PULSATILE FLOW OF A CHEMICALLY-REACTING NON-LINEAR FLUID

A Thesis

by

RONALD CRAIG BRIDGES, II

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

May 2007

Major Subject: Mechanical Engineering

PULSATILE FLOW OF A CHEMICALLY-REACTING NON-LINEAR FLUID

A Thesis

by

RONALD CRAIG BRIDGES, II

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Approved by:

Chair of Committee,	K.R. Rajagopal
Committee Members,	Jay Humphrey
	John Criscione
	Peter Kuchment
Head of Department,	Dennis O'Neal

May 2007

Major Subject: Mechanical Engineering

ABSTRACT

Pulsatile Flow of a Chemically-Reacting Non-Linear Fluid. (May 2007)

Ronald Craig Bridges, II, B.S., Texas A&M University

Chair of Advisory Committee: Dr. K.R. Rajagopal

Many complex biological systems, such as blood and polymeric materials, can be approximated as single constituent homogeneous fluids whose properties can change because of the chemical reactions that take place. For instance, the viscosity of such fluids could change because of the chemical reactions and the flow. Here, I investigate the pulsatile flow of a chemically-reacting fluid whose viscosity depends on the concentration of a species (constituent) that is governed by a convection-reaction-diffusion equation and the velocity gradient, which can thicken or thin the fluid. I study the competition between the chemical reaction and the kinematics in determining the response of the fluid.

The solutions to the equations governing the steady flow of a chemically-reacting, shear-thinning fluid are obtained analytically. The solution for the velocity exhibits a parabolic-type profile reminiscent of the Newtonian fluid profile, if the fluids are subject to the same boundary conditions. The full equations associated with the fluid undergoing a pulsatile flow are studied numerically. A comparison of the shear-thinning/chemical-thinning fluid to the shear-thinning/chemical-thickening fluid using a new non-dimensional parameter–the *competition number* (CN) shows that both the shear-thinning effects and the chemical-thinning/thickening effects play a vital role in determining the response of the fluid. For the parameter values chosen, the effects of chemical-thinning/thickening dominate the majority of the domain, while the effects due to shear-thinning are dominant only in a small region near the boundary.

ACKNOWLEDGMENTS

TABLE OF CONTENTS

LIST OF FIGURES

CHAPTER I

INTRODUCTION*

There are many important technological problems that concern the flow of chemically-reacting fluid mixtures. Many biological fluid systems are examples of such mixtures. For example, blood is a complex mixture of plasma, proteins, cells, and a variety of other chemicals that is modeled usually in a homogenized sense as a single constituent fluid. Blood is maintained in a delicate balance by a variety of chemical reactions, some that aid its coagulation and others its dissolution. Complicated models have been proposed to describe the biochemical reactions and the complex interplay between the rheology and biochemistry of flowing blood (see Kuharsky and Fogelson [1], Anand et al. [2]). The more recent models entail dozens of convection-reaction-diffusion equations coupled to the equations for the balance of mass and the balance of linear momentum. Unfortunately, such systems are far too complicated to be amenable to either mathematical or numerical analysis. A simplification, albeit rather drastic, that can provide useful insight into the problem is to approximate systems such as blood by coupling the balance of mass and the balance of linear momentum for a single component fluid to a single convection-reaction-diffusion equation, the viscosity of the fluid depending on the concentration of another species that is governed by the convection-reaction-diffusion equation. Within the context of a full mixture theory that allows for the interconversion between the various constituents one can account systematically for all the interactions that take place and also enforce the balance laws for each

of the constituents (see Truesdell [3], [4], Samohyl [5], Rajagopal and Tao [6]), but such an approach has its own attendant problems such as the increased level of complexity and an inherent difficulty in specifying appropriate boundary and initial conditions.

