24th COBEM - 2017

24th ABCM International Congress of Mechanical Engineering
December 3-8, 2017, Curitiba, PR, Brazil

COBEM-2017-1490
APPLICATION OF THE KBKZ-PSM INTEGRAL MODEL TO AXISYMMETRIC FLOWS

Caroline Viezel
Juliana Bertoco
Murilo Francisco Tomé
Department of Applied Mathematics and Statistics, University of São Paulo, Av. Trabalhador São Carlense, 400, São Carlos, Brazil
cviezel@usp.br, jubert@icmc.usp.br, murilo@icmc.usp.br

Michael Vynnycky
Division of Processes, Department of Materials Science and Engineering, KTH Royal Institute of Technology, Brinellvägen 23, 100 44 Stockholm, Sweden
michaelv@kth.se

Abstract. *This work deals with the application of the integral KBKZ-PSM constitutive equation to axisymmetric flow problems. The mass and momentum equations are solved by a finite difference technique presented by Tomé and co-workers. The Finger tensor is modeled by the deformation fields method proposed by Hulsen and co-workers while the integral KBKZ equations describing the components of the extra-stress tensor are solved by a second-order quadrature formula. The methodology employed is applied to simulate tube flows and is verified by using mesh refinement and an analytic solution for fully developed axisymmetric flow in a tube.*

Keywords: *KBKZ integral model, deformation fields method, axisymmetric flows, finite difference.*

1. INTRODUCTION

The KBKZ integral model was originally developed using ideas from rubber elasticity theory in a general framework accounting for the strain free energy associated with the elastic strain imposed on the material (see Bernstein *et al.* (1963)). This equation is known to approximate well the rheology of polymer melts and has motivated many researchers to tackle viscoelastic flows using integral models (e.g (Papanastasiou *et al.*, 1983; Goublomme and Crochet, 1993; Mitsoulis, 2013; Luo and Mitsoulis, 1990; Konaganti *et al.*, 2015, 2016)). A recent review of works using this constitutive equation is presented by Mitsoulis (2013), who provides an up-to-date review of the research on numerical methods for solving KBKZ integral models. This constitutive equation has been applied to solve viscoelastic flows using the finite element method and Tomé *et al.* (2007, 2016) have demonstrated that the finite difference method can also handle this integral model for two-dimensional confined and free surface flows.

In this work the KBKZ-PSM model proposed by Papanastasiou-Scriven-Macosko is adopted (see Papanastasiou *et al.* (1983)). The ideas of the *deformation fields method* (see Hulsen *et al.* (2001)) are applied to store the deformation history, on which the Finger tensor is computed by solving an appropriate evolution equation. The governing equations for axisymmetric flows are solved by the finite difference method on a staggered grid using the ideas of the GENSMAC methodology (see Tomé *et al.* (2007)). Tube flow is solved and verification and convergence results, using an analytical solution, are provided.

2. GOVERNING EQUATIONS

The mass and momentum conservation equations, in dimensionless form, for isothermal incompressible flows can be written as (for details, see Tomé *et al.* (2007))

$$\nabla \cdot \mathbf{v} = 0 \,, \tag{1}$$

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot (\mathbf{v}\mathbf{v}) = -\nabla p + \frac{1}{Re}\nabla^2 \mathbf{v} + \nabla \cdot \mathbf{\Phi} + \frac{1}{Fr^2}\mathbf{g} \,. \tag{2}$$

In these equations, $Re = \dfrac{\rho_0 U R}{\eta_0}$ is the Reynolds number and $Fr = \dfrac{U}{\sqrt{R\,g}}$ is the Froude number, where U and R are velocity and length scales and g, η_0, ρ_0 are the gravity acceleration, fluid viscosity and fluid density, respectively.

The non-Newtonian tensor $\mathbf{\Phi}$ is related to the extra-stress tensor $\boldsymbol{\tau}$ and is calculated through the following EVSS transformation (Rajagopalan *et al.*, 1990):

$$\mathbf{\Phi} = \boldsymbol{\tau} - \frac{2}{Re}\mathbf{D}\ , \text{ where } \mathbf{D} = \frac{1}{2}\Big[\nabla\mathbf{v} + (\nabla\mathbf{v})^{\mathrm{T}}\Big]. \tag{3}$$

The rheological behavior of the fluid flow is described by the KBKZ-PSM integral constitutive equation (for details, see Mitsoulis (2013))

$$\boldsymbol{\tau}(t) = \int_{-\infty}^{t} M(t-t')H(I_1, I_2)\mathbf{B}_{t'}(t)dt'\ , \tag{4}$$

where

$$M(t-t') = \sum_{k=1}^{m_1} \frac{a_k}{\lambda_k Wi} e^{-\frac{t-t'}{\lambda_k Wi}}, \tag{5}$$

and

$$H(I_1, I_2) = \frac{\alpha}{\alpha - 3 + \beta I_1 + (1-\beta)I_2}. \tag{6}$$

In the memory function, Eq. (5), λ_k, a_k, m_1 are relaxation times, relaxation modules and the number of relaxation modes, respectively, and $Wi = \lambda_{ref}\frac{U}{R}$ is the Weissenberg number, where λ_{ref} is a reference relaxation time. The function $H(I_1, I_2)$ in Eq. (6) is the Papanastasiou-Scriven-Macosko damping function, where the parameters α and β are obtained from a curve fitting to the rheological properties of the fluid (see Papanastasiou *et al.* (1983)). In Eq. (4), $\mathbf{B}_{t'}(t)$ is the Finger tensor and $I_1 = tr[\mathbf{B}_{t'}(t)]$ and $I_2 = \frac{1}{2}\left((I_1)^2 - tr[\mathbf{B}_{t'}^2(t)]\right)$ are the first and second invariants of $\mathbf{B}_{t'}(t)$, respectively.

