Semi-analytical solution for the problem of extended Pom-Pom fluid flow in a round pipe

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Abstract. A semi-analytical solution to the problem of the steady flow of viscoelastic single equation eXended Pom-Pom (XPP) fluid in a round pipe using the four-mode rheological equation of state of XPP is presented. An original parametric method for solving the set problem is used. The resulting method is applicable for solving a similar problem in a flat slit. The developed solution method is tested by comparing it with numerical results and experimental data. Using a polyacrylamide solution as an example, the influence of the Weissenberg number on the axial velocity profiles and the components of normal stresses is studied.

1. Literature survey
The flow of polymeric fluids is characterized by the presence of complex nonlinearly viscous and viscoelastic properties, and the analysis of the behavior of such media during their processing is an important link between production and the properties of the final product. A rheological model must satisfy a number of parameters, and the main condition for its applicability is an adequate description of the flow and emerging effects. One of the main problems in constitutive modeling is to obtain a correct description of the transient nonlinear behavior in elongated and shear flows simultaneously [1]. Some well-known and widely used rheological mono- and multimode models, for example, the Phan-Thien-Tanner and Giesekus models, are being replaced by others [2]. For example, such a model is the Pom-Pom model presented by McLeish and Larson [3]. Using only a single-mode model, it is possible to qualitatively predict the behavior during both shear and elongation of the low-density polyethylene melt. However, this model has three disadvantages: solutions in steady-state elongation show discontinuities, the orientation equation is unlimited for high strain rates, and the model does not have a second normal difference of stresses in shear. These disadvantages are eliminated by introducing the so-called local offset of the branching point [4]. The modified Pom-Pom model is called an eXtended Pom-Pom (XPP) [5]. We use this model for the mathematical description of the steady viscoelastic fluid flow in a round pipe. Based on the analysis of the published data, we can conclude that the literature contains only numerical solutions to the problems of the XPP fluid flow in channels with different geometries. These results are compared with existing experimental results. Due to the complexity of the XPP model, we have not found analytical or semi-analytical solutions, which necessitates the development of such methods. In this work, we have developed a semi-analytical method for solving the problem of a steady XPP liquid flow in a round pipe, the results of which can be used as a validation of numerical methods, as well as for setting boundary conditions at the inlet and outlet of the channel containing various obstacles inside, for example, a cylinder.
2. Problem statement

Let us consider the isothermal steady state flow of a viscoelastic Single equation eXtended Pom-Pom (XPP) fluid in a round pipe using the n-mode constitutive equation of XPP with the Newtonian stress component as [5]:

$$\sigma = \sigma_N + \sum_{k=1}^{n} \sigma_k, \quad \sigma_N = \mu_N D$$  \hspace{1cm} (1)

$$f(\sigma_k) \sigma_k + \frac{\lambda_k}{\mu_k} (\nabla \cdot \sigma_k) + \frac{\mu_k}{\lambda_k} \left( \frac{f(\sigma_k) - 1}{\epsilon_k} \right) I = 2\mu_k D,$$  \hspace{1cm} (2)

where

$$f(\sigma_k) = \frac{2}{e^{\Lambda_k}} \frac{(\Lambda_k)^{-\frac{1}{2}}}{\Lambda_k} \left( \frac{\alpha_k \lambda_k t}{3\mu_k} \right) \sigma_k,$$

$$\Lambda_k = \frac{1}{1 + \frac{\lambda_k t \sigma_k}{3\mu_k}}$$

is the backbone stretch, $\epsilon_k = \frac{\lambda_k}{\lambda_k}$, $k = 1, \ldots, n$; $k$ is current mode number, $n$ is the total number of modes;

$\sigma$ is the extra stress tensor; $\sigma_N$ is the Newtonian part of extra stress tensor;

$\nabla \sigma = \frac{d\sigma}{dt} - \sigma \cdot \nabla V - \nabla \cdot \sigma = \frac{\partial \sigma}{\partial t} + \nabla \sigma \cdot V - \sigma \cdot \nabla V - \nabla \cdot \sigma$ is the upper convective derivative of a tensor $\sigma$; $I$ is the unit tensor; $p$ is the pressure, $\mu_N$ is the solvent viscosity; $D = (\nabla V + (\nabla V)^T)/2$ is the rate of deformation tensor; $V$ is the velocity; $\sigma_k$ is the elastic part of extra stress tensor corresponding to each mode; $\lambda_k$ is the relaxation time; $\mu_k$ is the polymeric viscosity; $q$ is the number of arms at the backbone extremity of the Pom-Pom molecule; and $\alpha_k$ and $\epsilon_k$ are the rheological parameters [6].

