data and the predictions by the second order and the isotropic models for the trace of NLT_{ij} is shown in **Fig. 40**. The quality of the predictions is better than that of NLT_{11} , the largest contribution to the trace by far, because the underprediction of NLT_{33} partially compensates for the overprediction of NLT_{11} (cf. **Fig. 37**). Regarding the prediction of NLT_{kk} , the "isotropic" model performs less well than the "second-order" closure, because of the stronger overprediction of NLT_{11} in the former.

Having shown the predictive capabilities of the new closures regarding NLT_{kk} the remaining issue is whether the model developed by Pinho et al. [4] for the viscoelastic stress work also applies to HDR. The transport equation for the turbulent kinetic energy (k) of a FENE-P fluid is equation (128), where there is dissipation of k by two different components, the solvent (Newtonian) contribution and the polymeric (viscoelastic) contribution, both of which are defined below equation (129). The Newtonian part is given by the classical rate of dissipation of k (denoted ε^N), which needs to be calculated by an appropriate transport equation. The viscoelastic counterpart (ε^V) is actually called viscoelastic stress work as it is not everywhere of dissipative nature, and an adequate closure needs to be developed for it. This viscoelastic stress work is also defined in terms of the conformation tensor components below equation (129) taken from [4].

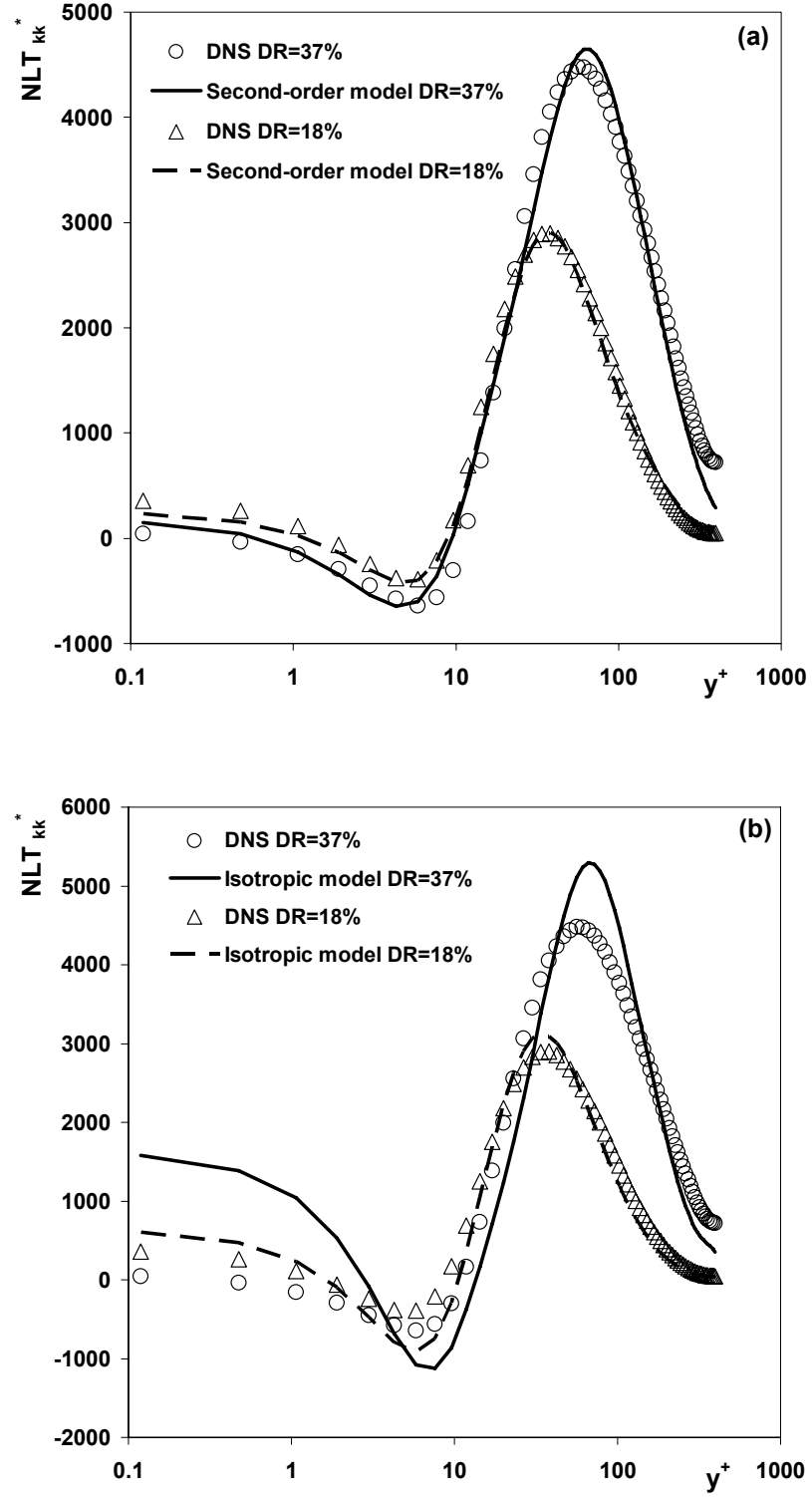
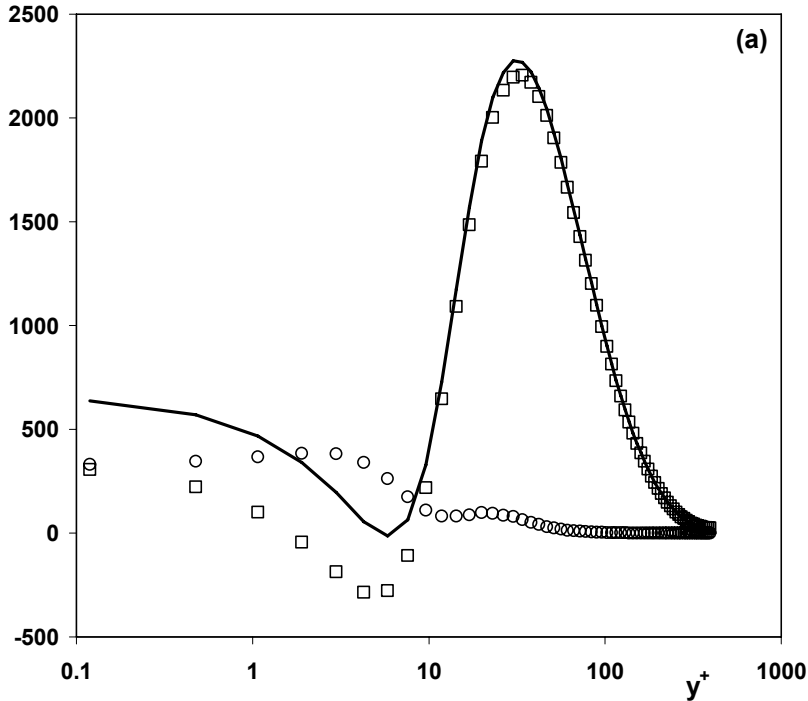


Fig. 40. Comparison between the DNS data and models for the trace of NLT_{ij} for $Re_{\tau_0} = 395$, $L^2 = 900$, $\beta = 0.9$ with $We_{\tau_0} = 25$ (18% DR) and $We_{\tau_0} = 100$ (37% DR): (a) second-order model of NLT_{ij} (Eq. (153)) and (b) isotropic model of NLT_{ij} (Eq. (157))

For DR=18% Pinho et al. [4] have shown that the double correlation is negligible by comparison with the triple correlation, $\overline{C_{ik} f(\hat{c}_{mm}) \frac{\partial u_i}{\partial x_k}} \ll \overline{c_{ik} f(\hat{c}_{mm}) \frac{\partial u_i}{\partial x_k}}$. The same applies at higher drag reductions, even though by a slight lesser amount as can be seen in **Fig. 41**. As the Weissenberg number increases the magnitude of the double correlation term increases in absolute and relative terms, but far from the wall the underlying approximation essentially remains valid. Close to the wall the double correlation is as important as the triple correlation, but ε^V is negligible in comparison to three other relevant terms of the transport equation of k , namely the rate of dissipation by the Newtonian solvent, the production of turbulence and the molecular diffusion of k , cf. Pinho et al. [4]. Therefore the same simplification, embodied in equation (166), can be used at HDR with no negative effects upon the balance equation of k .

$$\varepsilon^V \approx \frac{\eta_p}{\rho\lambda} \left[\overline{c_{ik} f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}} \right]. \quad (166)$$



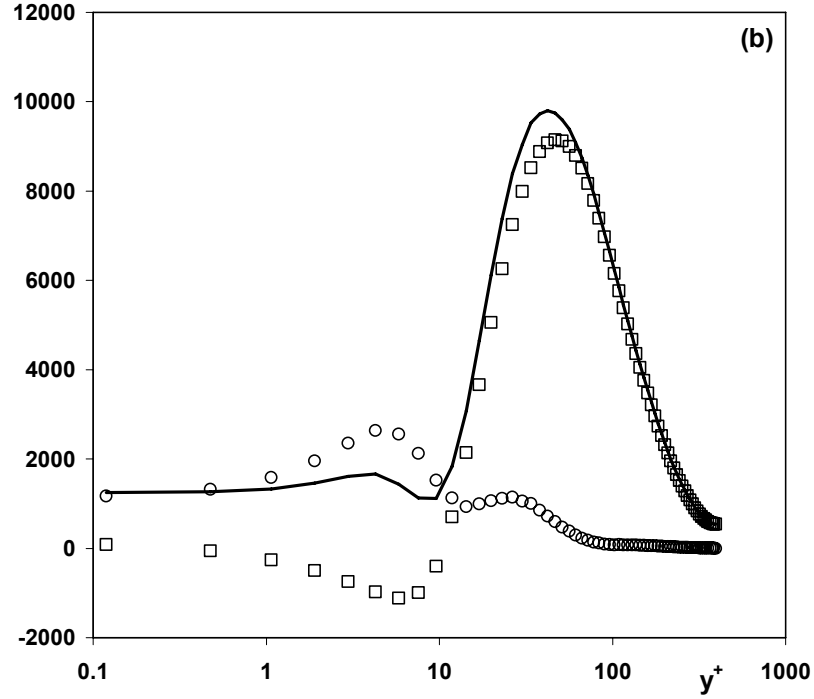


Fig. 41. Transverse profiles of the different contributions to $\varepsilon^{V+} \text{Re}_{\tau 0}^{-2}$ (equation (129)), $(\circ) \overline{C_{ik} f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}}$, $(\square) \overline{c_{ik} f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}}$ and the sum (—) for the channel flow of a FENE-P with $\text{Re}_{\tau} = 395$, $L^2 = 900$, $\beta = 0.9$: (a) $We_{\tau 0} = 25$, $\text{DR} = 18\%$ and (b) $We_{\tau 0} = 100$, $\text{DR} = 37\%$.

Following the methodology of Pinho et al. [4], the triple correlation is decoupled into a product of the double correlation NLT_{kk} with the function $f(C_{kk})$ of the time-averaged trace of the conformation tensor and then corrected by a multiplicative parameter. To account for a small Weissenberg number dependence a corrective function is also introduced leading to the final form of the model for the viscoelastic stress work given by equation (167)

$$\varepsilon^V ; \frac{\eta_p}{\rho\lambda} \left[\overline{c_{ik} f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}} \right] \approx \frac{\eta_p}{\rho\lambda} \left[f(C_{mm}) \overline{c_{ik} \frac{\partial u_i}{\partial x_k}} \right] = C_{\varepsilon^V} \left(\frac{We_{\tau 0}}{25} \right)^{n-1} \frac{\eta_p}{\rho\lambda} \left[f(C_{mm}) \frac{NLT_{mm}}{2} \right] \quad (167)$$

where $C_{\varepsilon^V} = 1.27$ and $n = 1.15$. In **Fig. 42** four sets of data are plotted: the DNS data for ε^V , the predictions by the model of equation (167) using directly the DNS data for NLT_{kk} and finally the predictions of equation (167) using the NLT_{kk} as given by the two

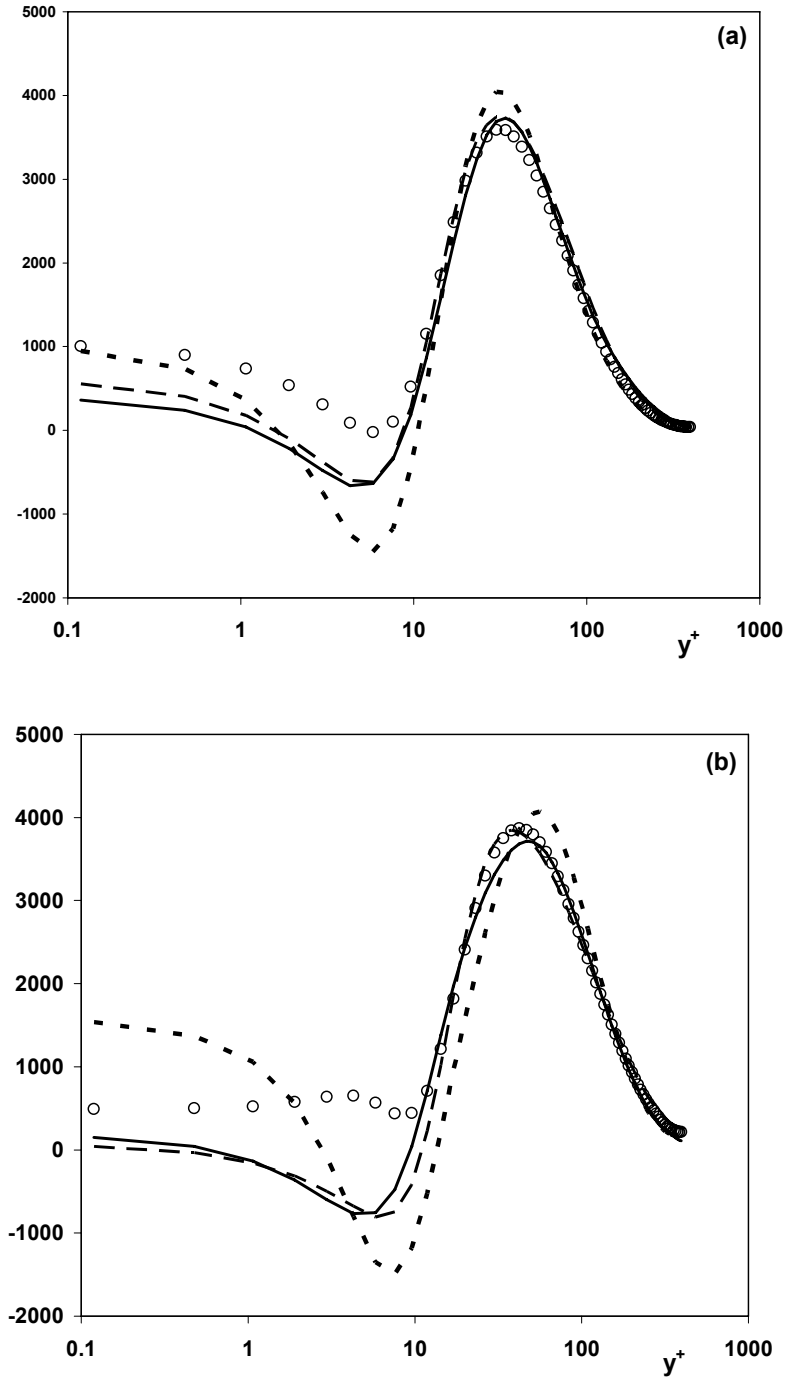


Fig. 42. Comparison between DNS data of $\varepsilon^{V+} \text{Re}_{\tau_0}^{-2}$ ($\circ$) and the models of equation (167) using NLT_{kk}^* DNS data (—), NLT_{kk}^* from the second-order NLT_{ij}^* model (—) and from the "isotropic" NLT_{ij}^* model (---) for $\text{Re}_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$ as a function of drag reduction: (a) $We_{\tau_0} = 25$ (18% DR) and (b) $We_{\tau_0} = 100$ (37% DR).

closures developed in Sections 5.2.2.5 and 5.2.2.6, namely the complete NLT_{ij} model and the "isotropic" NLT_{ij} model. It is clear that the model of equation (167) is good where it should be, i.e. in the buffer and log law layers and that the correct prediction of the viscoelastic stress work in these regions requires a good prediction of NLT_{kk} . It is also clear that the use of the "isotropic" model to predict NLT_{kk} is not as good as the general closure, but it is still satisfactory. The discrepancy between ε^V and any of the models is strong in the viscous sublayer, but in this region the viscoelastic stress work is negligible by comparison with three other contributions, as explained, hence such discrepancy will have a negligible impact in the predictions.

Due to the simplifications made in the modelling it is necessary to calibrate it, and for this reason the final model of viscoelastic dissipation can be observed in Eq. (168). The closure developed by Pinho et al. [4] for the viscoelastic stress work at low DR, is adopted and extended to include also the high DR regime.

$$\varepsilon^V \equiv \frac{1}{\rho} \overline{\tau'_{ik,p} \frac{\partial u_i}{\partial x_k}} \approx 1.37 \times f_{DR}^1 \frac{\eta_p}{\rho \lambda} f(C_{mm}) \frac{NLT_{mm}}{2} \quad (168)$$

The modification of ε^V is embodied by function $f_{DR}^1 = \left[1 - \exp\left(-\frac{We_{\tau 0}}{6.25}\right) \right]^4 \times \left[\frac{We_{\tau 0}}{25} \right]^{0.095}$, which essentially corrects the existing coefficient 1.37 to take into account the non-linear dependence on the Weissenberg number. Obviously, there is a second modification in the model relative to the original closure of Pinho et al. [4]. Since ε^V is modelled by the trace of NLT_{ij} , the new closure of Eq. (159) also has an effect.

5.4.1.2. *Viscoelastic turbulence transport model for the turbulent kinetic energy transport equation*

The viscoelastic turbulence transport, denoted Q^V , is the second new term in the transport equation of k . It is exactly given by

$$Q^V = \frac{\eta_p}{\lambda} \frac{\partial}{\partial x_k} \left[c_{ik} f(\hat{c}_{mm}) u_i + C_{ik} f(\hat{c}_{mm}) u_i \right], \text{ and although it is not very important at low}$$

DR, Pinho et al [4] nevertheless developed a closure for it neglecting the effect of the second term (double correlation) and modelling only the first term (triple correlation). However, the second term becomes important as DR increases, as is shown in **Fig. 43**, where $(\overline{c_{ik} f(\hat{c}_{mm}) u_i} + C_{ik} \overline{f(\hat{c}_{mm}) u_i})$ and the triple correlation $(\overline{c_{ik} f(\hat{c}_{mm}) u_i})$ plotted. The difference between the sum and the triple correlation corresponds to $(\overline{C_{ik} f(\hat{c}_{mm}) u_i})$, which increases significantly when DR varies from 18% to 37%. Consequently, in this work we provide a new closure for Q^v , which incorporates the model for the triple developed by Pinho et al [1], modified to account also for Weissenberg number effects, and denoted as $(CU)_{iik}$, and the new model for the double correlation, denoted as $(FU)_i$, which is developed below. Prior to explaining the model for $(FU)_i$ it is advantageous to rewrite Q^v as

$$Q^v = \frac{\eta_p}{\lambda} \frac{\partial}{\partial x_k} (CU)_{iik} + \frac{\eta_p}{\lambda} \frac{\partial}{\partial x_k} [C_{ik} (FU)_i] \quad (169)$$

A fluctuating strain rate is usually related to purely turbulent velocity and length scales, but for the purpose of modelling the viscoelastic turbulent transport we consider a combined viscoelastic turbulent length scale (L_λ), such that the fluctuating strain rate is the ratio between velocity fluctuations and the viscoelastic length scale leading to an estimate of the velocity fluctuations that involves L_λ , as in equation (171).

$$\frac{\partial u}{\partial x} \sim \frac{u}{L_\lambda} \rightarrow u \sim L_\lambda \frac{\partial u}{\partial x}. \quad (170)$$

The viscoelastic turbulent length scale is defined as the length travelled by a fluid particle due exclusively to the fluctuating turbulent flow for a period of the order of the relaxation time of the polymer, i.e.,

$$L_\lambda \sim u \times \lambda \quad (171)$$

Back-substituting u and L_λ into the double correlation of Q^v we get

$$\overline{f(\hat{c}_{mm}) u} \sim \lambda \times \overline{f(\hat{c}_{mm}) u \frac{\partial u}{\partial x}} \quad (172)$$

Since by definition

$$\overline{2u_i \frac{\partial u_i}{\partial x_j}} = \overline{\frac{\partial u_i u_i}{\partial x_j}} \quad (173)$$

and considering that $\sqrt{c_{kk}^2} \ll C_{kk}$ and the arguments above on the behaviour of function $f(\hat{c}_{mm})$, using equation (173) and decoupling we arrive at the following closure for the double correlation in Q^v

$$(FU)_i = \overline{f(\hat{c}_{mm})u_i} \approx \frac{C_{FU}}{2} \times \lambda \times f(C_{mm}) \times \overline{\frac{\partial u_n u_n}{\partial x_i}} \quad (174)$$

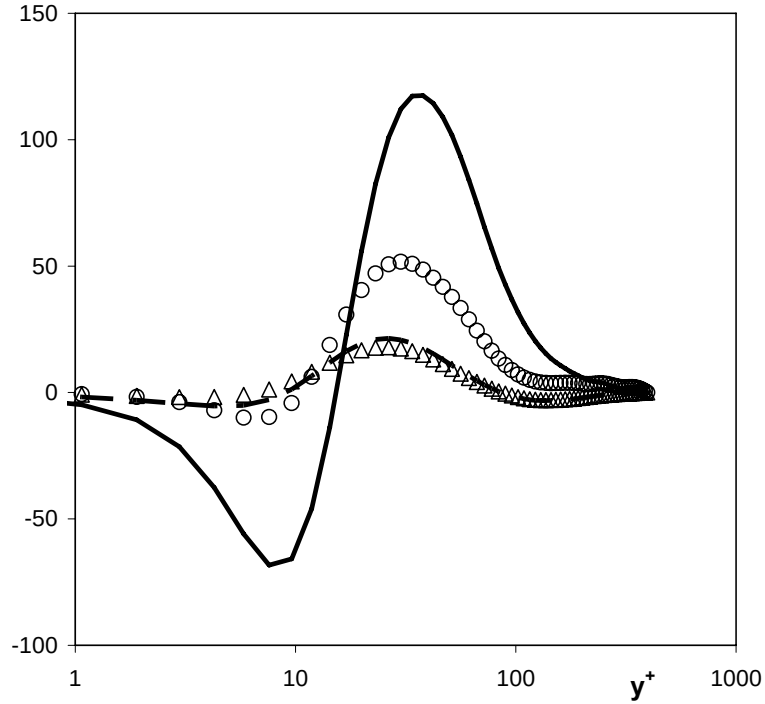


Fig. 43. Comparison between DNS data of $\overline{c_{ik}f(C_{mm} + c_{mm})u_i^+}$ (symbols) and $\overline{c_{ik}f(C_{mm} + c_{mm})u_i^+} + C_{ik}f(C_{mm} + c_{mm})u_i^+$ (lines) for channel flow of a FENE-P at $Re_\tau = 395$, $L^2 = 900$ and $\beta = 0.9$: (---) and (Δ) for $We_\tau = 25$, DR=18%; (—) and ($\circ$) for $We_\tau = 100$, DR=37%.

