Using Comsol Multiphysics to Model Viscoelastic Fluid Flow

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Viscoelastic fluids have first normal stress differences even in rectilinear flow. Thus, they are more complicated than purely viscous non-Newtonian fluids modeled as a power-law model or Carreau model. Viscoelastic effects must be included when modeling the flow of polymer melts and concentrated polymer solutions in situations for which the normal stresses matter. Such problems include the classic ones of stick-slip, extrudate swell, hole pressure, 4:1 contraction, and exit pressure. Both hole pressure and exit pressure problems provide means for measuring the normal stress differences.[1 2] The extrudate swell problem involves a free surface whose location must be obtained such that it is a streamline in the jet. This paper describes some key parameters of polymers, creates some models of viscoelastic fluids, and shows how to use Comsol Multiphysics to solve such models.

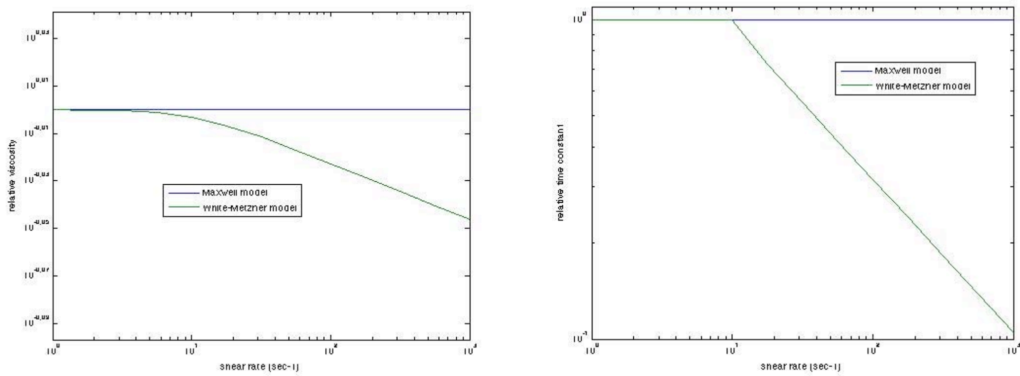
1. Introduction

Polymer properties. When a polymer is flowing between two flat plates in Couette flow the shear rate is constant across the layer. The shear stress is constant, too; since the viscosity is the shear stress divided by the shear rate, the viscosity is constant, too, in that flow. The viscosity of polymers varies with shear rate, though, so that different viscosities are obtained with different velocities (shear rates) in the Couette flow. Such fluids are called purely viscous non-Newtonian fluids. Polymer melts and concentrated polymer solutions exhibit an additional effect known as a first (and second) normal stress difference. This is the cause of swelling when a polymer comes out of a die, or the reason a polymer climbs a rotating rod. For these fluids, it is necessary to also model the normal stresses, which are elastic in nature. Typical plots of viscosity and first normal stress differences are shown in Figure 1 for a Maxwell model and for a 9% solution of polystyrene in dioctyl phthalate ($\hat{M}_w$ =153,000). The viscosity, η, and time constant, λ, are related to the shear stress and first normal stress by the following equations, valid for an Olydroyd model (see below).[3]

$$\tau = \eta\dot{\gamma}, \quad N_1 = 2\eta\lambda\dot{\gamma}^2, \ \text{or} \quad \eta = \frac{\tau}{\dot{\gamma}}, \ \lambda = \frac{N_1}{2\eta\dot{\gamma}^2}.$$

Rheological models. There are a variety of models for the viscoelasticity, from the upper convected Maxwell model,[3] which is the same as an Olydroyd-B[4] model with a = 1 and b = 0, to White-Metzner models, to Phan-Thien-Tanner[5] models. The equations for an upper-convected Maxwell model with are

[1] Higashitani, K. and W. G. Pritchard, *Trans. Soc. Rheol.* **16** 687 (1972).
[2] Tuna, N. Y. and B. A. Finlayson, *J. Rheology*, **28**79-93 (1984).
[3] Owens, R. G. and T. N. Phillips, *Computational Rheology*, Imperial College Press (2002).
[4] Oldroyd, J. G., *Proc. Roy. Soc. Lond. A*, **200** 523-541 (1950).
[5] Phan-Thien, N. and R. I. Tanner, *J. Non-Newtonian Fluid Mech.* **2** 353-365 (1977).