Here, we allow for the viscosity of the fluid to vary in virtue of the changes in the concentration of the second species that co-exists with the fluid of interest. We interpret the change in the concentration of this species as leading to a change in the viscosity of the fluid. We shall, however, require the fluid to undergo only isochoric motions, i.e., the flows meet $\text{div}(\mathbf{v}) = 0$. In a single component fluid, the above condition is a consequence of the balance of mass and incompressibility, and in a homogenous fluid this implies that the density is a constant. However, in an inhomogeneous fluid it means that the density of a specific material point is a constant. We, on the other hand, have a situation wherein the fluid under consideration can be viewed as being incompressible in that its own density is a constant. It is assumed to co-exist with another constituent whose concentration (defined as the ratio of the density of the reactant to the sum of the density of the fluid and the reactant) changes, and this in turn changes the viscosity of the fluid. We shall, however, not concern ourselves with the balance laws for the reactant, or the fact that its density is changing. This is akin to problems such as flow through porus media wherein the equations for the porous solid matrix are ignored while those for the fluid are taken cognizance of. One could also view the problem as the flow of a fluid wherein the effect of a chemical reaction can be captured by an internal variable that is governed by a convection-reaction-diffusion equation. Thus, the quantity considered to be the concentration can be viewed as an internal variable.

CHAPTER II

KINEMATICS[*]

Let $\kappa_o(\beta)$ denote the reference configuration of the body β. By a motion, we mean a sequence of placers, parameterized by time, that assigns to a particle at a point $\mathbf{X} \in \kappa_o(\beta)$ a point $\mathbf{x}$ in the current configuration $\kappa_t(\beta)$. This implies the existence of a one-to-one mapping $\boldsymbol{\chi}_{\kappa_o}$ for each instant of time $t \in \mathbb{R}$ such that

$$\mathbf{x} = \boldsymbol{\chi}_{\kappa_o}(\mathbf{X}, t). \tag{2.1}$$

We shall assume the mapping $\boldsymbol{\chi}_{\kappa_o}$ to be sufficiently smooth. For the purpose of this work we shall require the definition of some kinematical tensors, namely the Rivlin-Ericksen tensors (see Rivlin and Ericksen [7]). The first Rivlin-Ericksen tensor is defined as:

$$\mathbf{A}_1 = \left[\frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}} \right)^T \right] = 2\mathbf{D}, \tag{2.2}$$

where

$$\mathbf{v} = \frac{\partial \boldsymbol{\chi}_{\kappa_o}}{\partial t}, \tag{2.3}$$

and $\mathbf{D}$ is the symmetric part of the velocity gradient. The higher order Rivlin-Ericksen tensors are defined through the recurrence relationship:

$$\mathbf{A}_i = \frac{d\mathbf{A}_{i-1}}{dt} + \mathbf{A}_{i-1} \frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}} \right)^T \mathbf{A}_{i-1}, \ \ i \geq 2. \tag{2.4}$$

As stated in the introduction, we wish to study the behavior of a fluid that thickens or thins due to chemical reactions, and thus the viscosity changes with the concentration as well as the shear-rate. Here we define the concentration in the

following manner:

$$c = \frac{\rho_r}{\rho_r + \rho}.$$

<div align="right">(2.5)</div>

The quantities ρ and ρ_r denote the densities of the fluid and the co-existing reacting fluid, respectively. On the other hand, as mentioned in the introduction, 'c' could denote an internal variable on which the viscosity depends. Since the fluid is assumed to be incompressible we are interested in studying only isochoric motions.

CHAPTER III

GOVERNING EQUATIONS[*]

We shall study the behavior of isotropic fluids of the differential type. For such fluids, the Cauchy stress has the following representation (see Truesdell and Noll [8]):

$$\mathbf{T} = \mathbf{f}(\mathbf{A}_1, \mathbf{A}_2, ..., \mathbf{A}_i, \rho). \tag{3.1}$$