Calibration against the DNS data provides the numerical value of $C_{FU} = 1$ and introduces a Weissenberg number correction that makes this double correlation stronger as the

Weissenberg number increases (cf. **Fig. 43**) so that the final form of the model for the second term on the RHS of equation (169) is

$$C_{ik}(FU)_i = \frac{C_{FU}}{2} \sqrt{\frac{We_{\tau 0}}{25}} \times C_{ik} \times \lambda \times f(C_{mm}) \times \frac{\partial \overline{u_n u_n}}{\partial x_i} \quad (175)$$

The model of Pinho et al [4] for $(CU)_{ik}$ is a contraction from the more general model of $(CU)_{ijk}$, which was here modified to account for the Weissenberg number dependence as is given by

$$(CU)_{ijk} = -C_{\beta 1} \sqrt{\frac{25}{We_{\tau 0}}} \frac{\lambda}{f(C_{mm})} \left(\overline{u_i u_m} \frac{\partial C_{kj}}{\partial x_m} + \overline{u_j u_m} \frac{\partial C_{ik}}{\partial x_m} \right) - C_{\beta 2} \left(\frac{We_{\tau 0}}{25} \right)^{1.661} \left[\pm \sqrt{\overline{u_j^2}} C_{ik} \pm \sqrt{\overline{u_i^2}} C_{jk} \right] \quad (176)$$

with parameters $C_{\beta 1} = 0.6$ and $C_{\beta 2} = 0.05$.

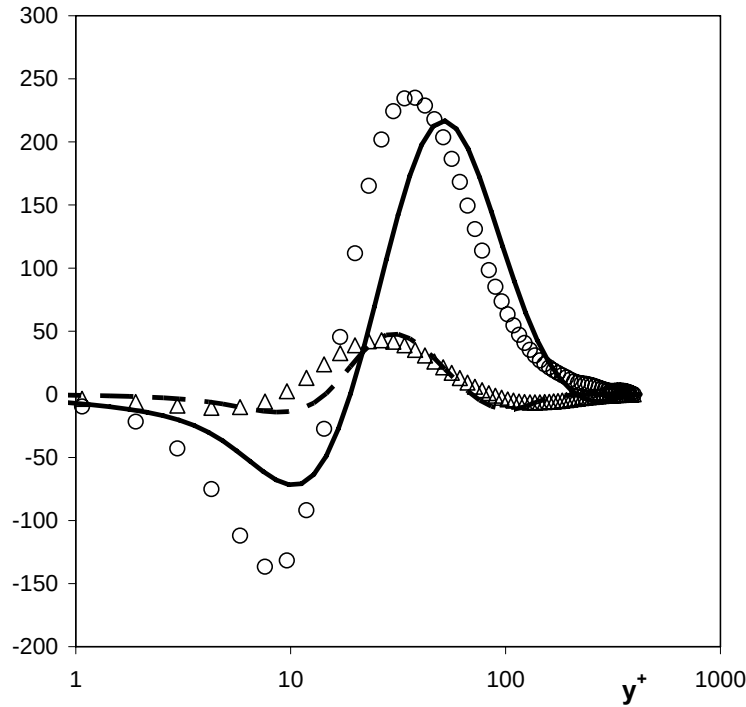


Fig. 44. Comparison between model predictions of $\overline{c_{ik} f(C_{mm} + c_{mm}) u_i^+} + C_{ik} \overline{f(C_{mm} + c_{mm}) u_i^+}$ (lines) and DNS data (symbols) for channel flow of FENE-P fluids at $Re_\tau = 395$, $L^2 = 900$ and $\beta = 0.9$: (—) and (Δ) for $We_\tau = 25$, DR=18%; (—) and ($\circ$) for $We_\tau = 100$, DR=37%.

The performance of the full closure for Q^V against DNS data is shown in **Fig. 44** for 18% and 37% of drag reduction. The model compares well with the DNS and captures all its main features. A small shift is observed in the sloping increase in the buffer layer at DR= 38%, but the impact of this is negligible since Q^V is not a major term in the balance of turbulent kinetic energy.

5.4.1.3. *Viscoelastic model for the rate of dissipation of the turbulent kinetic energy transport equation*

Previous models for viscoelastic fluids ([4, 39, 85]) neglected the extra term E_{τ_p} appearing in the transport equation of $\tilde{\varepsilon}^N$ due to the viscoelastic nature of the rheological constitutive equation. One of the consequences for the model of Pinho et al. [4] was an overprediction of $\tilde{\varepsilon}^N$ and this also lead to an underprediction of k and some deficiencies in the prediction of $-\overline{uv}$, although the underprediction of k was not only caused by the overprediction of $\tilde{\varepsilon}^N$. The reduction of $\tilde{\varepsilon}^N$ with DR reported in the literature requires a direct influence of the polymer in reducing $\tilde{\varepsilon}^N$, which formally exists as term E_{τ_p} , therefore we assumed that E_{τ_p} is a destruction type term in order to allow the model to behave accordingly, i.e., to reduce $\tilde{\varepsilon}^N$. A major contribution of this work is exactly in providing, for the first time, a model for this new term. In developing a model for E_{τ_p} , and assuming that it plays the role of a destruction term it was also assumed that it should depend on the same quantities as the classical Newtonian destruction term, i.e., it should be proportional to ε^2/k , with ε here representing any of the stress work terms ($\tilde{\varepsilon}^N$ or ε^V). The viscoelastic destruction term is modelled as in Eq. (177) and has two contributions, both of which are proportional to viscoelastic quantities.

$$E_{\tau_p} = -f_s \times f_{DR} \times \frac{(1-\beta)}{(L^2-3)} \times \frac{\tilde{\varepsilon}^{N^2}}{k} \left[\frac{C_{\varepsilon F1}}{We_{\tau_0}^{0.437}} \times \frac{\varepsilon^V}{\tilde{\varepsilon}^N} \times (L^2-3)^2 + \frac{C_{\varepsilon F2}}{We_{\tau_0}^{2.374}} \times C_{mm}^2 \times f(C_{mm})^2 \right] \quad (177)$$

This closure includes a wall damping function $f_s = [1 - \exp(-y^+/50)]$, a Weissenberg number corrector function $f_{DR} = [1 - \exp(-We_{\tau_0}/6.25)]^4$, and the numerical coefficients $C_{\varepsilon F1} = 0.0867$ and $C_{\varepsilon F2} = 39.75$.

5.4.2 Summary of the present model

It is helpful at this stage to summarise and present the complete set of equations that need to be solved to arrive at a solution for turbulent flow of a FENE-P fluid in the context of RANS/RACE. The continuity and momentum equations, (178) and (179), respectively, the polymer stress tensor is calculated with equation (180), the conformation tensor by equation (181) and the required NLT_{ij} model is that of equation (182). The Reynolds stress tensor is calculated by Eq. (184), defined by the inclusion of the polymeric effect in the eddy viscosity, eq. (185). The transport equations of kinetic energy and this dissipation are Eq. (187) and Eq. (192), respectively, the corresponding viscoelastic closures are defined by Eq. (189), Eq. (190) and Eq. (194).

- Continuity equation:

$$\frac{\partial U_i}{\partial x_i} = 0 \quad (178)$$

- Momentum equation:

$$\rho \frac{\partial U_i}{\partial t} + \rho U_k \frac{\partial U_i}{\partial x_k} = -\frac{\partial \bar{p}}{\partial x_i} + \eta_s \frac{\partial^2 U_i}{\partial x_k \partial x_k} - \frac{\partial}{\partial x_k} (\rho \overline{u_i u_k}) + \frac{\partial \bar{\tau}_{ik,p}}{\partial x_k} \quad (179)$$

- Polymeric stress tensor:

$$\bar{\tau}_{ij,p} = \frac{\eta_p}{\lambda} [f(C_{kk})C_{ij} - f(L)\delta_{ij}] \quad (180)$$

- Tensor conformation equation:

$$\left(\frac{\partial C_{ij}}{\partial t} + U_k \frac{\partial C_{ij}}{\partial x_k} - C_{jk} \frac{\partial U_i}{\partial x_k} - C_{ik} \frac{\partial U_j}{\partial x_k} \right) - \underbrace{\left(c_{kj} \frac{\partial u_i}{\partial x_k} + c_{ik} \frac{\partial u_j}{\partial x_k} \right)}_{NLT_{ij}} = - \frac{\bar{\tau}_{ij,p}}{\eta_p} \quad (181)$$

with

$$\begin{aligned} NLT_{ij} \equiv \overline{c_{kj} \frac{\partial u_i}{\partial x_k}} + \overline{c_{ik} \frac{\partial u_j}{\partial x_k}} &\approx C_{F1} \left(0.0552 \frac{We_{\tau 0}}{25} + 0.116 \right) \times \frac{C_{ij} \times f(C_{mm})}{\lambda} - C_{F2} We_{\tau 0}^{0.743} \left[C_{kj} \frac{\partial U_i}{\partial x_k} + C_{ik} \frac{\partial U_j}{\partial x_k} \right] \\ &+ \frac{\lambda}{f(C_{mm})} \left[C_{F3} \times \left(\frac{25}{We_{\tau 0}} \right)^{0.718} \times \left(\frac{\partial U_j}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + \frac{\partial U_i}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} \right. \right. \\ &\left. \left. + \frac{\partial U_k}{\partial x_n} \frac{\partial U_m}{\partial x_k} \left(C_{jn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + C_{in} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} \right) \right) \right] \\ &+ \frac{\lambda}{f(C_{mm})} \left[\frac{C_{\varepsilon_F}}{We_{\tau 0}} \frac{4}{15} \times \frac{\varepsilon^N}{(\nu_s + \nu_r)} \times \beta C_{mm} \times f_{F2} \times \delta_{ij} \right] \\ &- \frac{\lambda}{f(C_{mm})} \times f_{F1} \times C_{F4} \times \left(\frac{25}{We_{\tau 0}} \right)^{0.7} \times \left[C_{jn} \frac{\partial U_k}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{in} \frac{\partial U_k}{\partial x_n} \frac{\partial U_j}{\partial x_k} + C_{kn} \frac{\partial U_j}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{kn} \frac{\partial U_i}{\partial x_n} \frac{\partial U_j}{\partial x_k} \right] \end{aligned} \quad (182)$$

where the damping functions and parameters are in Eq. (183) and Table 8.

$$\begin{aligned} f_{F1} &= \left(1 - 0.8 \exp \left(- \frac{y^+}{30} \right) \right)^2 ; \quad f_{F2} = \left(1 - \exp \left(- \frac{y^+}{25} \right) \right)^4 \\ \text{and } f_{DR}^1 &= \left[1 - \exp \left(- \frac{We_{\tau 0}}{6.25} \right) \right]^4 \times \left[\frac{We_{\tau 0}}{25} \right]^{0.095} \end{aligned} \quad (183)$$

Table 8. Parameters of the NLT_{ij} model of Eq. (182).

C_{F1}	C_{F2}	C_{F3}	C_{F4}	C_{ε_F}
1.0	0.0105	0.046	1.05	2

- Reynolds stress tensor:

$$-\rho \overline{u_i u_j} = 2\rho \nu_T S_{ij} - \frac{2}{3} \rho k \delta_{ij} \quad (184)$$

with the following turbulent viscosity

$$\nu_T = C_\mu \times f_\mu \times \frac{k^2}{\tilde{\varepsilon}^N} \left(1 - C_\mu^P \times f_\mu^P \times f_{DR}^P \times C_{mm} \right). \quad (185)$$

The parameters are $C_\mu = 0.09$ and $C_\mu^P = 0.00045$ and the damping functions are defined by Eq. (186).

$$f_\mu = \left[1 - \exp\left(-\frac{y^+}{26.5}\right) \right]^2; \quad f_\mu^P = \left[1 + 2.55 \times \exp\left(-\frac{y^+}{44}\right) \right]$$

$$\text{and } f_{DR}^P = \left[1 - \exp\left(-\frac{We_{\tau 0}}{6.25}\right) \right]^4 \times \left[\frac{25}{We_{\tau 0}} \right]^{0.1232} \quad (186)$$

- The transport equation for the turbulent kinetic energy

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho U_i k}{\partial x_i} = -\rho \overline{u_i u_k} \frac{\partial U_i}{\partial x_k} + \frac{\partial}{\partial x_i} \left[\left(\eta_s + \frac{\rho f_i \nu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + \eta_s \frac{\partial^2 k}{\partial x_i \partial x_i} - \rho \tilde{\varepsilon}^N - \rho D + Q^V - \rho \varepsilon^V \quad (187)$$

where

$$D = 2(\nu_s + \nu_{\tau p}) \left(\frac{d\sqrt{k}}{dy} \right)^2 \text{ and } \nu_{\tau p} = \frac{\tau_{12}^P}{\frac{\partial U}{\partial y}} \quad (188)$$

$$\varepsilon^V \equiv \frac{1}{\rho} \overline{\tau'_{ik,p} \frac{\partial u_i}{\partial x_k}} \approx 1.37 \times f_{DR}^P \frac{\eta_p}{\rho \lambda} f(C_{mm}) \frac{NLT_{mm}}{2} \quad (189)$$

and $Q^V \equiv \frac{\partial \overline{\tau'_{ik,p} u_i}}{\partial x_k} \approx \frac{\eta_p}{\lambda} \frac{\partial}{\partial x_k} \left[f(C_{mm}) \left(\frac{C_{ik} F U_i + C U_{iik}}{2} \right) \right]$ where

$$C U_{ijk} = -C_{\beta 1} \sqrt{\frac{25}{We_{\tau 0}}} \frac{\lambda}{f(C_{mm})} \left(\overline{u_i u_m} \frac{\partial C_{kj}}{\partial x_m} + \overline{u_j u_m} \frac{\partial C_{ik}}{\partial x_m} \right) - C_{\beta 7} \left(\frac{We_{\tau 0}}{25} \right)^{1.661} \left[\pm \sqrt{u_j^2} C_{ik} \pm \sqrt{u_i^2} C_{jk} \right]$$

$$C_{ik}FU_i = \frac{C_{FU}}{2} \sqrt{\frac{We_{\tau 0}}{25}} \times C_{ik} \times \lambda \times f(C_{mm}) \times \frac{\partial \overline{u_n u_n}}{\partial x_i} \quad (190)$$

The parameters of Q^V are $C_{\beta 1} = 0.6$; $C_{\beta 2} = 0.05$ and $C_{FU} = 0.5$.

The turbulent diffusion term contains a variable Prandtl number via function

$$f_T = 1 + 3.5 \exp\left(-\left(\frac{Re_T}{150}\right)^2\right) \quad (191)$$

- The transport equation for the rate of dissipation of the turbulent kinetic energy

$$\frac{\partial \rho \tilde{\varepsilon}^N}{\partial t} + \frac{\partial \rho U_i \tilde{\varepsilon}^N}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\left(\eta_s + \frac{\rho f_t \nu_T}{\sigma_\varepsilon} \right) \frac{\partial \tilde{\varepsilon}^N}{\partial x_i} \right] + f_1 C_{\varepsilon 1} \frac{\tilde{\varepsilon}^N}{k} P_k - f_2 C_{\varepsilon 2} \rho \frac{\tilde{\varepsilon}^{N^2}}{k} + \rho E + E_{\tau_p} \quad (192)$$

where

$$E = \nu_s \nu_T (1 - f_\mu) \left(\frac{\partial^2 U_i}{\partial y \partial y} \right)^2 \quad (193)$$

$$E_{\tau_p} \sim -f_5 \times f_{DR}^\varepsilon \times \frac{(1 - \beta)}{We_{\tau 0} (L^2 - 3)} \frac{\tilde{\varepsilon}^N}{k} \left[C_{\varepsilon F1} \times (L^2 - 3)^2 \times \varepsilon^V + C_{\varepsilon F2} \times \tilde{\varepsilon}^N \times C_{mm}^2 \times f(C_{mm})^2 \right] \quad (194)$$

The Newtonian and the viscoelastic damping functions are defined in Eq. (195) and Eq. (196), respectively.

$$f_1 = 1 \text{ and } f_2 = 1 - 0.3 \exp\left(-(\text{Re}_T)^2\right) \quad (195)$$

$$f_5 = \left[1 - \exp(-y^+/50) \right], \quad f_{DR}^\varepsilon = \left[1 - \exp(-We_{\tau 0}/6.25) \right]^4,$$

$$C_{\varepsilon F1} = 0.531 (We_{\tau 0}/25)^{0.563} \text{ and } C_{\varepsilon F2} = 0.477 (25/We_{\tau 0})^{1.374} \quad (196)$$

The remaining constant Newtonian parameters, associated to the transport equations of kinetic energy and dissipation are $\sigma_k = 1.1$, $\sigma_\varepsilon = 1.3$, $C_{\varepsilon 1} = 1.45$ and $C_{\varepsilon 2} = 1.9$.

5.5 Results and discussion

In this section we evaluate the performance of the full turbulence model against the DNS data sets for fully-developed turbulent channel flow with 18% and 37% drag reduction. Then, we also provide results of parametric studies for different values of the independent parameters. The numerical calculations were carried out using the same finite-volume code as in Pinho et al. [4], which had been modified for the FENE-P fluid. Non-uniform meshes mapping the channel from wall to wall with 99 cells were used, with about 8 cells located inside each of the viscous sublayers in order to provide mesh independent results to within 0.5% for the mean velocity and the friction factor.

Fig. 45 - (a) and (b) compares the predicted velocity profiles with DNS data and includes predictions at Weissenberg numbers other than those used for calibration. For the specific 18% and 37% DR flows the agreement is good with improvements in the buffer layer relative to the previous model of Pinho et al. [4]. This improvement is essentially associated with the inclusion of a polymeric contribution in the eddy viscosity model. The earlier model [1] also predicted a drag increase at low values of the Weissenberg number ($We_{\tau 0} < 20$), i.e., a profile below the log-law, and this deficiency has now been corrected as shown.

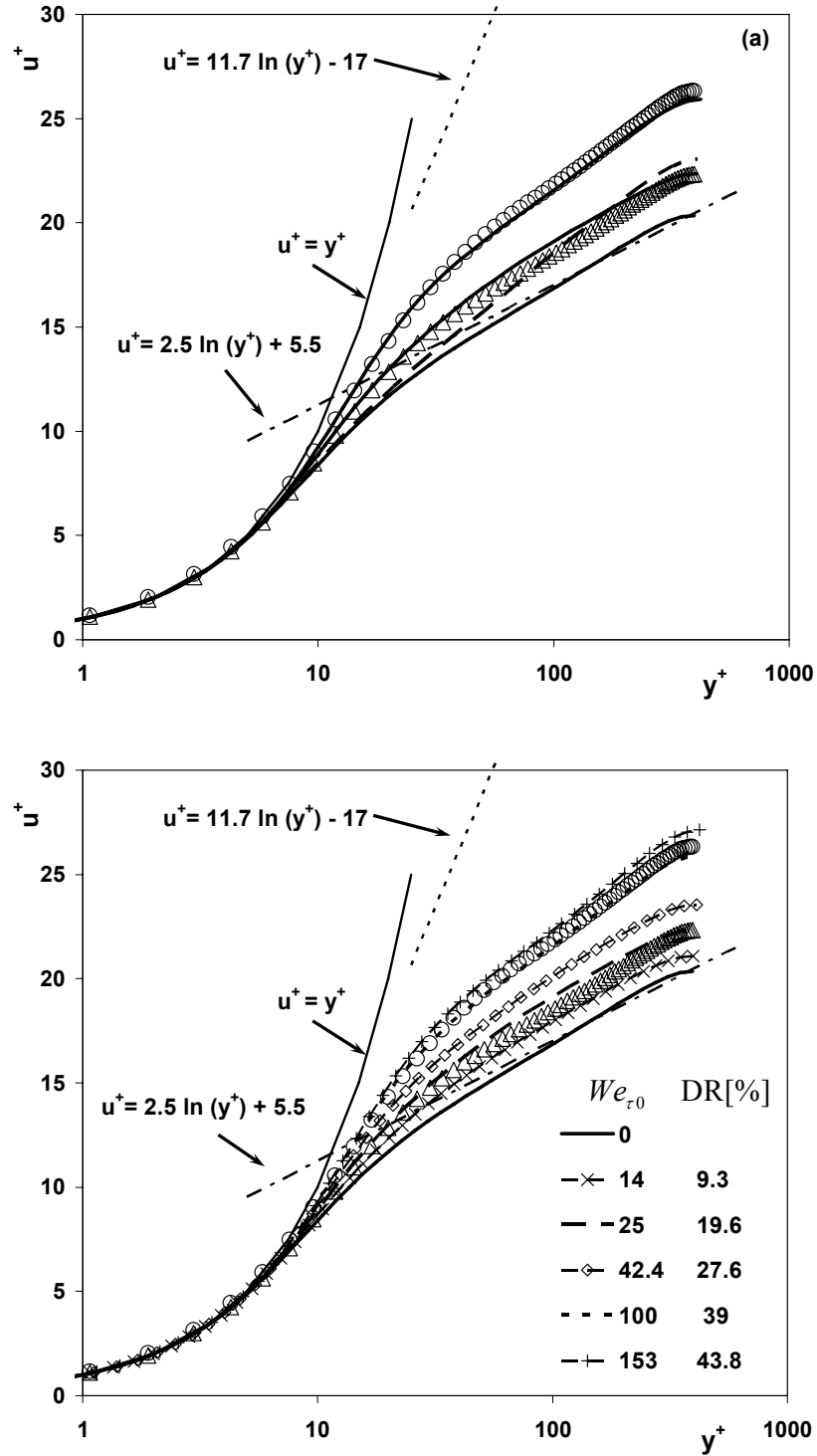


Fig. 45. Normalised velocity profile in wall coordinates for Newtonian and FENE-P flows, at $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$: (a) Comparison with DNS data sets for Δ 18% DR data and $\circ$ 37% DNS data; full lines predictions; dashed line: Pinho et al. [4]; (b) variation with Weissenberg number.

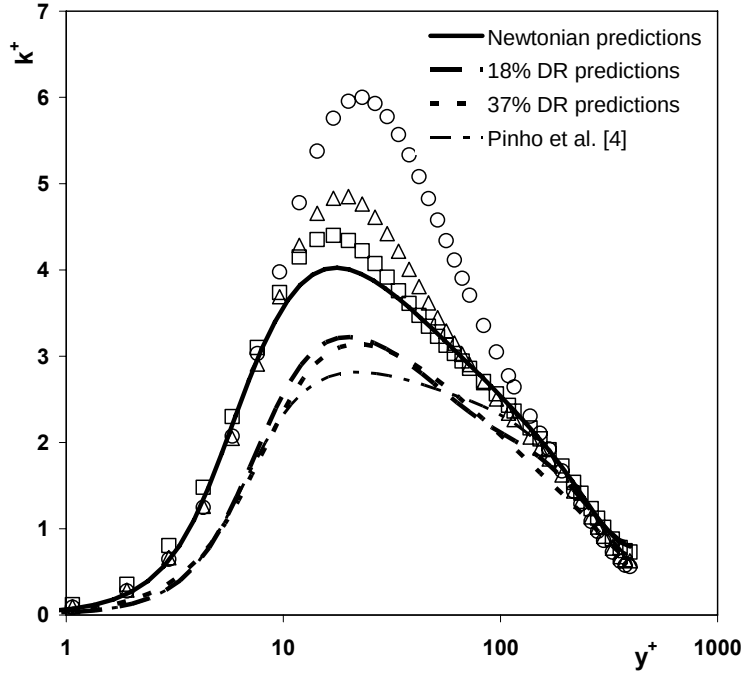


Fig. 46. Comparison between predictions and DNS data of the turbulent kinetic energy for turbulent channel flow with $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$: $\square$ Newtonian, Δ DR= 18% and $\circ$ DR=37%.

