PIPE FLOW OF MULTIMODE PTT FLUIDS

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Abstract. *In this work a semi analytical procedure for the calculation for fully developed pipe flow of a multimode formulation based on the Simplified Phan Thien-Tanner rheology is presented. Both the exponential and the linear versions of the multimode SPTT model will be analyzed. As will be shown, the proposed solution partially relies on the corresponding single-mode solution. The methodology described can be extended to other fluids or flow conditions.*

Keywords*: Multimode model, viscoelasticity, pipe flow, PTT model.*

1. Introduction

Nonlinear differential constitutive equations are increasingly being used to describe the rheology of viscoelastic fluids and in solving fluid mechanics problems of relevance to polymer melts and solutions. Analytical solutions can be obtained with simple constitutive equations or under rather simplifying flow conditions where such assumptions as symmetry or fully-developed conditions lead to integrable expressions. As a consequence, most of the studies concern single-mode models. Many examples abound, but here we just give a few: Beris *et al.* (1983) for concentric and eccentric annular flow of Maxwell, White- Metzner and CEF fluids, Cruz and Pinho (2003) for skewed Poiseuille-Couette flows of PTT fluids, Oliveira (2002) for pipe and channel flow of a FENE-P fluid, pipe and channel flow of Giesekus fluid, Schleiniger and Weinacht (1991) or the various works of Oliveira *et al.* (2004) and Coelho *et al.* (2003 and 2004), on isothermal and non-isothermal pipe and channel flow of PTT and FENE-P fluids (Oliveira *et al.*, 2004 and Oliveira and Pinho, 2000), and lately of Hashemabadi (2003a and 2003b).

However, very often the rheology of polymer melts and concentrated polymer solutions is more complex than predicted by such single mode models, and multimode models become necessary for their adequate description.

In this paper we develop semi-analytical solutions for fully-developed pipe and channel flows of multimode models based on the Phan-Thien - Tanner rheology, henceforth called PTT model. As will be shown, this partially relies on the corresponding single-mode solution and consequently we predict that the methodology described can probably be extended to other fluids or flow conditions.

In the next section we present the governing equations necessary to solve for the pipe and channel flow of the multimode linear and exponential PTT models and describe in the following section the method to obtain the corresponding solutions. This is followed by a presentation and discussion of results that shows the application of the method developed and illustrates the differences between a single mode and a multimode solution.

2. Governing Equations

For fully-developed pipe flow the momentum equation in the *z*-direction simplifies to

$$\frac{1}{r}\frac{d}{dr}\left(r\tau_{rz,T}\right)-\frac{dp}{dz}=0 \tag{1}$$

where *r* and *z* designate the radial and axial coordinate, *p* is the pressure and τ_{rz} is the *rz* stress component. Subscript T indicates that the total *rz* extra stress component is being considered, *i.e.*, in a multimode model the total *ij* extra stress component is the sum of the N individual polymer ($\tau_{ij,I}$) and one solvent ($\tau_{ij,S}$) contributions,

$$\tau_{ij,T}=\sum_{I=1}^{N}\tau_{ij,I}+\tau_{ij,S} \quad . \tag{2}$$

The use of a solvent contribution in combination with a PTT constitutive equation is required when dealing with some polymer solutions.

The fluid dynamical solution is unique and is well characterized by a velocity profile in the z-direction (u), the radial and tangential velocities being null.

The multimode constitutive equation is given by Eq. (2), with each mode $\tau_{ij,I}$ obeying the PTT equation of Phan-Thien and Tanner (1977). Here, the simplified version of the PTT model with a zero second normal stress difference is being considered ($\xi = 0$), and it is given by Eq. (3) for each mode I.

$$f\left(\tau_{kk,I}\right)\tau_{ij,I} + \lambda_I \overset{\nabla}{\tau}_{ij,I} = 2\eta_I D_{ij} \tag{3}$$

