A NUMERICAL INVESTIGATION OF THE THIXOTROPIC EFFECTS IN A STRUCTURED FLUID FLOW AROUND A CYLINDER CONFINED BETWEEN TWO PARALLEL PLATES

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Abstract. *Many materials with industrial applications exhibit a thixotropic behavior. Thixotropic fluid has as main feature the breaking of the structure by applying a shear and a restructuring with the removal of this stress. This process is reversible and occurs isothermally. This article aims to study the behavior of these materials, using a model recently proposed by de Souza Mendes, 2009. The equations used in this model is solved by a stabilized finite element method (GLS method). A sensitivity analysis is presented to a creeping flow around a cylinder in a confined planar channel, where the parameters relevant to the model is scanned in order to study their influences.*

Keywords: *viscoplastic fluids, Thixotropy, structured fluids, complex flows.*

1. INTRODUCTION

Modeling the behavior of materials has always been of interest to researchers and scientists. The interest is even greater when these materials are present in industrial activities. Materials that exhibit a thixotropic behavior are among the materials of great interest to researchers and industries. Examples of such materials can be mentioned: emulsions, paints, nano-composites, gels, drilling fluids, foods and minerals.

Even with the aforementioned reasons, there is still a great shortage of models that describe this type of material. Some researchers have presented alternative models that describe such materials. Are among the most recent Mujumdar et al., 2002, which developed a model to describe the rheological behavior of thixotropic fluids with yield stress and elasticity, based on the kinetic process responsible for structure changes in the fluid. A structure parameter that indicates the level of structure of the material was defined. Petera and Kotynia, 2004, proposed a modified Maxwell model to predict the viscoelastic and thixotropic behavior of semi-solid alloys, and tested the model using an available experiment in the literature, with good results. Recently de Souza Mendes, 2009, presented an interesting model for thixotropic fluids. The constitutive equation is based on the upper-convected Maxwell constitutive equation, modified to include structuring level dependence in both the elastic modulus and the viscosity. The structure parameter is governed by an evolution equation that is purely hyperbolic in steady flows.

The aim of the present article is to analyze the performance in complex flow of the constitutive equation for elasto-viscoplastic thixotropic fluids recently proposed by de Souza Mendes . A numerical investigation is performed for the permanent flow of a fluid structured around a cylinder between two parallel plates. The relationship between the channel height and diameter of the cylinder is held fixed. Inertia is neglected and elastic effects are assessed by a relevant set of governing parameters. All numerical results proved to be physically meaningful and according to the related literature, indicating that constitutive equation is capable of giving a good prediction of the mechanical behavior of the thixotropic fluid.

2. MATERIAL BEHAVIOR

The model used herein describes a thixotropic fluid with elasticity. To compound the thixotropic and elastic effects, a constitutive equation proposed (de Souza Mendes, 2009) is developed starting from an equation to describe an elastic fluid, Maxwell-B model, with modifications. Here, viscosity and elastic modulus are functions of a parameter to represent the level of structure of the material. An evolutionary equation is developed to describe this parameter, which is taken into account effects of time and which is a function of shear stress applied, property which determines the breakdown of the structure.

2.1 Constitutive equation

The constitutive equation used to describe the behavior of a thixotropic material have which base the Maxwell-B equation for the viscoelastic fluids modified, where a structural viscosity and elastic modulus are dependent on a parameter for the material structure. This parameter is described by an evolutive equation presents in the following section. Thus, we have:

$$\boldsymbol{\tau}+\theta(\lambda)\overset{\nabla}{\boldsymbol{\tau}}=2\eta_v(\lambda)\mathbf{D}(\mathbf{u}) \tag{1}$$

where $\boldsymbol{\tau}$ is extra-stress tensor, **D** is the strain rate tensor. The structural viscosity, η_v, and modulus of elasticity, G_s are described respectively by:

$$\eta_v(\lambda)=\left(\frac{\eta_0}{\eta_\infty}\right)^{\lambda}\eta_\infty \quad \text{and} \quad G_s(\lambda)=\frac{G_0}{\lambda^m} \tag{2}$$

where η_o is the viscosity of the fluid in its state of highest structuring level ($\lambda = 1$); and η_∞ is the viscosity of the fluid in its state of lowest structuring level ($\lambda = 0$).