Fig. 47 plots the normalized rate of dissipation of k by the Newtonian solvent (ε^{N+}) and here an excellent agreement with DNS data is found except very close to the wall. This difference at the wall also exists for Newtonian fluids, i.e., it is a known deficiency of k - ε type models and is unrelated to the viscoelastic closures, the correction of which involves the use of better behaved quantities, such as the specific rate of dissipation (ω) in the so-called k - ω models, since ω is better behaved near the wall than ε . Elsewhere the predictions of $\tilde{\varepsilon}^N$ are excellent and this is due to the inclusion of the viscoelastic destruction term in the transport equation of $\tilde{\varepsilon}^N$, which decreases $\tilde{\varepsilon}^N$ as flow viscoelasticity increases. This is a major improvement over the model of Pinho et al. [4], who considered $E_{\tau}=0$. The inclusion of this contribution into the model improves its behaviour in the logarithmic region and is also responsible for a smoother variation of the velocity profile with the Weissenberg number. In the previous model of Pinho et al. [4] there was initially (at low We_{τ}) a downshift in the velocity profile (going below

the Newtonian log-law) followed by a quick upshift as the Weissenberg increased and subsequently the code would diverge, a problem which has now been eliminated.

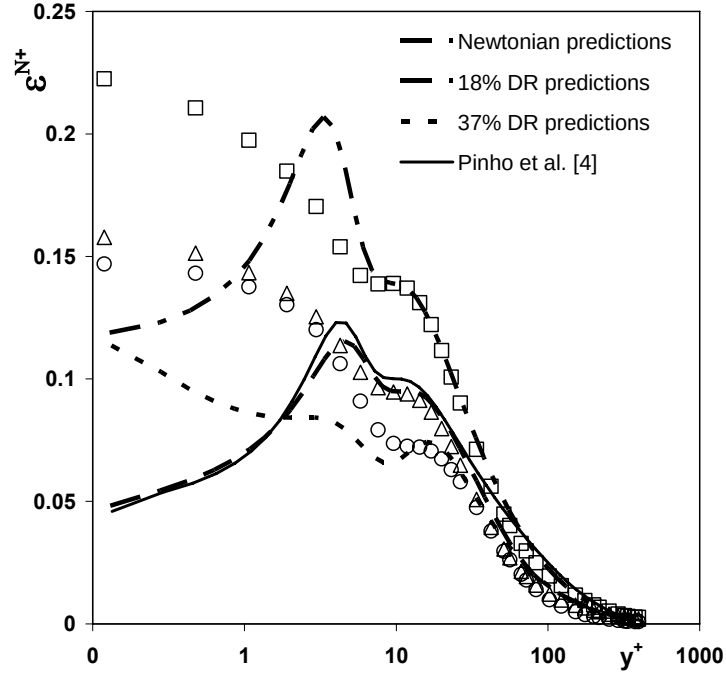


Fig. 47. Comparison between the predictions and DNS data of $\mathcal{E}^{N+}$ for turbulent channel flow with $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$: $\square$ Newtonian, Δ DR= 18% and $\circ$ DR= 37%.

The predictions of the viscoelastic stress work are plotted in **Fig. 48** and show that this closure is good and capable of capturing the lower peak at the buffer-log law edge, a feature absent from Pinho et al.'s [4], even though the match with DNS is not that good. The differences between DNS and predictions in the viscous and buffer layers are not so important because, as shown in Pinho et al [4] for DR= 18%, and similarly for DR= 37%, in these two regions the viscoelastic stress work has a negligible impact on the balance of k . However, ε^V is an important contribution to the balance of k in the inertial sublayer where it acts as a dissipative term, lowering the value of k . It would be easy to match the predictions of ε^V with the DNS data, but this would entail a higher dissipation and a concomitant reduction in k , which is already underpredicted, especially at DR=37%. The solution of this problem is most probably the adoption of a

second order closure, where there is an extra mechanism at play, which by its nature must be strongly affected the presence of the polymeric additives, the pressure strain, contributing to the enhanced Reynolds stress anisotropy.

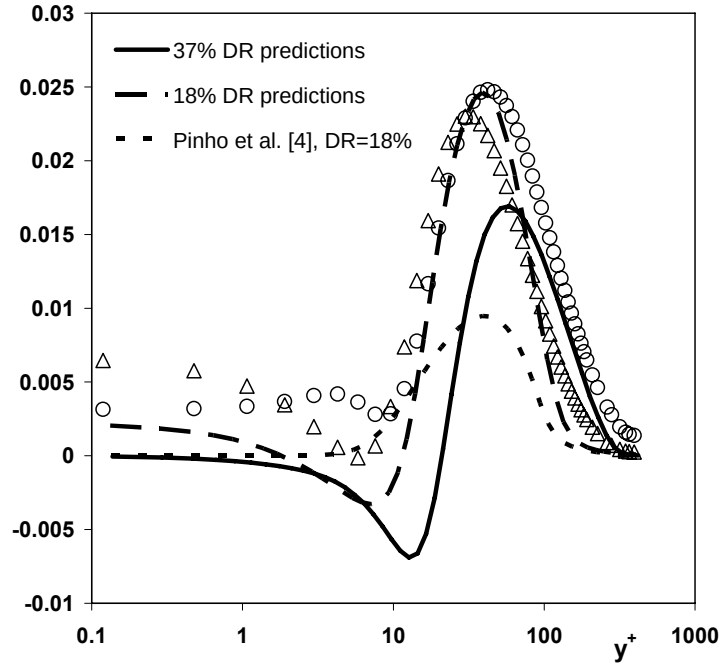
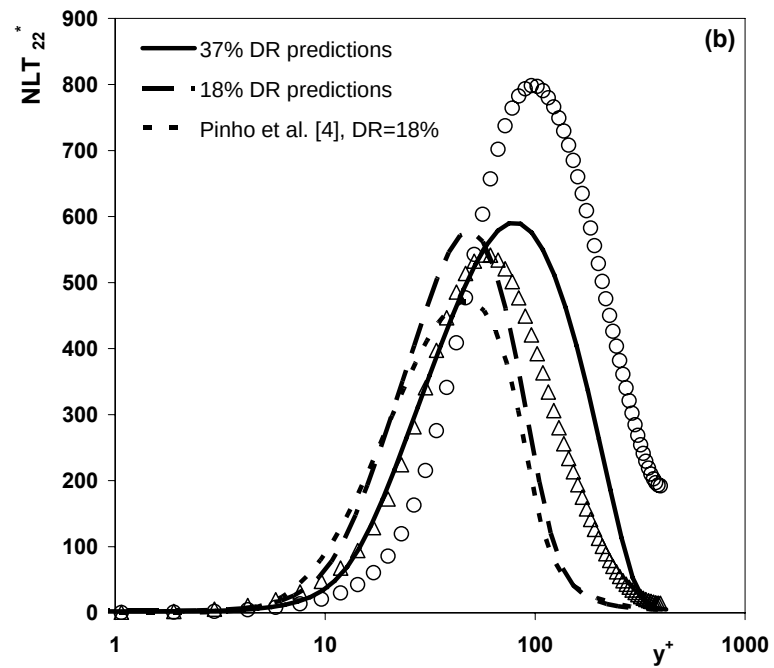
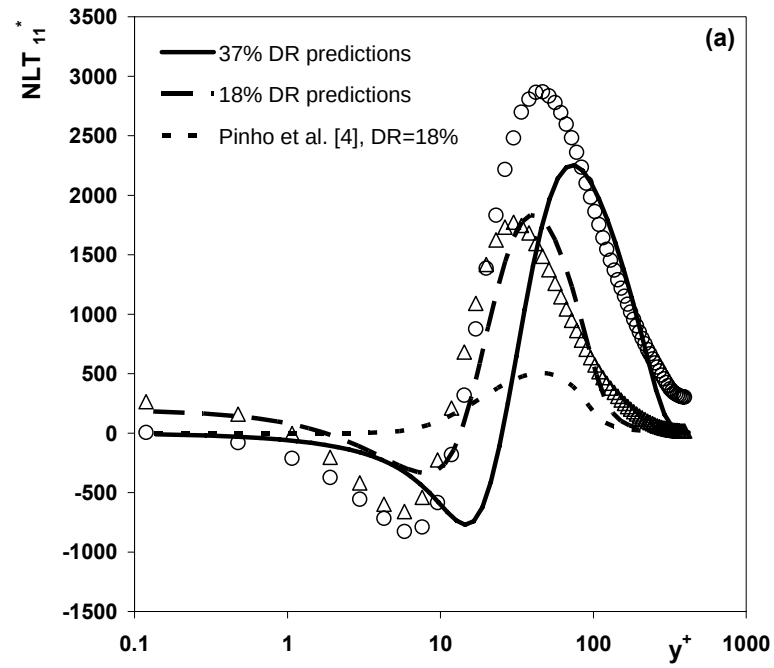
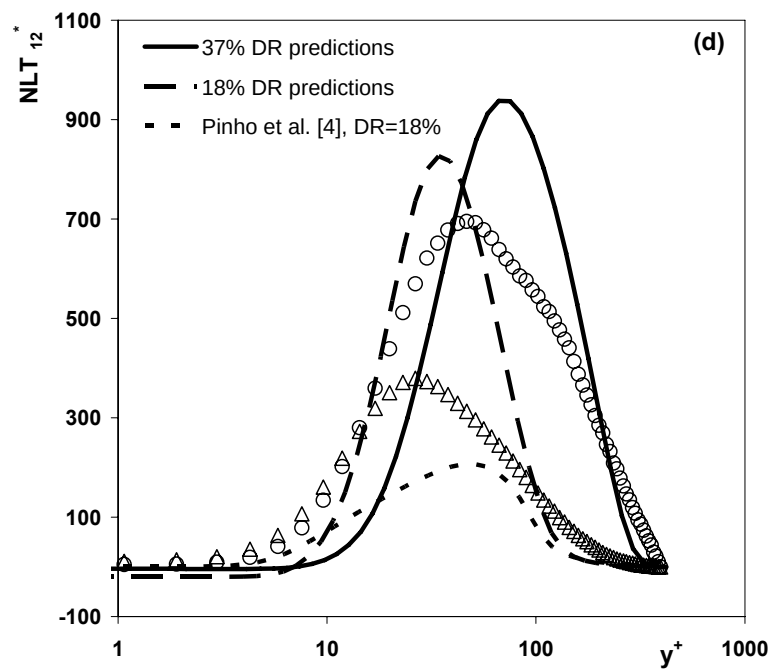
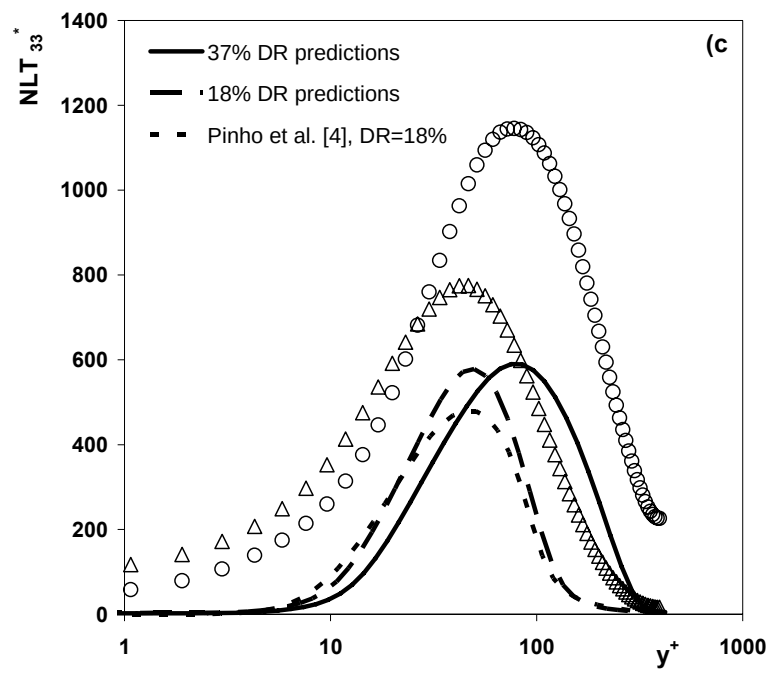


Fig. 48. Comparison between predictions and DNS data of ε^{V+} for turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$: Δ DR=18% and $\circ$ DR=37%.

The predictions of NLT_{ij} by the full turbulence model are compared with DNS data in **Fig. 49 – (a) to (e)**, including shear component. There are some differences between the predictions and the DNS data, especially at high DR, with underpredictions of peak values, but the model captures well all main features, such as the increase in NLT with DR, the shift of the peak location to higher values of y^+ as DR increases and the existence of the negative peaks of NLT_{11} in the buffer layer. All these features impact on the behaviour of NLT_{kk} , **Fig. 49 – (e)**, which is part of the model for ε^V .





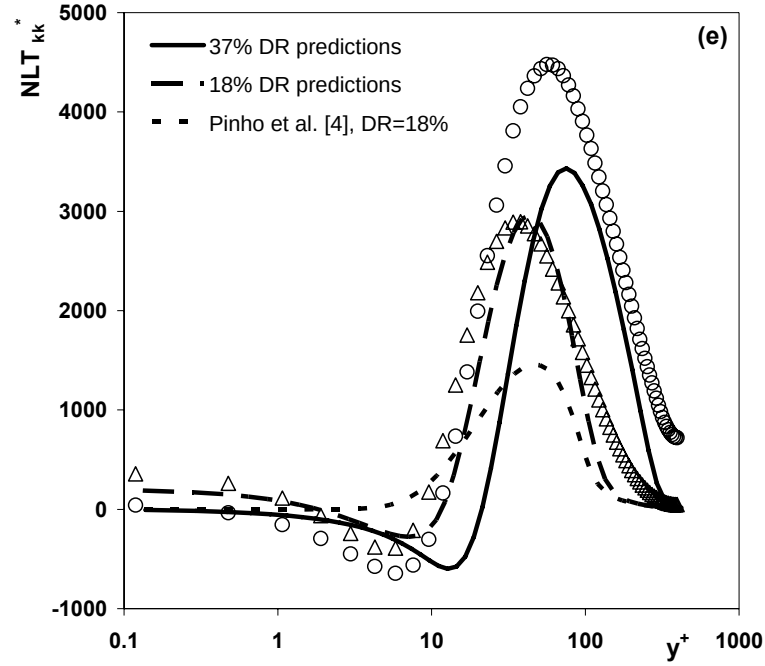
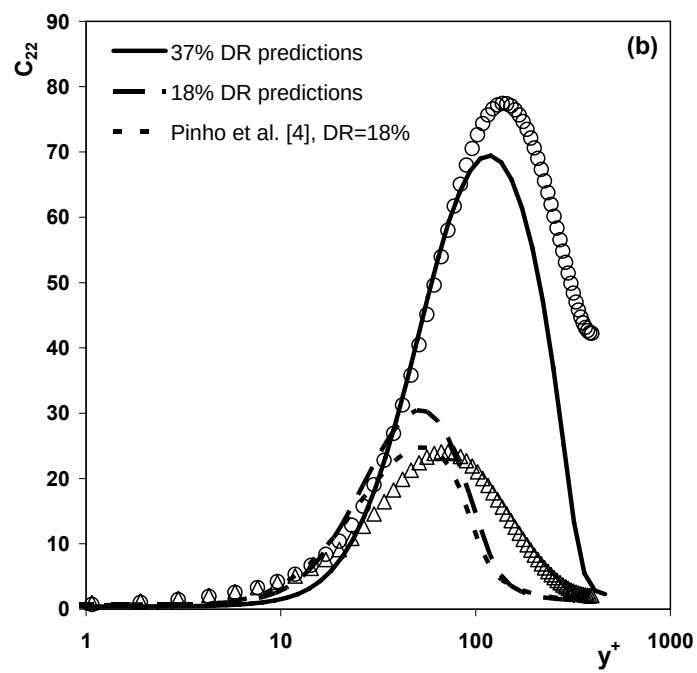
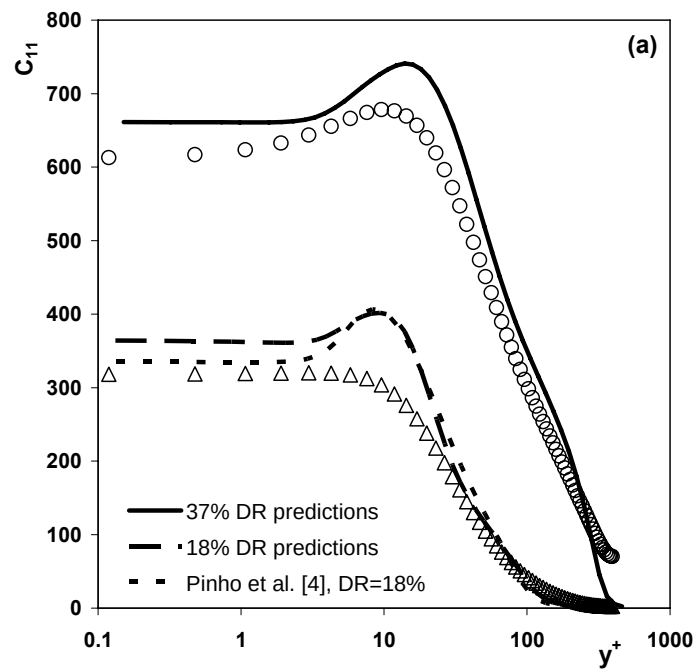
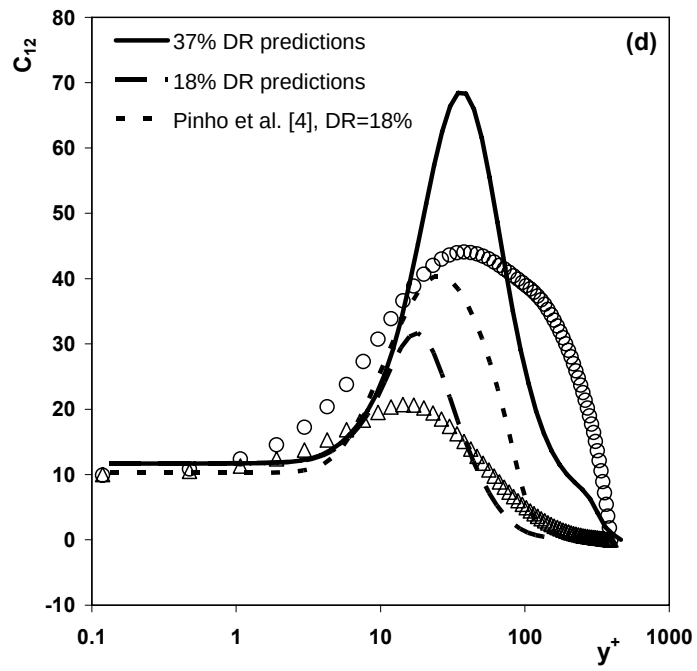
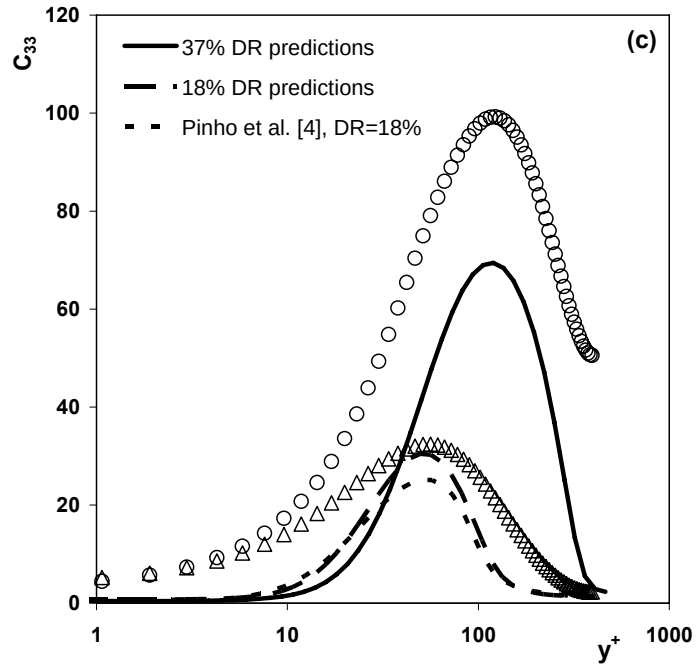


Fig. 49. Comparison between the predictions and DNS data of NLT_{ij} for turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$: Δ DR= 18% and $\circ$ DR=37%.

The correct predictions of NLT_{ij} have a direct impact on the prediction of the conformation tensor, as is obvious from Eq. (124-a), especially regarding the two transverse normal components and the shear component (C_{22} , C_{33} and C_{12}), whereas it is not so important in the prediction of the C_{11} component, Kim et al. [54]. The profiles of C_{ij} are plotted in **Fig. 50 – (a) to (e)**, and they only show improvements relative to the corresponding predictions of Pinho et al. [4] for the shear component. The quality of the comparison in C_{ij} is similar to the quality of the comparison of NLT_{ij} whenever NLT_{ij} is a major contribution to the balance of C_{ij} as for the C_{22} and C_{33} components, and is better when the impact of NLT_{ij} is smaller and C_{ij} is also determined by the other terms of the evolution equation for C_{ij} (Eq. (124-a)) which are exact. In addition, two terms of the RACE equation are negligible at low DR, but there are some DNS results suggesting they may need to be considered at higher and maximum drag reductions and this may improve predictions, something to be investigated in the future.