Fluids that can be represented by this model are often referred to as a Rivlin-Ericksen fluids of complexity i, and such fluids are frame-indifferent as the tensors $\mathbf{A}_i$ are frame-indifferent. It follows from standard representation theorems for an isotropic tensor-valued function that the Cauchy stress in a Rivlin-Ericksen fluid of complexity 1 has the form:

$$\mathbf{T} = \alpha_0\mathbf{1} + \alpha_1\mathbf{A}_1 + \alpha_2\mathbf{A}_1^2, \tag{3.2}$$

where α_0, α_1 and α_2 are all functions of $\mathrm{tr}\mathbf{A}_1$, $\mathrm{tr}\mathbf{A}_1^2$ and $\mathrm{tr}\mathbf{A}_1^3$. Here we wish to study a special sub-class of (3.2) that is often referred to as an incompressible, generalized Newtonian fluid. For such a fluid, equation (3.2) reduces to:

$$\mathbf{T} = -\pi\mathbf{1} + \mu_a(\mathbf{A}_1)\mathbf{A}_1, \tag{3.3a}$$

where $-\pi\mathbf{1}$ denotes the indeterminate part of the stress due to the constraint of incompressibility. Fluids belonging to the sub-class (3.3a) with an apparent viscosity μ_a of the form:

$$\mu_a(\mathbf{A}_1) = \mu\left[1 + \alpha\mathrm{tr}(\mathbf{A}_1^2)\right]^n \tag{3.3b}$$

---

have been used in modelling the flows of polymeric liquids [9]. The main characteristic of this non-linear model is that it captures the ability of a fluid to shear-thin or shear-thicken in shear flows through the material parameters n and α. If the shear-index $n < 0$ this model characterizes the behavior of a shear-thinning fluid while if $n > 0$ it characterizes the behavior of a shear-thickening fluid. If $n = 0$ this model reduces to the linearly viscous fluid model. The quantity μ is called the zero shear-rate viscosity and is defined as:

$$\mu = \lim_{\kappa \to 0} \mu_a(\kappa), \tag{3.4}$$

where κ is the shear-rate. The mathematical properties pertaining to existence and uniqueness of the equations governing the flows of a fluid characterized by (3.3) have been studied in great detail (see Malek et al. [10]), and the stability of such flows has been studied by Malek, Rajagopal and Ruzicka [11]. The Lagrange multiplier π is, in general, a function of r, θ, z and t, and since $\text{tr}\mathbf{A}_1 = 2\text{div}(\mathbf{v}) = 0$, π is equal to the mean hydrostatic pressure. This is not the case with most (incompressible) non-linear models as the trace of the 'extra stress' is non-zero. The fluid is assumed to be thermally uniform and is assumed to undergo isothermal processes. Consequently, the rate of dissipation ξ reduces to:

$$\xi = \mathbf{T} \cdot \mathbf{D}, \tag{3.5}$$

where the scalar product between the Cauchy stress and the symmetric part of the velocity gradient is often referred to as the stress-power. The 2nd law of thermodynamics requires the rate of dissipation, and in this case the stress-power, to be non-negative. If the stress power is to be non-negative for all n, then we conclude that $\alpha \geqq 0$. We note that such a model can also be developed as a trivial case within the framework recently proposed by Rajagopal and Srinivasa [12].

We are interested in the viscosity depending on the concentration 'c', and thus the model that we shall consider has the representation:

$$\mathbf{T} = -\pi\mathbf{1} + \mu(c, \mathbf{A}_1)\mathbf{A}_1, \tag{3.6a}$$

where

$$\mu(c, \mathbf{A}_1) = \mu^{\star}(c)\left[1 + \alpha\mathrm{tr}(\mathbf{A}_1^2)\right]^n. \tag{3.6b}$$

Henceforth, we shall drop the star for convenience.

As the fluid is incompressible, it can undergo only isochoric motions and thus:

$$\mathrm{div}(\mathbf{v}) = 0. \tag{3.7}$$

On substituting the constitutive relation (3.6) into the balance of linear momentum:

$$\mathrm{div}(\mathbf{T}) + \rho\mathbf{b} = \rho\frac{d\mathbf{v}}{dt}, \tag{3.8}$$

we obtain:

$$-\frac{\partial\pi}{\partial\mathbf{x}} + \mathbf{A}_1\frac{\partial}{\partial\mathbf{x}}\left[\mu(c, \mathbf{A}_1)\right] + \mu(c, \mathbf{A}_1)\Delta\mathbf{v} = \rho\frac{d\mathbf{v}}{dt}, \tag{3.9}$$

on using (3.7) and on neglecting the body force $\rho\mathbf{b}$. The governing relationship for the concentration is the convection-reaction-diffusion equation:

$$\frac{\partial c}{\partial t} + \mathrm{div}(c\mathbf{v}) = \mathrm{f}. \tag{3.10}$$