The stress coefficient function $f(\tau_{kk})$ takes either the exponential form in Eq. (4) or its linearised form given in Eq. (5) form,

$$f\left(\tau_{kk,I}\right) = \exp\left(\frac{\lambda_I \varepsilon_I}{\eta_I}\tau_{kk,I}\right) \tag{4}$$

$$f\left(\tau_{kk,I}\right) = 1 + \frac{\lambda_I \varepsilon_I}{\eta_I}\tau_{kk,I} \tag{5}$$

Parameters λ, η and ε are the relaxation time, the viscosity coefficient and a parameter limiting the extensional viscosity, respectively. D_{ij} is the rate of deformation tensor defined in Eq. (6) and $\overset{\nabla}{\tau}_{ij}$ represents Oldroyd's upper convected derivative defined in Eq. (7).

$$D_{ij} = \frac{\left(\nabla u\right)_{ij} + \left(\nabla u\right)_{ij}^T}{2} \tag{6}$$

$$\overset{\nabla}{\tau}_{ij} = \frac{\partial \tau_{ij}}{\partial t} + u_k \frac{\partial \tau_{ij}}{\partial x_k} - \tau_{ik}\frac{\partial u_j}{\partial x_k} - \tau_{kj}\frac{\partial u_i}{\partial x_k}\,. \tag{7}$$

The Newtonian solvent contribution is

$$\tau_{ij,S} = 2\eta_s D_{ij} \tag{8}$$

3. Method of Solution

For fully-developed pipe flow the rheological equation for each polymer mode simplifies to the following set, with Eq. (9c) accounting for the solvent stress contribution

$$\tau_{rz,I} = \frac{\eta_I}{f\left(\tau_{kk,I}\right)}\frac{\partial u}{\partial r} \tag{9a}$$

$$\tau_{zz,I} = \frac{2\lambda_I \eta_I}{f\left(\tau_{kk,I}\right)^2}\left(\frac{\partial u}{\partial r}\right)^2 \tag{9b}$$

$$\tau_{rz,S} = \eta_s \frac{\partial u}{\partial r} \tag{9c}$$

These equations are identical to the equations for a single mode, regardless of the stress function $f\left(\tau_{kk,I}\right)$, except that the shear rate is the same for all modes. Inspection of the equation for τ_{rr} shows $\tau_{rr,I} = 0$ and $\tau_{\theta\theta,I} = 0$ due to symmetry. Note the introduction of subscript I to emphasize that we are dealing here with a multimode model. As for the single mode solution of Oliveira and Pinho (1999), both non-zero stresses are related via

$$\tau_{rz,I} = \sqrt{\frac{\eta_I \tau_{zz,I}}{2\lambda_I}} \tag{10}$$

In agreement with the single mode solution of Oliveira and Pinho (1999), the solution for the multimode fluid involves the coupling between the normal and shear stresses, but it is possible to relate the velocity and pressure gradients only with the normal stress via back-substitution. Consideration of a multimode model leads to a more complex relationship which requires a numerical solution, but conceptually the procedure is identical to that for a single mode model.

We will rewrite any modal normal stress as a function of a single normal stress which we will refer to as the principal stress $\tau_{zz,p}$. For convenience, the principal normal stress will always be the normal stress of the first mode ($\tau_{zz,1}$). Since the velocity profile is the same for all modes, Eq. (9b) gives the relationship between the principal stress and the normal stress for a mode written in the form of Eq. (11), thus defining what is called function ϕ_p. For compactness, $f_p \equiv f\left(\tau_{zz,p}\right)$ and $f_I \equiv f\left(\tau_{zz,I}\right)$.

$$\phi_p = \frac{\tau_{zz,p} f_p^2}{\lambda_p \eta_p} = \frac{\tau_{zz,I} f_I^2}{\lambda_I \eta_I} \tag{11}$$

Henceforth, Eq. (11) is used to solve for $\tau_{zz,1}$ as a function of ϕ_p. Then, from the relationship between the shear and normal stresses, Eq. (10), we use the momentum equation, Eq. (1) and Eq. (9b) to arrive at integrable expressions for the principal normal stress and the velocity gradient, respectively. The integration of these final equations to determine $\tau_{zz,p}$ and *u* must be carried out numerically. The solutions for the linearized and exponential PTT models are slightly different and are presented separately, in the next section.