(a) **(b)**

Figure 1. Typical normalized (a) viscosity and (b) time constant as a function of shear rate

$$\boldsymbol{\tau} + \lambda \frac{\Delta_{10}\boldsymbol{\tau}}{\Delta t} = \eta \mathbf{d}, \ \ \mathbf{d} \equiv \nabla \mathbf{v} + \nabla \mathbf{v}^T, \ \ \frac{\Delta_{10}\boldsymbol{\tau}}{\Delta t} \equiv \mathbf{v} \bullet \nabla \boldsymbol{\tau} - \nabla \mathbf{v}^T \bullet \boldsymbol{\tau} - \boldsymbol{\tau} \bullet \nabla \mathbf{v}$$

The White-Metzner model is obtained by allowing the time constant and viscosity to vary with shear rate. Another constitutive equation was developed by Phan-Thien and Tanner (PTT)[6,7] to exhibit shear thinning (viscosity decreases as the shear rate increases) and a finite extensional viscosity. The form used here is

$$\boldsymbol{\tau} + \lambda \frac{\Delta_{10}\boldsymbol{\tau}}{\Delta t} + \varepsilon \frac{\lambda}{\eta} \mathrm{tr}(\boldsymbol{\tau})\boldsymbol{\tau} = \eta \mathbf{d}$$

For polymer melts the Reynolds number is so small (typically 10^{-6} to 10^{-3}) that the inertial term in the momentum equation is neglected. The equations are difficult to solve because the stress equations are hyperbolic and strong singularities are developed at corners.[3,8] Special techniques have been developed to handle these difficulties, including the Explicitly Elliptic Momentum Equation (EEME),[9] several different Petrov-Galerkin methods,[10] and Elastic-Viscous-Split-Stress (EVSS) methods.[11] The finite element representation of the stress tensor terms is also important, and bilinear, biquadratic, bicubic, and biquartic polynomials have all been used as well as schemes dividing an element into 16 sub-elements with the stress a constant on each sub-element. An EVSS method is used here and described below.

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[6] Phan-Thien, N., *Trans. Soc. Rheol.* **22** 259-283 (1978).
[7] Phan-Thien, N. and R. I. Tanner, *J. Non-Newtonian Fluid Mech.* **2** 353-365 (1977).
[8] Keunings, R., *Comp. Fluid Dynamics J.*, **9** 449-458 (2001).
[9] King, R. C., M. R. Apelian, R. C. Armstrong and R. A. Brown, *J. Non-Newtonian Fluid Mech.* **20** 187 (1989).
[10] Crochet, M. J. and R. Keunings, *J. Non-Newtonian Fluid Mech.* **42** 283-299 (1992).
[11] Rajagoplan, D., R. C. Armstrong, and R. A. Brown, *J. Non-Newtonian Fluid Mech.* **36** 135-157 (1990).

2. Applications

Two problems are treated here. The first is a classic problem, called the stick-slip problem, shown in Figure 2. The difficulties in this problem include the viscoelastic fluid as well as difficulties inherent in the Newtonian problem as well: a singularity at the corner where the no-slip surface changes to a slip surface. It is known that the velocity along the free surface goes as $x^{0.5}$ for a Newtonian fluid, which means the velocity gradient goes as $x^{-0.5}$, where x is measured from the end of the no-slip surface. Thus, as x approaches zero the shear rate approaches infinity.

The second problem is the hole pressure problem, shown in Figure 3. This problem was developed because the first normal stress difference can be measured by measuring the pressure difference between the bottom of the hole and the top surface opposite.[1] This problem is solved for a specific polymer which exhibits mild shear thinning and has a time constant which varies with shear rate. Experimental data is also available for comparison.