The relaxation time of the fluid, θ, therefore, is also a implicit function of λ and given by:

$$\theta(\lambda)=\frac{\eta_v(\lambda)}{G_s(\lambda)} \tag{3}$$

In a brief analysis, it is noted that for higher structure levels, high values of relaxation times are also obtained and in consequence, elasticity effects are shown. For an unstructured material, the behavior shown is similar to a generalized Newtonian fluid.

2.2 Evolutive equation for the structure parameter

According to the expression proposed by de Souza Mendes (2009), it is assumed that the equation for the evolutive parameter structure, λ, follows the following structure:

$$\mathbf{u}\cdot\nabla\lambda=\frac{1}{t_{eq}}\left[(1-\lambda)^a-(1-\lambda_{eq})^a\left(\frac{\lambda}{\lambda_{eq}}\right)^b\left(\frac{\tau}{\eta_v(\lambda)\dot{\gamma}}\right)^c\right] \tag{4}$$

where a and b are positive scalar coefficients, τ is the stress modulus applied on the fluid and **u** the velocity vector. In the evolution equation, the left side represents the rate of change of structure in time. On the right side, the first term represents the accumulation or growth of the structure, and the second term determines the break of structure. The parameter t_{eq} is called equilibrium time. It has the function of the time scale for the process of accumulation of the microstructure. It is important to note that the function associated with the break term is dependent of the stress module applied to the fluid, where the stress level that produces the breakdown of the material structure. When a particle fluid is subjected to a constant stress for a time long enough, the structure of the material tends to reach an equilibrium level on this stress. This structure in a state of equilibrium is given by the following expression:

$$\lambda_{eq}(\dot{\gamma})=\frac{\ln\eta_{eq}(\dot{\gamma})-\ln\eta_\infty}{\ln\eta_0-\ln\eta_\infty} \tag{5}$$

where η_∞ is the viscosity of the material unstructured and η_0 is the viscosity of the completely structured material. The viscosity in a equilibrium state, η_{eq}, is given by the equation proposed in Mendes de Souza (2004) for viscoplastic fluids.

By definition, the structure parameter of the material ranges between 0 and 1. For structure parameter equal to 0 have a material with a structure completely broken. As for a material with the structure parameter equal to 1, we can say that he is fully structured.

3. NUMERICAL MODELING

Numerical solutions were obtained via stabilized finite element approximations of the mass and momentum balance equations, constitutive equation for the material behavior and a new evolutive equation for the structure parameter. Here, GLS (Galerkin Least-squares) method is applied in terms of the structure parameter, extra- stress, pressure and velocity. Thus, we can establish the following problem of boundary condition: Find the quadruple such that $\forall(\phi, \mathbf{S}, q, \mathbf{v}) \in \Lambda\times\mathbf{\Sigma}\times P\times\mathbf{V}$