3.1. Linear PTT Model

For the linear PTT model, Eq. (11) is a cubic equation in $\tau_{zz,I}$ written as

$$\tau_{zz,I}^3 + a_1 \tau_{zz,I}^2 + a_2 \tau_{zz,I} + a_3 = 0 \tag{12}$$

with coefficients

$$a_1 = \frac{2\eta_I}{\varepsilon_I \lambda_I}\ ; \quad a_2 = \frac{\eta_I^2}{\varepsilon_I^2 \lambda_I^2}\ ; \quad a_3 = -\frac{\eta_I^3}{\varepsilon_I^2 \lambda_I}\phi_p \tag{13}$$

The real solution of this cubic equation is given by

$$\tau_{zz,I} = \sqrt[3]{R_I + \sqrt{Q_I^3 + R_I^2}} + \sqrt[3]{R_I - \sqrt{Q_I^3 + R_I^2}} - \frac{1}{3}a_1 \tag{14}$$

with

$$R_I = \frac{9a_1 a_2 - 27a_3 - 2a_1^3}{54} = \frac{1}{2}\frac{\eta_I^3}{\lambda_I \varepsilon_I^2}\phi_p + \frac{1}{27}\frac{\eta_I^3}{\lambda_I^3 \varepsilon_I^3} \tag{15a}$$

$$Q_I = \frac{3a_2 - a_1^2}{9} = -\frac{1}{9}\frac{\eta_I^2}{\lambda_I^2 \varepsilon_I^2} \tag{15b}$$

The radial variation of $\tau_{zz,p}$ is obtained after integration of the momentum equation, Eq. (1) into

$$\frac{dp}{dz}\frac{r}{2} = \sum_{I=1}^{N} \tau_{ij,I} + \tau_{ij,S} \tag{16}$$

and using Eqs. (10) and (11), i.e.

$$\frac{dp}{dz}\frac{r}{2} = \sqrt{\frac{\eta_p \tau_{zz,p}}{2\lambda_p}} + \sum_{I=2}^{N} \sqrt{\frac{\eta_I}{2\lambda_I}\tau_{zz,I}} + \eta_s \frac{du}{dr} \tag{17}$$

where the velocity gradient is calculated from Eq. (9b) with the principal normal stress

$$\frac{du}{dr} = \sqrt{\frac{\tau_{zz,p}}{2\lambda_p \eta_p}}\left(1 + \frac{\varepsilon_p \lambda_p}{\eta_p}\tau_{zz,p}\right) \tag{18}$$

The numerical solution of Eq. (17) provides the relationship between $\tau_{zz,p}$ and the pipe radius, whereas the velocity profile is obtained by numerical integration of Eq. (18).

3.2. Exponential PTT Model

For the exponential PTT model one cannot obtain an explicit expression for $\tau_{zz,I}$ and an iterative process is required. From Eq. (11)

$$\phi_p = \frac{\tau_{zz,p}}{\lambda_p \eta_p}\exp\left(\frac{\varepsilon_p \lambda_p}{\eta_p} 2\tau_{zz,p}\right) = \frac{\tau_{zz,I}}{\lambda_I \eta_I}\exp\left(\frac{\varepsilon_I \lambda_I}{\eta_I} 2\tau_{zz,I}\right) \tag{19}$$

and now it is a matter of rewriting this equation as

$$\tau_{ij,I}^{(n)} = \tau_{zz,p}\frac{\lambda_I \eta_I}{\lambda_p \eta_p}\exp\left(2\frac{\varepsilon_p \lambda_p}{\eta_p}\tau_{zz,p} - 2\frac{\varepsilon_I \lambda_I}{\eta_I}\tau_{ij,I}^{(n-1)}\right) \tag{20}$$

where the superscripts (n) and (n-1) designate the level of iteration. As a first guess of $\tau_{ij,I}$, we use the linearised version of Eq. (14).