We assume that the velocity vector has only one non-zero axial component $V^z$, which depends on variable $r$ (cylindrical coordinate system, $z$-axial coordinate). The no-slip boundary condition is set on the pipe wall.

Under the assumptions made, the system of equations for the momentum transfer and continuity will take the form

$$0 = -\frac{\partial P}{\partial r} + \frac{1}{r} \frac{d}{dr} \left( r \sigma_{op} \right) \sigma_{op}, \quad 0 = -\frac{\partial P}{\partial \varphi} + \frac{1}{r} \frac{d}{dr} \left( r \sigma_{oz} \right) \sigma_{oz}, \quad 0 = -\frac{\partial P}{\partial z} + \frac{1}{r} \frac{d}{dr} \left( r \sigma_{oz} \right) \sigma_{oz} = 0.$$  \hspace{1cm} (3)

where $P$ is the pressure; and $\sigma_{ij}^{\text{op}}, i, j = r, \varphi, z$ are the contravariant components of extra stress tensor. The solution to the system of equations of motion and continuity can be represented as

$$\frac{\partial P}{\partial z} = C_0 = \text{const} = -|C_0|, \quad \sigma_{oz} = \sigma_{oz}^{\text{N}} + \sum_{k=1}^{n} \sigma_{oz}^{\text{k}} = -|C_0|/2 |r|.$$  \hspace{1cm} (4)

Let us introduce the non-dimensional variable $\eta = r/R$, where $R$ is the pipe radius. We introduce the physical dimensionless components of the elastic stress tensor in the form

$$\sigma_{oz}^{\text{k}} = \frac{\chi_k}{\beta_k \lambda_0} \tau_{oz}^{\text{k}}, \quad \sigma_{op}^{\text{k}} = \frac{\chi_k}{\beta_k \lambda_0 r^2} \tau_{op}^{\text{k}}, \quad \sigma_{oz}^{\text{zz}} = \frac{\chi_k}{\beta_k \lambda_0} \tau_{oz}^{\text{zz}}, \quad \sigma_{oz}^{\text{k}} = \frac{\chi_k}{\beta_k \lambda_0} \tau_{oz}^{\text{k}}.$$  \hspace{1cm} (5)

where $\chi_k = \mu_k / \mu_0$, $\chi_s = \mu_s / \mu_0$, $\beta_k = \lambda_k / \lambda_0$ and the expression for the dimensionless shear rate gradient $\dot{\gamma}_k = \lambda_k dV_z / dr$ in the form

$$\dot{\gamma}_k = \lambda_k dV_z / dr.$$  \hspace{1cm} (6)
\[
\dot{\gamma}_k = \lambda_k \frac{dV_z}{dr} = \frac{\lambda_0}{R} \frac{\lambda_0 V_a}{\mu} \frac{dv^z}{d\eta} = \beta_k We \frac{dv^z}{d\eta} = \beta_k We \frac{g}{\gamma},
\]

(6)

where \( \lambda_0 = \sum_{k=1}^{N} \lambda_k \), \( \mu = \mu_N + \sum_{k=1}^{N} \mu_k \), \( \frac{dV_z}{dr} = \frac{\lambda_0 V_a}{R} \frac{1}{\lambda_0} \frac{dv^z}{d\eta} = We \dot{\gamma} \), \( We = \frac{\lambda_0 V_a}{R} \) is the Weissenberg number.