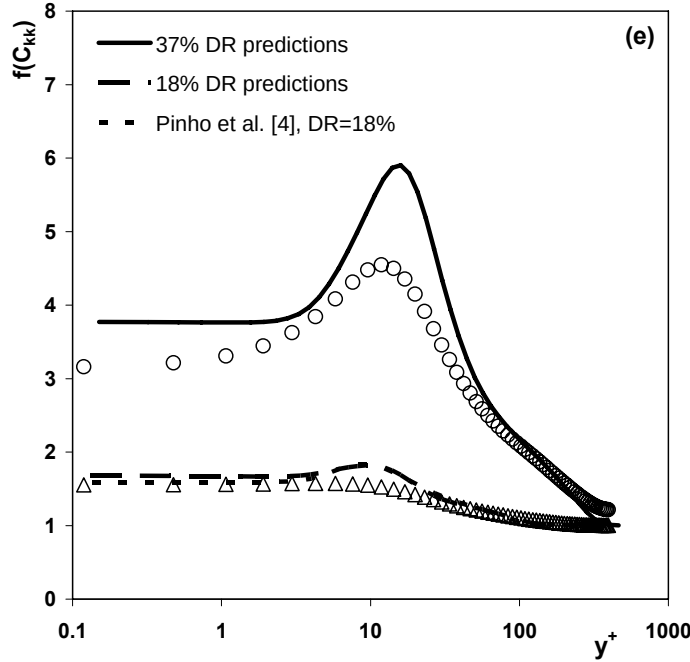
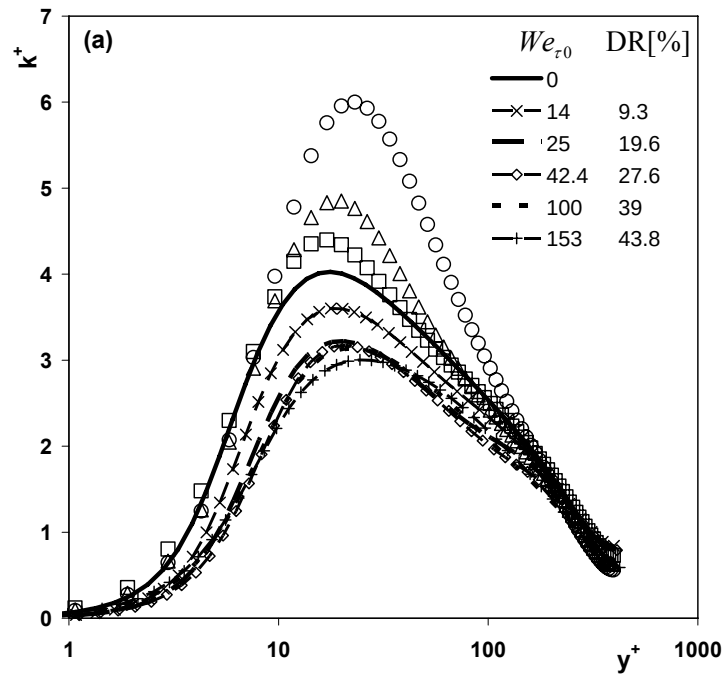


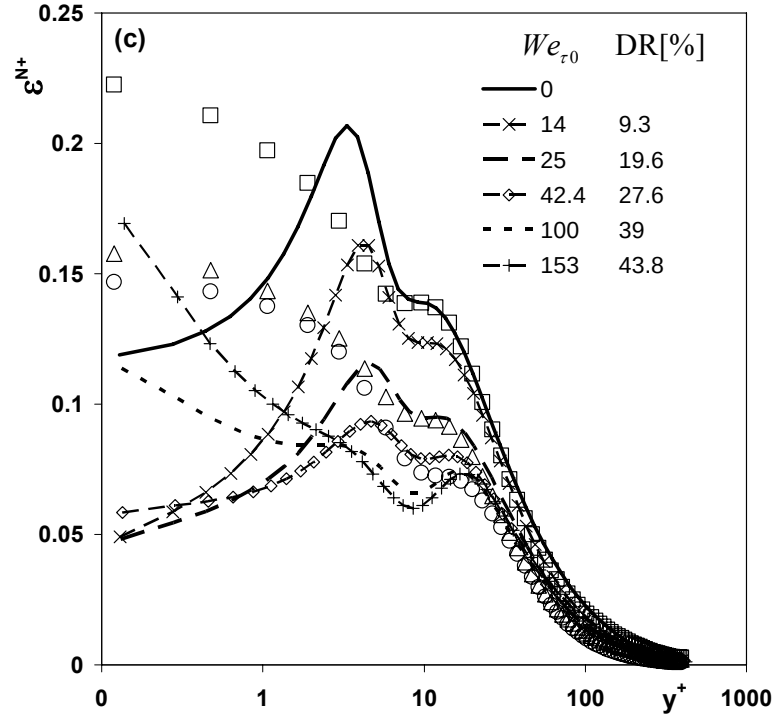
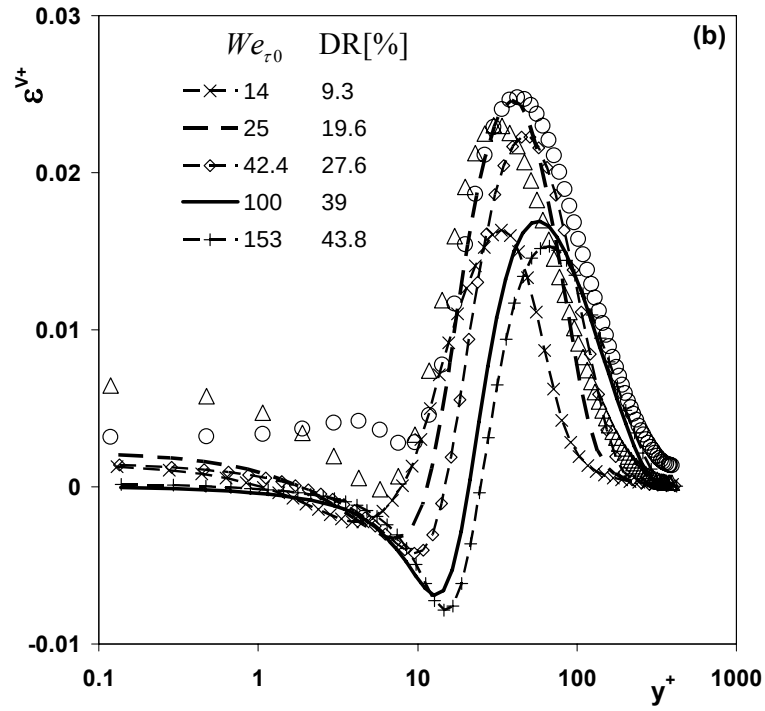
Fig. 50. Comparison between the predictions and DNS data of the conformation tensor for turbulent channel flow with $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$: Δ DR= 18% and $\circ$ DR= 37%.

In **Fig. 51** predictions at values of Weissenberg number other than those of the DNS have also been included to see that they evolve correctly on going from low to high DR, but the reader should be warned that the behaviour at values of DR higher than 45% needs further investigation, because the closures developed have not yet been tested against data at higher values of We and for different values of L^2 and β . This is quite important because DR is characterized by an asymptotic behaviour, whereas by considering only two data sets in our calibration procedure, the nonlinear variation of some coefficients/ functions with We has not yet been taken into account. This issue will also be addressed in the future. In any case, at this point it is already possible to visualize the saturation phenomenon of drag reduction in some quantities, as for example with the turbulent kinetic energy, **Fig. 51 - (a)**, even though we have seen that this quantity is being underpredicted and requires future improvements. Another quantity where saturation with drag reduction is oversed is NLT_{kk} : it increases rapidly from 18% to 37% DR and then it tends to stabilise at DR= 44%, as shown in **Fig. 51 - (d)**. However and somewhat surprisingly, in the viscoelastic stress work plotted in **Fig.**

51 - (b), which is direct related with the NLT_{kk} , we do not see this effect, simply because of the increase of $f(C_{nn})$ with the Weissenberg number/ DR (cf. **Fig. 50 – (e)**). The evolution of the Newtonian dissipation is well predicted as We is increased, **Fig. 51 - (c)**, giving further credence to the developed closure for the viscoelastic destruction of ε^N .

Finally it is worth analysing the distribution of all shear stresses across the channel and we do that separately for DR = 18% in **Fig. 52 – (a)** and DR = 37% in **Fig. 52 – (b)**. The solvent stress is always very well captured as a consequence of the good prediction of the velocity profile and its exact definition. The Reynolds shear stress is well predicted but we always see an overprediction of the peak and an underprediction close to the wall. Since there are only three stresses, that their sum is by definition well predicted in this flow calculation and the solvent stress is correct, the compensation for the deficiencies in the Reynolds shear stress must come from an opposite deficiency in the polymer shear stress. Indeed, we observe that $\bar{\tau}_{12,p}^+$ is overpredicted very close to the wall and underpredicted farther away as a consequence of the predictive behaviour of the shear component of the conformation tensor (C_{12}), c.f. **Fig. 50 – (d)**.





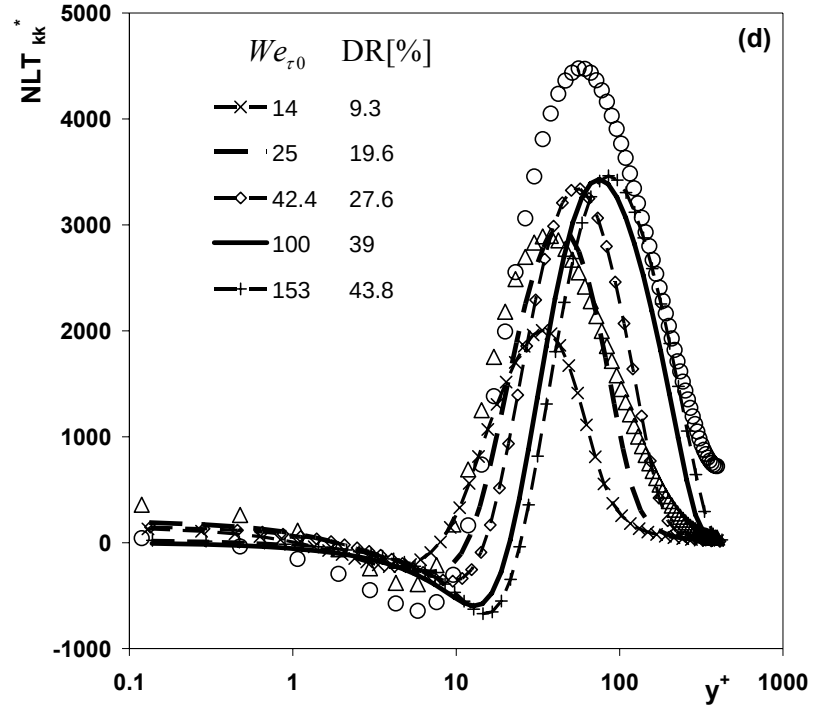
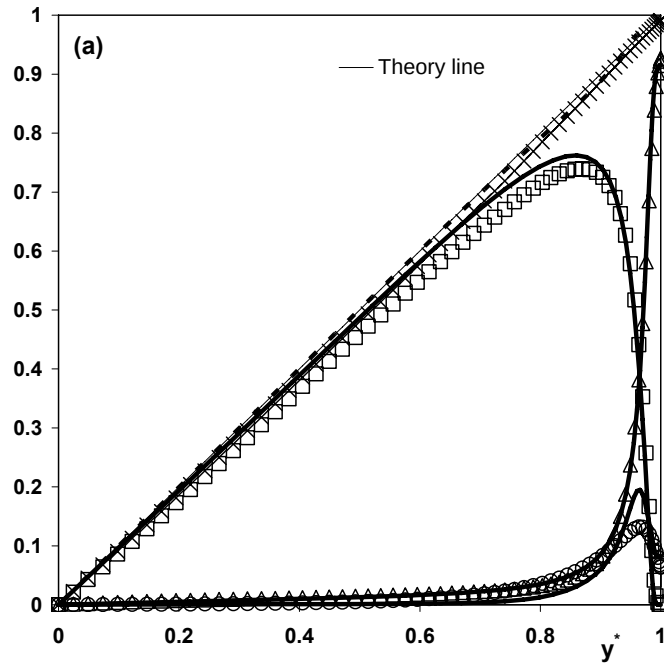


Fig. 51. Effect of Weissenberg number on predictions for turbulent channel flow at $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$. Predictions (lines), DNS DR= 18% (Δ) and DNS DR=37% ($\circ$): (a) k^+ ; (b) ε^{V+} ; (c) ε^{N+} ; (d) NLT_{kk}^* .



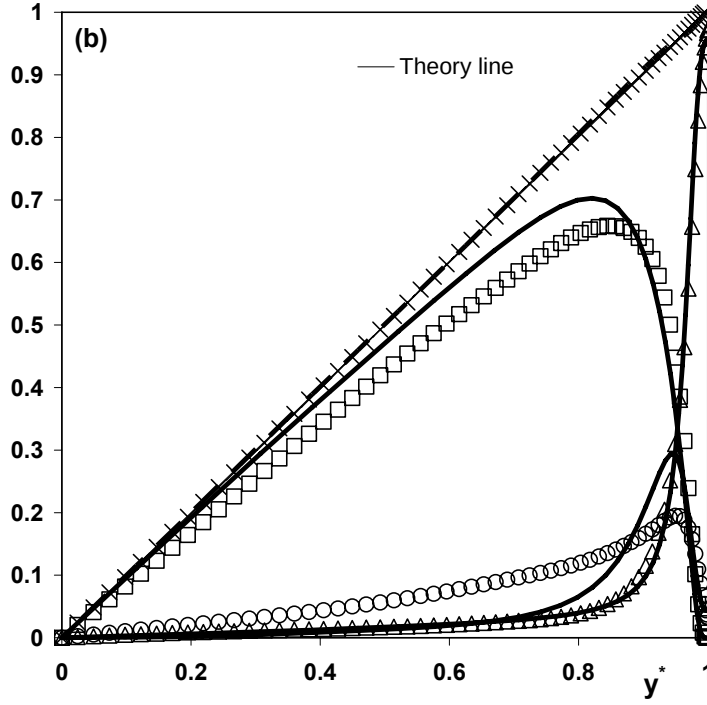


Fig. 52. Comparison between the predictions (lines) and DNS data (symbols) for normalized shear stresses (τ_N^+ , τ_p^+ , $-\overline{u_1 u_2}^+$) in turbulent channel flow with $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$. (Δ and line) τ_N^+ , ($\circ$ and line) τ_p^+ , ($\square$ and line) $-\overline{u_1 u_2}^+$; ($\times$ and dashed line) sum of stresses: (a) DR=18%; (b) DR=37%.

5.6 Conclusions

A new k - ε low-Reynolds-number turbulence model is developed here for turbulent flow of dilute polymer solutions represented by the FENE-P rheological constitutive equation. It constitutes a major improvement over the previous model of Pinho et al. [4] since several of its components have been modified and in addition the new model is valid not only at low drag reductions but also at high drag reduction.

The main features of this new model are completely new closures for the Reynolds-averaged non-linear term of the polymer conformation equation (denoted NLT_{ij}), for the eddy viscosity, the inclusion of a viscoelastic destruction term in the

transport equation of the rate of dissipation of k by the Newtonian solvent, and an extra contribution to the viscoelastic turbulent diffusion, previously neglected, in addition to other improvements as for the viscoelastic stress work model and the extension to the high drag reduction regime.

Arguably, the most important modification was the development of the closure for NLT_{ij} , which started from its exact equation and simplification on the basis of various simplifying physical arguments, such as homogeneous isotropic turbulence, and an order of magnitude analysis. Out of this came two NLT_{ij} models: the first closure was developed in the context of second-order turbulence models and the other, designated by "isotropic" model, considered an isotropic distribution of the Reynolds stresses and of the rate of dissipation tensor by the Newtonian solvent and is typically to be used in the context of the k - ε and k - ω turbulence models. The two models behave similarly at low drag reduction, but show differences at large drag reduction, with the simpler model performing slightly less well. In any case both models captured the main features of the individual components of tensor NLT_{ij} , and in particular their variations with drag reduction.

The new eddy viscosity closure directly incorporated a polymer contribution to the Reynolds stress tensor calculation. It behaves quite well, but the fact that it is now a difference between two contributions is a cause of concern and may have to be further modified when the model is tried in more complex flows to remove its inherent stability problems. The deficiencies of the previous model of Pinho et al. [4] in predicting the rate of dissipation of k by the Newtonian solvent were largely eliminated by developing a closure for the new term appearing in the transport equation of ε^N , which accounts for the direct impact of the polymer additives. This new term was considered as a destruction term, because without it we always had an overprediction of ε^N . The goodness of the viscoelastic stress work (ε^V) closure developed by Pinho et al. [4] was confirmed and here this model was extended to deal with low as well as high drag reduction using the corresponding DNS data. Finally, an extra term of the definition of the viscoelastic turbulent diffusion, which had previously been neglected at low DR, was now incorporated and the performance of the model for the viscoelastic stress work was also enhanced so that its predictions could be improved.

As a consequence of all these changes to the new turbulence model shows better predictions for all quantities, and especially for the mean velocity, Newtonian rate of dissipation, NLT_{ij} distribution, conformation tensor distribution and the polymer and Reynolds shear stresses. However, the improvements in the prediction of k were small and k remained underpredicted. We think this problem is essentially associated to the assumption of turbulence isotropy inherent to the k - ε model. Comparing with the model of Pinho et al. [4] the increase in the maximum value of k seen now is due to the improved capacity of the new model to predict more accurately the evolution of NLT_{ij} in the buffer layer, where it captures the lower peak of NLT_{kk} profile. This enters the viscoelastic stress work, where it acts as a production in part of the buffer layer, thus increasing the turbulent kinetic energy. Finally the model needs to be extended to the maximum drag reduction regime and to deal with fluids having a different maximum extensibility and viscosity solvent ratio.

Chapter 6

***k*- ω model for the FENE-P constitutive equation**

This chapter is based on the manuscript *Development of a low k - ω model closure for FENE-P fluids*, which is about to be submitted to an archival journal

This chapter presents a k - ω turbulence model based on the FENE-P rheological constitutive equation, and uses most of the viscoelastic closures developed in chapter 6, for the k - ε model. Here, the governing equations will be written based on the ω definition introduced by Wilcox [55] and the performance of the k - ω turbulence model in turbulent channel flow is assessed against the same set of previous DNS data used in chapter 6.

6.1 Governing equations

In what follows upper-case letters and overbars denote Reynolds-averaged quantities, whereas lower-case letters and primes denote fluctuations. A caret is used to identify instantaneous quantities. The equations are written in the indicial notation of Einstein, with $\delta_{ij} = 0$ when $i \neq j$ and $\delta_{ij} = 1$ for $i = j$.

In the context of Reynolds average turbulent flow calculations, solving for a turbulent flow problem of an incompressible FENE-P fluid requires the solution of the continuity and momentum Eqs. (120) and (121), respectively,

$$\frac{\partial U_i}{\partial x_i} = 0 \quad (197)$$

$$\rho \frac{\partial U_i}{\partial t} + \rho U_k \frac{\partial U_i}{\partial x_k} = -\frac{\partial \bar{p}}{\partial x_i} + \eta_s \frac{\partial^2 U_i}{\partial x_k \partial x_k} - \frac{\partial}{\partial x_k} (\overline{\rho u_i u_k}) + \frac{\partial \bar{\tau}_{ik,p}}{\partial x_k}, \quad (198)$$

where $\bar{\tau}_{ik,p}$ is the Reynolds-averaged polymer stress, U_i is the velocity vector, $\bar{p}$ is the mean pressure, ρ is the fluid density and $-\overline{\rho u_i u_k}$ is the Reynolds stress tensor. The fluid rheology is described by the FENE-P model, where the extra stress is the sum of a Newtonian solvent contribution of viscosity η_s with a polymeric contribution, as in Eq. (122) below.

$$\bar{\tau}_{ij} = \eta_s \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + \bar{\tau}_{ij,p} \quad (199)$$

This total extra stress has already been incorporated into the momentum Eq. (121). The mean polymer stress $\bar{\tau}_{ij,p}$ results from Reynolds-averaging the rheological FENE-P constitutive equation relating the instantaneous stress and conformation tensors and is given by Eq. (123). The mean conformation tensor (C_{ij}) is determined by Reynolds averaging its instantaneous evolution equation leading to equation (201), where the first-term inside the brackets on the left-hand-side is Oldroyd's upper convected derivative of C_{ij} .

$$\bar{\tau}_{ij,p} = \frac{\eta_p}{\lambda} \left[f(C_{kk}) C_{ij} - f(L) \delta_{ij} \right] + \frac{\eta_p}{\lambda} \overline{f(C_{kk} + c_{kk}) c_{ij}} \quad (200)$$

$$\left[\frac{\partial C_{ij}}{\partial t} + U_k \frac{\partial C_{ij}}{\partial x_k} - \underbrace{\left(C_{jk} \frac{\partial U_i}{\partial x_k} + C_{ik} \frac{\partial U_j}{\partial x_k} \right)}_{M_{ij}} \right] + \underbrace{u_k \frac{\partial c_{ij}}{\partial x_k}}_{CT_{ij}} - \underbrace{\left(c_{kj} \frac{\partial u_i}{\partial x_k} + c_{ik} \frac{\partial u_j}{\partial x_k} \right)}_{NLT_{ij}} = - \frac{\bar{\tau}_{ij,p}}{\eta_p} \quad (201)$$

The functions appearing in these equations are

$$f(C_{kk}) = \frac{L^2 - 3}{L^2 - C_{kk}} \text{ and } f(L) = 1 \quad (202)$$

where L^2 denotes the maximum extensibility of the dumbbell model. Alternative formulations of these functions are possible, but the issue is largely irrelevant here [4].

The other parameters of the rheological constitutive equation are the relaxation time of the polymer λ and its viscosity coefficient η_p . Below Eq. (201) the specific designations of the terms on the left-hand-side are presented and include the viscoelastic cross-correlations for which adequate closures are developed in this work, namely NLT_{ij} and CT_{ij} .

The Reynolds stress tensor appearing in the momentum equation is modelled by invoking the Boussinesq turbulent stress-strain relationship (203)

$$-\overline{\rho u_i u_j} = 2\rho \nu_T S_{ij} - \frac{2}{3} \rho k \delta_{ij} \quad (203)$$

where k is the turbulent kinetic energy and ν_T is the eddy viscosity. This is where this work differs from those of Pinho et al. [4] and the k - ε model of chapter 5 (C5) where the eddy viscosity closures were based on the turbulent kinetic energy (k) and its rate of dissipation by the Newtonian solvent (ε^N). Here, instead of ε^N the eddy viscosity closure uses the specific rate of dissipation (ω^N) as in Eq. (204),

$$\nu_T = g() \frac{k}{\omega^N}, \quad (204)$$

where the specific form of the dimensionless function $g()$ is discussed in section 3.1. The quantities k and ω^N need to be obtained from their transport equations.

The transport equation for the turbulent kinetic energy is a contraction of the Reynolds stress transport equation written originally by Dimitropoulos et al. [37] and given by Eq. (128)

$$\rho \frac{Dk}{Dt} + \overline{\rho u_i u_k} \frac{\partial U_i}{\partial x_k} = -\overline{\rho u_k} \frac{\partial k}{\partial x_k} - \frac{\partial \overline{p' u_i}}{\partial x_i} + \eta_s \frac{\partial^2 k}{\partial x_k^2} - \eta_s \frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_k} + \frac{\partial}{\partial x_k} \left(\overline{\tau_{ik}^p u_i} \right) - \left(\overline{\tau_{ik}^p} \frac{\partial u_i}{\partial x_k} \right) \quad (205)$$

Introducing the definition of instantaneous polymer stress (see [4]), Eq. (128) is rewritten as

$$\begin{aligned} \rho \frac{Dk}{Dt} = & \underbrace{-\overline{\rho u_i u_k} \frac{\partial U_i}{\partial x_k}}_{\rho P_k} - \underbrace{\left(\overline{\rho u_k} \frac{\partial k}{\partial x_k} + \frac{\partial \overline{p' u_i}}{\partial x_i} \right)}_{\rho Q_k} + \underbrace{\eta_s \frac{\partial^2 k}{\partial x_k^2}}_{\rho D_k^N} - \underbrace{\eta_s \frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_k}}_{\rho \varepsilon^N} + \\ & \underbrace{\frac{\eta_p}{\lambda} \frac{\partial}{\partial x_k} \left[\overline{C_{ik} f(C_{mm} + c_{mm}) u_i} + \overline{c_{ik} f(C_{mm} + c_{mm}) u_i} \right]}_{\rho Q^V} - \\ & \underbrace{\frac{\eta_p}{\lambda} \left[\overline{C_{ik} f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}} + \overline{c_{ik} f(C_{mm} + c_{mm}) \frac{\partial u_i}{\partial x_k}} \right]}_{\rho \varepsilon^V} \end{aligned} \quad (206)$$

The left-hand side of Eq. (129) represents the advection of k and the remaining terms on the right-hand side have the following meaning, using the notation of Dimitropoulos et al. [17]: P_k - rate of production of k ; Q_k - turbulent transport of k by velocity and pressure fluctuations; D_k^N - molecular diffusion of k associated with the

Newtonian solvent; ε^N - direct viscous dissipation of k by the Newtonian solvent; Q^V - viscoelastic turbulent transport and finally ε^V - viscoelastic stress work, which can be positive or negative, acting as a dissipative or a productive mechanism, respectively.