3. NUMERICAL METHOD

The governing equations (Eqs. (1-6)), written in cylindrical coordinates (r, z), are solved by the finite difference method on a staggered grid. The projection method is employed to uncouple the velocity and pressure fields from Eqs. (1) and (2) and then, the velocity $\mathbf{v}(r,z) = \big(u(r,z), w(r,z)\big)$ and the pressure $p(r,z)$ are calculated based on the methodology presented by Tomé *et al.* (2007). In summary, a tentative velocity field $\widetilde{\mathbf{v}}(r,z)$ is obtained from an explicit Euler scheme discretization of Eq. (2) while the final velocity field is computed by adding a gradient of a potential function $\mathbf{v}(r,z) = \widetilde{\mathbf{v}}(r,z) - \nabla\psi(r,z,t)$ that obeys a Poisson equation to ensure incompressibility everywhere. For details see Tomé *et al.* (2007).

To compute the extra-stress tensor, $\boldsymbol{\tau}$ it is necessary to track the Finger tensor at the past times t'_j using the ideas of the *deformation fields method* (Hulsen *et al.*, 2001). In this method, the Finger tensor $\mathbf{B}_{t'_j(t)}(\mathbf{x}, t)$ is evolved in time by the convection equation,

$$\frac{\partial}{\partial t}\mathbf{B}_{t'_j(t)}(\mathbf{x},t) + \mathbf{v}(\mathbf{x},t)\cdot\nabla\mathbf{B}_{t'_j(t)}(\mathbf{x},t) = [\nabla\mathbf{v}(\mathbf{x},t)]^T\cdot\mathbf{B}_{t'_j(t)}(\mathbf{x},t) + \mathbf{B}_{t'_j(t)}(\mathbf{x},t)\cdot\nabla\mathbf{v}(\mathbf{x},t)\ . \tag{7}$$

where t'_j are given past times in $[0,\ t_{n+1}]$. This equation is resolved by the modified Euler method while t'_j are obtained from a geometric progression discretization of the interval $[0,\ t_{n+1}]$ into $2N$-subintervals $[t'_{j-1},\ t'_j], j = 1, 2, \cdots, 2N$. The integral in Eq. (4) is computed assuming that $\mathbf{B}_{t'}(t_{n+1}) = \mathbf{B}_0(t_{n+1}), \forall\, t' < 0$ and applying a second order quadrature formula on each interval $[t'_j,\ t'_{j+2}]$. For details see Tomé *et al.* (2016).

4. POISEUILLE FLOW

The pressure-driven flow (*Poiseuille flow*) is often used for verification of numerical methodologies in CFD because in this flow type the momentum and constitutive equations are simplified and an analytic or semi-analytic solution can be obtained.

To verify the numerical technique used in this work, an analytic solution for steady state tube flows of an one-module KBKZ fluid has been developed. This analytic solution is an extension of the solution for Poiseuille flows in a channel presented in Tomé *et al.* (2016).

4.1 Analytic solution

By considering fully-developed flow of a 1-mode KBKZ fluid in a cylinder of radius R (see Fig. 1), the following assumptions are made:

$$r \in [0,\ 1], \quad u = 0, \quad w = w(r), \quad \dot{\gamma} = \frac{\partial w}{\partial r}, \quad \mathbf{B} = \begin{bmatrix} 1 & 0 & \dot{\gamma}(t-t') \\ 0 & 1 & 0 \\ \dot{\gamma}(t-t') & 0 & 1+\dot{\gamma}^2(t-t')^2 \end{bmatrix}, \tag{8}$$

leading to the following invariants I_1 and I_2 that are required in the Papanastasiou function $H(I_1, I_2)$:

$$I_1 = I_2 = 3 + \dot{\gamma}^2(t-t')^2, \tag{9}$$

and the equations for the components of the extra-stress tensor become

$$\tau^{rz} = \frac{a_1\alpha}{Wi}\int_{-\infty}^{t} \frac{\dot{\gamma}(t-t')e^{-(t-t')/Wi}}{\alpha + \dot{\gamma}^2(t-t')^2}dt' \ , \tag{10}$$

$$\tau^{zz} = \frac{a_1\alpha}{Wi}\int_{-\infty}^{t} \frac{\left[1+\dot{\gamma}^2(t-t')^2\right]e^{-(t-t')/Wi}}{\alpha + \dot{\gamma}^2(t-t')^2}dt' \ , \tag{11}$$

$$\tau^{rr} = \tau^{\theta\theta} = \frac{a_1\alpha}{Wi}\int_{-\infty}^{t} \frac{e^{-(t-t')/Wi}}{\alpha + \dot{\gamma}^2(t-t')^2}dt' \ . \tag{12}$$

and making the transformation $s = t - t'$, these equations become

$$\tau^{rz}(r) = \frac{a_1\alpha}{Wi}\int_{0}^{\infty} \frac{\dot{\gamma}se^{-s/Wi}}{\alpha + \dot{\gamma}^2 s^2}ds, \tag{13}$$

$$\tau^{zz}(r) = \frac{a_1\alpha}{Wi}\int_{0}^{\infty} \frac{\left[1+\dot{\gamma}^2 s^2\right]e^{-s/Wi}}{\alpha + \dot{\gamma}^2 s^2}ds, \tag{14}$$

$$\tau^{rr}(r) = \tau^{\theta\theta} = \frac{a_1\alpha}{Wi}\int_{0}^{\infty} \frac{1\, e^{-s/Wi}}{\alpha + \dot{\gamma}^2 s^2}ds. \tag{15}$$

