ANALYSIS OF PLANE EXTRUDATE SWELL WITH AN ALGEBRAIC VISCOELASTIC CONSTITUTIVE EQUATION

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Abstract. *Free surface flows on non Newtonian liquids occur in different industrial processes, such as coating, polymer extrusion, and many others. The complete understanding of the liquid flow is vital to the optimization of these important manufacturing processes. The use of appropriate constitutive models to describe the mechanical behavior of the liquid and the presence of the free surface make the problem highly complex. In this work, the performance of an algebraic viscoelastic model that is still able to predict elastic phenomenona, such as normal stress difference and variable extensional and shear viscosity in the flow exiting a slot is analyzed. It is well known that viscoelastic liquids present an exaggerated "swelling" as it exits the slot, phenomenon known as extrudate swell. The differential equations that describe the problem, i.e. the momentum, continuity and mesh generation equations for the unknown physical domain, were solved by the Galerkin's / finite element method. The resulting non-linear algebraic system was solved by Newton's method. The results show that the use of the appropriate algebraic model can capture the main features of the well studied elastic phenomenon at a much smaller computational cost.*

Keywords: *Viscoelastic liquids, extrudate swell, finite element method.*

1. INTRODUCTION

Free surface flow of non Newtonian liquids occur in many different industrial processes, such as coating, polymer extrusion, fiber spinning, and many others. The complete understanding of the liquid flow is vital to the optimization of these important manufacturing processes.

Theoretical models of such flows are complex. The presence of the free surface makes the problem highly non linear, even in the case of Newtonian liquids. The physical domain where the flow occurs is unknown a priori and it is part of the solution. Moreover, the behavior of polymer solutions in complex flows is very sensitive to the local kinematics.

Polymer molecules behave quite differently in flow regions where the liquid is persistently stretched along the orientation of the molecules and in flow zones where the straining is oblique to molecular orientation. Some differential constitutive models can qualitatively describe the interaction of flow kinematics and polymer conformation in complex flows. However, the numerical solution of the momentum equation coupled with the differential constitutive relation is computationally expensive and challenging in flows where corners or contact lines introduce singularities in the velocity gradient. An alternative approach is to use algebraic models that relate stress to the rate-of-strain and relative-rate-of-rotation. They are perhaps the simplest and computationally most economical attempt at capturing the different behavior of polymer molecules in extension-dominated and shear-dominated flow zones. Recent advances in this class of models (Thompson et al, 1999) have produced a constitutive relation that describes shear thinning and normal stress differences in simple shear flow and extensional thickening in extensional flows.

This work analyzes the performance of the algebraic constitutive model presented by Thompson et al. (1999) in the flow of viscoelastic liquid exiting a slot, known as the extrudate swell flow. It is well known that viscoelastic liquid present an exaggerated swelling as it exits the slot. Several differential models have been used to predict swell ratios (Reddy and Tanner, 1978; Papanastasiou et al., 1987; Wesson et al., 1989; Wen-Yen and Goang-Ding, 1988).

The differential equations that describe the problem, i.e. the momentum, continuity and the mesh generation equation for the unknown physical domain were solved by the Galerkin's /finite element method. The results of the simpler and less expensive algbraic model are compared with the predictions of different differential constitutive equations.

2. GOVERNING EQUATIONS AND SOLUTION METHOD

Figure 1 shows the flow domain and boundary conditions used in the analysis. The velocity and pressure field of creeping flow are governed by the momentum and continuity equations, which in dimensionless form are

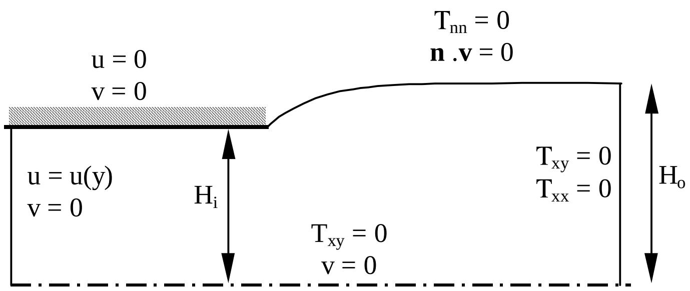

Figure 1: Sketch of flow domain and boundary conditions.

$$\nabla \cdot \mathbf{T} = 0 \quad \text{and} \quad \nabla \cdot \mathbf{v} = 0 . \tag{1}$$

The total stress $\mathbf{T}$ is the sum of pressure and viscous stress. Its relation with the flow kinematics is a function of the constitutive model used to describe the mechanical behavior of the liquid.