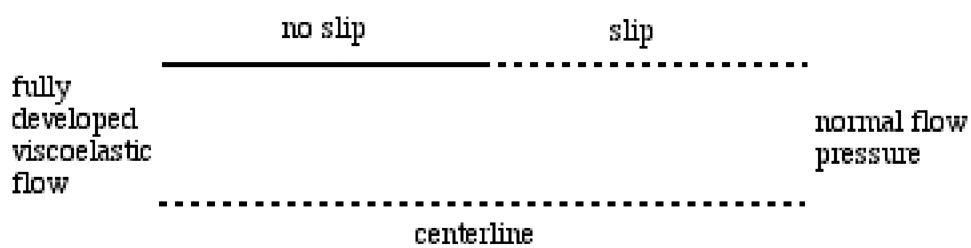

Figure 2. Stick-slip problem

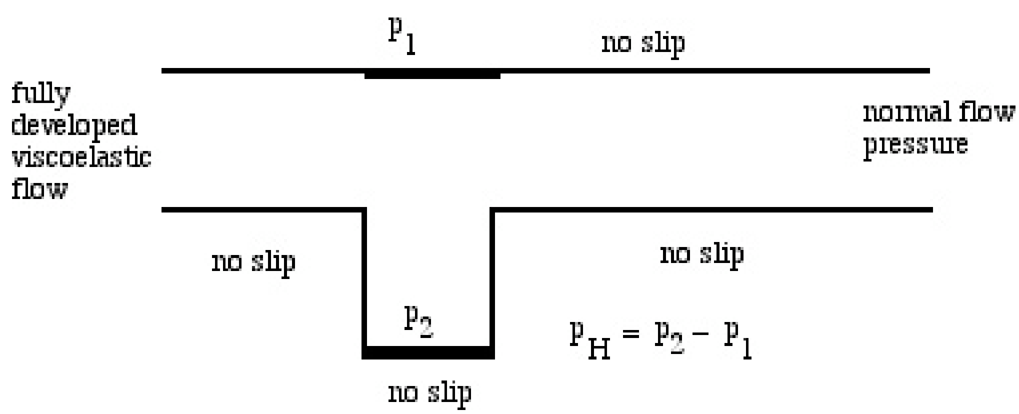

Figure 3. Hole pressure problem

3. Numerical methods

The differential models used here all exhibit hyperbolic behavior, since equations for the three stress components are all hyperbolic. This makes the problems hard to solve with the finite element method. Early work used the Galerkin method, with expansions of velocity as P^2-C^0, pressure as P^1-C^0, and stress components as P^1-C^0 or P^2-C^0. In the 1980s the Petrov-Galerkin method was introduced to solve the stress equations, using either the streamwise upwinding Petrov-Galerkin method (SUPG) or the inconsistent Petrov-Galerkin method (SU). In the later case, the Petrov-Galerkin weighting function was used only on the convective terms in the stress equation. That method (SU) converges much better than others, but it may converge to the wrong solution; it is not used here. Here the Galerkin method and Petrov-Galerkin method (SUPG) are applied to the momentum equation and stress equations using an extra-stress formulation. In dimensionless terms, it is

$$Re\,\mathbf{u} \bullet \nabla \mathbf{u} = -\nabla p + \nabla^2 \mathbf{u} + \nabla \bullet \tau^e, \;\; \nabla \bullet \mathbf{v} = 0, \;\; \tau \equiv \mathbf{d} + \tau^e$$

$$\boldsymbol{\tau} + We\,\frac{\Delta_{10}\boldsymbol{\tau}}{\Delta t} = \mathbf{d}, \;\; \mathbf{d} \equiv \nabla \mathbf{v} + \nabla \mathbf{v}^T, \;\; \frac{\Delta_{10}\boldsymbol{\tau}}{\Delta t} \equiv \mathbf{v} \bullet \nabla \boldsymbol{\tau} - \nabla \mathbf{v}^T \bullet \boldsymbol{\tau} - \boldsymbol{\tau} \bullet \nabla \mathbf{v}$$

The stress equations (for τ_{xx}, τ_{xy}, τ_{yy}) are solved using three mass transfer/convection and diffusion equations, with $D = 0$ and Petrov-Galerkin artificial diffusion. The extra stresses are defined using

$$\boldsymbol{\tau}^e = \boldsymbol{\tau} - \mathbf{d}$$

in a subdomain expression and these are then used to define the appropriate terms in the momentum equation, which are introduced as body forces.