The momentum equations reduce to

$$-\frac{\partial p}{\partial r} + \frac{1}{r}\frac{\partial}{\partial r}(r\tau^{rr}) - \frac{\tau^{\theta\theta}}{r} = 0 \ , \tag{16}$$

$$-\frac{\partial p}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}(r\tau^{rz}) = 0. \tag{17}$$

Integrating Eq. (16) yields

$$p(r,z) = \int^{r} \frac{1}{x}\frac{\partial}{\partial x}(x\tau^{rr})dx - \int^{r} \frac{\tau^{\theta\theta}}{x}dx + F(z) \quad \Longrightarrow \quad \frac{\partial p}{\partial z} = F'(z) \tag{18}$$

and Eq. (17) can be rewritten as

$$\frac{1}{r}\frac{\partial}{\partial r}(r\tau^{rz}) = F'(z), \tag{19}$$

where the prime denotes differentiation with respect to z. We see that, since the left-hand-side of Eq. (19) is a function of r, F' must be a constant which we denote by $C = dp/dz$; hence we have

$$\tau^{rz}(r) = \frac{1}{2}Cr + \frac{h(z)}{r}, \tag{20}$$

and since the fact that $\tau^{rz}(r = 0)$ must be finite implies that $h(z) = 0$, we must have

$$\tau^{rz}(r) = \frac{1}{2}Cr. \tag{21}$$

Thus, Eq. (13) can be written as

$$\frac{1}{2}Cr = \frac{a_1\alpha}{Wi}\int_{0}^{\infty} \frac{\dot{\gamma}se^{-s/Wi}}{\alpha + \dot{\gamma}^2 s^2}ds, \tag{22}$$

The constant C is determined from the boundary condition at the tube entrance where a velocity profile $w^{in}(r)$ is prescribed by

$$w^{in}(r) = 1 - r^2 \quad \text{so that} \quad w^{in}(0) = 1 \text{ and } w^{in}(1) = 0, \tag{23}$$

and we have

$$\int_0^1 r w^{in} dr = \int_0^1 r(1 - r^2) dr = \frac{1}{4}. \tag{24}$$

By conservation of mass, we must therefore have

$$\int_0^1 r\, w(r) dr = \frac{1}{4}, \tag{25}$$

and integrating by parts gives

$$\int_0^1 r\, w(r) dr = \Big[\frac{1}{2} r^2 w(r)\Big]_0^1 - \frac{1}{2}\int_0^1 r^2 \dot{\gamma} dr, \tag{26}$$

so that

$$\int_0^1 r^2 \dot{\gamma} dr = -\frac{1}{2}. \tag{27}$$

Therefore, for a given value of C, we compute $\dot{\gamma}(r)$ from Eq. (22) and check if

$$F(C) = \int_0^1 r^2 \dot{\gamma} dr + \frac{1}{2} = 0 \tag{28}$$

is satisfied.

The procedure for calculating the analytical solution is given by:

Step 1 An interval $\big[C_0,\ C_1\big]$ can be calculated where $F(C_0) * F(C_1) < 0$;

Step 2 By using the bisection method on the interval $\big[C_0,\ C_1\big]$, a value of C and $\dot{\gamma}(r)$ are computed such that $|F(C)| < eps$ where eps is the accuracy required. For this, Eq. (22) is evaluated by a 12-point-Gauss-Laguerre formulae and the integral in Eq. (28) is computed by the Simpson 1/3 quadrature rule.

Step 3 Calculate $\tau^{rz}(r), \tau^{rr}(r), \tau^{zz}(r)$ from Eqs. (21), (14) and (15), respectively.

4.2 Results

The numerical method described in Section 3. was applied to simulate tube flow of a 1-module KBKZ fluid using the following data:

- Velocity scale: $U = 0.025$ m s^{-1}.
- Length scale: tube radius $R = 0.01$m, tube length: $H = 10R = 0.1$m.
- Relaxation time and module: $\lambda_1 = \lambda_{ref} = 0.1396$s, $a_1 = 1.6648$ Pa.
- Dynamic viscosity: $\eta_0 = \lambda_1 \times a_1 = 0.2324$ Pa.s, density: $\rho_0 = 801.5$ kg m^{-3}.
- Papanastasiou parameters: $\alpha = 10.0$ and $\beta = 1.0$.
- Number of *deformation fields* $N = 100$.
- Reynolds and Weissenberg numbers: $Re = \dfrac{\rho U R}{\eta_0} = 0.8622$, $Wi = \lambda_{ref}\dfrac{U}{R} = 0.3490$.

