Modeling Viscoelastic Flow Through a Quarter Circle Contraction

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Introduction

The purpose of this project was to determine the first normal stress difference of an elastic polymer flowing through a geometry with a hyperbolic contraction. The first normal stress difference has been known to characterize the elasticity of complex fluids, and although the normal stress difference is difficult to measure in reality, we can take advantage of virtual tools and solve for the normal stress difference using a computer aided model.

The geometry used is shown below in Figure 1. It consisted of a rectangle with a quarter circle contraction and was inspired by Dr. Gareth McKinley, Professor of Mechanical Engineering at the Massachusetts Institute of Technology, and his presentation entitled Extensional Rheometry on a Chip: Flows of Dilute Polymer Solutions in Microfluidic Contractions, given at the American Institute of Chemical Engineers (AICHE) conference in November 2006.

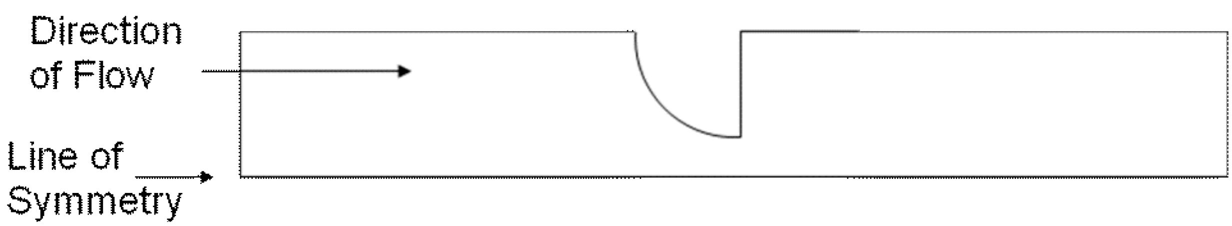

Figure 1. Outline of geometry used to model the polymeric fluid.

Method and Materials

The geometry was created in COMSOL Multiphysics 3.3 and contained 1800 elements and 3997 degrees of freedom. As shown in Figure 2, the geometry had a length of 40, a height of 1 at the sides, and a height of 0.2 at the narrow region.

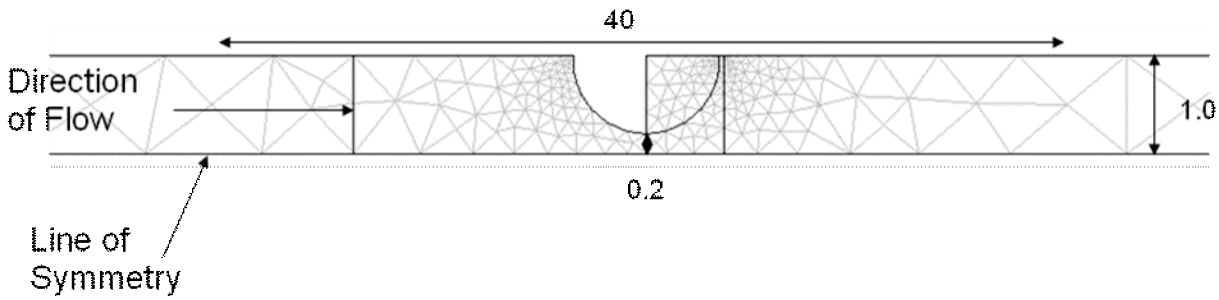

Figure 2. Geometry created in COMSOL Multiphysics showing dimensions and mesh pattern.

The viscoelastic fluid parameters were provided by Dr. Bruce Finlayson, Professor Emeritus of Chemical Engineering at the University of Washington (See Appendix 1 for equations).

For the Maxwell model, parameters were made dimensionless and boundary conditions were set so that the average velocity in the narrow portion was equal to one. For the Phan-Thien-Tanner model, the average velocity in the entrance region was set equal to one. The viscosity was also set equal to one and the density was set equal to zero. In order to find the first normal stress difference, we desired to know the pressure drop that took place through the geometry. To solve for this, the predicted pressure drop was calculated using Eq. (1):

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

where $\Delta p/L$ is the calculated pressure drop, ε is equal to 0 for the Maxwell model and 0.02 for the Phan-Thien-Tanner model, and the We is the Weissenberg number, which represents the ratio relaxation time over specific process time.