Then the rheological equation of state (1) - (2) in the selected coordinate system, taking into account that \( \sigma_{k^{op}} = \sigma_{k^{oz}} = 0 \), will be written as

\[
f\left(\tau_k\right) \tau_k^{rr} + \alpha_k \left(\left(\tau_k^{rr}\right)^2 + \left(\tau_k^{rr}\right)^2\right) + \left(f\left(\tau_k\right) - 1\right) = 0,
\]

(7)

\[
f\left(\tau_k\right) \tau_k^{rr} - \gamma_k \tau_k^{rr} + \alpha_k \left(\tau_k^{rr} + \tau_k^{zz}\right) \tau_k^{zz} = \gamma_k,
\]

(8)

\[
f\left(\tau_k\right) \tau_k^{pp} + \alpha_k \left(\tau_k^{pp}\right)^2 + \left(f\left(\tau_k\right) - 1\right) = 0,
\]

(9)

\[
f\left(\tau_k\right) \tau_k^{zz} - 2 \gamma_k \tau_k^{zz} + \alpha_k \left(\tau_k^{rr} + \tau_k^{zz}\right) + \left(f\left(\tau_k\right) - 1\right) = 0,
\]

(10)

\[
f\left(\tau_k\right) = \frac{2\lambda_k}{\lambda_{vol}} e^{\frac{2(\Lambda_k - 1)}{q}} \left(1 - \frac{1}{\Lambda_k}\right) + \frac{1}{\Lambda_k^2} \left(1 - \frac{\alpha_k I_z}{3}\right),
\]

(11)

where \( \Lambda_k = \sqrt{1 + \frac{I_z}{3}} \), \( I_1 = \left(\tau_k^{rr} + \tau_k^{pp} + \tau_k^{zz}\right) \), \( I_2 = \left(\tau_k^{rr}\right)^2 + \left(\tau_k^{pp}\right)^2 + 2\left(\tau_k^{rr}\right)^2 + \left(\tau_k^{zz}\right)^2 \).

Let us introduce the parameter \( \rho_k \) and new variables

\[
\tau_k^{pp} = -\rho_k, \tau_k^{zz} = \frac{\xi_k + \zeta_k}{2}, \tau_k^{rr} = \frac{\xi_k - \zeta_k}{2}, \xi_k = \tau_k^{zz} + \tau_k^{rr}, \xi_k = \tau_k^{zz} - \tau_k^{rr},
\]

(12)

As the analysis of the obtained dependences has shown, the value of \( \rho_k \) is in the range from 0 to 1, which greatly simplifies the obtaining of the final solution of the original problem.

After simple algebraic operations, we can obtain an equation that determines the dependence of \( \Lambda_k \) on the parameter \( \rho_k \)

\[
2f\left(\rho_k\right) \xi_k \left(\Lambda_k, \rho_k\right) + \alpha_k \left(\xi_k \left(\Lambda_k, \rho_k\right)^2 + \frac{2\Omega_k \left(\Lambda_k\right) \left(\xi_k \left(\Lambda_k, \rho_k\right) + 2\right)}{f\left(\rho_k\right) + \alpha_k \xi_k \left(\Lambda_k, \rho_k\right)}\right)
\]

\[
+ 4\left(f\left(\rho_k\right) - 1\right) - 4\Omega_k \left(\Lambda_k\right) = 0,
\]

(13)

where \( f\left(\rho_k\right) = \frac{1 - \alpha_k \rho_k^2}{1 - \rho_k} \), \( \xi_k \left(\Lambda_k, \rho_k\right) = \rho_k + 3\Lambda_k^2 - 3 \), \( \Omega_k \left(\Lambda_k\right) = \frac{3}{\xi_k} e^{\frac{2(\Lambda_k - 1)}{q}} \Lambda_k \left(\Lambda_k - 1\right) \).

Further, the dependencies \( \tau_k^{rr} \left(\rho_k\right) \), \( \tau_k^{zz} \left(\rho_k\right) \), \( \tau_k^{rc} \left(\rho_k\right) \), \( \tau_k^{cz} \left(\rho_k\right) \), \( \gamma_k \left(\rho_k\right) \) can be expressed as follows

\[
\Omega_k \left(\rho_k\right) = \frac{3}{\xi_k} e^{\frac{2(\Lambda_k - 1)}{q}} \Lambda_k \left(\rho_k\right) \left(\Lambda_k \left(\rho_k\right) - 1\right), \xi_k \left(\rho_k\right) = \rho_k + 3\Lambda_k \left(\rho_k\right)^2 - 3
\]