To verify mesh independence results, this problem was simulated using the various meshes defined in Tab. 1. The explicit calculation of the momentum equations leads to a time-step restriction based on the Reynolds number given by $\delta t < Re\,\dfrac{1}{4}\delta r^2$ where uniform meshes ($\delta r = \delta z$) were used. Therefore, for reasons of accuracy, the time-step employed in the simulations, for each mesh used, are given in Tab. 1.

Table 1. Meshes employed in the tube flow simulations.

Mesh	$(\delta_r = \delta_z)/R$	Mesh size	$\delta_t * (U/R)$
M10	0.1000	(10x100)	2.1554x10^{-4}
M20	0.0500	(20x200)	5.3887x10^{-5}
M30	0.0333	(30x300)	2.3949x10^{-5}
M40	0.0250	(40x400)	1.3471x10^{-5}

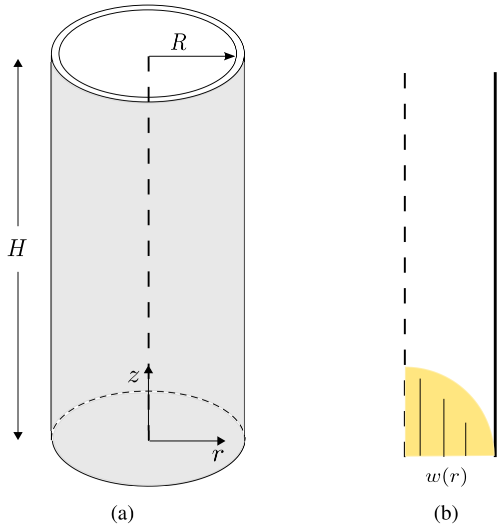


Figure 1. Description of flow domain (a) and the computational domain (b).

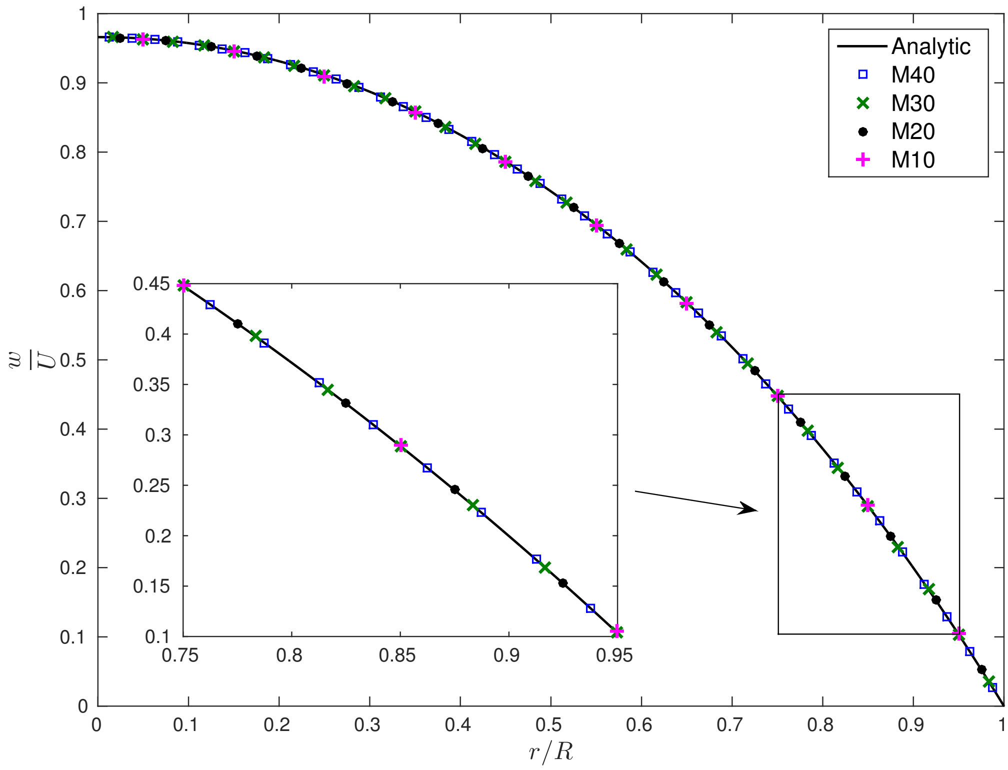
The simulations were started at $t = 0$ and were carried out until $t = 250$, when it was assumed that at this time, steady state has been established. The analytic value of the pressure gradient found by the bisection method was $dp/dz = -4.0239142$ while the numerical values obtained on each mesh employed were -4.003365, -4.016398, -4.020535, -4.022304, respectively. The results obtained for $w(r)$ and $\partial w(r)/\partial r$ are plotted in Fig. 2 while the results for the tensor components are displayed in Figs. 3 and 4. In Figs. 2 - 4, it is seen that the numerical solutions on meshes M10, $\cdots$, M40 agree well with the corresponding analytic solutions. In addition, the errors calculated by Eq. (29) are shown in Tab. 2 and plotted in Fig. 5, which confirms the decay of the error with mesh refinement. In Tab. 2 it is also possible to verify that the pressure gradient obtained by the numerical results approximates well the pressure gradient obtained by the analytic solution.

$$E(\cdot) = \sqrt{h\left[(\cdot)_{analytic} - (\cdot)_{numerical}\right]^2}, \quad h = \delta_r = \delta_z. \tag{29}$$