By changing the Weissenberg number and the calculated pressure drop, different solutions were obtained. The outlet pressure was assumed to be zero, so the excess pressure drop could be calculated using Eq. (2):

$$\Delta p_{excess} = \Delta p_{measured} - \Delta p_{@We=0} \tag{2}$$

The first normal stress could be calculated from the calculated pressure drop and Eq. (3)

$$\tau_{xx,w} = 2\frac{\lambda}{\eta}\left(\frac{\Delta p}{L}\cdot H\right)^2 \tag{3}$$

where λ is a number chosen to fit a model to the experimental data, Δp/L is the calculated pressure drop, H is the height of the geometry, and η is the viscosity and can be calculated using Eq. (4):

$$\eta = \frac{\Delta p}{L}\frac{H^2}{3 < u >} \tag{4}$$

where Δp/L is the calculated pressure drop, H is the height of the geometry, <u> is the average velocity in the x-direction.

Results

Figure 3 below shows a solution obtained for the pressure drop solved for the Maxwell model at a Weissenberg number of 0.06. The red lines represent the stream velocity and the color represents the pressure concentration.

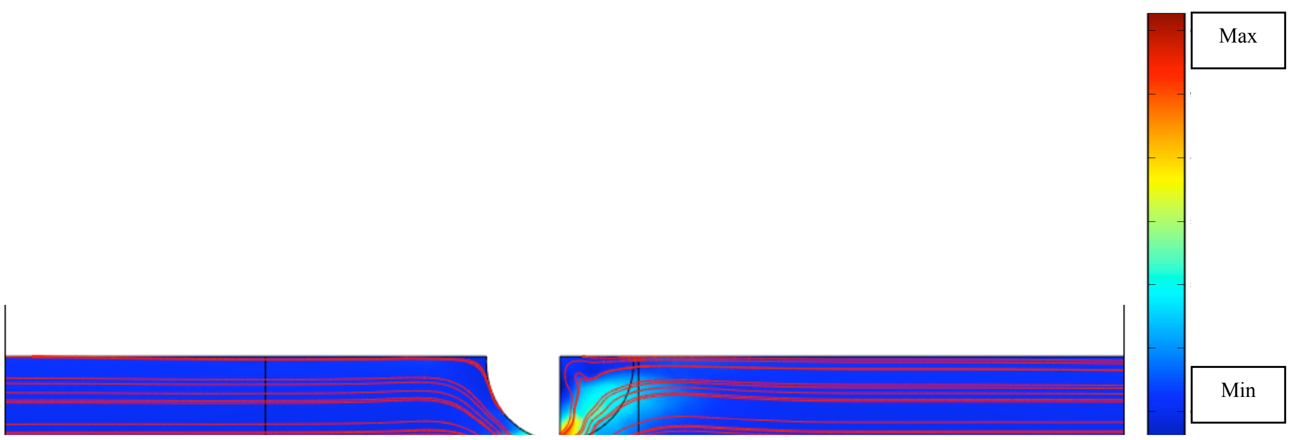

Figure 3. Sample solution for the Maxwell model.

After the excess pressure drop was computed, the normal stress was calculated using Eq. (3). Figures 4 and 5 display plots of the first normal stress differences as a function of the pressure drop for increasing values of the Weissenberg number.