The specific rate of dissipation by the Newtonian solvent (ω^N) is defined as

$$\omega^N = \frac{\varepsilon^N}{C_k k}. \quad (207)$$

The transport equation of ω^N for a FENE-P fluid can be obtained from this definition and the transport equations for k and ε^N . The exact form of the transport equation for the rate of dissipation of turbulent kinetic energy is Eq. (130), originally derived by Pinho et al. [4] for a FENE-P fluid.

$$\begin{aligned} \rho \frac{\partial \varepsilon^N}{\partial t} + \rho U_k \frac{\partial \varepsilon^N}{\partial x_k} = & -2\eta_s \left[\frac{\partial U_i}{\partial x_m} \frac{\partial u_i}{\partial x_m} \frac{\partial u_i}{\partial x_k} + \frac{\partial U_i}{\partial x_k} \frac{\partial u_i}{\partial x_m} \frac{\partial u_k}{\partial x_m} \right] - 2\eta_s \frac{\partial^2 U_i}{\partial x_m \partial x_k} \overline{u_k \frac{\partial u_i}{\partial x_m}} \\ & - 2\eta_s \frac{\partial u_i}{\partial x_m} \frac{\partial u_i}{\partial x_k} \frac{\partial u_k}{\partial x_m} - \frac{\partial}{\partial x_k} \left[\overline{\rho u_k \varepsilon^{N'}} + 2\nu_s \frac{\partial p'}{\partial x_m} \frac{\partial u_k}{\partial x_m} \right] + \eta_s \frac{\partial^2 \varepsilon^N}{\partial x_k \partial x_k} - 2\eta_s \nu_s \frac{\partial^2 u_i}{\partial x_m \partial x_k} \frac{\partial^2 u_i}{\partial x_m \partial x_k} \\ & + 2\nu_s \frac{\eta_p}{\lambda(L^2 - 3)} \frac{\partial u_i}{\partial x_m} \frac{\partial}{\partial x_k} \left\{ \overline{\frac{\partial}{\partial x_m} \left[f(C_{nn}) f(\hat{C}_{pp}) c'_{qq} C_{ik} \right]} \right\} \end{aligned} \quad (208)$$

The last term on the right-hand-side denoted $E_{\varepsilon^N}^V$ is a viscoelastic contribution, whereas all other terms exist also in the corresponding equation for a Newtonian fluid. This equation is used in a modelled form, so it is adequate to rewrite it as in Eq. (164).

$$\begin{aligned} \frac{\partial \rho \tilde{\varepsilon}^N}{\partial t} + \frac{\partial \rho U_i \tilde{\varepsilon}^N}{\partial x_i} = & \underbrace{f_1 C_{\varepsilon_1} \frac{\tilde{\varepsilon}^N}{k} P_k + \eta_s \nu_T (1 - f_\mu) \left(\frac{\partial^2 U_i}{\partial y \partial y} \right)^2}_{\rho P_{\varepsilon^N}} + \\ & \underbrace{\frac{\partial}{\partial x_i} \left[\left(\eta_s + \frac{\rho f_i \nu_T}{\sigma_\varepsilon} \right) \frac{\partial \tilde{\varepsilon}^N}{\partial x_i} \right]}_{\rho (D_{\varepsilon^N}^N + Q_{\varepsilon^N})} - \underbrace{f_2 C_{\varepsilon_2} \rho \frac{\tilde{\varepsilon}^{N^2}}{k}}_{\rho \Phi_{\varepsilon^N}} + E_{\varepsilon^N}^V \end{aligned} \quad (209)$$

where for compactness we denote P_{ε^N} as the rate of production of ε^N , Q_{ε^N} as the turbulent transport of ε^N by velocity and pressure fluctuations, $D_{\varepsilon^N}^N$ as the molecular diffusion of ε^N by the Newtonian solvent and Φ_{ε^N} as the destruction. $E_{\varepsilon^N}^V$ is the viscoelastic term, which is here assumed as a destruction term since the DNS data has shown that ε^N decreases with the viscoelasticity (measured through the Weissenberg number) and drag reduction.

Following Bredberg et al. [61], deriving Eq. (207) gives

$$\frac{D\omega^N}{Dt} = \frac{D}{Dt} \left(\frac{\varepsilon^N}{C_k k} \right) = \frac{1}{C_k k} \frac{D\varepsilon^N}{Dt} - \frac{\omega^N}{k} \frac{Dk}{Dt}. \quad (210)$$

Back-substituting the transport equations of k and ε^N into this expression, the following transport equation of ω^N is obtained

$$\frac{D\omega^N}{Dt} = P_{\omega^N} - \Phi_{\omega^N} + Q_{\omega^N} + D_{\omega^N}^N + E_{\omega^N}^V, \quad (211)$$

where the various terms are defined as

$$P_{\omega^N} = \frac{1}{C_k k} P_{\varepsilon^N} - \frac{\omega^N}{k} P_k \quad (212)$$

$$\Phi_{\omega^N} = \frac{1}{C_k k} \Phi_{\varepsilon^N} - \frac{\omega^N}{k} \varepsilon^N \quad (213)$$

$$D_{\omega^N}^N = \frac{1}{C_k k} D_{\varepsilon^N}^N - \frac{\omega^N}{k} D_k^N = \frac{2\nu_s}{k} \frac{\partial \omega^N}{\partial x_i} \frac{\partial k}{\partial x_i} + \nu_s \frac{\partial^2 \omega^N}{\partial x_i^2} \quad (214)$$

$$\begin{aligned} Q_{\omega^N} &= \frac{1}{C_k k} Q_{\varepsilon^N} - \frac{\omega^N}{k} Q_k = \frac{1}{C_k k} \frac{\partial}{\partial x_i} \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} \frac{\partial \varepsilon^N}{\partial x_i} \right) - \frac{\omega^N}{k} \frac{\partial}{\partial x_i} \left(\frac{\nu_T}{\sigma_k} \frac{\partial k}{\partial x_i} \right) \\ &= \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} - \frac{\nu_T}{\sigma_k} \right) \frac{\omega^N}{k} \frac{\partial^2 k}{\partial x_i^2} + \frac{\omega^N}{k} \frac{\partial}{\partial x_i} \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} - \frac{\nu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_i} + \frac{\partial}{\partial x_i} \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} \frac{\partial \omega^N}{\partial x_i} \right) \\ &\quad + 2 \frac{\nu_T}{\sigma_{\varepsilon^N}} \frac{1}{k} \frac{\partial \omega^N}{\partial x_i} \frac{\partial k}{\partial x_i} \end{aligned}$$

or

$$\begin{aligned}
&= \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} - \frac{\nu_T}{\sigma_k} \right) \frac{\omega^N}{k} \frac{\partial^2 k}{\partial x_i^2} + \frac{\partial}{\partial x_i} \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} \frac{\partial \omega^N}{\partial x_i} \right) + \frac{1}{k} \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} + \frac{\nu_T}{\sigma_k} \right) \frac{\partial \omega^N}{\partial x_i} \frac{\partial k}{\partial x_i} \\
&+ \frac{1}{k} \frac{\partial k}{\partial x_i} \frac{\partial}{\partial x_i} \left[\left(\frac{\nu_T}{\sigma_{\varepsilon^N}} - \frac{\nu_T}{\sigma_k} \right) \omega^N \right]
\end{aligned} \tag{215}$$

$$E_{\omega^N}^V = \frac{1}{C_k k} E_{\varepsilon^N}^V - \frac{\omega}{k} Q^V + \frac{\omega}{k} \varepsilon^V \tag{216}$$

The direct viscoelastic contribution to the balance of ω^N is given in Eq. (216) and has three components: the viscoelastic turbulent diffusion and the viscoelastic stress work from the k - equation and the viscoelastic destruction term from the ε^N - equation. The final form of the transport equation of ω^N is given by Eq. (217).

$$\begin{aligned}
\frac{D\omega^N}{Dt} &= \left[\frac{1}{C_k k} P_{\varepsilon^N} - \frac{\omega^N}{k} P_k \right] - \left[\frac{1}{C_k k} \Phi_{\varepsilon^N} - \frac{\omega^N}{k} \varepsilon^N \right] \\
&+ \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} - \frac{\nu_T}{\sigma_k} \right) \frac{\omega^N}{k} \frac{\partial^2 k}{\partial x_i^2} + \frac{\partial}{\partial x_i} \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} \frac{\partial \omega^N}{\partial x_i} \right) + \frac{1}{k} \frac{\partial k}{\partial x_i} \frac{\partial}{\partial x_i} \left[\left(\frac{\nu_T}{\sigma_{\varepsilon^N}} - \frac{\nu_T}{\sigma_k} \right) \omega^N \right] \\
&+ \left[\nu_s \frac{\partial^2 \omega^N}{\partial x_i^2} \right] + \underbrace{\frac{1}{k} \left(\frac{\nu_T}{\sigma_{\varepsilon^N}} + \frac{\nu_T}{\sigma_k} \right) \frac{\partial \omega^N}{\partial x_i} \frac{\partial k}{\partial x_i} + \frac{2\nu_s}{k} \frac{\partial \omega^N}{\partial x_i} \frac{\partial k}{\partial x_i}}_{\text{cross diffusion term}} + E_{\omega^N}^V
\end{aligned} \tag{217}$$

The k - ω model of Bredberg et al. [61] keeps the viscous and turbulent cross-diffusion term, singled-out as the penultimate set of terms in Q_{ω^N} , Eq. (217), which Wilcox [56] neglected. By including the cross diffusion term the k - ω model describes better the asymptotic near-wall behaviour of k and ω , which vary as $k \sim y^2$ and $\omega \sim y^{-1}$, without the need to a specific damping function. The remaining damping function in the ω^N equation depends on the turbulent Reynolds number, defined as $\text{Re} = k/(\nu_s \omega)$, avoiding the ambiguity of defining a distance to a wall in complex geometries.

6.2 Non-dimensional numbers and DNS cases

The development of the various closures is carried out with the assistance of DNS data for fully developed turbulent channel flow of FENE-P fluids. In this exercise various non-dimensional numbers are used, which are defined as follows: the Reynolds number $Re_{\tau_0} \equiv hu_{\tau}/\nu_0$ is based on the friction velocity (u_{τ}), the channel half-height (h) and the zero shear-rate kinematic viscosity of the solution, which is the sum of the kinematic viscosities of the solvent and polymer ($\nu_0 = \nu_s + \nu_p$). The Weissenberg number is given by $We_{\tau_0} \equiv \lambda u_{\tau}^2/\nu_0$ and β ($\beta \equiv \nu_s/\nu_0$) is the ratio between the solvent viscosity and the solution viscosity at zero shear rate.

The two DNS data sets are characterized by a Reynolds number of $Re_{\tau_0} = 395$, a solvent to total zero-shear-rate viscosities ratio of $\beta = 0.9$ and a maximum extensibility $L^2 = 900$. The Weissenberg numbers are $We_{\tau_0} = 25$ and $We_{\tau_0} = 100$, corresponding to drag reductions of 18% and 37%, respectively. The former is typical of the low drag reduction (LDR) regime and latter is at the low end of the high drag reduction (HDR) regime.

6.3 Closures of the viscoelastic turbulence model

6.3.1 Momentum equation

The variation of the Reynolds stress with drag reduction has been established long ago in experiments, like those of Ptasinski et al. [16], and is also quantified in direct numerical simulations.

The Reynolds stress closure was introduced in Eq. (203) and relies on a model for the eddy viscosity. Not all components of the Reynolds stress tensor decrease with DR, but most do and in particular the shear Reynolds stress. In order to incorporate better the influence of the DR on the Reynolds stress in their k - ε turbulence model for FENE-P

fluids, chapter 5 showed the need to modify the eddy viscosity model, which is divided into Newtonian (ν_T^N) and polymeric (ν_T^P) contributions as in Eq. (218).

$$\nu_T = \nu_T^N + \nu_T^P \quad (218)$$

The Newtonian contribution is modelled by the classical low Reynolds number turbulent viscosity model, now modified by the use of the specific rate of dissipation as in Eq. (219) for the k - ω model (Wilcox [55]), i.e.,

$$\nu_T^N = C_\mu \times f_\mu \times \frac{k}{\omega^N}, \quad (219)$$

where the Newtonian parameters and damping functions are similar to those of Bredberg et al. [61] presented in Eq. (220). Here, the coefficient 25 of the damping function f_μ was slightly changed to 28 for improved predictions of velocity in Newtonian turbulent channel flow.

$$C_\mu = 1.0 \text{ and } f_\mu = 0.09 + \left(0.91 + \frac{1}{R_t^3}\right) \left[1 - \exp\left\{-\left(\frac{R_t}{28}\right)^{2.75}\right\}\right] \text{ with } R_t = \frac{k}{\omega \cdot \nu_s} \quad (220)$$

Following on the steps of chapter 5, the polymeric contribution to the eddy viscosity has the same physical dependency, but also incorporates viscoelastic quantities, namely the trace of the conformation tensor. Additionally, and in order to better represent the variation of the eddy viscosity with wall distance and drag reduction, the k - ε model of chapter 5 found it necessary to correct the model with a function $f(We_{\tau_0}, y^+)$ incorporating wall damping and Weissenberg number effects, so that ν_T^P is given by Eq. (221)

$$\nu_T^P = f(We_{\tau_0}, y^+) \times C_{mm} \times C_\mu \times f_\mu \times \frac{k}{\omega^N}, \quad (221)$$

$$\text{where } f(We_{\tau_0}, y^+) = f_\mu^P \times f_{DR}^P \text{ with } f_\mu^P = 0.00045 \left[1 + 2.55 \times \exp\left(-\frac{y^+}{44}\right)\right] \text{ and}$$

$$f_{DR}^P = \left[1 - \exp\left(-\frac{We_{r0}}{6.25}\right) \right]^4 \times \left[\frac{25}{We_{r0}} \right]^{0.1232}. \quad (222)$$

This function from chapter 5 is used here without any modification. The eddy viscosity model is capable of predicting the correct evolution shown by the DNS data in both LDR and HDR, namely a decrease in ν_T as DR increase, visualized in **Fig. 53**. As can also be observed the discrepancies at large y^+ are inherent to the original Newtonian model and not a consequence of viscoelastic modelling. To close the eddy viscosity model transport equations are solved for k and ω^N , discussed in sections 4.3 and 4.4. The Reynolds-average polymer stress is provided by the Reynolds- average constitutive equation, discussed next.

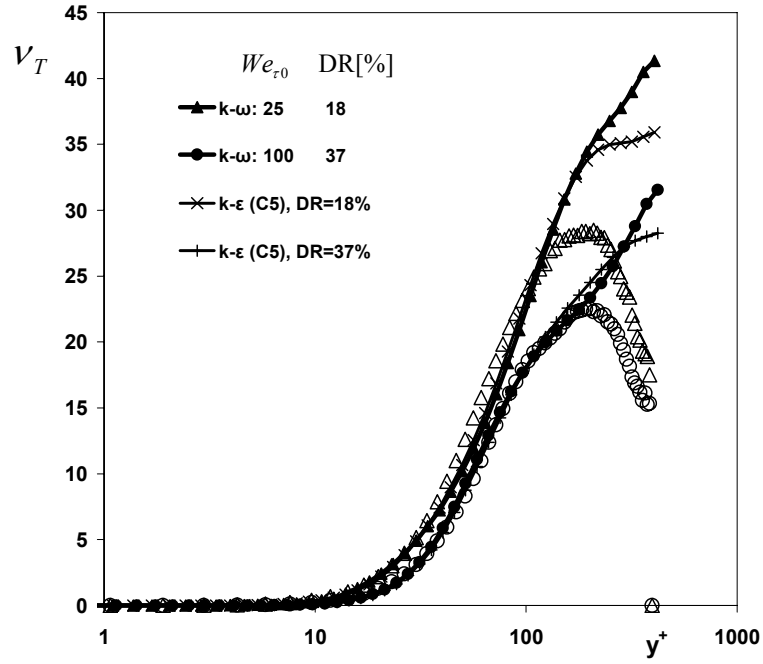


Fig. 53. Comparison between the model predictions (lines with close symbols) of the turbulent viscosity normalized by ν_0 and DNS data (open symbols), for turbulent channel flow with $Re_{r0} = 395$, $L^2 = 900$ and $\beta = 0.9$: Δ DR=18% and $\circ$ DR=37%.

6.3.2 Constitutive equation

The Reynolds-averaged polymer stress is given in Eq. (123) and is a function of the average conformation tensor and of a double correlation involving fluctuations of the conformation tensor. Pinho et al. [4] have shown the impact of this double correlation to be small at low drag reduction. Even though k - ε model of chapter 5 found it to be non-negligible at high drag reduction (HDR), it was still fairly small in the low range of HDR and consequently it is neglected here also. Consequently, the Reynolds-averaged polymer stress is given by Eq. (223) and is a function of the Reynolds-averaged conformation tensor.

$$\bar{\tau}_{ij,p} \approx \frac{\eta_p}{\lambda} \left[f(C_{kk}) C_{ij} - f(L) \delta_{ij} \right] \quad (223)$$

To determine the Reynolds-averaged conformation tensor it is necessary to solve Eq. (201), which contains two turbulent terms (CT_{ij} and NLT_{ij}) requiring appropriate closures. The CT_{ij} term is negligible at low and high DR in comparison with the remaining terms of the equation [4] and to calculate NLT_{ij} chapter 5 developed a new closure in the context of k - ε , which is adopted here without any modification. This closure is given by Eq. (224).

$$\begin{aligned} NLT_{ij} \equiv \overline{c_{kj} \frac{\partial u_i}{\partial x_k}} + \overline{c_{ik} \frac{\partial u_j}{\partial x_k}} \approx C_{F1} \left(0.0552 \frac{We_{\tau 0}}{25} + 0.116 \right) \times \frac{C_{ij} \times f(C_{mm})}{\lambda} - \\ - C_{F2} We_{\tau 0}^{0.743} \left[C_{kj} \frac{\partial U_i}{\partial x_k} + C_{ik} \frac{\partial U_j}{\partial x_k} \right] + \end{aligned}$$

$$\begin{aligned}
& + \frac{\lambda}{f(C_{mm})} \left[C_{F3} \times \left(\frac{25}{We_{\tau_0}} \right)^{0.718} \times \left(\frac{\partial U_j}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + \frac{\partial U_i}{\partial x_n} \frac{\partial U_m}{\partial x_k} C_{kn} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + \right. \right. \\
& \quad \left. \left. + \frac{\partial U_k}{\partial x_n} \frac{\partial U_m}{\partial x_k} \left(C_{jn} \frac{\overline{u_i u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} + C_{in} \frac{\overline{u_j u_m}}{\nu_0 \sqrt{2S_{pq} S_{pq}}} \right) \right) \right] - \\
& - \frac{\lambda}{f(C_{mm})} \times f_{F1} \times C_{F4} \times \left(\frac{25}{We_{\tau_0}} \right)^{0.7} \times \left[C_{jn} \frac{\partial U_k}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{in} \frac{\partial U_k}{\partial x_n} \frac{\partial U_j}{\partial x_k} + \right. \\
& \quad \left. C_{kn} \frac{\partial U_j}{\partial x_n} \frac{\partial U_i}{\partial x_k} + C_{kn} \frac{\partial U_i}{\partial x_n} \frac{\partial U_j}{\partial x_k} \right] + \\
& + \frac{\lambda}{f(C_{mm})} \left[\frac{C_{\varepsilon_F}}{We_{\tau_0}} \frac{4}{15} \times \frac{\varepsilon^N}{(\nu_s + \nu_{\tau_p}) \times \beta} C_{mm} \times f_{F2} \times \delta_{ij} \right] \quad (224)
\end{aligned}$$

The parameters and damping functions of the NLT_{ij} model are listed in Table 9.

Table 9. Parameters and damping functions of the NLT_{ij} model.

C_{F1}	C_{F2}	C_{F3}	C_{F4}	C_{ε_F}
1.0	0.0105	0.046	1.05	2
$f_{F1} = \left(1 - 0.8 \exp\left(-\frac{y^+}{30}\right) \right)^2$		$f_{F2} = \left(1 - \exp\left(-\frac{y^+}{25}\right) \right)^4$		

6.3.3 Transport equation of turbulent kinetic energy

The transport equation of turbulent kinetic energy is Eq. (129) with adequate closures for Q_k , ε^N , ε^V and Q^V , whereas the exact terms are obviously carried over and do not need any modelling. Strictly speaking, in the context of the k - ω model there is no need to modify the transport equation of k , except on what concerns the change from the dissipation rate (ε^N) to the specific dissipation rate (ω^N) considering Eq. (207), i.e., one could import the modelled transport equation for a particular k - ε model and turn it into the k equation for a k - ω model just invoking $\varepsilon^N = C_k k \omega^N$. However,

for improved performance modifications are admissible and often necessary, but here will be kept to a minimum.

For the present k - ω model the closures for the turbulent transport of k by velocity and pressure fluctuations (Q_k) and for the viscoelastic stress work (ε^V) are those developed in the previous low Reynolds number k - ε models for FENE-P fluids [4] and chapter 5, namely

$$Q_k = \frac{\partial}{\partial x_i} \left(\frac{\nu_T}{\sigma_k} \frac{\partial k}{\partial x_i} \right) \quad (225)$$

and

$$\varepsilon^V \equiv \frac{1}{\rho} \overline{\tau'_{ik,p} \frac{\partial u_i}{\partial x_k}} \approx 1.37 \times f_{DR}^{-1} \frac{\eta_p}{\rho \lambda} f(C_{mm}) \frac{NLT_{mm}}{2}, \quad (226)$$

where the drag reduction function $f_{DR}^{-1} = \left[1 - \exp\left(-\frac{We_{\tau 0}}{6.25}\right) \right]^4 \times \left[\frac{We_{\tau 0}}{25} \right]^{0.095}$ corrects the behaviour for different Weissenberg numbers (cf. chapter 5).

Finally, regarding the remaining contribution, the viscoelastic turbulent transport (Q^V), the closure developed originally by Pinho et al. [4] and improved by chapter 5 was again modified, as explained next.