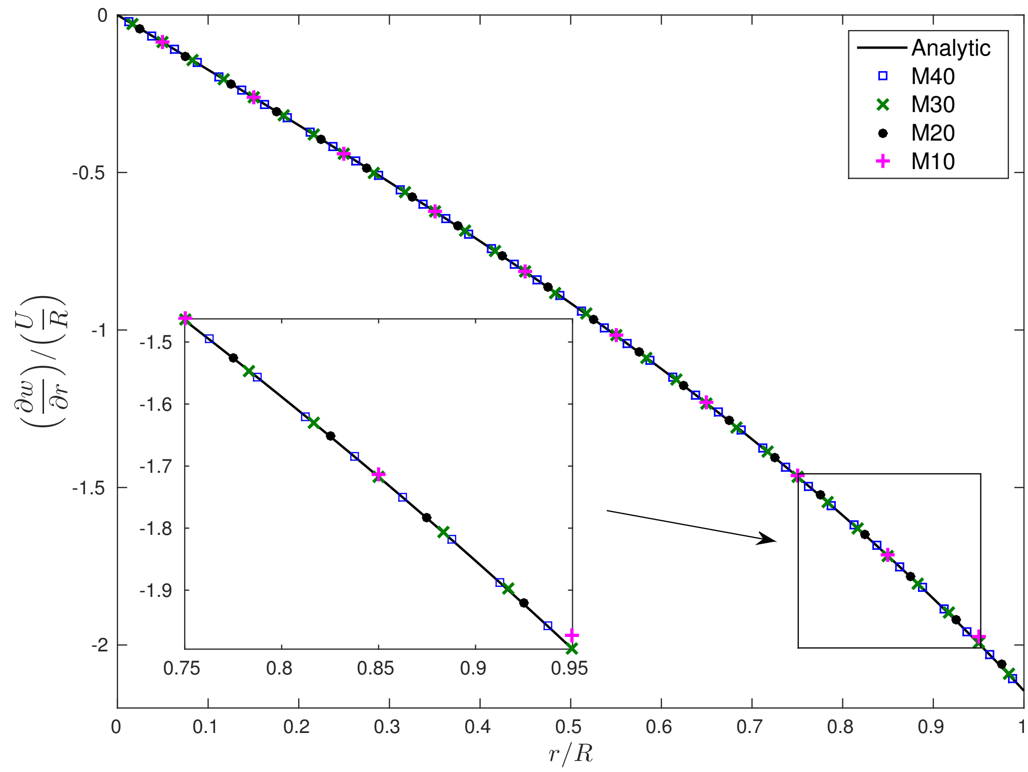
These results verify the convergence of the numerical method for tube flows when the mesh is refined.

Table 2. Errors between analytic and numerical solutions calculated on meshes M10, M20, M30 and M40.

Mesh	$E(w)$	$E(dw/dr)$	$E(\tau^{rz})$	$E(\tau^{zz})$	$E(dp/dz)$
M10	$1.3612e^{-3}$	$7.0306e^{-3}$	$4.9284e^{-3}$	$1.2002e^{-2}$	$6.4979e^{-3}$
M20	$4.6185e^{-4}$	$1.8021e^{-3}$	$1.4624e^{-3}$	$3.1720e^{-3}$	$1.6804e^{-3}$
M30	$2.1185e^{-4}$	$7.8236e^{-4}$	$8.3103e^{-4}$	$2.0075e^{-3}$	$6.1689e^{-4}$
M40	$1.2880e^{-4}$	$4.4901e^{-4}$	$4.9009e^{-4}$	$1.7629e^{-3}$	$2.5455e^{-4}$