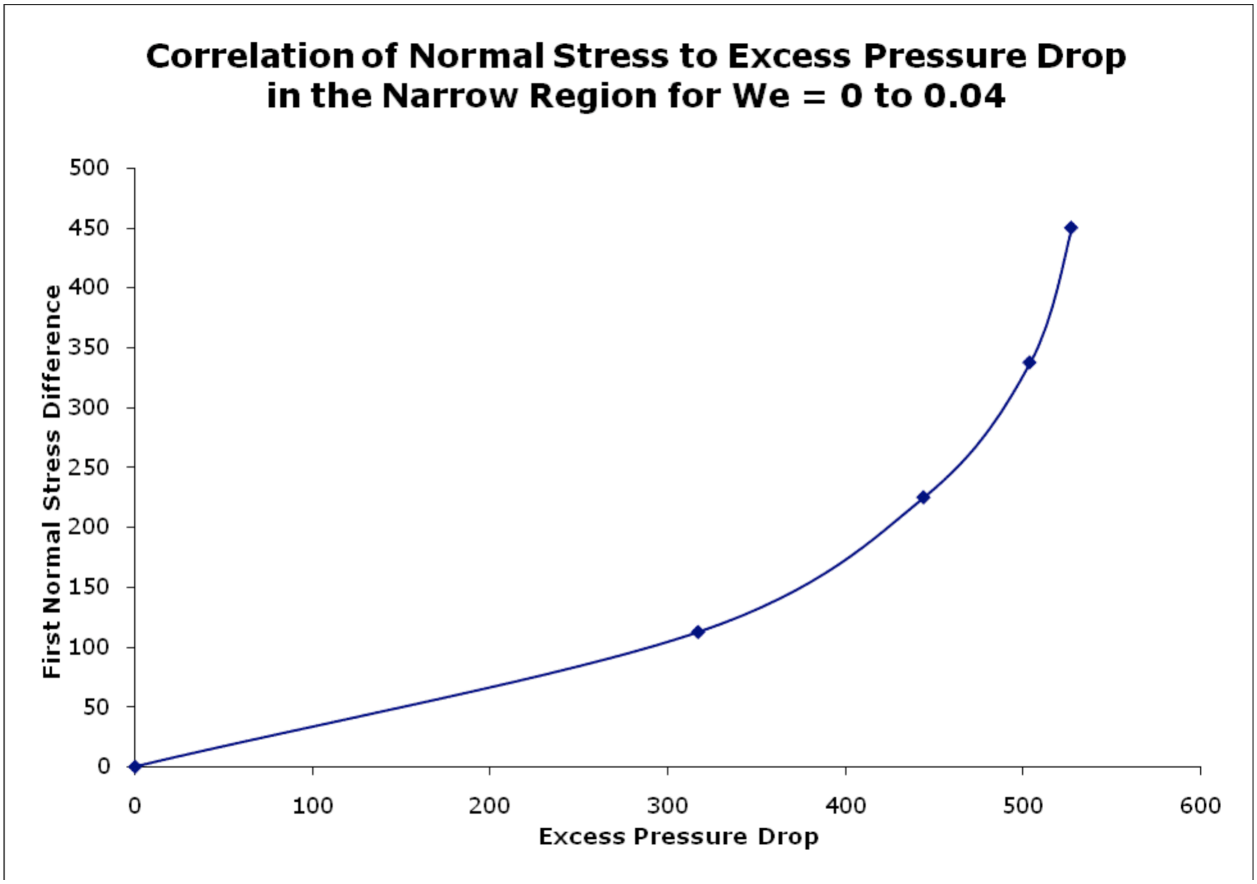

Figure 4. Correlation of the First Normal Stress Difference to the Excess Pressure Drop for the Maxwell Model.