As in other k - ε low Reynolds number models for Newtonian fluids, in the models for FENE-P fluids of Pinho et al. [4] and chapter 5 ε^N was split into a pseudo-dissipation ($\tilde{\varepsilon}^N$) and a wall correction (D) according to $\varepsilon^N = D + \tilde{\varepsilon}^N$. In Pinho et al. [4] D is proportional to the Newtonian solvent viscosity, but this was found to be inadequate especially at low Weissenberg numbers, leading to predictions of drag increase rather than drag reduction (or to no change in relation to the Newtonian flow). Actually, this deficiency is not so severe as one might think; the Weissenberg number is usually decreased by reducing the relaxation time, but for FENE-P fluids the relaxation time and the polymer viscosity coefficient are related by $\eta_p \rightarrow nk_B T \lambda L^2 / (L^2 + 5)$ in the limit of small Weissenberg numbers, i.e., at small We both parameters must be reduced and when this is done the model deficiency is reduced. However, the exact equation

relating λ and η_p is unknown so there is a real problem at small We as We is reduced without the concomitant change in Re , which chapter 5 solved by making D proportional to the local shear viscosity of the fluid ($\eta_s + \eta_{\tau_p}$, where $\eta_{\tau_p} = \tau_{xy}^p / \dot{\gamma}$).

By using ω^N instead of ε^N this wall correction D term naturally disappears and the problem of predicting a drag increase at low We reappears. The solution of this problem is a modification of the original closures for the viscoelastic turbulent diffusion of k and ω^N in a way that impacts only the wall region, as was the case of term D in k - ε . This modification specifically consists of the direct incorporation of an extra molecular diffusion associated with the local shear polymer viscosity in the transport equations of k and of ω^N , the former being denoted Q_D^V and the latter to be discussed in Section 4.3. Consequently, the closure for Q^V is now

$$Q^V \equiv \frac{\partial \overline{\tau'_{ik,p} u_i}}{\partial x_k} \approx \underbrace{\frac{\eta_p}{\lambda} \frac{\partial}{\partial x_k} \left[f(C_{mm}) \left(\frac{C_{ik} F U_i + C U_{iik}}{2} \right) \right]}_{Q_\tau^V} + \underbrace{\eta_{\tau_p} \frac{\partial^2 k}{\partial x_k^2}}_{Q_D^V}, \quad (227)$$

where Q_τ^V is the former Q^V (as in chapter 5). Q_D^V together with the molecular diffusion by the Newtonian solvent ($\eta_s \partial^2 k / \partial x_i \partial x_i$) results in a molecular diffusion by the whole solution, since $\eta_s + \eta_{\tau_p}$ is the local shear viscosity of the FENE-P fluid. Incidentally, the k - ε v^2 - f viscoelastic turbulence model of Iaccarino et al. [49] also has a molecular diffusion term proportional to the fluid viscosity, $\eta_s + \eta_{\tau_p}$. The closures for $C U_{iik}$ and $C_{ik} F U_i$ are given by equations (228) and (229), respectively,

$$C U_{iik} = -C_{\beta 1} \sqrt{\frac{25}{We_{\tau 0}}} \frac{\lambda}{f(C_{mm})} \left(2 \overline{u_i u_m} \frac{\partial C_{ki}}{\partial x_m} \right) - C_{\beta 7} \left(\frac{We_{\tau 0}}{25} \right)^{1.661} \left[\pm 2 \sqrt{\overline{u_i^2}} C_{ik} \right] \quad (228)$$

$$C_{ik} F U_i = \frac{C_{FU}}{2} \sqrt{\frac{We_{\tau 0}}{25}} C_{ik} \frac{\partial \overline{u_n u_n}}{\partial x_i} \quad (229)$$

with coefficients $C_{\beta 1} = 0.6$, $C_{\beta 2} = 0.05$ and $C_{FU} = 1$, i.e., identical to those in chapter 5. In addition to solving the problem of drag increase at very low We , this closure of Q^V provides an onset of drag reduction at $We_{\tau_0} \approx 5.5$, which is close to the value of $We_{\tau_0} \approx 6.25$ obtained by DNS.

The final form of the transport equation of turbulent kinetic energy is

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho U_i k}{\partial x_i} = -\overline{\rho u_i u_k} \frac{\partial U_i}{\partial x_k} + \frac{\partial}{\partial x_i} \left[\left(\eta_s + \rho \nu_{\tau_p} + \rho \frac{\nu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] - \rho C_k \omega k + Q_T^V - \rho \varepsilon^V \quad (230)$$

The values of the turbulent Prandtl number and of the Newtonian parameter are based on Bredberg et al's. [61] model, with $\sigma_k = 1.0$ and $C_k = 0.09$, respectively.

6.3.4 Transport equation of the specific dissipation rate

The starting point for the transport equation for the specific dissipation rate is Eq. (217), which was obtained by application of the definition of Eq. (210) and incorporates the viscous cross-diffusion neglected originally by Wilcox [55]. Below we discuss the model adopted for $E_{\omega^N}^V$ and one other modification to arrive at the final form of the modelled ω^N equation. The solvent contribution to Eq. (217) is modelled as in the Bredberg et al. [61], and so the modelled transport equation becomes

$$\begin{aligned} \frac{\partial \rho \omega}{\partial t} + \frac{\partial \rho U_i \omega}{\partial x_i} = & \frac{\partial}{\partial x_i} \left[\left(\eta_s + \rho \nu_{\tau_p} + \rho \frac{\nu_T}{\sigma_\varepsilon} \right) \frac{\partial \omega}{\partial x_i} \right] + C_{\omega_1} \frac{\omega}{k} P_k - \\ & \underbrace{C_{\omega_2} \rho \omega^2 + \rho \frac{C_\omega}{k} \left(\frac{\eta_s}{\rho} + \nu_{\tau_p} + \nu_T \right) \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i}}_{\text{cross diffusion term}} + \rho E_{\omega^N}^V. \end{aligned} \quad (231)$$

Term $E_{\omega^N}^V$ given in Eq. (232) differs from $E_{\omega^N}^V$ in the viscoelastic turbulent diffusion contribution to the k equation.

$$E_{\omega^N}^V = \frac{1}{C_k k} E_{\varepsilon^N}^V - \frac{\omega}{k} Q_T^V + \frac{\omega}{k} \varepsilon^V \quad (232)$$

In fact, Q^V was given as $Q^V = Q_T^V + Q_D^V$ in Eq. (227) and the closure for Q_D^V (diffusion of k by the local polymer viscosity ν_{τ_p}) was put together with the solvent molecular diffusion and eddy diffusion of k , so it now appears in the cross-diffusion term of the ω^N equation (231) as a consequence of equation (210). The incorporation of Q_D^V in the transport equation of k was part of the solution to avoid drag increase at low Weissenberg number flows, but the solution to this problem also involved adding to the transport equation of ω^N a similar molecular diffusion of ω^N by the local polymer viscosity (second contribution to the first term on the rhs of equation (231)).

Regarding Equation (232), the viscoelastic closures for ε^V and Q_T^V are those given by Eq. (226) and Eq. (227), respectively. The $E_{\varepsilon^N}^V$ term is a viscoelastic destruction of ε^N , exactly given by Eq. (233) and requiring a closure.

$$E_{\varepsilon^N}^V = 2\eta_s \frac{\eta_p}{\lambda(L^2 - 3)} \frac{\partial u_i}{\partial x_m} \frac{\partial}{\partial x_k} \left\{ \frac{\partial}{\partial x_m} \left[f(C_{mm}) f(\hat{C}_{pp}) c'_{qq} C_{ik} \right] \right\} \quad (233)$$

In principle, we could use for $E_{\varepsilon^N}^V$ the closure developed by chapter 5, but a correction to the constants values is necessary to improve its performance. The reason for this correction is due to the different capacity of the turbulence models to predict the same Newtonian dissipation quantity, ε^N . This is accomplished through a change in the parameters values of $C_{\varepsilon F1}$ and $C_{\varepsilon F2}$. More details on the development of the closure of $E_{\varepsilon^N}^V$ can be found in chapter 5. In this case, the closure for $E_{\varepsilon^N}^V$ has the same form as previously and is given by Equation (234).

$$E_{\varepsilon^N}^V \approx -f_5 f_{DR}^{\varepsilon} \frac{(1-\beta)}{We_{\tau_0}(L^2 - 3)} \frac{\varepsilon^{N^2}}{k} \left[C_{\varepsilon F1} \frac{\varepsilon^V}{\varepsilon^N} (L^2 - 3)^2 + C_{\varepsilon F2} C_{mm}^2 f(C_{mm})^2 \right] \quad (234)$$

The two viscolastic damping functions of $E_{\varepsilon^N}^V$ remain unchanged as $f_5 = [1 - \exp(-y^+/50)]$ and $f_{DR} = [1 - \exp(-We_{\tau 0}/6.25)]^4$, but the function coefficients $C_{\varepsilon F1}$ and $C_{\varepsilon F2}$ were slightly modified to become $C_{\varepsilon F1} = 0.44(We_{\tau 0}/25)^{0.724}$ and $C_{\varepsilon F2} = 1.0(25/We_{\tau 0})^{1.558}$ for improved predictions.

The capacity of this closure to predict well in both the k - ε and k - ω turbulence models, with small adjustments in the coefficients due to the capacity of the Newtonian turbulence model in predict correctly ε^N , suggests the fairness of the assumptions invoked by chapter 5 in its developments.

The remaining Newtonian parameters are $C_\omega = 1.0$, $C_{\omega_1} = 0.49$, $C_{\omega_2} = 0.072$ and $\sigma_\omega = 1.8$, with a correction in the coefficient C_ω for which we use 1.0 rather than 1.1. Note that this change in C_ω is with the same principle used before in damping function f_μ , to improve the Newtonian predictions.

6.4 Summary of the present model

Summarizing, the complete set of equations that need to be solved to arrive at a solution for turbulent flow of a FENE-P fluid in the context of this RANS/RACE k - ω model are: the continuity and momentum equations (120) and (121), respectively, with the polymer stress tensor calculated by equation (235) with the functions $f(L)$ and $f(C_{kk})$ given by equations (202).

$$\bar{\tau}_{ij,p} = \frac{\eta_p}{\lambda} [f(C_{kk})C_{ij} - f(L)\delta_{ij}] \quad (235)$$

The time-average conformation tensor is determined by equation (236)

$$\left(\frac{\partial C_{ij}}{\partial t} + U_k \frac{\partial C_{ij}}{\partial x_k} - C_{jk} \frac{\partial U_i}{\partial x_k} - C_{ik} \frac{\partial U_j}{\partial x_k} \right) - NLT_{ij} = -\frac{\bar{\tau}_{ij,p}}{\eta_p} \quad (236)$$

and the required NLT_{ij} model is that of equation (224), with the coefficients and the functions of Table 9.

The Reynolds stress tensor appearing in the momentum equation and in the NLT_{ij} model is calculated by Eq. (203), with the new eddy viscosity model given by equation (218) where the Newtonian and polymeric contributions are given by equations (219) and (221), respectively. The corresponding coefficients and damping functions are defined in Eq. (220) and (222).

The transport equation of turbulent kinetic energy is the following equation (237),

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho U_i k}{\partial x_i} = -\overline{\rho u_i u_k} \frac{\partial U_i}{\partial x_k} + \frac{\partial}{\partial x_i} \left[\left(\eta_s + \rho \nu_{\tau_p} + \rho \frac{\nu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] - \rho C_k \omega k + Q^V - \rho \varepsilon^V \quad (237)$$

The required model for the viscoelastic stress work appears in equation (226) with the corresponding drag reduction function. The viscoelastic turbulent transport term, Q^V_T , is defined in equation (227) with the models for $(CU)_{iik}$ and $C_{ik}(FU)_i$ given by equations (228) and (229), respectively.

The transport equation for the specific rate of dissipation of the turbulent kinetic energy by the Newtonian solvent is equation (238).

$$\begin{aligned} \frac{\partial \rho \omega^N}{\partial t} + \frac{\partial \rho U_i \omega^N}{\partial x_i} &= \frac{\partial}{\partial x_i} \left[\left(\eta_s + \rho \nu_{\tau_p} + \rho \frac{\nu_T}{\sigma_\varepsilon} \right) \frac{\partial \omega^N}{\partial x_i} \right] + C_{\omega_1} \frac{\omega^N}{k} P_k - \\ &C_{\omega_2} \rho \omega^{N^2} + \rho \frac{C_\omega}{k} \left(\frac{\eta_s}{\rho} + \nu_{\tau_p} + \nu_T \right) \frac{\partial k}{\partial x_i} \frac{\partial \omega^N}{\partial x_i} + \rho E_{\omega^N}^V, \end{aligned} \quad (238)$$

where the viscoelastic contribution is defined by equation (232) with the model for the viscoelastic destruction ($E_{\varepsilon^N}^V$) given in equation (234) with the corresponding coefficients and functions. The remaining Newtonian coefficients of the k and ω^N equations are given in Table 10, based on Bredberg et al's. [61] model.

Table 10. Newtonian parameters of the turbulence model.

C_μ	C_k	C_ω	C_{ω_1}	C_{ω_2}	σ_k	σ_ω
1.0	0.09	1.0	0.49	0.072	1.0	1.8

6.5 Method of solution and boundary conditions

To evaluate the performance of the model calculations are carried out for fully-developed channel flow using a finite-volume code specifically developed for walls confined flows and it was modified for FENE-P fluids. The code uses staggered meshes to ensure pressure-velocity- stress coupling and the TDMA solver is used to calculate the solution of the discretized algebraic governing equations.

The usual no-slip boundary conditions are used at the wall for mean and turbulent velocities, $U=0$ and $k=0$. Regarding the specific rate of dissipation, the wall value is infinity but ω follows a well defined asymptotic behavior. According to Wilcox [55], near a wall ω obeys the asymptotic behaviour of Eq. (239), and its numerical implementation requires the use of a fine mesh inside the viscous sublayer having at least 5 computational cells for $y^+ < 2.5$, in order to guarantee numerical accuracy. In our case we ensured between 5 and 10 points existed in that region where this expression was imposed.

$$\omega \rightarrow \frac{2\nu}{C_k \cdot y^2} \quad (239)$$

Since the FENE-P polymer solution has a viscosity given by the sum of the solvent and polymer viscosity, Wilcox's [55] asymptotic expression for Newtonian fluids was modified to incorporate the local total shear viscosity by the inclusion of the corresponding kinematic polymeric contribution (ν_{τ_p}).

$$\omega^N \rightarrow \frac{2(\nu_s + \nu_{\tau_p})}{C_k \cdot y^2} \quad (240)$$

6.6 Results and discussion

The turbulence model was tested against DNS data for FENE-P fluids in a viscoelastic turbulent channel flow at 18% and 37% drag reduction ($We_{\tau_0} = 25$ and $We_{\tau_0} = 100$, respectively), all other parameters being constant, namely the Reynolds number ($Re_{\tau_0} = 395$), maximum extension of the conformation tensor ($L^2 = 900$) and the viscosity ratio ($\beta = 0.9$). To obtain results with an estimated accuracy of $\pm 1\%$, a mesh of 99 non-uniform computational cells from wall to wall was used, containing about 10 cells within each viscous sublayer.

The predictions are compared with the DNS data for the following proprieties: velocity, turbulent kinetic energy, conformation tensor, NLT_{ij} tensor, Reynolds shear stress and the polymer stress tensor, respectively. A parametric analysis was also carried out to assess the capabilities of the turbulence model. Its results are compared with the predictions of the function developed by Li et al. [39] based on the DNS data, by changing the Wesseinberg and the Reynolds numbers for the same L^2 and β .

In **Fig. 54** the predicted mean velocity profiles are compared with DNS data for DR=18% and 37% and with the predictions of the k - ε model of chapter 5. The k - ω predictions coincide with those of the previous k - ε model and show good agreement with the DNS data. The monotonic shift of the log-law region with the DR is well captured as is the correct evolution in the buffer-layer.

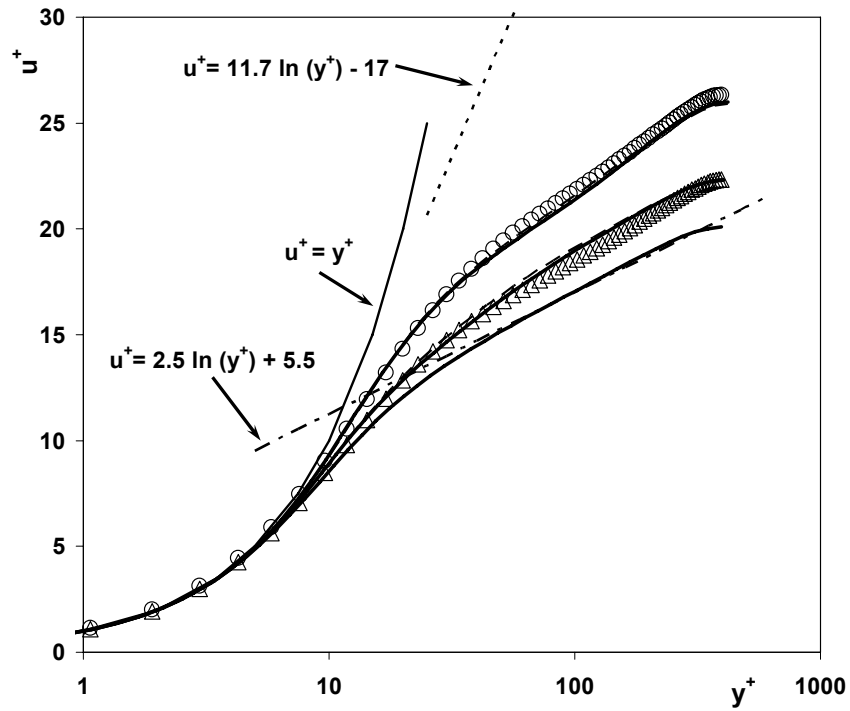


Fig. 54. Comparison between the velocity predictions of the (—) present model, (---) $k-\epsilon$ model of chapter 5 (C5) and DNS data (symbols), for turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$: Δ DR=18% and $\circ$ DR=37%.

The impact of the Weissenberg number variation on the prediction of the velocity profile and the limits of the model can be observed **Fig. 55**, where the turbulence model is able to reach a DR=50% in high regime of DR, with computation stability.

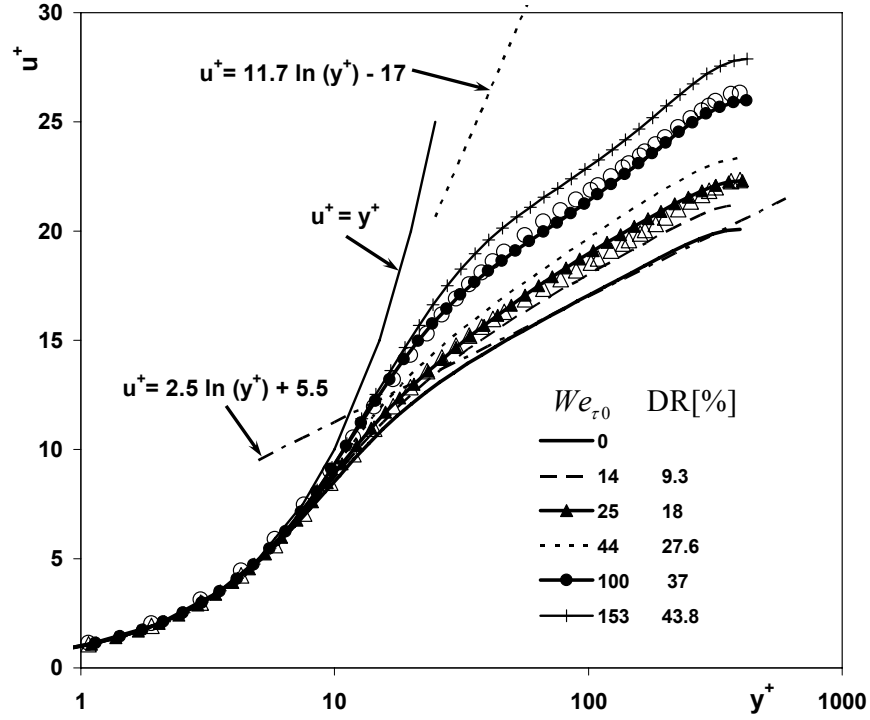


Fig. 55. Comparison between the predictions (lines with close symbols) and DNS data (open symbols) of the velocity for turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$ and different Weissenberg numbers: Δ DR= 18% and $\circ$ DR= 37%.

It is possible to quantify this through a comparison with Equation (241), developed by Li et al. [39], which allows the determination of the drag reduction intensity as a function of the Weissenberg number (We_{τ_0}), the Reynolds number (Re_{τ_0}) and the maximum molecular extensibility of the dumbbell (L), where $We_{\tau_0,c} = 6.25$ and $Re_{\tau_0,r} = 125$. In Table 11 the drag reduction predicted by the $k-\omega$ model is compared with that of Eq. (241) and DNS data for several values of the Weissenberg number, all other nondimensional numbers (Re_{τ_0} , L^2 and β) being constant. This equation represents DR as a function of We_{τ_0} and Re_{τ_0} as obtained in a large set of DNS simulations. While there is a fairly good agreement for large We_{τ_0} , at low We_{τ_0} there is an underprediction of DR of about 30% for 18% DR when comparing with DNS data, this can be explain by the underprediction of the equation for low regime of DR, more details can be found in Li et al. [39].

$$DR = 80 \left[1 - \exp(-0.0275L) \right] \left\{ 1 - \exp \left[-0.025 \left(We_{\tau_0} - We_{\tau_0,c} \right) \left(\frac{Re_{\tau_0}}{Re_{\tau_0,r}} \right)^{-0.225} \right] \right\} \quad (241)$$

Table 11. Comparison between the DR (%) of the present model with Li et al.'s [39] equation for $L^2 = 900$, $Re_{\tau_0} = 395$ and $\beta = 0.9$.

We_{τ_0} $DR(\%)$	14	25	44	100	153
Present model	9.3	18	27.6	37	43.8
Li et al. [39] equation	6.2	13.6	23.3	37.6	42.3
DNS data	-	18	-	37	-

The turbulent kinetic energy are plotted in **Fig. 56**. The predicted peak values decrease with DR, in contrast with the DNS data, and this represents a deficiency of the model. The data of k - ε model of chapter 5 show the same deficiency, but the k - ω model has always better predictions especially for the Newtonian fluid. The evolution of the predictions of k with We_{τ_0} is shown in **Fig. 57** where we observe a continuous reduction in k , a defect of the present model also present in the k - ε model of chapter 5. This deficiency limits the application of this model to a maximum drag reduction of about 50%.

This deficiency is related to the inherent incompatibility between the eddy viscosity closure used and the physics of the drag reducing fluids. As the Weissenberg number is increased the Reynolds shear stress decreases, but the turbulent kinetic energy increases. Since the eddy viscosity closure models the Reynolds shear stress in proportion to k (the turbulent velocity scale used in the closure), a reduction in the Reynolds shear stress requires a reduction in this turbulent velocity scale, but it actually increases. In an attempt to solve this problem Pinho et al. [4] incorporated the viscoelastic stress work in the turbulence length scale, whereas the k - ε model of chapter 5 and the present work consider instead a polymeric contribution to the eddy viscosity

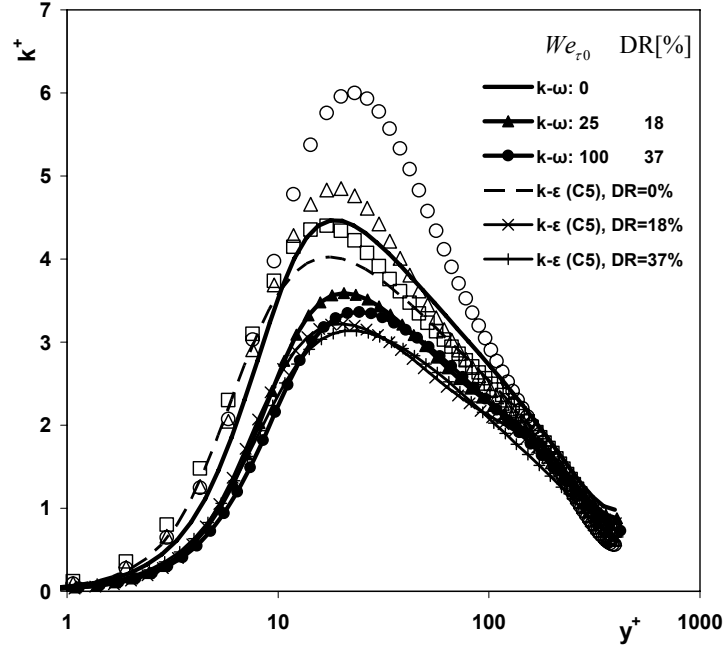


Fig. 56. Comparison between the kinetic energy predictions (lines with close symbols) of the present model, $k-\varepsilon$ model of chapter 5 (C5) and DNS data (open symbols), for turbulent channel flow with $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$: $\square$ Newtonian, Δ DR=18% and $\circ$ DR=37%.