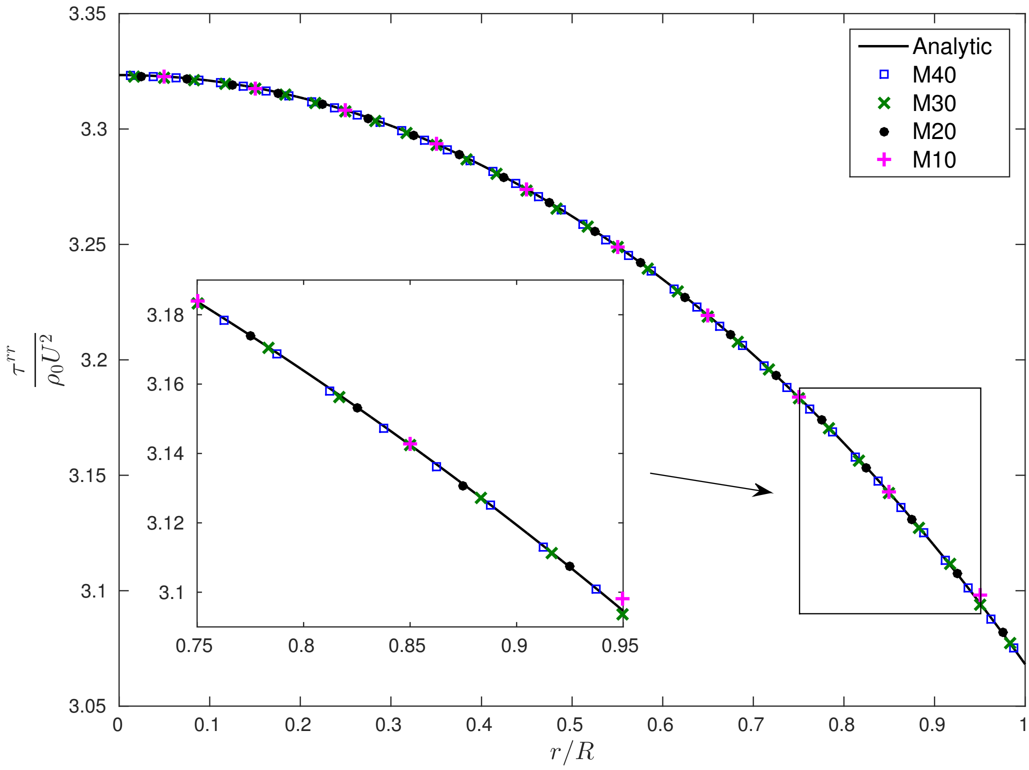


(a)

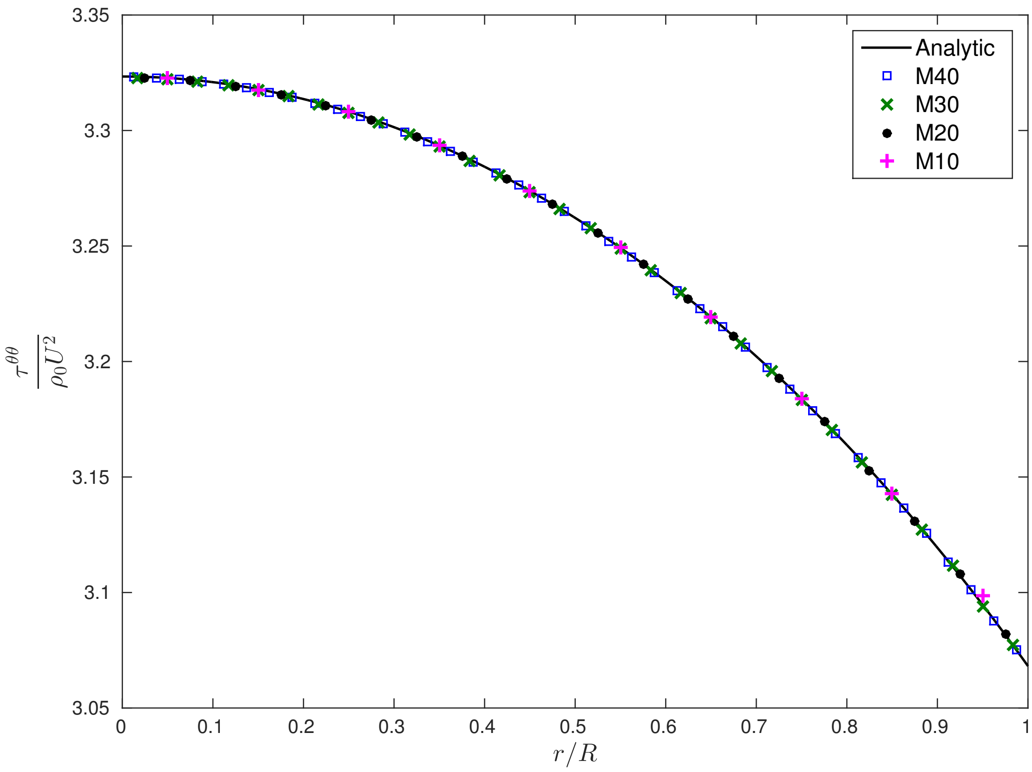


(b)

Figure 2. Numerical and analytic solutions of fully developed tube flow using mesh refinement. (a) $w(r)$ and (b) $\partial w(r)/\partial r$.