We shall assume f to be of the special form:

$$\mathrm{f} = -\mathrm{div}(\mathbf{p}), \tag{3.11}$$

where $\mathbf{p}$ is a flux vector that is related to the reactions that take place within the fluid. We assume the flux vector $\mathbf{p}$ is given by a constitutive relation that is similar

to that used in Fick's assumption, i.e.,

$$\mathbf{p} = -K\frac{\partial c}{\partial \mathbf{x}}, \qquad (3.12)$$

where K is a scalar-valued function of the first Rivlin-Ericksen tensor. Therefore, the reaction-convection-diffusion equation reduces to:

$$\frac{\partial c}{\partial t} + \text{div}(c\mathbf{v}) = \text{div}\left[K(\mathbf{A}_1)\frac{\partial c}{\partial \mathbf{x}}\right]. \qquad (3.13)$$

Thus, in general, the balance of mass (3.7), the balance of linear momentum (3.9) and the convection-reaction-diffusion equation (3.13) are coupled, and one must solve them together for the velocity 'v' and the concentration 'c'.

CHAPTER IV

THE BOUNDARY VALUE PROBLEM[*]

Let us consider the pulsating flow of a reacting fluid in the domain Ω: $0 \leqq r \leqq R_i$, $0 \leqq \theta < 2\pi$ and $-\infty < z < \infty$, where (r, θ, z) is a cylindrical-polar coordinate system that is placed such that $r = R_i$ is the inner wall of the tube, and $r = 0$ is the axis of symmetry. We shall employ a semi-inverse approach and seek a velocity field of the form:

$$\mathbf{v} = v_z(r, t)\mathbf{e}_z, \tag{4.1}$$

where $\mathbf{e}_z$ denotes the base vector in the z coordinate direction. On substituting (4.1) into (3.9), expressed in a cylindrical-polar coordinate system in view of the specific boundary value problem under consideration, yields:

$$-\frac{\partial \pi}{\partial r} = 0, \tag{4.2a}$$

$$-\frac{1}{r}\frac{\partial \pi}{\partial \theta} = 0, \tag{4.2b}$$

and

$$\frac{1}{r}\frac{\partial}{\partial r}\left\{r\mu(c)\left[1 + 2\alpha\left(\frac{\partial v_z}{\partial r}\right)^2\right]^n \frac{\partial v_z}{\partial r}\right\} - \frac{\partial \pi}{\partial z} = \rho\frac{\partial v_z}{\partial t}. \tag{4.2c}$$

Equation (4.2a) implies the pressure is independent of r. Similarly, equation (4.2b) reveals the pressure is not a function of θ. It would then be natural to assume, since we shall consider a fully-developed, pulsating flow, an axial pressure gradient of the form:

$$\frac{\partial \pi}{\partial z} = -[A_o + B_o\sin(\omega t)], \tag{4.3}$$

where A_o and B_o are constants, and ω is the frequency of the pulsation. Combining (4.2c) and (4.3) we obtain:

$$\frac{1}{r}\frac{\partial}{\partial r}\left\{r\mu(c)\left[1+2\alpha\left(\frac{\partial v_z}{\partial r}\right)^2\right]^n\frac{\partial v_z}{\partial r}\right\}+A_o+B_o\mathrm{sin}(\omega t)=\rho\frac{\partial v_z}{\partial t}. \quad (4.4)$$

The solution to equation (4.4) depends on the particular choice for μ, namely how it depends on the concentration 'c'.

Due to the structure of the domain Ω and the pulsatility of the flow, the concentration is assumed to have the form:

$$c = \hat{c}(r, t). \quad (4.5)$$

On appealing to equation (3.7) and the assumption (4.5), equation (3.13) reduces to:

$$\frac{\partial \hat{c}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\mathbf{K}(\mathbf{A}_1)\frac{\partial \hat{c}}{\partial r}\right]. \quad (4.6)$$

We shall assume the diffusivity to be of the special form:

$$\mathbf{K}\left(\mathbf{A}_1\right) = \eta\|\mathbf{A}_1\|^2 = \psi\left(\frac{\partial v_z}{\partial r}\right)^2, \quad (4.7)$$

where η and ψ are constants and $\|\cdot\|$ denotes the trace-norm.