Henceforth the process is similar to that for the linear PTT, i.e., Eq. (17) gives the principal normal stress as a function of the pipe radius, with the adequate modifications of the stress coefficient, and the following equation provides the velocity gradient.

$$\frac{du}{dr} = \sqrt{\frac{\tau_{zz,p}}{2\lambda_p \eta_p}}\exp\left(\frac{\varepsilon_p \lambda_p}{\eta_p}\tau_{zz,p}\right) \tag{21}$$

The numerical integration of Eq. (21) provides the velocity profile for a given pressure gradient.

4. Results and Discussion

To evaluate this procedure we calculated the pipe flow for a multimode PTT fluid. The fluid chosen was a modification of the shear-thinning solution of 500 ppm of polyacrilamide in a glycerin-water mixture (hence called PAA500) characterised by Alves et al (2004). Alves et al (2003) obtained the linear viscoelastic spectrum for PAA500 fluid and predicted well its steady shear viscosity using a four mode linear PTT model with constant $\varepsilon = 0.02$ and $\xi = 0.04$ plus a Newtonian solvent. The viscoelastic spectrum is listed in Table 1, but for our solution we have set the parameter ξ to zero (simplified PTT model). We refer to this as Fluid 1, and we also calculated the pipe flow solution for Fluid 1b, which is identical to Fluid 1 except for the absence of the Newtonian solvent.

Fluid 1b allowed comparison of its pipe flow solution with that for the single mode PTT fluid having the same linear viscoelastic spectrum, and for which Oliveira and Pinho (1999) provided an analytical solution. To obtain the parameters η and λ of the single mode PTT model having the same linear viscoelastic spectrum of the multimode fluid, the following equations are used

$$\eta = \eta_{solvent} + \sum_{k \neq solvent} \eta_k \tag{22}$$

$$\lambda = \frac{\sum_{k \neq solvent} \lambda_k \eta_k}{\sum_{k \neq solvent} \eta_k} \tag{23}$$

which gave λ = 20.48 s and η= 4.07 Pa.s for Fluid 1 and λ = 20.48 s and 3.8 Pa.s for Fluid 1b.

Table 1 - Linear viscoelastic spectrum for Fluid 1 (PAA500) (from Alves *et al.*, 2003)

Mode	λ_k [s]	η_k [Pa.s]
1	30	2.5
2	3	0.9
3	0.3	0.3
4	0.03	0.1
Solvent	-	0.27

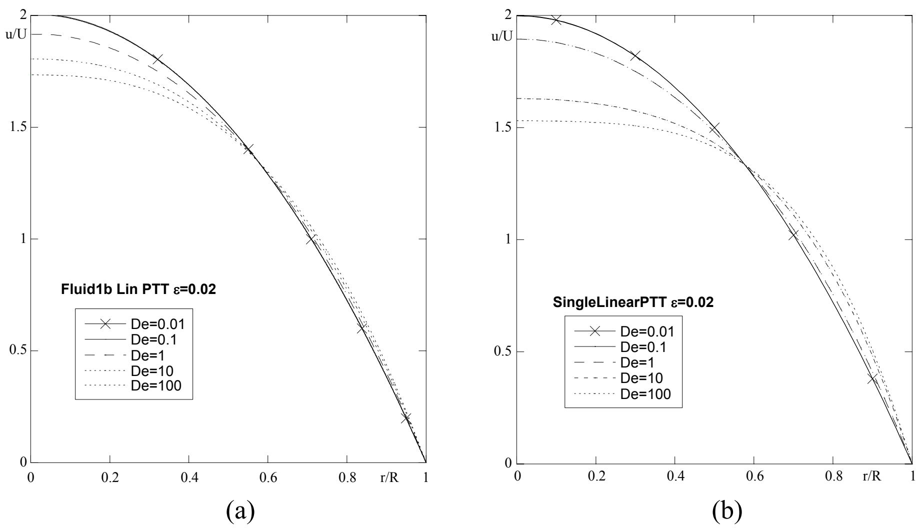


Figure 1. Effect of Deborah number on the normalized velocity profile for simplified PTT model with linear stress coefficient and $\varepsilon = 0.02$ (Fluid 1b): (a) 4 mode model; (b) Equivalent single mode model.