As seen below, such a method will converge only for low Weissenberg numbers. While the parametric solver and mesh refinement techniques in Comsol Multiphysics are an improvement over early work, they are not sufficient to overcome the numerical difficulties inherent in the problem. Here we apply the Discrete Elastic-Viscous-Split-Stress (DEVSS) method,[12] a version of the EVSS method. In this method the shear rate components are approximated directly by a finite element expansion rather than calculating them as derivatives of the velocity finite element approximation. The result is that the shear rate is continuous across element boundaries. The equations are presented here in their weighted residual form.[3] The variables are $(\mathbf{u}_\delta,\; p_\delta,\; \boldsymbol{\tau}_\delta, \dot{\boldsymbol{\gamma}}_\delta)$ and the weighting functions are $(\mathbf{v}_\delta,\; q_\delta,\; \mathbf{S}_\delta, \mathbf{G}_\delta)$.

$$\int \nabla \bullet \mathbf{u}_\delta \; q_\delta \; d\boldsymbol{\Omega} = 0$$

$$\int \alpha(\dot{\boldsymbol{\gamma}}(\mathbf{u}_\delta) - \dot{\boldsymbol{\gamma}}_\delta) : \nabla \mathbf{v}_\delta \; d\boldsymbol{\Omega} + \int \boldsymbol{\tau}_\delta : \nabla \mathbf{v}_\delta \; d\boldsymbol{\Omega} - \int \nabla \bullet \mathbf{v}_\delta \; p_\delta \; d\boldsymbol{\Omega} - \int \mathbf{b} \bullet \mathbf{v}_\delta \, d\boldsymbol{\Omega} = 0$$

$$\int [\boldsymbol{\tau}_\delta + \lambda \frac{\Delta_{10}\boldsymbol{\tau}_\delta}{\Delta t} - \eta\,\dot{\boldsymbol{\gamma}}_\delta(\mathbf{u}_\delta)] : \mathbf{S}_\delta \;\; d\boldsymbol{\Omega} = 0$$

€

$$\int (\dot{\boldsymbol{\gamma}}_\delta(\mathbf{u}_\delta) - \dot{\boldsymbol{\gamma}}) : \mathbf{G}_\delta \; d\boldsymbol{\Omega} = 0$$

This equation is used in Comsol Multiphysics as follows. The continuity equation is handled the same as in the Navier-Stokes formulation. The second equation is put into the Navier-Stokes equation by including the second integral (involving stress) as an expression in the body force term. The terms involving pressure and body force are the same as in the Navier-Stokes equation. For the first term note that the first half of this is similar to the stress term, with stress

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[12] Guénette, R. and M. Fortin, *J. Non-Newtonian Fluid Mech.* **60** 27-52 (1995).

replaced by shear rate. This is the term that is usually the viscous term in the Navier-Stokes equation, since it uses the shear rate defined in terms of the velocity approximation. Thus, we take the viscosity in the Navier-Stokes equation as $\eta = \alpha$. Finally, the term involving the shear rate expressed in its finite element form is added to the equation in the body force term, using the same expressions (with different variables) as was done for stress. In particular, there are terms like: diff(*tauxx,x*), diff(*tauxx,y*), diff(*gdotxx,x*), diff(*gdotxx,y*), etc. The stress equations are developed by using a mass transfer/convection and diffusion equation for each component of stress (three for planar 2D geometry). The diffusion coefficient is set to zero, the Petrov-Galerkin option is chosen, and the other terms are included in the 'R' term, component by component. Finally, the final equation is developed using three mass transfer/diffusion equations. The diffusion coefficient was set to zero and all the terms were included in the 'R' term. The approximation spaces used in the DEVSS method were: velocity as P^2-C^0, pressure as P^1-C^0, and stress components as P^1-C^0. These have been shown by Fortin, *et al.*[13] to satisfy all compatibility conditions.

For the two applications given below, fully developed velocity and stress profiles are needed at the inlet. The upper-convected Maxwell model gives (in dimensionless notation)

$$u = 1.5(1-y^2), \quad \tau_{xy} = -3y, \quad \tau_{xx} = 18\,We\,y^2$$

where the domain is $0 \le y \le 1$. The White-Metzner model is more complicated, but since the interest in the hole pressure problem is downstream and the shear-thinning is modest, the inlet conditions are taken as the same as a Maxwell model. The PTT model is quite a bit more complicated. However, they can be arranged into the following form. Compute the pressure drop corresponding to the desired average velocity (taken as 1.0 in the non-dimensional version).

$$< u > = \frac{1}{3}\frac{\Delta p}{L} + \frac{2\varepsilon We^2}{5}\left(\frac{\Delta p}{L}\right)^3$$