(14)

\[
\zeta_k \left(\rho_k\right) = \frac{2\Omega_k \left(\rho_k\right)}{f\left(\rho_k\right) + \alpha_k \xi_k \left(\rho_k\right)}, \tau_k^{rr} \left(\rho_k\right) = \frac{\xi_k \left(\rho_k\right) + \zeta_k \left(\rho_k\right)}{2}, \tau_k^{zz} \left(\rho_k\right) = \frac{\xi_k \left(\rho_k\right) - \zeta_k \left(\rho_k\right)}{2}
\]

(15)
\[ \gamma_k = - \left( f (\rho_k) + \alpha_k \varepsilon_k (\rho_k) \right) \sqrt{ \frac{2\Omega_k (\rho_k)}{\left( \varepsilon_k (\rho_k) + 2 \left[ f (\rho_k) + \alpha_k \varepsilon_k (\rho_k) \right] - 2\Omega_k (\rho_k) \right)} }, \quad (16) \]

\[ \tau_k (\rho_k) = - \frac{\sqrt{\Omega_k (\rho_k)} \sqrt{ \left( \varepsilon_k (\rho_k) + 2 \left[ f (\rho_k) + \alpha_k \varepsilon_k (\rho_k) \right] - 2\Omega_k (\rho_k) \right)}}{\sqrt{2} \left( f (\rho_k) + \alpha_k \varepsilon_k (\rho_k) \right)} \]. \quad (17) \]

It should be noted that the values obtained for each of the modes depend only on two rheological constants \( \alpha_k \) and \( \varepsilon_k \). For a given flow rate, the condition for the normalization of the velocity vector can be represented as

\[ \int_0^1 v_z \eta d\eta = 0.5 \quad \text{or} \quad \int_0^1 v_z d\eta^2 = - \frac{1}{\text{We} \beta_k} \int_0^1 \eta^2 \gamma_k d\eta = 1. \quad (18) \]

The parametric dependence may be obtained in the form \( v_z (\eta) = \{v_z (\rho_1), \eta (\rho_1)\} \), where the definition of the dimensionless velocity with subsequent integration over the parameter is used for the function \( v_z (\rho_1) \):

\[ v_z (\rho_1) = \int_{\rho_1}^{\rho_{\text{max}}} \gamma_k (\rho_1) / \beta_k d\rho_1. \quad (19) \]

To determine the dependence \( \eta (\rho_1) \) we use the solution of the momentum transfer equation (4), into which the dimensionless quantities are introduced.

\[ \eta (\rho_1) = - \left[ \frac{X_m \gamma_m (\rho_m)}{\beta_m} + \sum_{k=1}^{n} \frac{X_k \gamma_k (\rho_k)}{\beta_k} \right] / \text{Kri}, \quad (20) \]

where \( \text{Kri} = \frac{C_0}{2 R \mu_0} \).

Dependences \( \rho_k (\rho_1) \) can be obtained from the definition of the shear rate gradient

\[ \varepsilon = \frac{dv_z}{d\eta} = \frac{\varepsilon_1}{\text{We} \beta_1} = \frac{\varepsilon_2}{\text{We} \beta_2} = \ldots = \frac{\varepsilon_n}{\text{We} \beta_n}. \quad (21) \]

Thus, the calculation algorithm includes:

- setting a fixed value of \( \rho_{\text{max}} \),
- finding \( \rho_{\text{max}}, k = 1, 2, \ldots, n \) from the condition \( \varepsilon / \beta_1 = \varepsilon / \beta_2 = \ldots = \varepsilon / \beta_n \),
- calculating the \( \text{Kri} \) value from (49) and the Weissenberg number using the formula:

\[ \text{We} = - (\beta_k)^{-1} \int_0^1 \eta^2 \gamma_k d\eta, \]

- plotting the velocity profile using the formula:

\[ v_z (\eta_n) = (\text{We} \beta_k)^{-1} \int_{\eta_n}^1 \gamma_k d\eta. \]