We now proceed to non-dimensionalize the governing equations by introducing the mapping $(r, t) \rightarrowtail (\varepsilon, \tau)$ and parameters:

$$\epsilon = \frac{r}{R_i}, \qquad \tau = \frac{\overline{v}t}{R_i}, \qquad \lambda = \frac{v_z}{\overline{v}},$$

$$\gamma = \frac{A_oR_i}{\rho\overline{v}^2}, \qquad \beta = \frac{B_oR_i}{\rho\overline{v}^2}, \qquad \overline{\omega} = \frac{R_iw}{\overline{v}}, \qquad c = \hat{c}(r, t) = \varsigma(\epsilon, \tau), \quad (4.8)$$

$$\delta = 2\alpha\frac{\overline{v}^2}{R_i^2}, \qquad \phi = \psi\frac{\overline{v}}{R_i^3}, \qquad \widetilde{\mu} = \frac{\mu[\hat{c}(r, t)]}{\rho\overline{v}R_i} = \frac{\overline{\mu}[\varsigma(\epsilon, \tau)]}{\rho\overline{v}R_i},$$

where $\overline{v}$ is a representative velocity. Thus, the non-dimensional forms of the governing equations (4.4) and (4.6) are:

$$\frac{\partial \lambda}{\partial \tau} = \gamma + \beta \sin(\overline{\omega}\tau) + \frac{1}{\epsilon}\frac{\partial}{\partial \epsilon}\left\{\epsilon\widetilde{\mu}\left[1 + \delta\left(\frac{\partial \lambda}{\partial \epsilon}\right)^2\right]^n \frac{\partial \lambda}{\partial \epsilon}\right\}, \quad 0 < \epsilon < 1, \quad \tau > 0,$$

$$(4.9)$$

and

$$\frac{\partial \varsigma}{\partial \tau} = \frac{\phi}{\epsilon}\frac{\partial}{\partial \epsilon}\left[\epsilon\left(\frac{\partial \lambda}{\partial \epsilon}\right)^2 \frac{\partial \varsigma}{\partial \epsilon}\right], \quad 0 < \epsilon < 1, \quad \tau > 0, \tag{4.10}$$

respectively.

A.   The Zero Shear-Rate Viscosity

As stated earlier, we wish to study both chemical-thickening and thinning, and the zero shear-rate viscosity should either be a monotonically increasing or monotonically decreasing function, respectively, of the concentration. For simplicity, we choose the quadratic function:

$$\overline{\mu}(\varsigma) = k_1\varsigma^2 + k_2, \tag{4.11}$$

where k_1 and k_2 are constants.

To describe chemical-thickening, we require the following conditions to be satisfied:

$$\overline{\mu}(0) = 100\hat{\mu} \quad \text{and} \quad \overline{\mu}(1) = 500\hat{\mu}, \tag{4.12}$$

where $\hat{\mu}$ is a constant. $\varsigma = 0$ corresponds to the fluid prior to any reaction while $\varsigma = 1$ corresponds to a state in which the fluid is thicker and more viscous due to the chemical reactions. Application of these conditions to equation (4.11) yields:

$$\overline{\mu}(\varsigma) = \hat{\mu}\mathrm{g}_1(\varsigma) = 100\hat{\mu}(4\varsigma^2 + 1). \tag{4.13}$$

In the case of a fluid that thins due to the reactions we assume that:

$$\overline{\mu}(0) = 500\hat{\mu} \quad \text{and} \quad \overline{\mu}(1) = 100\hat{\mu}. \tag{4.14}$$

In this case, $\varsigma = 1$ implies the fluid has completely transformed to a thinner, less viscous fluid. The conditions in (4.14) require:

$$\overline{\mu}(\varsigma) = \hat{\mu}\mathrm{g}_2(\varsigma) = 100\hat{\mu}(5 - 4\varsigma^2). \tag{4.15}$$