$$\begin{aligned}
&B(\lambda^h, \boldsymbol{\tau}^h, p^h, \mathbf{u}^h, \phi^h; \mathbf{S}^h, q^h, \mathbf{v}^h) = (2\eta_p)^{-1}\int_\Omega \boldsymbol{\tau}^h\cdot\mathbf{S}^h d\Omega - \int_\Omega \mathbf{D}(\mathbf{u}^h)\cdot\mathbf{S}^h d\Omega + \int_\Omega \boldsymbol{\tau}\cdot\mathbf{D}(\mathbf{v}^h) d\Omega \\
&+ (2\eta_p)^{-1}\int_\Omega \theta(\lambda)(\nabla\boldsymbol{\tau}^h)\mathbf{u}^h\cdot\mathbf{S}^h d\Omega - (2\eta_p)^{-1}\int_\Omega \theta(\lambda)\nabla\mathbf{u}^h\boldsymbol{\tau}^h\cdot\mathbf{S}^h d\Omega - (2\eta_p)^{-1}\int_\Omega \theta(\lambda)\boldsymbol{\tau}^h\nabla(\mathbf{u}^h)^T\cdot\mathbf{S}^h d\Omega \\
&+ \int_\Omega \mathbf{u}^h\cdot\nabla\lambda^h\phi^h d\Omega + \int_\Omega t_{eq}^{-1}\left[\sum_{i=1}^{n}\binom{a}{i}\lambda_i^{h^i}\right]\phi^h d\Omega + \int_\Omega t_{eq}^{-1}\left[\left(\frac{\lambda}{\lambda_{ss}}\right)^b\left(\frac{\tau}{\eta_v(\lambda)\dot\gamma}\right)^c\right]\phi^h d\Omega \\
&- \int_\Omega t_{eq}^{-1}\left[\sum_{i=1}^{n}\binom{a}{i}\lambda_{ss}^i\left(\frac{\lambda^h}{\lambda_{ss}}\right)^b\left(\frac{\tau}{\eta_v(\lambda)\dot\gamma}\right)^c\right]\phi^h d\Omega - \int_\Omega p\,\mathrm{div}\,\mathbf{v}^h d\Omega - \int_\Omega \mathrm{div}\,\mathbf{u}^h q^h d\Omega \\
&+ \int_\Omega \delta(x)\,\mathrm{div}\,\mathbf{u}^h\,\mathrm{div}\,\mathbf{v}^h d\Omega + \sum_{K\in\Omega^h}\int_{\Omega_K}(\nabla p^h - \mathrm{div}\,\boldsymbol{\tau})\cdot\alpha(\boldsymbol{x})(-\nabla q^h + \mathrm{div}\,\mathbf{S}^h) d\Omega + \epsilon\int_\Omega p^h q^h d\Omega \\
&+ 2\eta_p\int_\Omega ((2\eta_p)^{-1}\boldsymbol{\tau}^h + (2\eta_p)^{-1}\theta(\lambda)((\nabla\boldsymbol{\tau}^h)\mathbf{u}^h - \nabla\mathbf{u}^h\boldsymbol{\tau}^h - \boldsymbol{\tau}^h\nabla(\mathbf{u}^h)^T) + \mathbf{D}(\mathbf{u})^h)\ \mathrm{x} \\
&\qquad \mathrm{x}\,\beta(\mathrm{De}_K)((2\eta_p)^{-1}\mathbf{S}^h + (2\eta_p)^{-1}\lambda((\nabla\mathbf{S}^h)\mathbf{u}^h - \nabla\mathbf{u}^h\mathbf{S}^h - \mathbf{S}^h\nabla(\mathbf{u}^h)^T) - \mathbf{D}(\mathbf{v})^h) d\Omega \\
&+ \int_\Omega\left[\mathbf{u}^h\cdot\nabla\lambda^h + \sum_{i=1}^{n}\binom{a}{i}\lambda_i^{h^i} + \left(\frac{\lambda^h}{\lambda_{ss}}\right)^b\left(\frac{\tau}{\eta_v(\lambda)\dot\gamma}\right)^c - \sum_{i=1}^{n}\binom{a}{i}\lambda_{ss}^i\left(\frac{\lambda^h}{\lambda_{ss}}\right)^b\left(\frac{\tau}{\eta_v(\lambda)\dot\gamma}\right)^c\right]\mathrm{x} \\
&\qquad \mathrm{x}\ \psi(\boldsymbol{x})\left[\mathbf{u}^h\cdot\nabla\lambda^h + \sum_{i=1}^{n}\binom{a}{i}\phi_i^{h^i} + \left(\frac{\phi^h}{\lambda_{ss}}\right)^b\left(\frac{\tau}{\eta_v(\lambda)\dot\gamma}\right)^c - \sum_{i=1}^{n}\binom{a}{i}\lambda_{ss}^i\left(\frac{\phi^h}{\lambda_{ss}}\right)^b\left(\frac{\tau}{\eta_v(\lambda)\dot\gamma}\right)^c\right] d\Omega \\
&= \int_\Omega \mathbf{f}\cdot\mathbf{v}^h d\Omega + \int_\Omega t_{eq}^{-1}\phi^h d\Omega + \int_{\Gamma_h}\mathbf{t}_h\cdot\mathbf{v}^h d\Gamma + \sum_{K\in\Omega^h}\int_{\Omega_K}\mathbf{f}\cdot\alpha(\boldsymbol{x})(-\nabla q^h + \mathrm{div}\,\mathbf{S}) d\Omega \\
&+ \sum_{K\in\Omega^h}\int_{\Omega_K} t_{eq}^{-1}\psi(\boldsymbol{x})\left[\mathbf{u}^h\cdot\nabla\lambda^h + \sum_{i=1}^{n}\binom{a}{i}\phi_i^{h^i} + \left(\frac{\phi^h}{\lambda_{ss}}\right)^b\left(\frac{\tau}{\eta_v(\lambda)\dot\gamma}\right)^c - \sum_{i=1}^{n}\binom{a}{i}\lambda_{ss}^i\left(\frac{\phi^h}{\lambda_{ss}}\right)^b\left(\frac{\tau}{\eta_v(\lambda)\dot\gamma}\right)^c\right] d\Omega
\end{aligned} \tag{6}$$