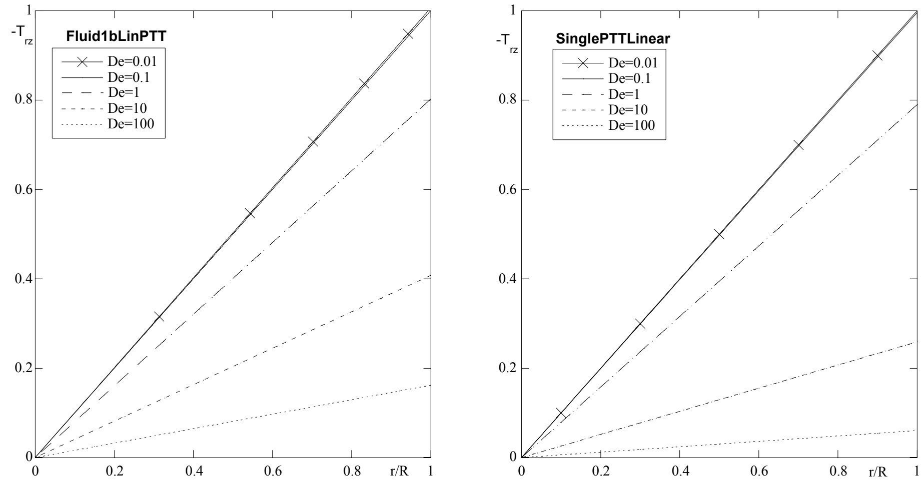
The Deborah number $De=\lambda U/D$ is based on the pipe diameter.

In Fig 1 we compare the velocity profiles for the 4-mode Fluid 1b with the equivalent single-mode solution. It is known from Oliveira and Pinho (1999) that the linear PTT model has a shear-thinning viscosity and that the flatness of the velocity profile in the centre of the pipe increases with ε and the flow Deborah number. The equivalent PTT model however, has an overall more intense degree of shear-thinning as is reflected in the larger variations of the velocity profile. In both cases, and for this small value of ε, the flows for $De \leq 0.1$ are basically Newtonian. This is also clear from the plots of normalized shear stress shown in Fig 2. The stresses are normalized as

$$T_{rz} = \frac{\tau_{rz}}{4\eta \frac{U}{R}} \tag{24}$$

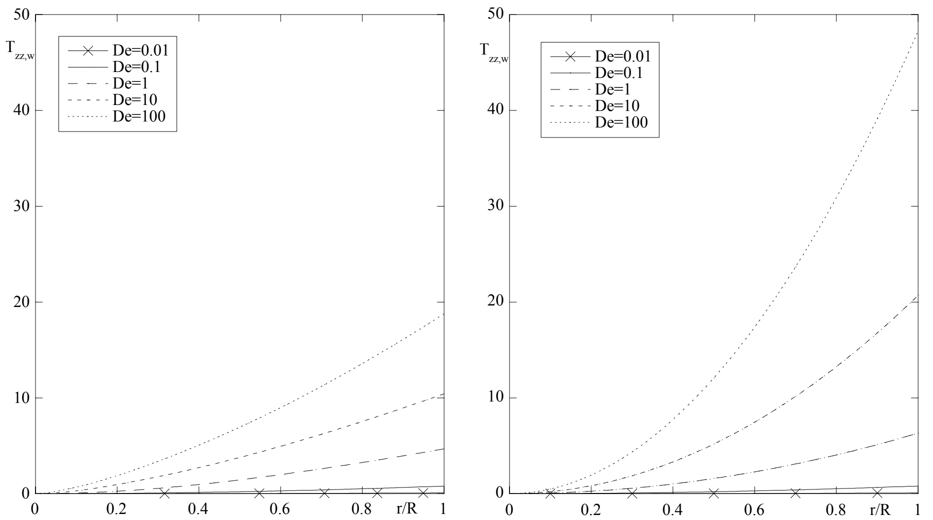
with the denominator representing the wall shear stress for a Newtonian fluid having the same total viscosity and flowing at the same flow rate. For $De \leq 0.1$ the normalized stresses vary linearly from 0 on axis to 1 at the wall and decrease with increasing Deborah numbers due to shear-thinning. The more intense shear-thinning of the equivalent single mode model is seen in the lower values of T_{rz} at identical values of *De*.