Then the other variables at the inlet are

$$u = \frac{1}{2}\frac{\Delta p}{L}(1-y^2) + \frac{\varepsilon We^2}{2}\left(\frac{\Delta p}{L}\right)^3(1-y^4)$$

$$\tau_{xy} = \frac{\Delta p}{L}y, \quad \tau_{xx} = 2We\left(\frac{\Delta p}{L}y\right)^2, \quad \tau_{yy} = 0$$

$$\dot{\gamma}_{xx} = 0, \quad \dot{\gamma}_{xy} = \frac{\Delta p}{L}y + 2\varepsilon We^2\left(\frac{\Delta p}{L}y\right)^3, \quad \dot{\gamma}_{yy} = 0$$

4. Stick-slip problem

The problem is solved for a Maxwell fluid using linear, quadratic, and quartic polynomials for the stress components τ_{xx}, τ_{xy}, τ_{yy}, but the results were similar and only the linear

[13] Fortin, M., R. Peyret, and R. Temam, *Comput. Meth. Appl. Mech. Engr.* **143** 79-95 (1997).

approximations are shown here. The stability limit (highest Weissenberg number) was not improved by changing the type of polynomial. The boundary conditions at the inlet are given above; the bottom surface was taken as a slip/symmetry surface. For the Navier-Stokes equation, the top surface was no slip for half of it and slip/symmetry for the second half. The outlet condition was normal velocity/pressure. For the stress components, the inlet conditions are given above. The top solid surface used zero flux or insulation/symmetry, and the free surface and bottom surface were taken as insulation/symmetry (in the convection and diffusion equation), and the outlet boundary condition was convective flux. These boundary conditions insured that extraneous finite element terms did not get introduced.

A typical mesh is shown in Figure 4, and it has been refined manually near the singularity. The velocity along the free surface is shown in Figure 5. The impact of the singularity is illustrated by plots of the pressure and τ_{xx}, τ_{xy}, τ_{yy} stresses along the top surface; see Figures 6-9, respectively. Clearly this is a difficult problem. Using straightforward techniques it is possible to solve for Weissenberg numbers up to 0.2, which is a very low value.

Next the DEVSS method was applied. The boundary conditions were the same as for the Maxwell fluid, but there are additional ones on the shear rate. At the inlet the fully developed shear rate was specified.

$$\dot{\gamma}_{xx} = 0, \quad \dot{\gamma}_{xx} = \frac{\Delta p}{L} y, \quad \dot{\gamma}_{yy} = 0$$

At the other boundaries, insulation/symmetry was used. Again, this insured that no extraneous terms appeared in the equations.

With the DEVSS method, it was possible to get solutions up to We = 0.45 easily, and sometimes higher. However, with this mesh, the solution began to oscillate for higher Weissenberg numbers. The solution for τ_{xx} is shown in Figures 10 (a). Solutions at higher Weissenberg numbers exist in the literature,[12,14] but only with a few hundred elements. It is well known that the critical Weissenberg number decreases as the mesh is refined.

Finally, the PTT model was applied and solutions were easily obtained up to Weissenberg number of 5. Those results are shown in Figure 10 (b).

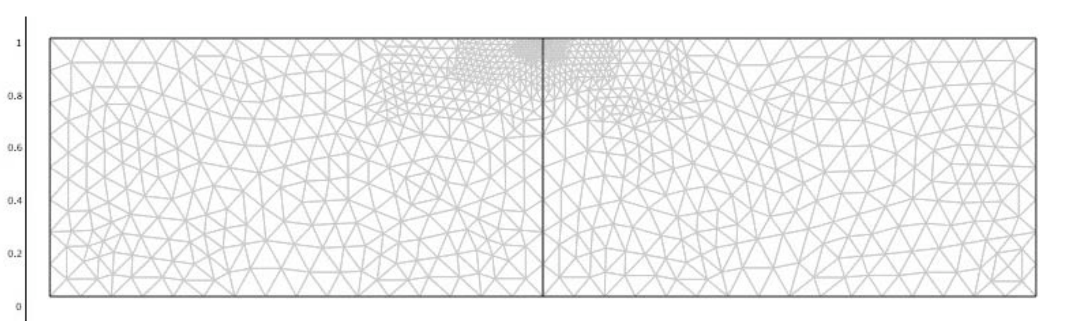

Figure 4. Mesh for stick-slip problem; 2102 elements, 13,082 dof (Maxwell), 16,412 dof (DEVSS); 2863 elements, 22829 dof (PTT)

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[14] Marchal, J. M. and M. J. Crochet, *J. Non-Newt. Fluid Mech.* **26** 77-114 (1987).