where the stability parameters α and δ are the ones proposed in Franca and Frey for constant viscosity fluids; ψ is the parameter introduced in Franca et al. in the context of the advection-diffusion equation; and the parameter β is set to 1, according to GLS error estimates established in Behr et al. Moreover, the non-linear system of equations obtained from the discretization of GLS formulation is solved by a quasi- Newton method. This algorithm makes use of a frozen Jacobian gradient strategy, updating the Jacobian matrix at each two or three iterations only.

4. DIMENSIONLESS PARAMETERS

This paper presents a non-dimensionalization proposed by de Souza Mendes (2007 and 2009), where the kinematic effects of the flow are decoupled from the rheological effects of the material.

Thus, the set of dimensionless variables below are considered

$$t^* = t\dot\gamma_1;\ \ \mathbf{x}^* = \frac{\mathbf{x}}{R};\ \ \mathbf{u}^* = \frac{\mathbf{u}}{\dot\gamma_1 R};\ \ \dot\gamma^* = \frac{\dot\gamma}{\dot\gamma_1};\ \ p^* = \frac{p}{\tau_{od}};\ \ \boldsymbol{\tau}^* = \frac{\tau}{\tau_{od}};\ \ \eta_v^*(\dot\gamma^*) = \frac{\eta_v(\dot\gamma)}{\eta_v(\dot\gamma_1)} = \frac{\eta_v(\dot\gamma)}{k\dot\gamma_1^{n-1}} \tag{7}$$

where the τ_{0d} is the dynamic yield stress .

From the group of dimensionless variables, we can write the dimensionless equations that govern the thixotropic fluid flow and its boundary conditions, giving rise to the following dimensionless groups that govern the flow:

$$\theta^* = \theta(\lambda)\dot\gamma_1 \Rightarrow \theta_0^* = \theta(1)\dot\gamma_1 = \frac{\tau_0}{G_0}(J+1);\quad U^* = \frac{u_c}{\dot\gamma_1 R};\quad J \equiv \frac{\dot\gamma_1 - \dot\gamma_0}{\dot\gamma_0} = \frac{\dot\gamma_1}{\dot\gamma_0} - 1;\quad t_{eq}^* = t_{eq}\dot\gamma_1 \tag{8}$$

In Eq. (8), the first equation is obtained from the dimensionless constitutive equation, where the elastic terms gives rise to a dimensionless relaxation time, that can also be considered as a version of rheological Deborah number. From the Dirichlet boundary condition for the dimensionless velocity arises the intensity flow U^*, which is the dimensionless parameter that takes into account the flow kinematic. From the dimensionless steady-state viscosity function, the jump number J appears. This number provides a relative measure for the plateau formed when the shear rate jumps from $\dot\gamma_{0_d} \equiv \tau_{0_d}/\eta_0$ to $\dot\gamma_1 \equiv (\tau_{0_d}/K)^{1/n}$. Finally, the evolution equation contributes to the analysis allowing defining a dimensionless time change of the material structure, t^*_{eq}, which does not take into account the kinematics of the flow, but only the rheological effects of the material.