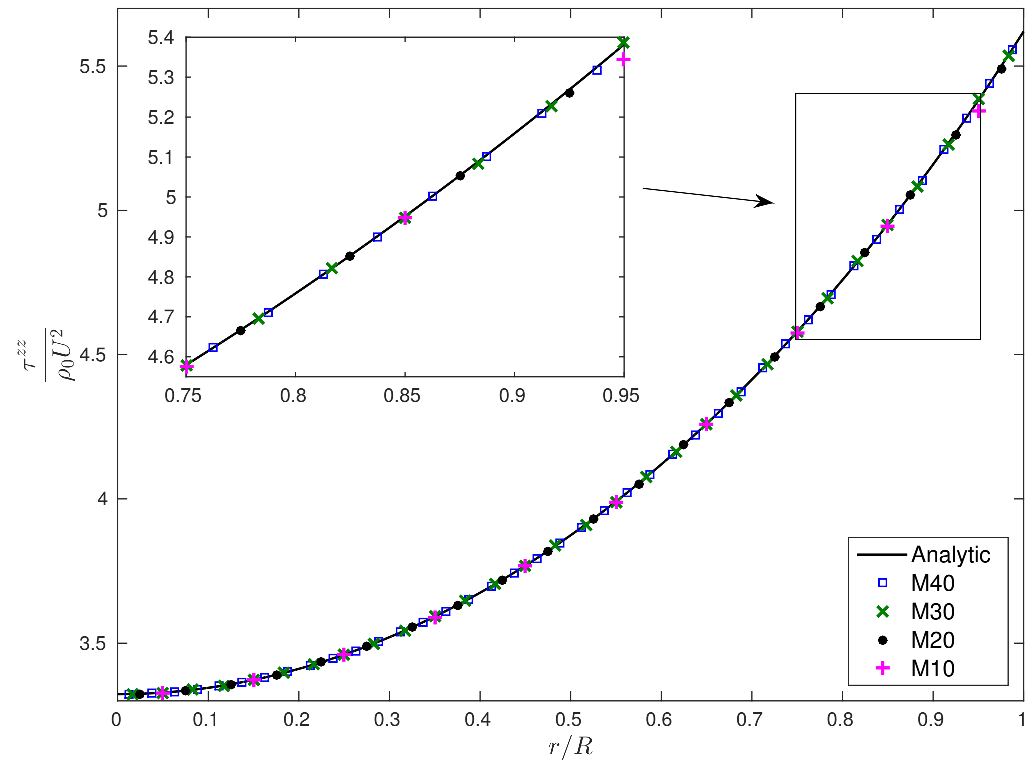


(a)



(b)

Figure 3. Comparison of (a) $\tau^{rr}(r)$ and (b) $\tau^{\theta\theta}(r)$ obtained on meshes M10, M20, M30 and M40 with the respective analytic solution.



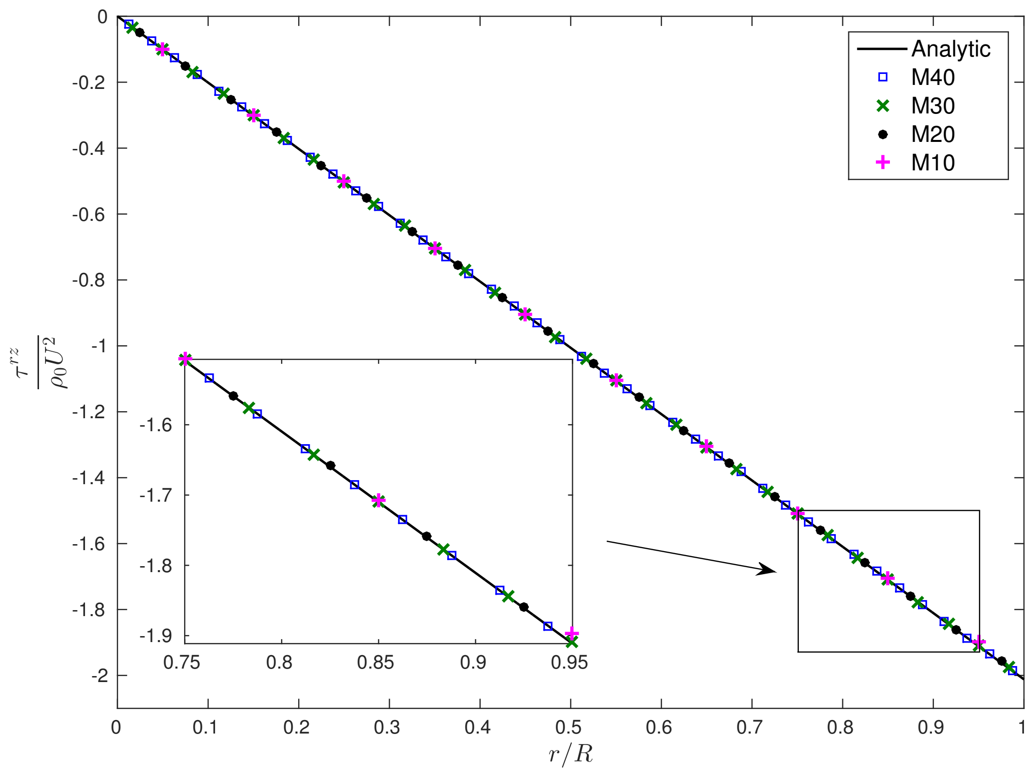


Figure 4. Comparison of (a) $\tau^{zz}(r)$ and (b) $\tau^{rz}(r)$ obtained on meshes M10, M20, M30 and M40 with the respective analytic solution.