3. Verification

The developed method is verified by the example of solving the problem of a stationary XPP fluid flow in a flat slit [1]. In this case, all the relationships obtained for the flow in a round pipe remain,
with the following exceptions: (a) \[ Kri = \lambda_0 |C_0| h/\mu_0, \] where \( h \) is half the width of the slit; (b) \[ We = (\lambda_0 V_a)/h; \] (c) relation (47) is replaced by the following relation: \[ (-1)(We\beta_k)^{-1}\int_0^1 \eta \gamma_k d\eta = 1. \]

Figure 1a shows a comparison of our calculated axial velocity profile in a flat slit with the literature data (we used the profile at \( x/R = -4 \) from the literature [1]). Note that we use the value \( We = (\lambda_0 V_a)/h = 1.45 \) that corresponds to the literature value \( We_{\text{liter data}} = (\lambda_0 V_a)/R_c = 2.9 \) [Viscoelastic analysis of complex polymer], since \( R_c = h/2 \) is the cylinder radius in [1]. As we can see from the figure, our results are in good agreement with both experimental data and numerical results obtained using the OpenFoam package. Note that the value of the axial velocity calculated on the axis of symmetry of the flat slot is equal to \( v_z(0) = 1.45 \).

In order to verify the obtained results, an additional comparison with the work [3] was carried out for the viscosity curve, which can be calculated by the formula

\[
\mu_{\text{eff}} = \sigma_{\text{rc}} (dV_z / dr)^{-1} = \left( \mu_N \frac{dV_z}{dr} + \sum_{k=1}^{n} \frac{\chi_k \mu_0}{\beta_k \lambda_0} \tau_k \right) \left( dV_z / dr \right) = \mu_N + \mu_0 \sum_{k=1}^{n} \left( \chi_k \tau_k \gamma_k \right). \] (22)

Figure 1b shows the dependence of the effective viscosity on the shear rate. It can be seen that the theoretical results obtained based on the developed analytical method are in good agreement with both the experimental viscometric data and the numerical results of the authors [1].

![Figure 1. Dimensionless axial velocity profiles (a) for slit flow (\( We_{\text{liter data}} = 2.9 \)) and viscosity curve (b).](image)

4. Results

Let us consider the 2500 ppm aqueous solution of polyacrylamide [7] (hereafter 2500ppm PAA) as a test liquid. The parameters of the XPP model (1) - (2) are obtained by approximating the flow curve when considering the twisting flow. Table 1 shows our calculated parameters of the rheological model, which adequately describes the viscosity curve.

| \( i \) | \( \lambda_i \) | \( \eta_i \) | \( \eta_N \) | \( q_i \) | \( \varepsilon_k \) | \( \alpha_i \) |
|---|---|---|---|---|---|---|
| 1 | 0.1043 | 0.2662 | 0.062 | 2 | 0.1 | 0.7 |
| 2 | 0.8716 | 1.9358 | - | 2 | 0.3 | 0.4 |
| 3 | 7.294 | 13.436 | - | 2 | 0.1 | 0.8 |
| 4 | 78.218 | 68.778 | - | 2 | 0.1 | 0.1 |
The figure shows the axial velocity profiles and normal stress for a steady flow of 5000 ppm PAA in a round tube. The influence of the Weissenberg number on the distribution of the axial velocity profile is consistent with the literature data, namely, an increase in the Weissenberg number leads to deformation of the velocity profile, which becomes flatted.

![Graphs of axial velocity and normal stress](image)

**Figure 2.** Nondimensional axial velocity (a) and normal stresses $\tau_{rr}$ (b) and $\tau_{zz}$ (c) for steady XPP fluid flow.

**Conclusions**

A semi-analytical method for solving the problem of a steady viscoelastic fluid flow in a round pipe using the eXtended Pom-Pom four-mode model has been developed. Approval of the developed method shows good agreement with the literature data. Using the nonlinear parameters of the XPP model for the 5000 ppm PAA, the axial velocity profiles and normal stress, which qualitatively agree with the well-known results have been analyzed.

**Acknowledgements**

The semi-analytical method was developed with the financial support by the RFBR No. 18-41-160007 and the Government of the Republic of Tatarstan in the framework of scientific project No. 18-41-160007. The determination of the non-linear parameter of the eXtended Pom-Pom model was developed with the financial support from RFBR №19-01-00375.

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