5. NUMERICAL RESULTS

In this section we present results obtained by numerical simulations using a four-field GLS method of a creeping flow around a cylinder confined between two flat plates. In the simulations, the aspect ratio provided by the channel height compared with the cylinder radius is equal to eight. The boundary conditions, described in Fig.1(a) are as follows: (i) no-slip and impermeability along the channel wall and on the cylinder surface ($\mathbf{u}$=0); (ii) symmetry along the channel centerline ($\tau_{12} =\partial_{x1}u_1=u_2=0$); (iii) uniform velocity and extra-stress profiles at the channel inlet ($\boldsymbol{\tau}$= 0, $u_1=\mathbf{U}$, u_2= 0); (iv) free-traction at the channel outlet ($[-p\mathbf{1} + 2\eta_v\ \mathbf{D}]\mathbf{n}=0$). Also, for the structure parameter, the following boundary conditions are imposed - (v) uniform profile along the channel inlet (λ=1); (vi) vanishing axial gradients along the other boundaries.

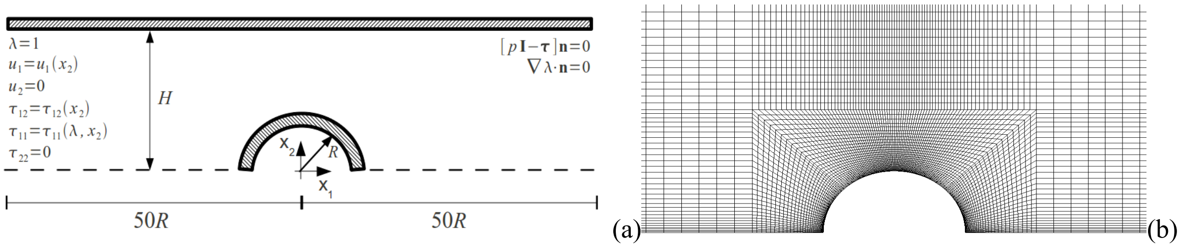


Figure 1 - Problem domain: (a) the geometry; (b) the mesh

The problem domain was discretized by three meshes with different refinements, using bi-linear quadrilateral elements. After a mesh independence study, using the drag coefficient as parameter, we choose a mesh with 5.830 Q1-elements. The mesh is more refined in the entrance, in the channel walls, and in surface of the cylinder, since these regions are subjected to severe boundary layers (Fig1(b)).

Figure 2 shows the structure parameter field, for U^*=1, n=0.5, J=200, θ_0^*=4 and t_{eq}^*=0.3-10. The equilibrium time t_{eq}^*, controls the intensity of the transport mechanism for the material structure level, since it multiplies the advective term of the evolution equation by the structure parameter. For low values of t_{eq}^*, the field of the structure parameter is approximately symmetrical. By increasing this parameter, the advection effect increases in both in the input channel as the surface of the cylinder.