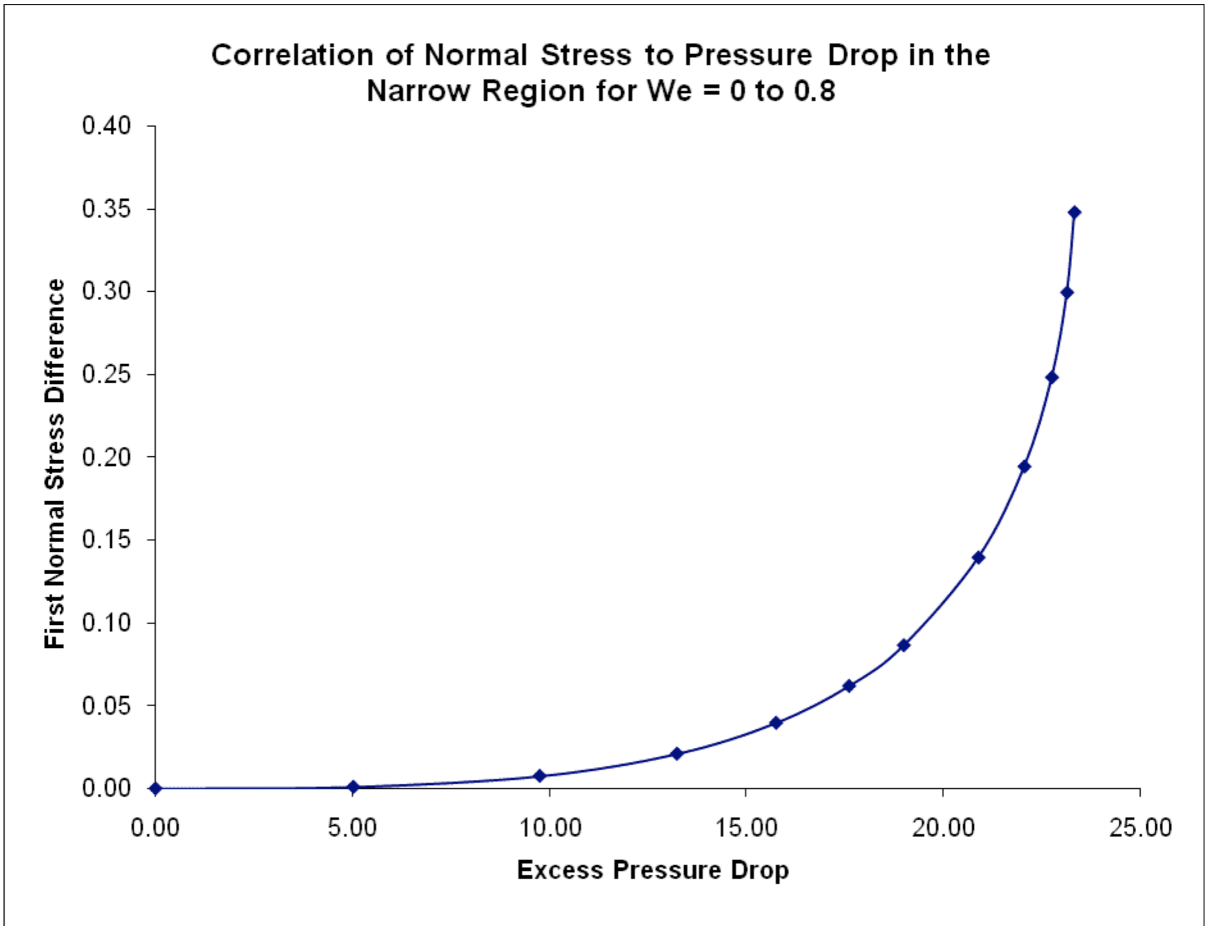

Figure 5. Correlation of the First Normal Stress Difference to the Excess Pressure Drop for the Phan-Thien-Tanner Model.

In Figure 6, the excess pressure drop was plotted as a function of the Weissenberg number. Thus, these charts become useful if one knows the Weissenberg number, because one can refer to Figure 6 and find the corresponding excess pressure drop, then go to Figure 4 or 5, depending on the value of epsilon, and find the first normal stress difference.