The differential equations (1) are posed in an unknown domain; the position of the liquid free surface is part of the solution. A simple way of solving this type of problem is to use a Picard iteration, i.e. solve the flow and the domain position separetely. To compute a free boundary problem, like this one, in a more efficient way, the set of differential equations posed in the unknown physical, domain has to be transformed to an equivalent set defined in a known reference domain, usually called computational domain. This transformation is done with the aid of the mapping $\mathbf{x} = \mathbf{x}(\xi)$. Here, the unknown physical domain is parametrized by the position **x**=(x,y), and the reference domain, parametrized by the position vector ξ=(ξ,η). The mapping is arbitrary, except that boundaries of the reference domain have to be continuously mapped onto the boundaries of the physical domain, and that the mapping has to be invertible. There are several ways to construct such mappings. Here, the inverse mapping is taken to satisfy the elliptic differential equation (see Santos, 1991):

$$\begin{aligned} \nabla \cdot \left[D_\xi \nabla \xi \right] = 0 \\ \nabla \cdot \left[D_\eta \nabla \eta \right] = 0 \end{aligned} . \qquad (2)$$

D_ξ and D_η control the spacing of the coordinates ξ and η of the reference domain. The differential equation (2) that describes the mapping between the unknown physical domain to the fixed reference domain is usually called the mesh generation equation.

In order to close the problem, the constitutive equation that relates the stress tensor with the liquid deformation has to be defined. The constitutive relation proposed by Thompson et al. (1999) is used here. The stress tensor **T** is a function of both the rate-of-deformation tensor **D** and the relative-rate-of-rotation tensor $\overline{\mathbf{W}}$. The latter is defined as

$$\overline{\mathbf{W}} = \mathbf{W} - \mathbf{\Omega},$$

where $\mathbf{W} \equiv \left[\nabla \mathbf{v} - \nabla \mathbf{v}^T \right] / 2$ is the vorticity tensor, and $\mathbf{\Omega}$ is a tensor related with the rate of rotation of the rate of strain $\mathbf{D} \equiv \left[\nabla \mathbf{v} + \nabla \mathbf{v}^T \right] / 2$ following the liquid particle motion. Based on the rate-of-deformation and relative-rate-of-rotation tensors, Astarita (1979) defined the flow classification index R to measure the degree to which the fluid particle avoids stretching. It is defined as

$$R \equiv \frac{\mathrm{tr}(\overline{\mathbf{W}}^2)}{\mathrm{tr}(\mathbf{D}^2)}.$$

The index takes the value of 0 in pure extension and 1 in shear flows. Moreover, as the motion approaches a rigid body motion, i.e. as $\mathbf{D} \to 0$, it approaches infinity.

As shown by Thompson et al. (1999), the simplified constitutive equation of this type that still has the capability of fitting independently rheological data for shear material functions and for extensional viscosity is

$$\mathbf{T} = -p\mathbf{I} + \alpha_1 \mathbf{D} + \alpha_2 \overline{\mathbf{W}}^2 + \alpha_4 \left(\mathbf{D} \cdot \overline{\mathbf{W}} - \overline{\mathbf{W}} \cdot \mathbf{D} \right). \qquad (3)$$

The coefficients α_i depend on the material functions of the liquid:

$$\begin{aligned} \alpha_1 &= 2\eta_s{}^R \eta_u{}^{(1-R)} \\ \alpha_2 &= -2 f(R) \left[\psi_1 + 2\psi_2 \right] \\ \alpha_4 &= f(R) \psi_1 \end{aligned}$$

The differential equations that govern the problem, i.e. equations (1) and (2), were solved all together with the finite element / Galerkin's method. The velocity, pressure and node position are represented in terms of basis functions:

$$u = \sum U_j \phi_j; \quad v = \sum V_j \phi_j; \quad p = \sum P_j \psi_j;$$
$$x = \sum X_j \phi_j; \quad y = \sum Y_j \phi_j$$

Because the stress tensor depends on the second derivative of the velocity field (through the definition of the index *R*), an additional variable **L** is introduced to represent the velocity gradient with a continuous interpolation. It is also represented in terms of basis functions:

$$L_{xx} = \sum Lxx_j \zeta_j; \quad L_{xy} = \sum Lxy_j \zeta_j; \quad L_{yy} = \sum Lyy_j \zeta_j$$