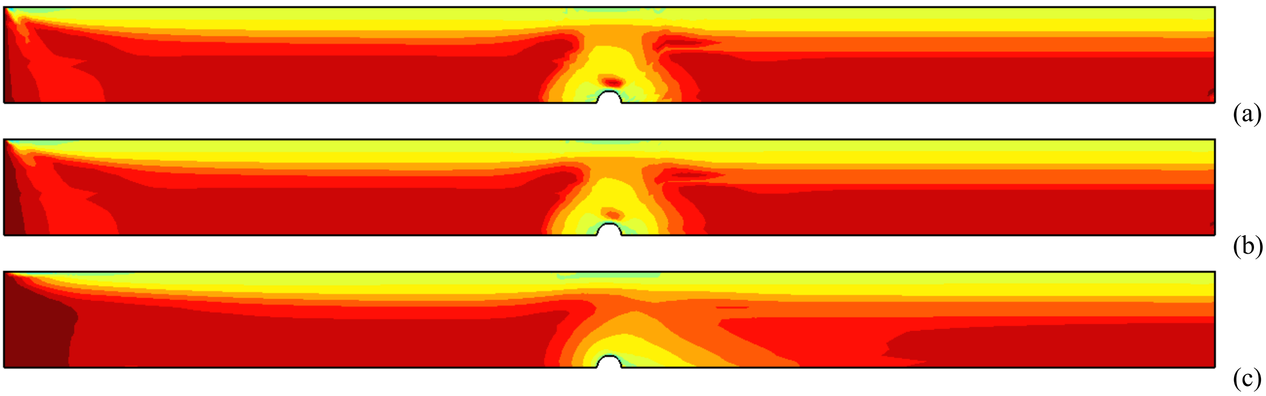
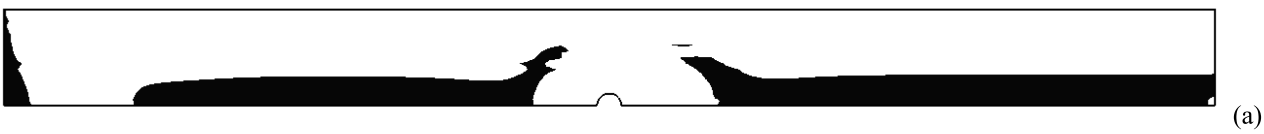
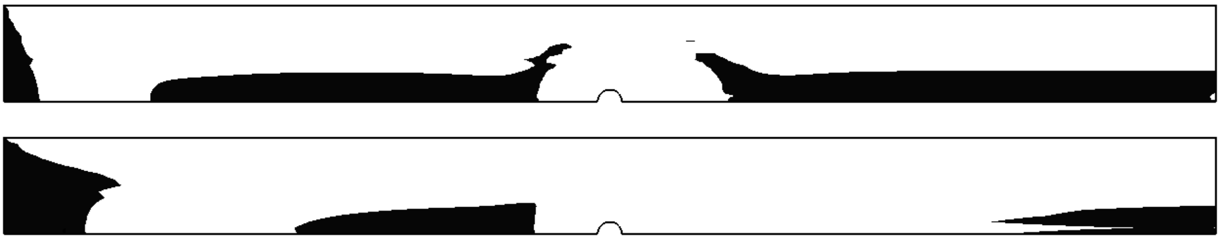


Figura 2 - Structure parameter field, for U^*=1, n=0.5, J=200 and θ_0^*=4: (a) t_{eq}^*=0.3; (b) t_{eq}^*=1; (c) t_{eq}^*=10.

In Fig.3 the unyielded regions are presented, for the same above described cases. The unyielded region is defined as the region where the material is considered structured. Therefore, we define the yield surface as the locus of points in which $\lambda_{ss}=\lambda_{ss}(\dot{\gamma}_0)\approx 0.9$. Thus, unyielded regions show the same pattern of the structure parameter field, being almost symmetric for low t_{eq}^*, and asymmetric due to the upwind effect experienced by its evolution equation.





(b)

(c)

Figura 3 - Unyielded regions, for U^*=1, n=0.5, J=200 and θ_0^*=4: (a) t_{eq}^*=0.3; (b) t_{eq}^*=1; (c) t_{eq}^*=10.

6. CONCLUSION

All the results confirmed the adequacy of the employed thixotropic model as an attractive alternative for modeling viscoplastic flows of materials presenting some degree of elasticity. Numerical modeling using a four-field GLS stabilizing procedure proved to be robust and efficient, even for an extremely complex mechanical model with nonlinear equations.

7. REFERENCES

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