Regarding fluid elasticity, the normal stresses $T_{zz,w}$ are compared in Fig. 3. Only in this figure, the stresses are normalized by the wall shear stress of the fluid ($T_{zz,w} = \tau_{zz} / (\tau_{rz})_{wall}$) in order to remove the non-monotonic behavior found by Oliveira and Pinho (1999). This refers to the cross-over of normal stresses at large Deborah numbers due to the intense shear-thinning of the fluids, which is eliminated when the normal stresses are normalized by the corresponding shear stresses (or the corresponding wall shear stresses). The normal stresses of the multimode model are lower than those of than the equivalent single mode model by a factor of 2.5, and the variation of $T_{zz,w}$ along the radius is also less non-linear.



(a) (b)

Figure 2. Effect of Deborah number on the normalized profile of total shear stress (T_{rz}) for simplified PTT model with linear stress coefficient and $\varepsilon = 0.02$ (Fluid 1b): (a) 4 mode model; (b) Equivalent single mode model.



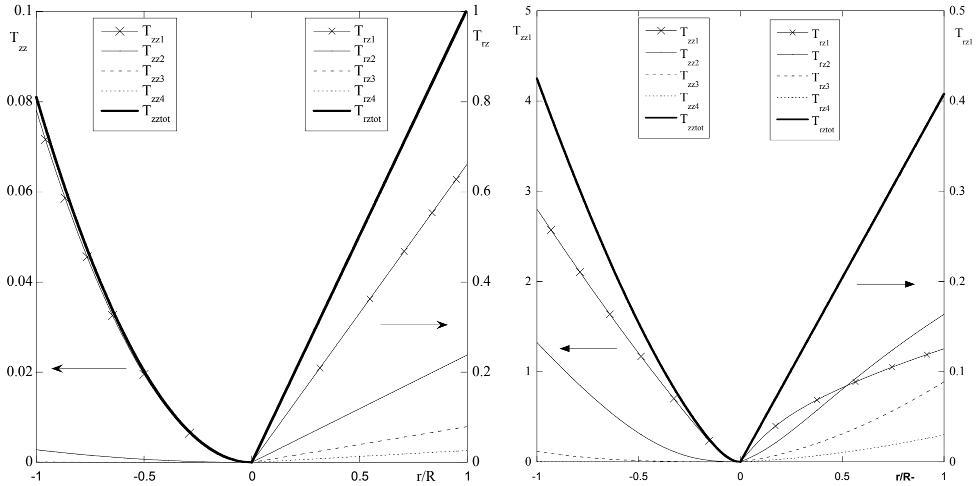
(a) (b)

Figure 3. Effect of De number on the normalized profile of total normal stress (Note the different normalization, ($T_{zz,w}$) for simplified PTT model with linear stress coefficient and $\varepsilon = 0.02$ (Fluid 1b)): (a) 4 mode model; (b) Equivalent single mode model.

Since the equivalence between the single mode and the multimode models is exclusively on the basis of the linear viscoelastic spectra, it is not surprising to find out that they behave differently in steady shear. It would have sufficed to compare the viscometric viscosity to arrive at similar conclusions. Therefore, we concentrate next in a more thorough analysis of the multimode solution.

On the right half of Fig. 4-(a) we plot the total shear stress and the shear stress of each individual mode shear stress for Fluid 1b represented by the 4-mode PTT equation, whereas on the left half the corresponding normal stresses are shown. All stresses have been normalized as in Eq. (24). Since this figure corresponds to the very low Deborah number of 0.01, all the shear stresses vary linearly, leading to the Newtonian parabolic shape shown in Fig. 2(a). The normal stresses are low but non-zero and vary quadratically as for a single mode model at very low Deborah numbers. In this case it is also clear that the lower modes are more important and this is especially so for the normal stress.