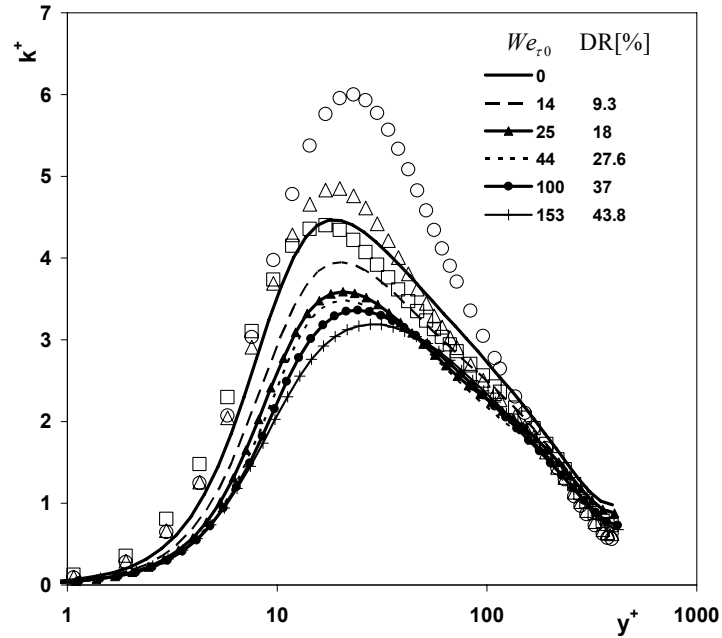


Fig. 57. Comparison between the predictions (lines with close symbols) and DNS data (open symbols) of the kinetic energy for turbulent channel flow with $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$ and different Weissenberg numbers: Δ DR= 18% and $\circ$ DR= 37%.

subtracting the standard Newtonian eddy viscosity. Both approaches were not enough to solve this problem. Incidentally, a fairly successful alternative is that of Durbin [100], who relate the turbulent velocity scale to the transverse normal Reynolds stress, and used by Iaccarino et al. [49], but this approach becomes difficult to implement in a geometry with more than one wall. The solution of this problem is certainly a major motivation for future work in these type of models.

The profiles of the predicted kinetic energy dissipation rate are presented in **Fig. 58**, including the DNS data and the predictions of chapter 5. In the buffer and log layers the predictions by both the $k\text{-}\omega$ model and $k\text{-}\varepsilon$ model of chapter 5 are similar and agree with the DNS data. Note that even for Newtonian fluids there are differences in the predictions of ε^N obtained with $k\text{-}\varepsilon$ and $k\text{-}\omega$ turbulence models. This difference forces a correction in the coefficient values of the $E_{\varepsilon^N}^V$ closure, which has a direct impact on the predictions of ε^N .

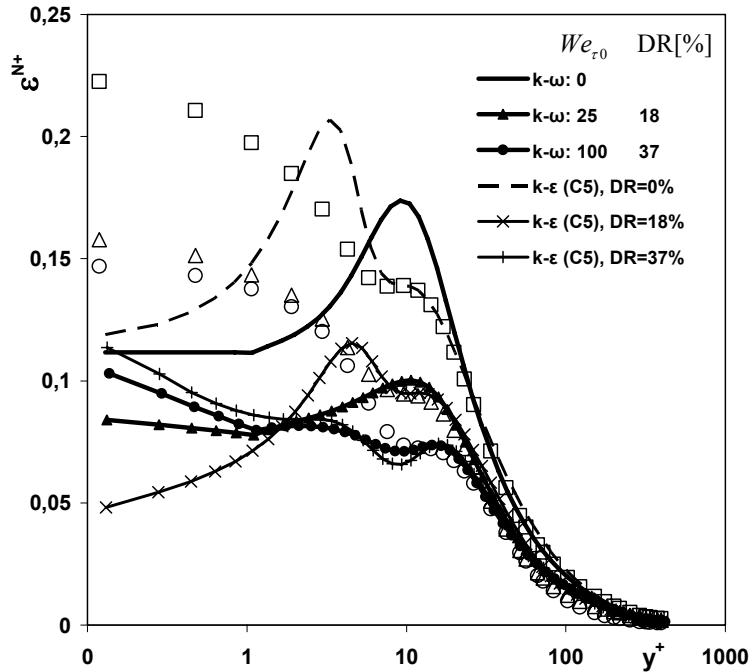


Fig. 58. Comparison between the kinetic energy dissipation predictions (lines with close symbols) of the present model, $k\text{-}\varepsilon$ model of chapter 5 (C5) and DNS data (open symbols), for turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$: $\square$ Newtonian, Δ DR=18% and $\circ$ DR=37%.

The behaviour of the rate of dissipation of k with We_{τ_0} is being well captured by the model in the log law, the buffer layers and especially near to the wall, as shown in **Fig. 59**. The saturation of ε^{N+} at large We_{τ_0} is also well captured: we observe that at large Weissenberg numbers ($We_{\tau_0}=100$ and 153) the profiles of ε^{N+} are essentially the same.

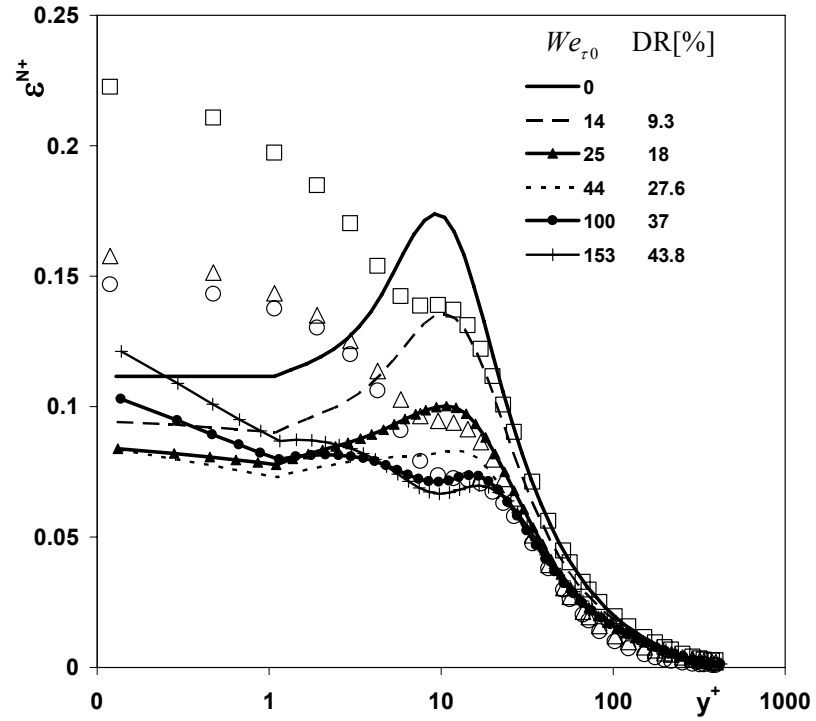
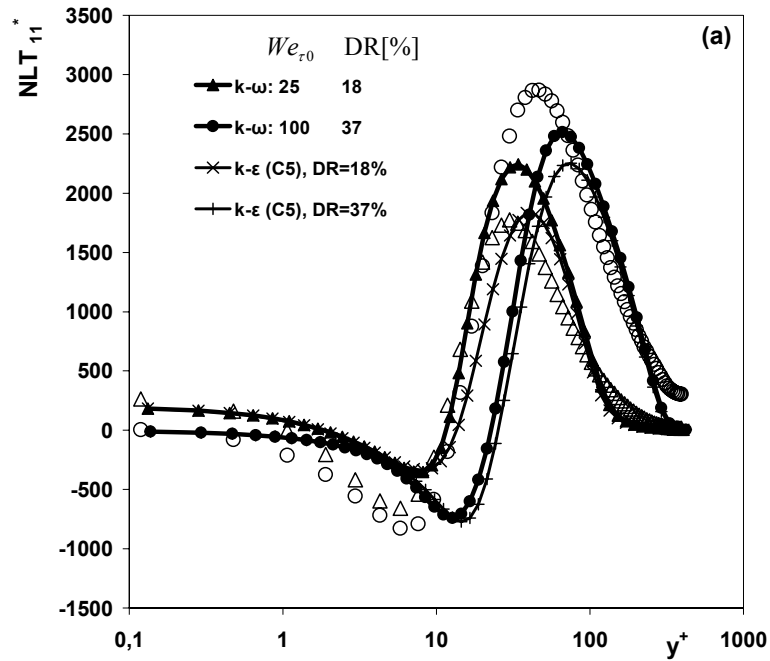
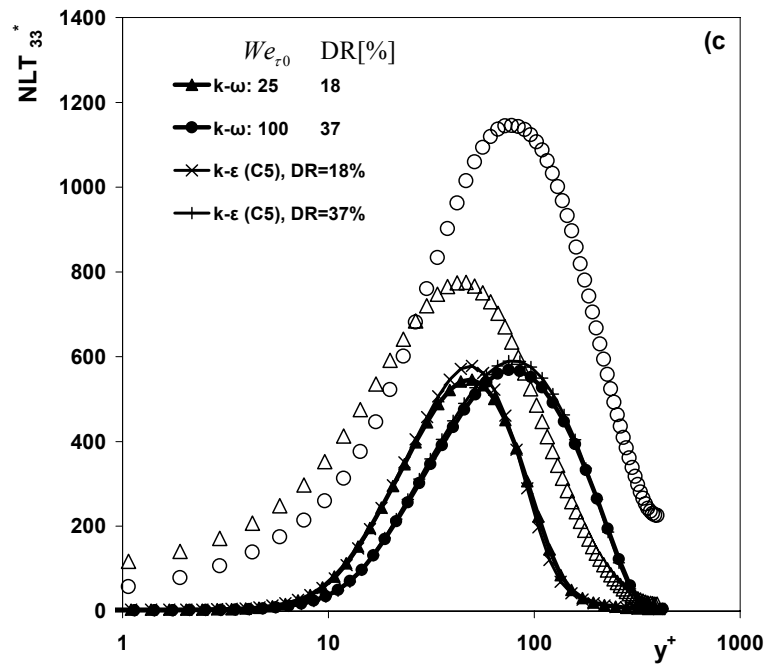
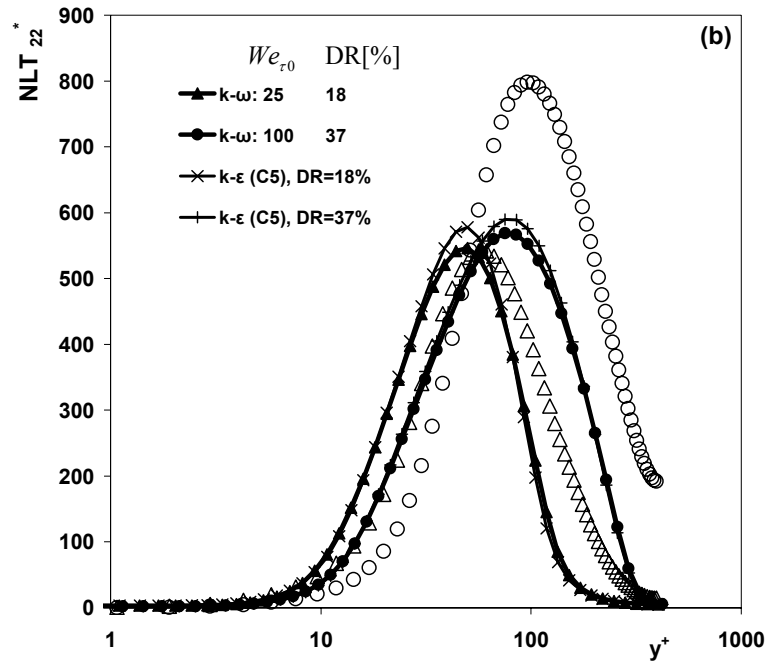


Fig. 59. Comparison between the predictions (lines with close symbols) and DNS data (open symbols) of ε^{N+} for turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$ and different Weissenberg numbers: Δ DR= 18% and $\circ$ DR= 37%.

Fig. 60 (a)-(e) compares the predictions of NLT_{ij} for both the k - ω and k - ε models for DR=18% and 37%. For each component the predictions by the two models are similar, with the former model showing better predictions than the latter for NLT_{11} and the trace NLT_{kk} and the other way for the other components. The main features of these predictions are the increase of the peak value of NLT_{ij} with DR and its shift away from

the wall, which becomes more intense in the log-zone. For all normal components there is an underprediction of the peak value for 37% DR, whereas for the shear component there is an overprediction. NLT_{22} (or NLT_{yy}) is the component of the NLT_{ij} tensor that has more impact in the calculation of the conformation tensor, except on C_{33} component and its variation with We_{τ_0} is shown in **Fig. 61 (a)**. There is a rapid increase at low DR ($DR < 30\%$), after which the maximum value of NLT_{22} decreases slowly to stabilize at high DR, as at $DR = 37\%$. The behaviour of the invariant NLT_{kk} is plotted in **Fig. 61 (b)** and shows also a rapid increase with We_{τ_0} at the low DR regime, followed by a slow increase and saturation at the high DR regime. Since the streamwise normal component is the main contribution to NLT_{kk} , NLT_{11} has a similar behavior and is not shown here for compactness.





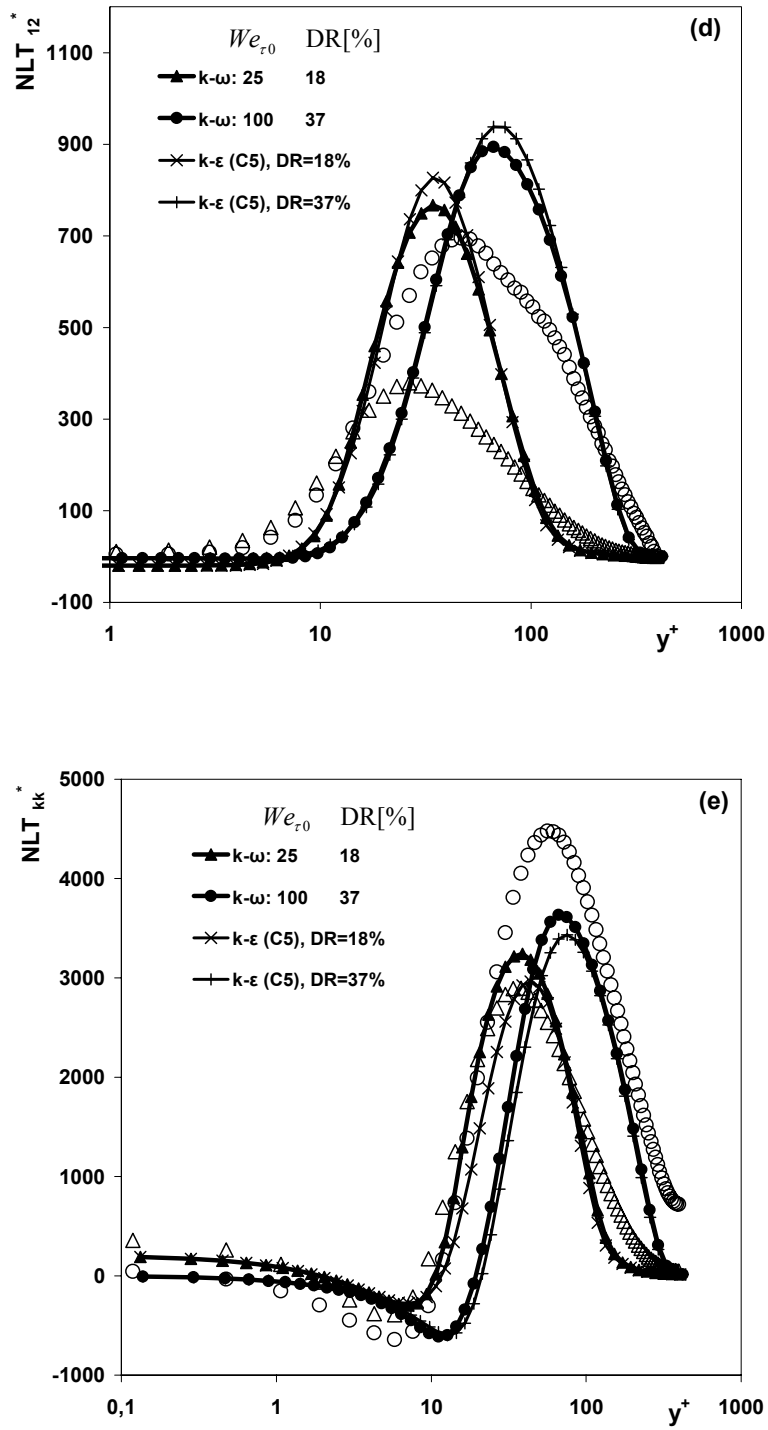


Fig. 60. Comparison between the NLT_{ij} model predictions (lines with close symbols) of the present model, $k-\epsilon$ model of chapter 5 (C5) and DNS data (Δ DR=18% and $\circ$ DR=37%), for turbulent channel flow with $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$: a) NLT_{11}^* ; b) NLT_{22}^* ; c) NLT_{33}^* ; d) NLT_{12}^* ; e) NLT_{kk}^* .

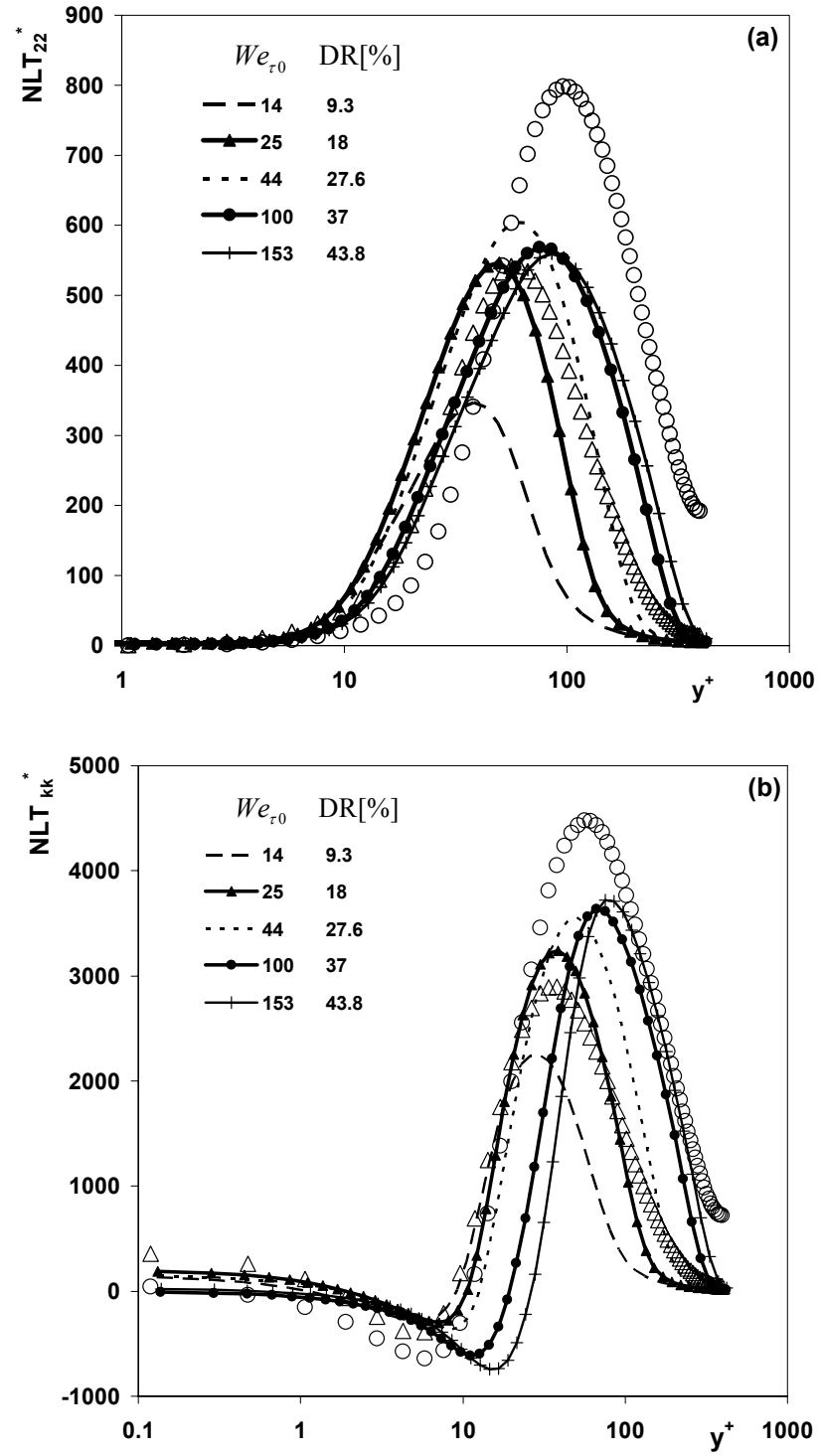


Fig. 61. Comparison between the predictions (lines with close symbols) and DNS data (open symbols) of NLT_{kk} for turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$ and different Weissenberg numbers: Δ DR= 18% and $\circ$ DR= 37%.

The predictions of the viscoelastic stress work in **Fig. 62** show higher values for the $k-\omega$ model than for the $k-\varepsilon$. This leads to a slight overprediction of ε^V for 37% DR, whereas at low DR both turbulence models continue to under-predict the DNS data. The variation of the viscoelastic stress work with We_{τ_0} is plotted in **Fig. 63** and exhibits a rapid increase at drag reductions, reaching a maximum at $We_{\tau_0} = 25$, (corresponds to DR= 18%), after which ε^{V+} decreases and its peak value moves away from the wall. In contrast, the DNS data shows that ε^{V+} always increases with We_{τ_0} . It is also possible to visualize a saturation effect, the reduction of the peak value variation as we increase DR from to 37% to 43.8%, which shows an asymptotic variation towards the maximum drag reduction.