The corresponding weighted residuals of the Galerkin's method are:

$$R^i_{mx} = \int_{\overline{\Omega}} \left\{ \rho\phi_i \left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} \right) + \frac{\partial \phi_i}{\partial x} T_{xx} + \frac{\partial \phi_i}{\partial y} T_{xy} \right\} \|\mathbf{J}\| d\overline{\Omega} - \int_{\overline{\Gamma}} \mathbf{e_x} \cdot (\mathbf{n} \cdot \mathbf{T}) \phi_i \frac{d\Gamma}{d\overline{\Gamma}} d\overline{\Gamma}$$

$$R^i_{my} = \int_{\overline{\Omega}} \left\{ \rho\phi_i \left(u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} \right) + \frac{\partial \phi_i}{\partial x} T_{xy} + \frac{\partial \phi_i}{\partial y} T_{yy} \right\} \|\mathbf{J}\| d\overline{\Omega} - \int_{\overline{\Gamma}} \mathbf{e}_y \cdot (\mathbf{n} \cdot \mathbf{T}) \phi_i \frac{d\Gamma}{d\overline{\Gamma}} d\overline{\Gamma}$$

$$R^i_{mx} = \int_{\overline{\Omega}} \left\{ \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \psi_i \right\} \|\mathbf{J}\| d\overline{\Omega}$$

$$R^i_L = \int_{\overline{\Omega}} \{ \mathbf{L} - \nabla \mathbf{u} \} \zeta_i \|\mathbf{J}\| d\overline{\Omega}$$

$$R^i_X = \int_{\overline{\Omega}} - \{ D_\xi \nabla \xi \cdot \nabla \phi_i \} \|\mathbf{J}\| d\overline{\Omega} + \int_{\overline{\Gamma}} D_\xi (\mathbf{n} \cdot \nabla \xi) \phi_i \frac{d\Gamma}{d\overline{\Gamma}} d\overline{\Gamma}$$

$$R^i_Y = \int_{\overline{\Omega}} - \{ D_\eta \nabla \eta \cdot \nabla \phi_i \} \|\mathbf{J}\| d\overline{\Omega} + \int_{\overline{\Gamma}} D_\eta (\mathbf{n} \cdot \nabla \eta) \phi_i \frac{d\Gamma}{d\overline{\Gamma}} d\overline{\Gamma}$$

Biquadratic basis functions were used for the velocity and nodes coordinates, bilinear basis functions were used for the interpolated velocity gradient, and linear discountinuous functions for the pressure. The domain was devided into 400 elements with 9904 degrees of freedom. A representative mesh is shown in Fig.2.

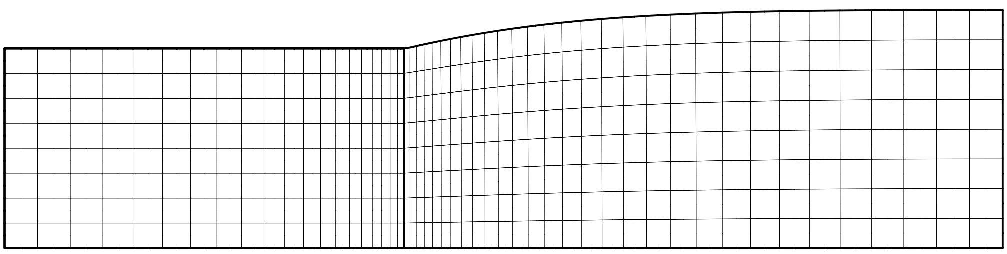

Figure 2: Representative mesh. The position of the free surface is the one predicted for the limiting case of Newtonian liquid. Number of elements = 400 and number of degrees of freedom = 9904.

Once the field variables are represented in terms of the basis functions, the system of partial differential equations become simultaneous algebraic equations for the coefficients of the basis functions.

$$\mathbf{R}(\mathbf{u})\,\mathbf{u} = 0$$

$\mathbf{u}$ is the solution vector. This set of equations is non-linear due to the constitutive relation and the unknown physical domain. The method of choice for this type of problem is Newton's method, which requires evaluation of the full Jacobian matrix, i.e.

$$\mathbf{J}\ \delta\mathbf{u} = -\mathbf{R}$$
$$\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \delta\mathbf{u}$$

$\mathbf{J}$ is the Jacobian matrix of sensitivities of the residuals to the unknowns, i.e. $J_{ij} = \partial R_i / \partial u_j$. The iteration procedure begins with an initial estimate $\mathbf{u}^{(0)}$ and continues until the system of equations (2) is nearly satisfied ($\|\mathbf{R}\| < 10^{-7}$). Free surface problems are strongly non-linear and a good initial guess is vital in order to Newton's method to converge. The solution at We = 0 was obtained using an initial guess that represented the solution of the flow in a fixed domain with perfectly slipery walls at the boundaries corresponding to the free surface. After that, zero order continuation on the Weissemberg number was used to obtain the the flow states presented here.