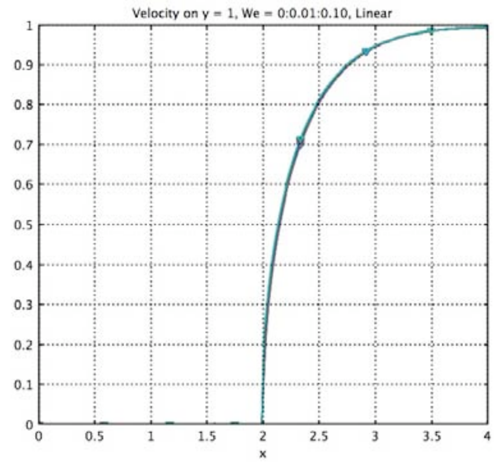


Figure 5. Velocity

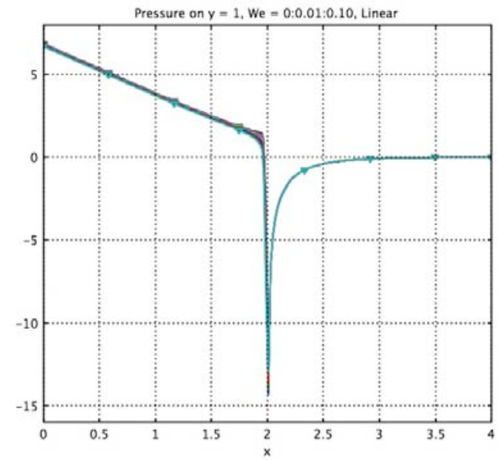


Figure 6. Pressure

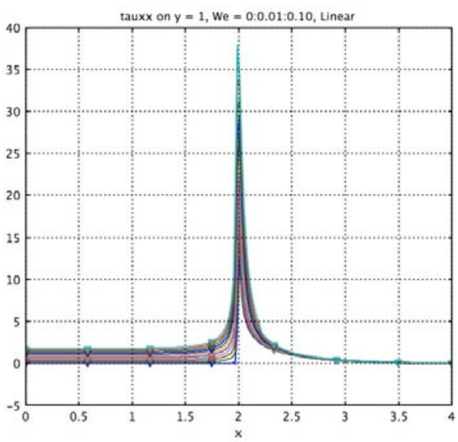


Figure 7. τ_{xx}

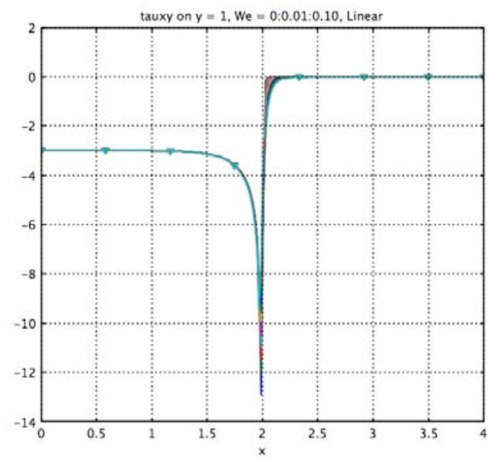


Figure 8. τ_{xy}

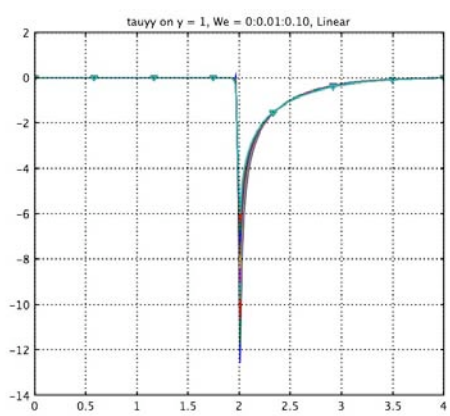
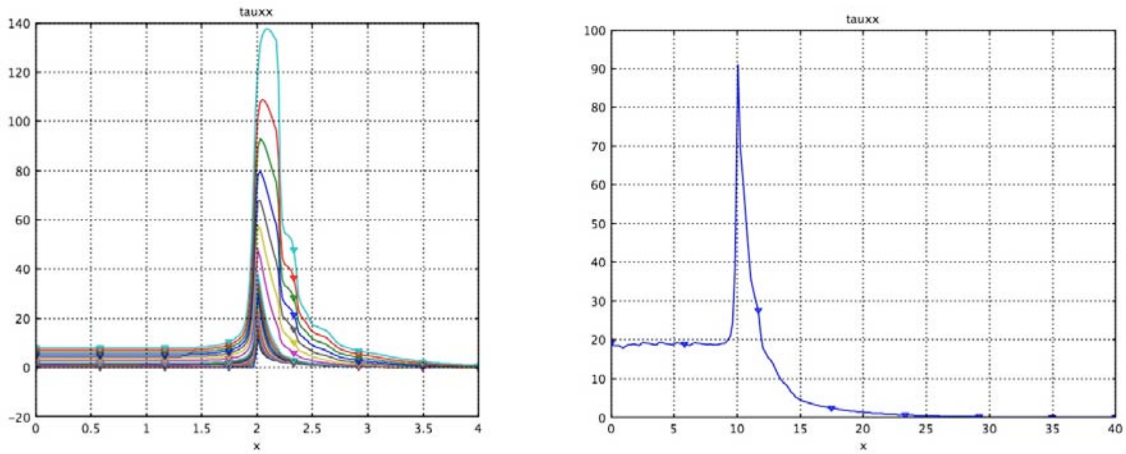


Figure 9. τ_{yy}



(a) **(b)**

Figure 10. (a) $\boldsymbol{\tau}_{xx}$ for DEVSS method, Maxwell fluid, We = 0:0.05:0.45 **(b) $\boldsymbol{\tau}_{xx}$ for DEVSS method, PTT fluid, We = 5**

5. Hole pressure problem

The second problem solved is the hole pressure problem. Experimental data exists for a 9% solution of polystyrene in dioctyl phthalate;[15] the normalized viscosity and time constant are shown in Figure 1 and the hole pressure results are in Baird.[15] This experiment was modeled first by Jackson and Finlayson using a White-Metzner model with the Galerkin method,[16] and it is modeled here using a White-Metzner model using the DEVSS formulation. The model was solved in the SI system, with a gap height of 0.003529 m, hole width of 0.003175 m, hole depth of 0.009526 m, in a region tat is 0.0254 m long. The calculations attained as high a flow rate as was obtained in the experiment; the highest flow rate corresponded to a shear rate at the wall in fully developed flow of 123 s^{-1}. The flow was planar flow, and the calculations are two-dimensional. The experiment used circular holes, so that the calculations do not strictly correspond to the experiment. The number of elements was 2976, with 23,385 dof. Figure 11 shows the experimental data, the results from the model, and the hole pressure estimated using the expression

$$p_H = -0.25\, N_1 = -0.25\, \tau_{xx}.$$

where the normal stress is the τ_{xx} stress from the calculations. This expression comes from the simplest theory of hole pressure. Figure 12 shows streamlines and stress concentrations.

6. Conclusions

Comsol Multiphysics is a versatile tool that can be used to solve complicated flow problems of polymers by combining the Navier-Stokes, convective diffusion, and diffusion equations. The DEVSS method can be used to stabilize the computations, thus enabling solutions at higher Weissenberg number than would otherwise be possible.

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[15] Baird, D. G., *J. Appl. Poly. Sci.* **20** 3155-3173 (1976).
[16] Jackson, N. R. and B. A. Finlayson, *J. Non-Newt. Fluid Mech.* **10** 71-84 (1982).