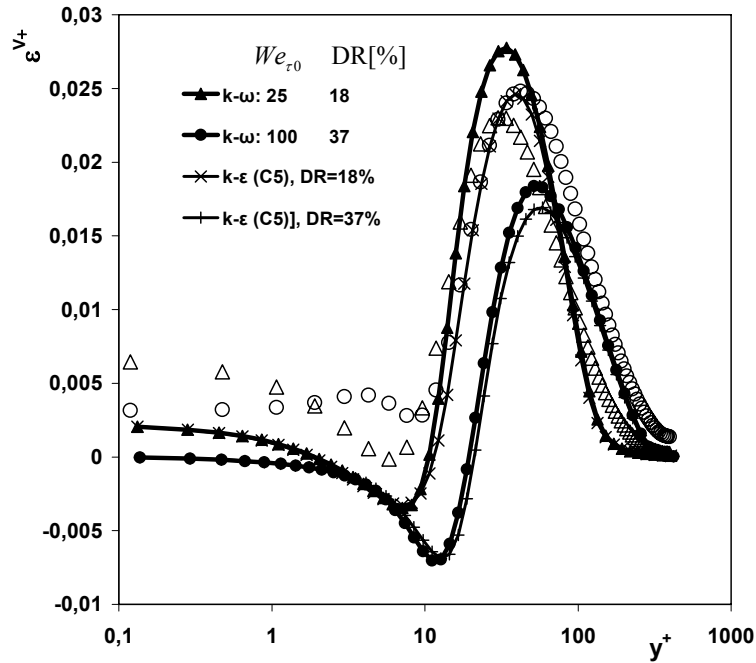


Fig. 62. Comparison between the viscoelastic dissipation model predictions (lines with close symbols) of the present model, $k-\varepsilon$ model of chapter 5 (C5) and DNS data (open symbols), for turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$: Δ DR=18% and $\circ$ DR=37%.

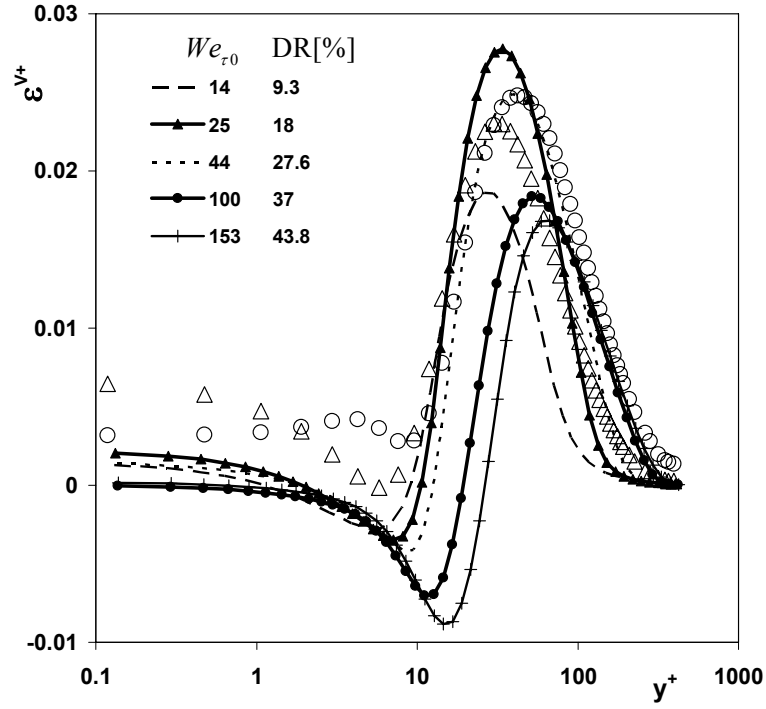
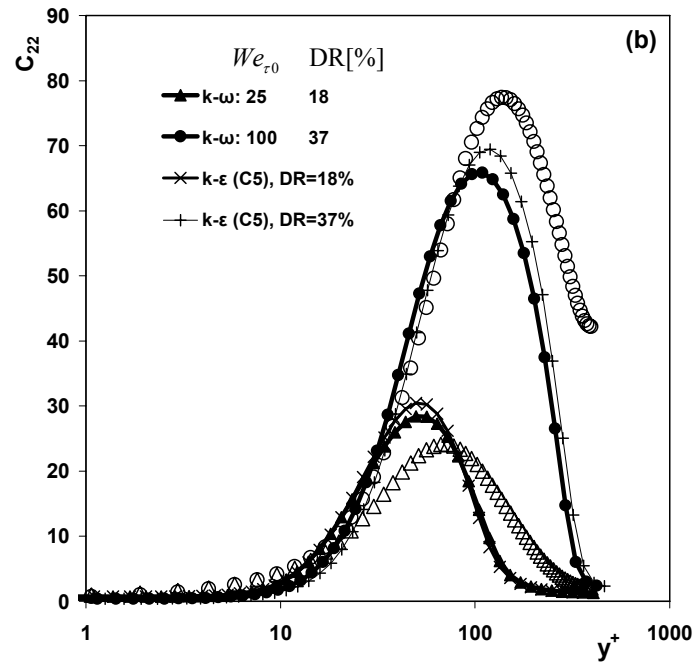
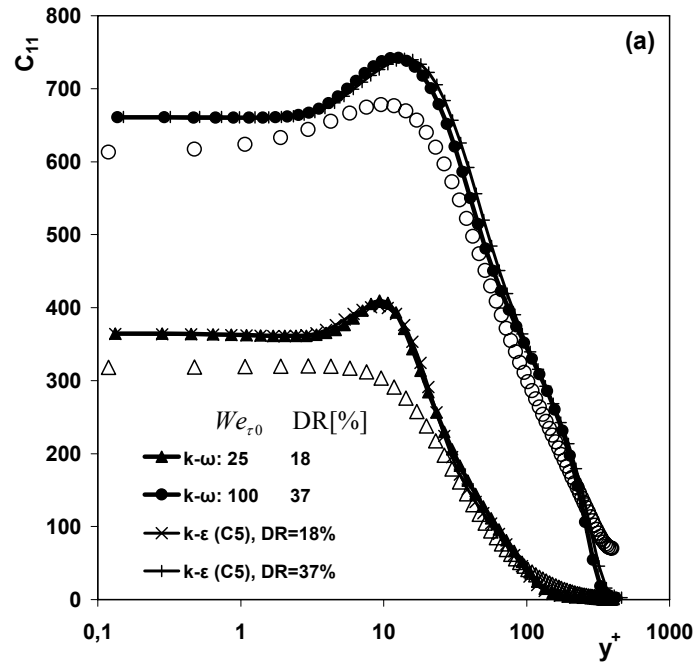
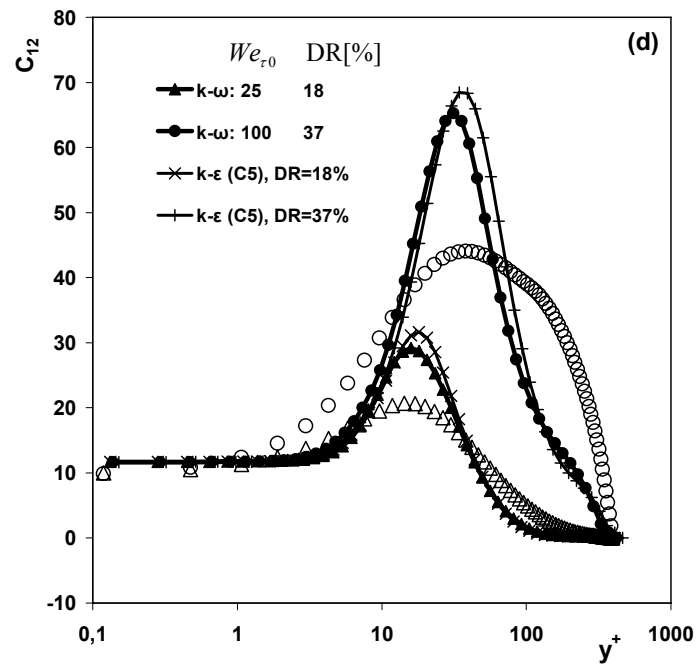
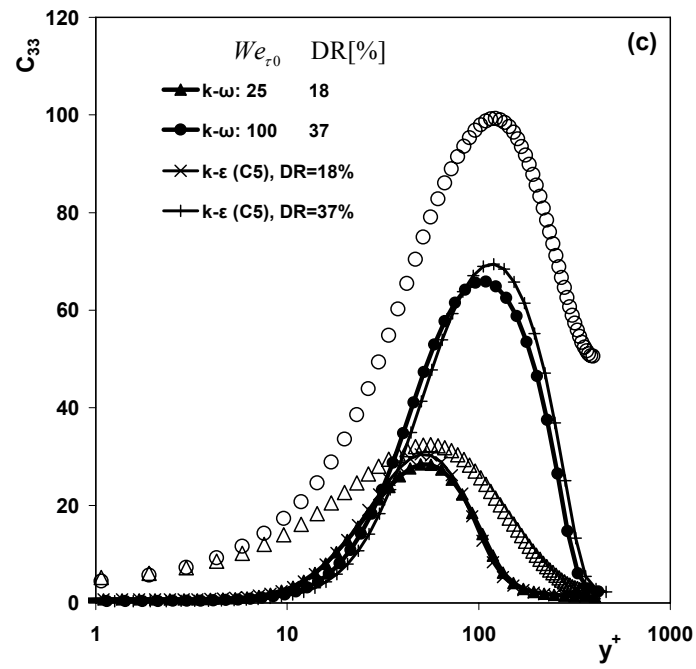


Fig. 63. Comparison between the predictions (lines with close symbols) and DNS data (open symbols) of ε^{V+} for turbulent channel flow with $Re_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$ and different Weissenberg numbers: Δ DR= 18% and $\circ$ DR= 37%.

The predictions of the NLT_{ij} tensor have a direct impact on the prediction of the conformation tensor according to Eq. (201), as can be observed in **Fig. 64 (a)-(d)**. The predictions of all components are fair except for C_{33} where there is a large deficit relative to the DNS data as a consequence of a deficit in the prediction of NLT_{33} . Again, we suspect this to be essentially a consequence of invoking turbulence isotropy to develop several closures within the model. An overprediction is observed for C_{11} , next to the wall, at 18% DR, which decreases when DR increases to 37%. For the C_{12} component there are also large discrepancies, with an overprediction next to the wall and a underprediction away from wall, which is stronger at large DR. The predictions of C_{22} are fair due to the correct prediction of NLT_{22} , but deficiencies observed with NLT_{22} are carried over to C_{22} , for example the underprediction of the maximum value of NLT_{22} is also detected in C_{22} . The behavior in terms of the trace C_{kk} can be assessed indirectly

through function $f(C_{kk})$ plotted in **Fig. 64 (e)**; there is an overprediction of the maximum value of $f(C_{kk})$ at both DR= 18% and 37%.





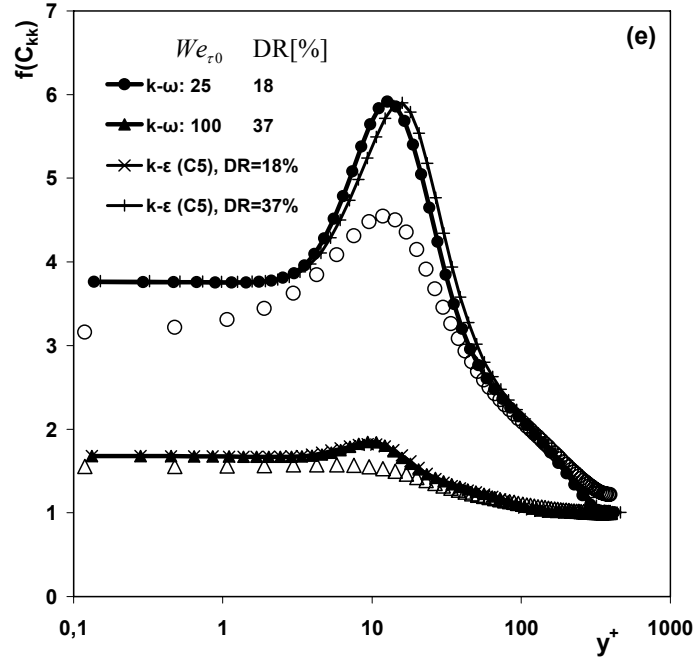


Fig. 64. Comparison between the conformation tensor predictions (lines with close symbols) of the present model, $k-\epsilon$ model of chapter 5 (C5) and DNS data (Δ DR=18% and $\circ$ DR=37%), for turbulent channel flow with $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$: .

The transverse distribution of the three shear stresses for DR= 18% and 37% is observed in **Fig. 65** and compared with the corresponding DNS data. The solvent stress is always well predicted and this is a consequence of the correct prediction of the velocity profile. The reduction of the Reynolds stress with DR and the simultaneously presence of a polymer stress is clear, but close to the wall there is an under-prediction of $-\overline{\rho uv}$ and an over-prediction of τ_{xy}^p , whereas away from the wall the opposite occurs. The polymer shear stress is calculated from the shear component of the conformation tensor and these differences are due to the corresponding predictions of C_{xy} . Then, the Reynolds shear stress must readjust in order for the total shear stress distribution to follow the straight line inherent to a fully-developed channel flow.

Ultimately, the evolution of the conformation and polymer stress tensors are based on the model used for NLT_{ij} . Since the closure used for this quantity was the same in both this turbulence model and in the $k-\epsilon$ model of chapter 5, it is no surprise that the stress distributions are essentially identical.

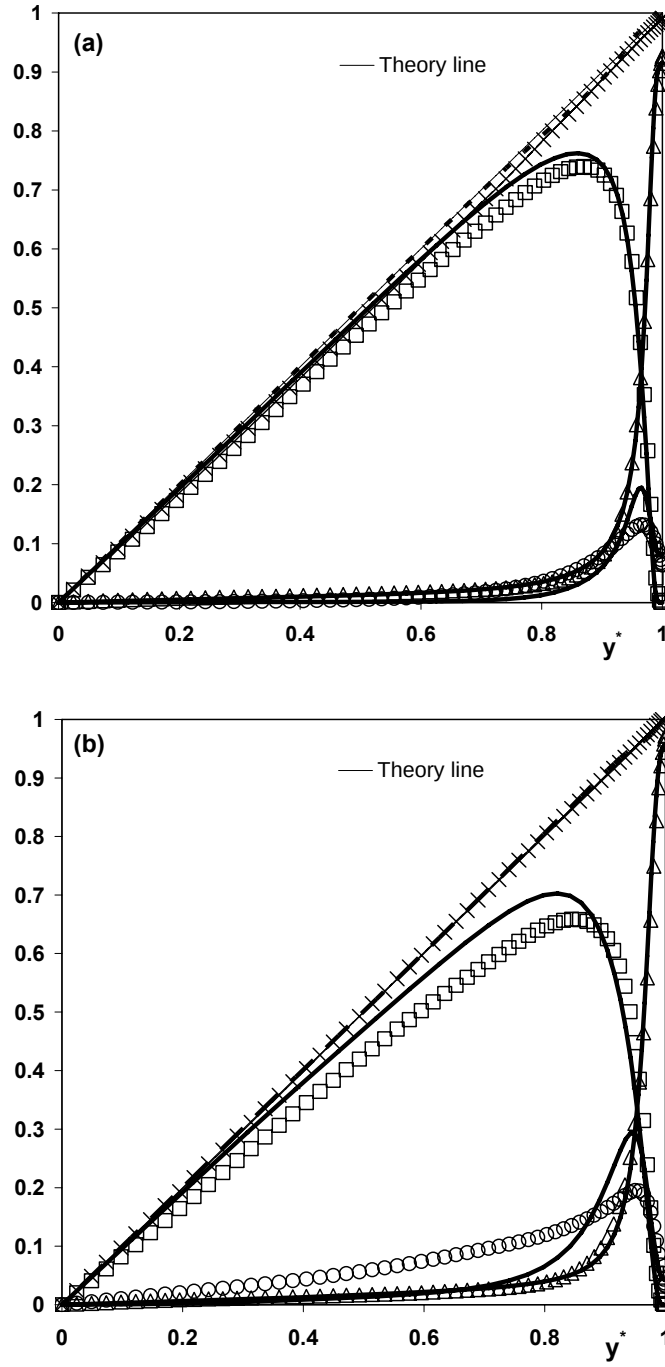


Fig. 65. Comparison between the predictions (lines) and DNS data (open symbols) for normalized shear stresses (τ_N^+ , τ_p^+ , $-\overline{u_1 u_2}^+$) in turbulent channel flow with $\text{Re}_{\tau_0} = 395$, $L^2 = 900$ and $\beta = 0.9$. (Δ and line) τ_N^+ , ($\circ$ and line) τ_p^+ , ($\square$ and line) $-\overline{u_1 u_2}^+$; ($\times$ and dashed line) sum of stresses: (a) DR=18%; (b) DR= 37%.

6.7 Conclusions

A k - ω turbulence model was developed for viscoelastic fluids described by the FENE-P rheological constitutive equation. The closures needed for the viscoelastic terms in the transport equations of k and ω were essentially identical to those used by the k - ε model of chapter 5 in the context of a low Reynolds number k - ε model, with a couple of exceptions. The advantage of this k - ω model in relation to the earlier k - ε model of chapter 5 is that it uses one less damping functions, since the specific rate of dissipation is better behaved near walls than ε . Generally speaking, the predictions by this k - ω turbulence model were better than those of chapter 5, but the main deficiency regarding the under-prediction of k remained an unsolved problem. This deficiency limits the application of this turbulence model to drag reductions not exceeding about 50%. Outside these conditions, the model severely under-predicts the turbulent kinetic energy. We believe this is a limitation of first order turbulence models associated with the assumption of turbulence isotropy, because there is an incompatibility between the variations of eddy viscosity and k with drag reduction: k increases and the eddy viscosity decreases at low DR, whereas this breed of turbulence models implies $\nu_T \propto k$. The solution of this deficiency requires closures that do not rely on turbulence isotropy, and more specifically that do not couple directly the eddy viscosity to the turbulent kinetic energy. This decoupling can be achieved through either the use of second order turbulence models or through first order models where the eddy viscosity closure is linked directly to a measure of turbulence that decreases with drag reduction, such as the normal transverse Reynolds stress. An example here is the k - ε ν^2 - f model of Iaccarino et al. [49].

The k - ω turbulence model here developed was also able to predict well the variation of the DR with Weissenberg number as given by the expression of Li et al. [39], which was developed from a large set of DNS data.

This work also showed that the various viscoelastic closures developed in the context of the k - ε model of chapter 5 can be used with minor modifications in the context of other first-order turbulence models.

Chapter 7

Conclusions and suggestions for future work

7.1 Conclusions

In this thesis new RANS turbulence models were developed for viscoelastic fluids described by two types of constitutive equation. More specifically, for a modified version of the generalized Newtonian constitutive equation (MGNF) a Reynolds stress model was developed. Subsequently, and in order to address the shortcomings of the generalised Newtonian constitutive equation, two other turbulence models were developed for a truly viscoelastic rheological constitutive equation, the FENE-P equation. These models are of first order type and are based on the eddy viscosity concept. They are a $k-\varepsilon$ and a $k-\omega$ turbulence model.

The performance of the two sets of turbulence models for viscoelastic fluids was assessed differently. For the MGNF model experimental data for turbulent pipe flow of four different dilute solutions was used, which includes rheology data obtained in steady and small oscillatory shear flow as well as in an extensional type of flow, the opposed jet rheometer. For the FENE-P fluid models two sets of DNS data for fully developed channel flow, corresponding to low and high drag reduction regimes, were used. These data sets were for $Re_{\tau 0} = 395$, $L^2 = 900$ and $\beta = 0.9$ for $We_{\tau 0} = 25$ (drag reduction of 18%) and $We_{\tau 0} = 100$ (drag reduction of 37%), respectively, in turbulent channel flow.

Generally speaking all turbulence models showed good predictions against the reference data. Specifically, the second order Reynolds stress model, which is better at predicting flows with recirculation, streamline curvature and other complex features than the first order models, predicted accurately the flow characteristics of viscoelastic fluids in turbulent pipe flow except for the normal Reynolds stresses for the 0.125% PAA, which were not so successful than those by the anisotropic $k-\varepsilon$ model of Resende et al. [3] also developed for MGNF fluids. However, the second order closure will certainly show its advantages when used in a complex geometry flow exhibiting the above features.

The two models for FENE-P fluids represent a significant improvement over the previous $k-\varepsilon$ model of Pinho et al. [4], because of several modifications in relevant parts

of the model. The new k - ε model has the capacity to accurately predict low and high regimes of drag reduction, in turbulent channel flow. Several viscoelastic closures were developed, in particular a new closure for the Reynolds-average non-linear term of the polymer conformation equation (denoted NLT_{ij}), the eddy viscosity saw the inclusion of a direct polymer contribution and a new viscoelastic destruction term was also included in the transport equation of the rate of dissipation of k by the Newtonian solvent. An extra contribution to the viscoelastic turbulent diffusion, previously neglected, was also considered in addition to other smaller improvements as in the viscoelastic stress work model and the extension to the high drag reduction regime.

Using the viscoelastic closures developed in chapter 5, in the context of a low Reynolds number k - ε turbulence model, a k - ω turbulence model was also developed for viscoelastic fluids described by the FENE-P model. The predictions of all quantities have a similar quality to those by the k - ε model, without the need to modify parameters or damping functions showing that the viscoelastic theories invoked to develop the partial closures of the full model captured the essential physics. So, it came as no surprise that in the end the k - ω turbulence model also underpredicted the turbulent kinetic energy and kept the model limit within 50% of the drag reduction, showing that turbulence isotropy assumptions can be insufficient to predict with accuracy viscoelastic fluids in turbulent flows, as previously suspected.

Both turbulent models for the FENE-P fluid were able to capture the essential effects of viscoelastic drag reduction, such as the increase of the maximum value of the conformation and NLT_{ij} tensors and their shift away from the wall with drag reduction. Although the velocity profile was always well predicted, the turbulent kinetic energy showed a decrease of its peak value with drag reduction in contrast to DNS results. This deficiency limits the turbulent model to 50% of DR and we suspect that this problem is associated with the assumptions of turbulence isotropy inherent to this type of turbulence models, something to be corrected in the near future.

7.2 Suggestions for future work

The development of RANS turbulence models for viscoelastic flows is indeed still in its infancy and much work needs to be done. Generally speaking none of the models present in the literature and in this thesis have been tested in flows other than the fully developed pipe or channel flow, so it is really necessary to extend their use to other canonical flows such as free jets, mixing layers or flows with recirculation, as the backward facing step or sudden expansion flows . This means that the new turbulence models must be implemented in more general computational codes and this applies to both models developed in the framework of the MGNF and the FENE-P constitutive equations. Probably, this will also require experimental and DNS data for those flows, which in most cases is unavailable (for the same MGNF fluids there are data sets for turbulent flow across sudden expansions).

Even for the fully-developed channel flow the developed turbulence models for FENE-P fluids need further improvements to extend their applicability to the higher range of high drag reduction as well as the maximum drag reduction, in addition to the capture of the effects of β and L^2 .

Nowadays Large Eddy Simulation (LES) models are ubiquitous for Newtonian fluids, but there is scarcely a good model for viscoelastic fluids. This is clearly an area of required research and the first step here will be the processing of existing or new DNS data for fully-developed channel flow for the purpose of developing the first reliable LES models.

Another area of future work is obviously the extension of RANS or LES type models to the prediction of heat transfer. At this moment we can reliably state that no turbulence models exist for any scalar fluxes for any type of viscoelastic fluids.

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