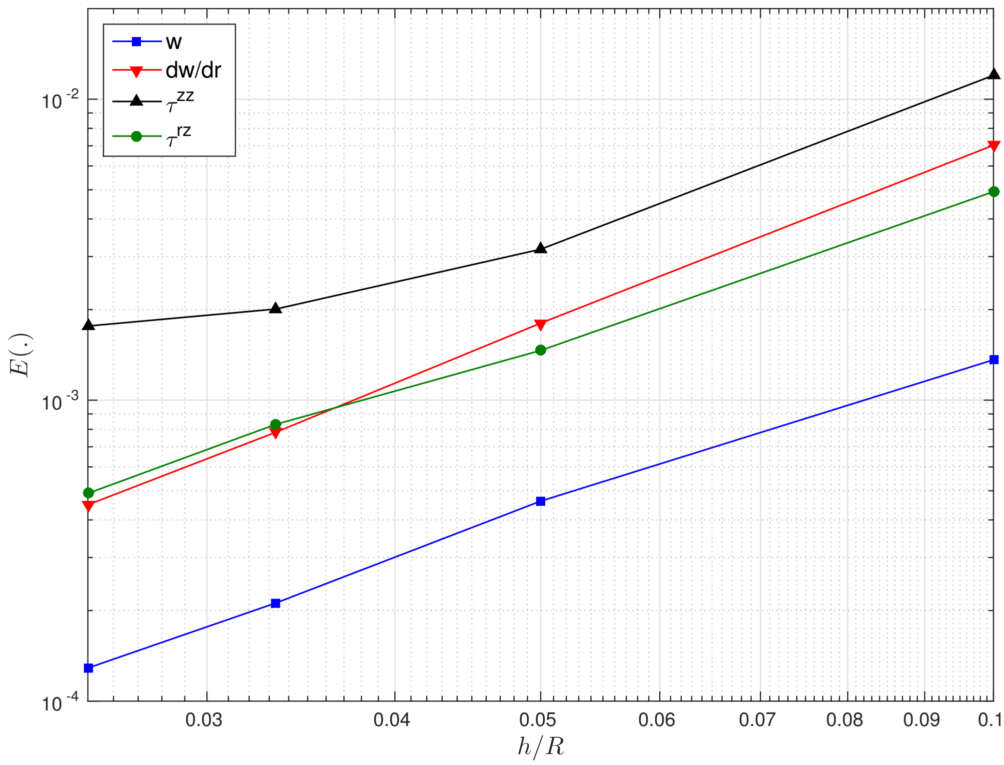


Figure 5. Decreasing of the error as function of mesh spacing h.

5. CONCLUSIONS

This work proposed a finite difference technique for solving viscoelastic flows governed by the integral constitutive KBKZ-PSM model. An analytic solution of a 1-mode KBKZ model for fully developed tube flows was developed. Tube flow was simulated on various meshes and verification results using the analytic solution demonstrated the convergence and mesh independence of the numerical method. As future work, this methodology will be improved by implementing an implicit method to solve the momentum equations and the calculation of the Finger tensor will be effected implicitly.

6. ACKNOWLEDGEMENTS

The authors would like to acknowledge the financial support given by the funding agencies: CNPq - Conselho Nacional de Desenvolvimento Científico e Tecnológico (Grant No. 306280/2014-0, 150282/2017-6 and 164517/2017-0), FAPESP - Fundação de Amparo a Pesquisa do Estado de São Paulo (Grant No. 2013/07375-0) (CEPID-CeMEAI project) and CAPES - Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (Grant No. PROEX-9259544/D). MV acknowledges the award of a visiting researcher grant within the Government of Brazil's "Science without Borders" programme, as well as a visiting researcher grant from the University of São Paulo.

7. REFERENCES

Bernstein, B., Kearley, E.A. and Zapas, L.J., 1963. "A study of stress relaxations with finite strain". *Transactions of the Society of Rheology*, Vol. 7, pp. 391–410.

Goublomme, A. and Crochet, M.J., 1993. "Numerical prediction of extrudate swell of a high-density polyethylene". *Journal of Non-Newtonian Fluid Mechanics*, Vol. 47, pp. 281–287.

Hulsen, M.A., Peters, E.A.J.F. and van den Brule, B.H.A.A., 2001. "A new approach to the deformation fields method for solving complex flows using integral constitutive equations". *Journal of Non-Newtonian Fluid Mechanics*, Vol. 98, pp. 201–221.

Konaganti, V.K., Ansari, M., Mitsoulis, E. and Hatzikiriakos, S.G., 2015. "Extrudate swell of a high-density polyethylene melt: II. modeling using integral and differential constitutive equations". *Journal of Non-Newtonian Fluid Mechanics*, Vol. 225, pp. 94–105.

Konaganti, V.K., Ansari, M., Mitsoulis, E. and Hatzikiriakos, S.G., 2016. "The effect of damping function on extrudate swell". *Journal of Non-Newtonian Fluid Mechanics*, Vol. 236, pp. 73–82.

Luo, X.L. and Mitsoulis, E., 1990. "A numerical study of the effect of elongational viscosity on vortex growth in contraction flows of polyethylene melts". *Journal of Rheology*, Vol. 34, pp. 309–342.

Mitsoulis, E., 2013. "50 years of the K-BKZ constitutive relation for polymers". *ISRN Polymer Science*, Vol. 2013.

Papanastasiou, A.C., Scriven, L.E. and Macosko, C.W., 1983. "An integral constitutive equation for mixed flows: viscoelastic characterization". *Journal of Rheology*, Vol. 27, pp. 387–410.

Rajagopalan, D., Armstrong, R.C. and Brown, R.A., 1990. "Finite element methods for calculation of steady, viscoelastic flow using constitutive equations with a Newtonian viscosity". *Journal of Non-Newtonian Fluid Mechanics*, Vol. 36, pp. 159–192.

Tomé, M.F., Bertoco, J., Oishi, C.M., Araujo, M.S.B., Cruz, D., Pinho, F.T. and Vynnycky, M., 2016. "A finite difference technique for solving a time strain separable K-BKZ constitutive equation for two-dimensional moving free surface flows". *Journal of Computational Physics*, Vol. 311, pp. 114–141.

Tomé, M.F., Grossi, L., Castelo, A., Cuminato, J.A., McKee, S. and Walters, K., 2007. "Die-swell, splashing drop and a numerical technique for solving the Oldroyd B model for axisymmetric free surface flows". *Journal of Non-Newtonian Fluid Mechanics*, Vol. 141, pp. 148–166.

8. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.