As the Deborah number increases to intermediate values (this depends on the numerical value of ε), as is the case here for De = 10 plotted in Fig. 4-(b), the non-dimensional normal stresses increase while the shear stresses decrease (notice the change in the ordinates). Except for the total stress, the shear stresses of the various modes no longer vary linearly and in relative terms the higher modes become more important. In the plot, we see that the stress of the first mode is lower than that of the second mode for $r/R > 0.5$. Similarly for the normal stress, in relative terms the relevance of the higher modes rises with Deborah number.



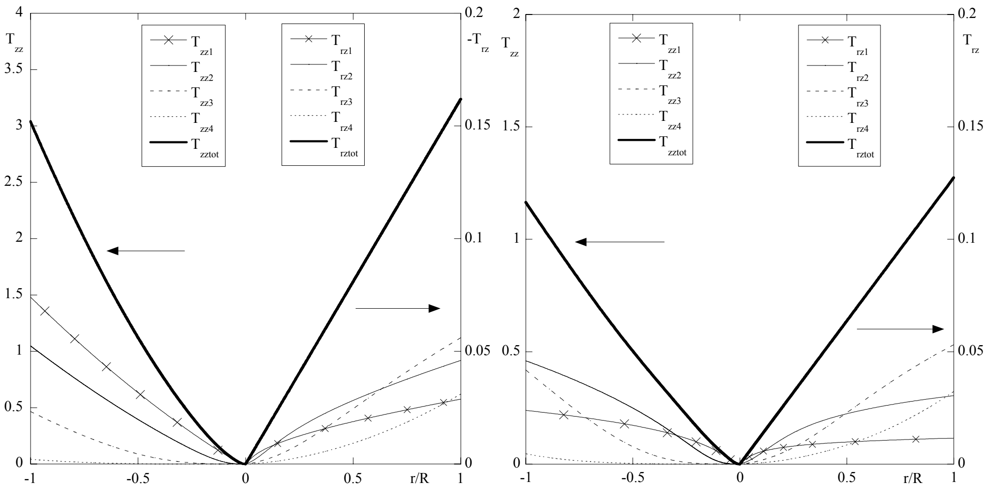
(a) (b)

Figures 4. Radial variation of the non-dimensional normal (T_{zz}) and shear (T_{rz}) stresses for all modes for the linear PTT model with $\varepsilon = 0.02$ (Fluid 1b): (a) De = 0.01; (b) De = 10.

At even higher values of the Deborah number, here represented by the plot at De = 100 in Fig. 5-(a), these trends are enhanced. Now, the most important contribution to the total shear stress near the wall comes from the third mode and only very close to the centerline the first mode is more important on account of the very low velocities of deformation. Near the wall, and in this flow case, the first mode is even less important that the fourth mode.

These observations have to be taken in relative terms since they depend on the specific values of the parameters chosen for the various modes. The important conclusion is that the relevance of the higher modes increase with the rates of deformation, so that it is possible for higher modes to become more relevant than lower modes.

The richer rheology of the exponential multimode PTT model, well known for the single mode version, leads to more complex and intense variations in terms of the contributions of the various modes to the total stresses, as is well shown in Fig. 5-(b). All parameters are identical to those used for the linear version in Fig 5-(a) and it pertains to De = 100. Now, even for the normal stress there is a cross-over of the various modes which also exhibit different concavities.



(a) (b)

Figures 5. Radial variation of the non-dimensional normal and shear stresses for all modes for the linear and exponential PTT model with $\varepsilon = 0.02$ (Fluid 1b) at De = 100: (a) T_{zz}; (b) T_{rz}.

5. Conclusion

In this work a semi analytical formulation was presented for the calculation of pipe flow of a multimode sPTT rheological model. It was shown that for small values of the Deborah number (De = 0.01)) all the shear stresses vary linearly, leading to the Newtonian parabolic shape, the normal stresses are low and vary quadratically as for a single mode model. For intermediate values of the Deborah number (*De* = 10), the various components of the shear stresses no longer vary linearly (except for the total stress), and in relative terms, the higher modes become more important.

It is worth noting that the procedure presented here can be extended to other non-Newtonian models leading to a generalized analytical-numerical formulation for multimode models.

6. Acknowledgements

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