3. RESULTS

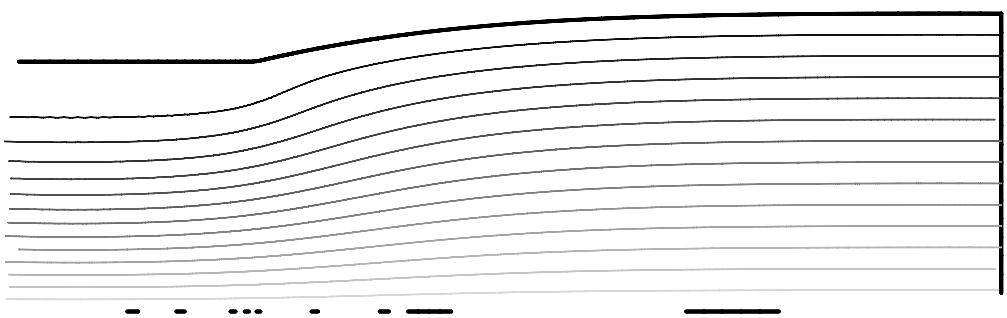

Figure 3: Streamlines of the extrudate swell flow for Newtonian liquid.

Figure 3 shows the streamlines for the limiting case of Newtonian liquids. The swell ratio, defined as H_0 / H_i, is a function of the capillary number $Ca \equiv \mu V / \sigma$ of the flow. In the case of vanishing surface tension, i.e. $Ca \to \infty$, there is an extrudate swell of approximately $H_0 / H_i = 1.2$, widely reported in the literature. The field of the flow classification index *R* of the Newtonian velocity field is shown in Fig.4. Inside the slot and close to the wall, the value of *R* is close to 1, indicating a pure shear flow. Close to the symmetry plane inside the slot, R approaches infinity, because there, the liquid is not deformed, i.e. there is a solid body motion. Far from the slot exit, the flow develops to a plug flow. As expected, R approaches infinity. Close to the slot exit, there is a region of extensional flow as the liquid particles are being stretched in the direction perpendicular to the flow. From the field of R, it can be noticed that the extrudate swell flow has three distinct regions where the fluid particles are deformed in different ways. The constitutive model used in the analysis has to be able to capture the behavior of the liquid in these different types of deformation.

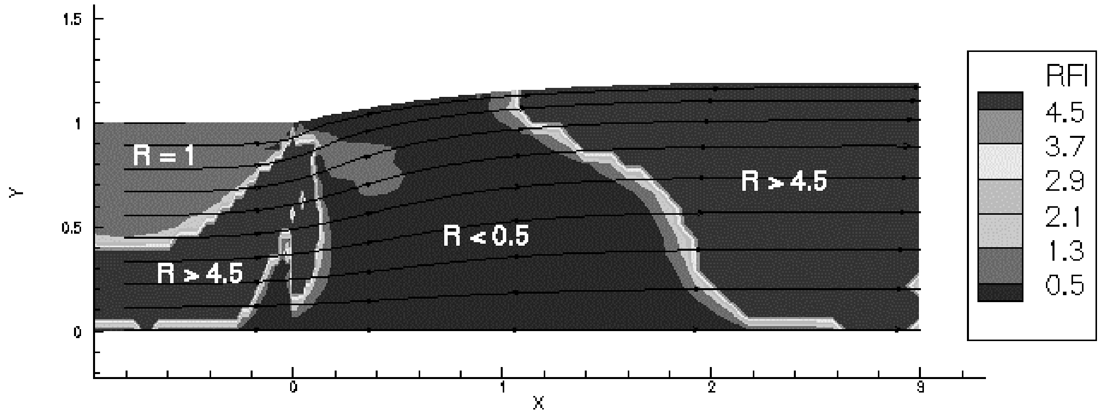

Figure 4: Field of the flow classification index R. R close to 1 indicates regions of shear predominant flow; R close to 0 indicates regions of extensional predominant flow

In order to calculate the coefficients α_i of the constitutive relation (3), the material functions of the liquid have to be defined. For simplification, it was assumed, in this first analysis, that the normal stress difference coefficients vanish, i.e. $\psi_1 = \psi_2 = 0$. The shear and extensional viscosity were chosen to follow a dependence on rate of deformation similar to the material functions yielded by the differential constitutive model of Giesekus (see Larson, 1988). In this case, the liquid is shear-thinning and extensional thicknenning. The parameters that define the material functions are η_0, β, λ and a. Fig.5 shows the shear and extensional viscosities for the case of $\eta_0 = 1, \beta = 0.59, \lambda = 0.1$ and $a = 0.1$.