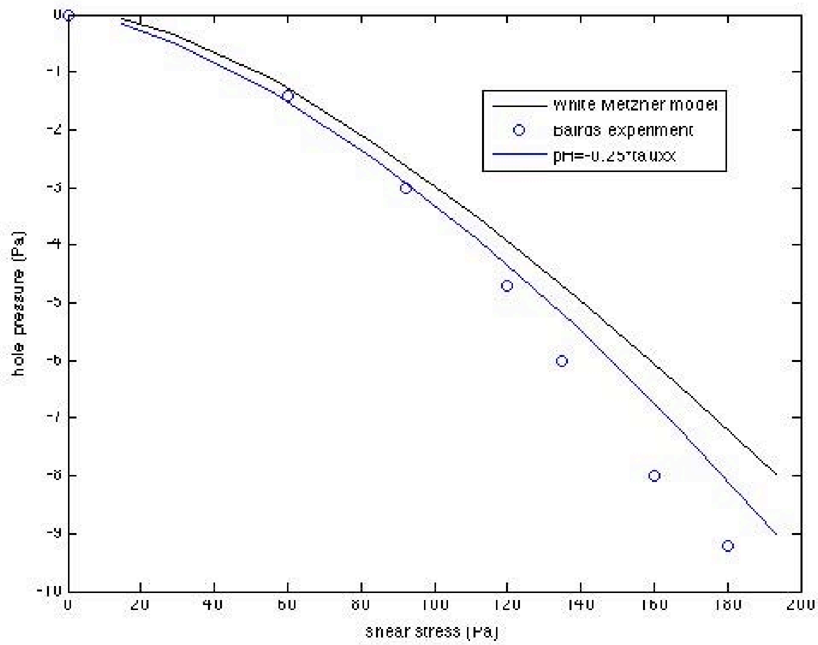

Figure 11. Hole Pressure Calculated with White-Metzner model — calculations, o Baird's experiment, $-N_1/4$

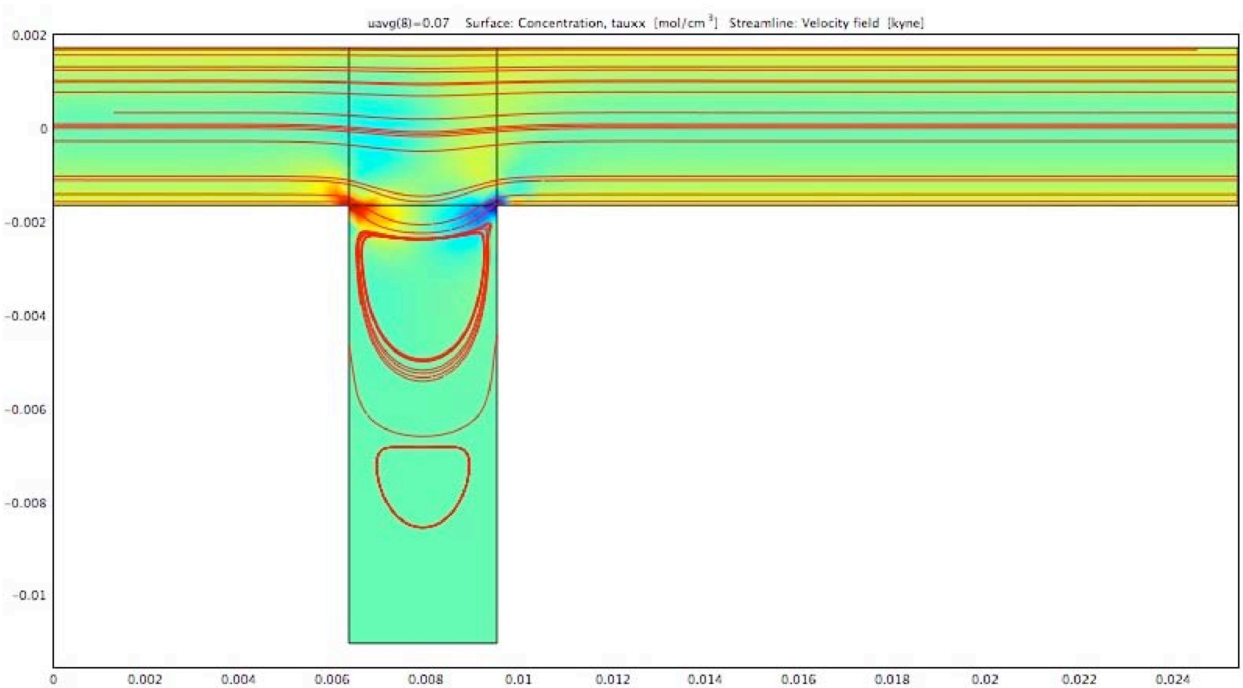

Figure 12. Streamlines and τ_{xx} for $\dot{\gamma}=123\ \mathrm{s}^{-1}$