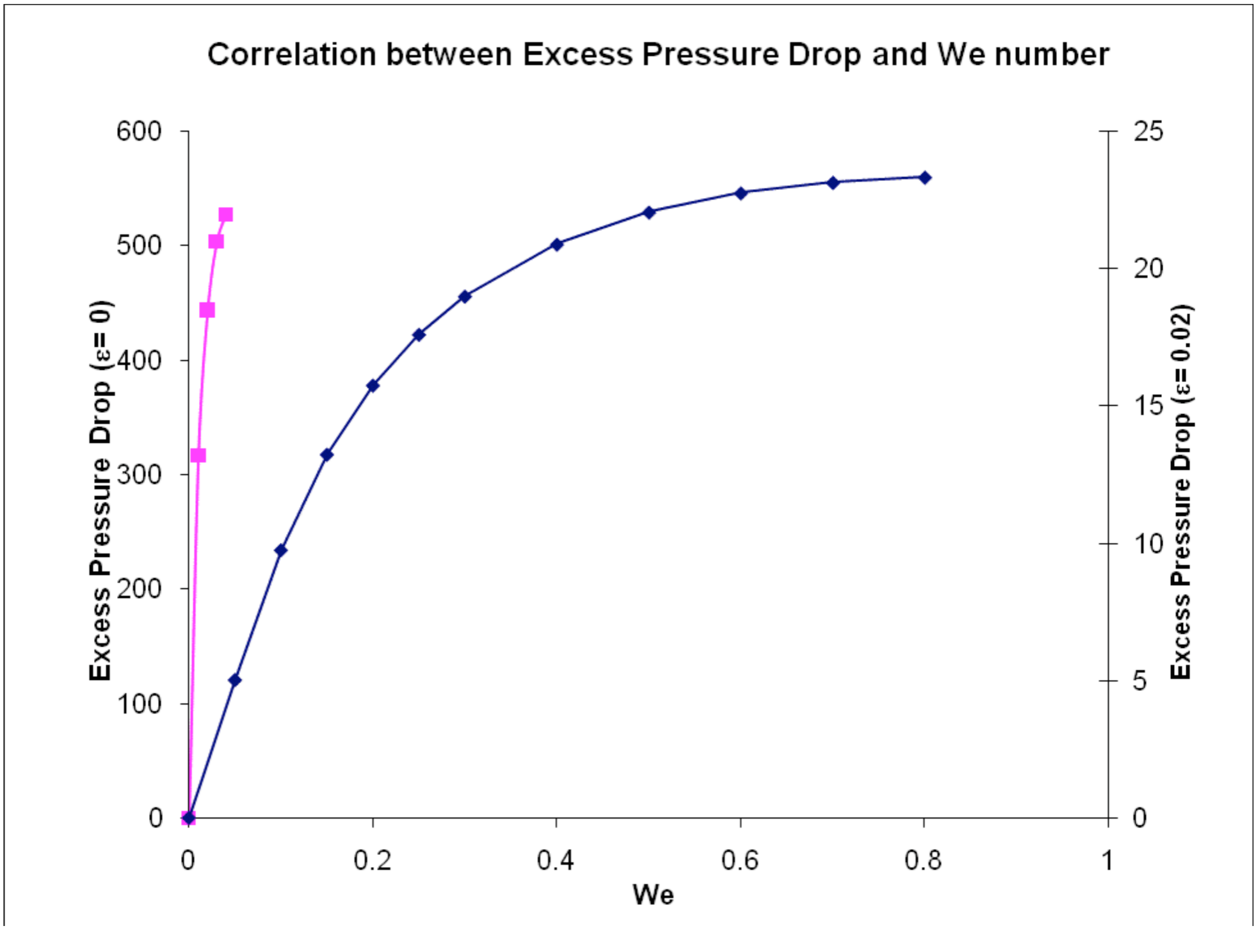

Figure 6. Correlation of the Weissenberg number to the Excess Pressure Drop for the Maxwell (ε = 0) and Phan-Thien-Tanner Models (ε = 0.02).

As a check, the average velocity was computed in COMSOL Multiphysics software to ensure that it was equal to one in the narrow region for the Maxwell model and equal to one in the entrance for the Phan-Thien-Tanner model.

Conclusions

The first normal pressure differences were obtained for various Weissenberg numbers for the Maxwell and Phan-Thien-Tanner models. For future experimentation, one could change the value of epsilon, find solutions for the pressure drop, and create more correlations between the Weissenberg number, the excess pressure drop, and the first normal stress difference.

Appendices

Appendix 1: Equations for Non-Newtonian Fluid

$$\mathrm{Re} \cdot u \cdot \nabla u = -\nabla p + \nabla \tau \text{ but Re} \rightarrow 0$$

$$\tau(1 + We \cdot \varepsilon \cdot t \cdot \tau) + We \frac{\Delta_{10}\tau}{\Delta t} = \nabla v + \nabla v^T$$

where $\frac{\Delta_{10}\tau}{\Delta t} = v \cdot \nabla \tau - \nabla v^T \cdot \tau - \tau \cdot \nabla v$, $\mathrm{Re} = \frac{\rho < u > x_s}{\mu}$, and $We = \frac{\lambda_0 \cdot u_s}{x_s}$

Appendix 2: Sample Calculations

<u>Calculating Δp excess:</u>

$$\Delta p_{excess} = \Delta p_{measured} - \Delta p_{@We=0}$$

$$\Delta p_{excess} = |1225 - 1543| = 317$$

<u>Calculating first normal pressure difference:</u>

$$\tau_{xx,w} = 2 \cdot We \cdot \left(\frac{\Delta p}{L}\right)^2$$ where λ = 1 η = 1 and H = 1

$$\tau_{xx,w} = 2 \cdot 0.01 \cdot \left(\frac{\Delta p}{L}\right)^2 = 2(317)^2 = 2012$$