The swell ratio is plotted as a function of the Weisemberg number in Fig.6. The Weisemberg number is defined as $We = \lambda V / H_i$, where V is the average velocity in the slot. The predictions obtained with the upper convected Maxwell differential constitutive model is also presented in the plot. The results obtained with the algebraic model tested here show that the swell ratio increases with Weissemberg number even for very small values of the dimensionless parameter. This behavior is not observed with the Maxwell model, the swell ratio first falls with *We* and then rises. Experimental measurements of Tanner (1970) were fitted to a monotonic curve on Weissemberg number, following the tendency predicted by the algebraic model.

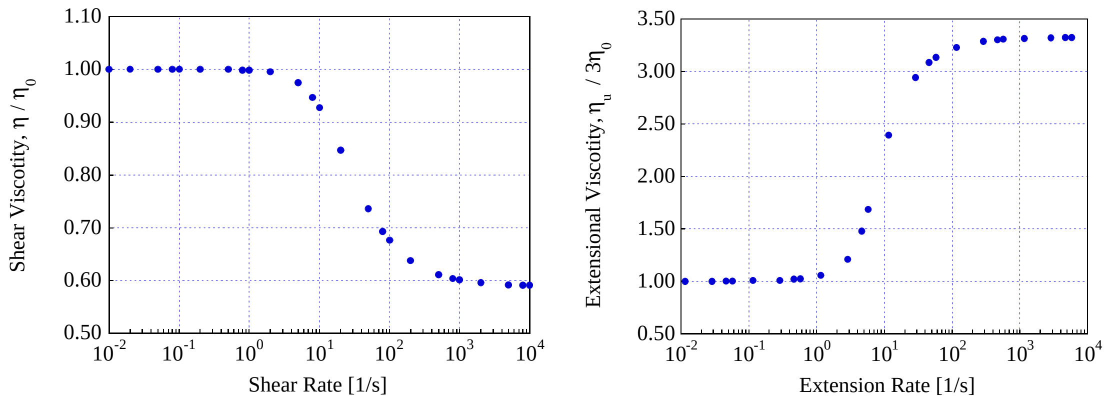

Figure 5: Shear and Extensional viscosity as function of deforamation rates.

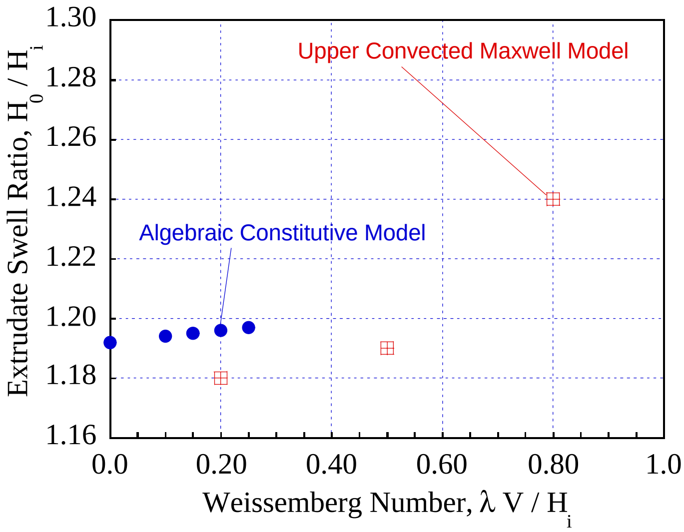

Figure 6: Extrudate Swell Ratio as a function of Weissember number.

The results obtained by the algebraic constitutive model are restricted to low Weissemberg numbers. Convergence problems are encountered at large values of the parameter. This issue is under investigation and it seems to be related with the precision of the linear solver used at each Newton step.

4. FINAL REMARKS

A free surface flow of a non Newtonian liquid was solved assuming an algebraic viscoelastic model proposed by Thompson et al. (1999) to describe the liquid behavior. This class of model is based on the flow classifiction index defined by Astarita (1979) and it is able to predict shear thinning and normal stress difference in shear flow and extensional thicknenning in extensional flow. The extrudate swell flow was investigated, and the results show that the flow has three distinct regions of deformation type: The flow inside the slot is predominantly a shear flow; close to the exit, it is mainly an extensional flow; and far from it, a solid body motion.

Although the predictions are still restricted to small values of Weissemberg number, the first results show that the tendency agrees with some experimental results and predictions by more complex and computationally expensive differential models.

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