B. Final Equations

Since $\overline{\mu}(\varsigma)$ is known in terms of the concentration, equation (4.9) is now stated in the more convenient form:

$$\frac{\partial \lambda}{\partial \tau} = \gamma + \beta \sin(\overline{\omega}\tau) + \frac{1}{(\mathrm{Re})\epsilon} \frac{\partial}{\partial \epsilon} \left\{ \epsilon \mathrm{g}_j(\varsigma) \left[1 + \delta \left(\frac{\partial \lambda}{\partial \epsilon} \right)^2 \right]^n \frac{\partial \lambda}{\partial \epsilon} \right\}, \tag{4.16}$$

where Re is the Reynolds number defined through:

$$\mathrm{Re} = \frac{\rho \overline{v} R_i}{\hat{\mu}}. \tag{4.17}$$

When $j = 1$ equation (4.16) is the governing relationship for a chemical-thickening fluid while if $j = 2$ it is the governing equation for a fluid that chemically thins.

We shall see that the flow-rate is an appropriate parameter for studying the thickening and thinning phenomena in these chemically-reacting fluids. We define the non-dimensional flow-rate through:

$$\overline{Q}(\tau) = 2\pi \int_0^1 \lambda(\epsilon, \tau)\epsilon d\epsilon \tag{4.18}$$

with respect to a cylindrical-polar coordinate system. From this point on, when physical quantities are mentioned it is with an understanding that they are non-dimensional.

CHAPTER V

SOLUTIONS[*]

Equations (4.10) and (4.16) constitute a non-linear system of partial differential equations that must be solved subject to initial conditions and boundary conditions, for both the velocity and the concentration, and we solve the system for a variety of physically interesting situations. Once the parameters and solution method are established, we solve the problem of a shear-thinning fluid that chemically thickens. Next, we study a fluid that has both shear-thinning and chemical-thinning characteristics. In each case, we compare the results to those obtained for a non-reacting Newtonian fluid.

A. Boundary and Initial Conditions

For fluids such as water flowing under normal conditions, it is customary to enforce the 'no-slip' boundary condition[‡]. Here, we shall enforce the no-slip boundary condition at the solid surface. We also need to prescribe a boundary condition for the concentration. For our problem, we shall require that no species enter or leave through the boundary. These two conditions can be stated as the following:

$$\lambda(1,\tau) = 0 \ \text{ and } \ \frac{\partial \varsigma}{\partial \epsilon}(1,\tau) = 0, \ \ \tau \geqq 0. \tag{5.1}$$

[‡]While the condition is supposed to have had the backing of Stokes, he was far from unequivocal about it. (see Stokes [14]). He advocated the condition for sufficiently slow flows.

Also, since the domain is axisymmetric, we require the following conditions at the center-line $\epsilon = 0$:

$$\frac{\partial \lambda}{\partial \epsilon}(0, \tau) = 0 \;\; \text{and} \;\; \frac{\partial \varsigma}{\partial \epsilon}(0, \tau) = 0, \;\; \tau \geqq 0. \tag{5.2}$$

Since the problem is unsteady, initial conditions must also be specified. This is always problematic when solving equations computationally since one does not know, especially in practical situations, the initial profile of the state variables, and these initial conditions can ultimately affect the solutions even once the transients have 'died-out'. However, the standard procedure is to prescribe a parabolic profile for the initial velocity. The initial profile for the concentration, congruent with the boundary conditions, is given by:

$$\varsigma(\epsilon, 0) = \epsilon^2(3 - 2\epsilon), \;\; 0 \leqq \epsilon \leqq 1. \tag{5.3}$$

This profile shows the initial concentration along the center-line is much less than that at the wall, and thus the reaction will begin very rapidly at the wall. However, it is possible that the rate of reaction will decrease, and this will ultimately depend on the solutions to the governing equations.

B. Parameter Values

There are a total of 7 non-dimensional parameters and the functions g_j in equations (4.10) and (4.16). Since we are interested in studying the interaction between the shear-thinning effects (n) and chemical-thinning/thickening effects (g_j) we assign typical values to the other non-dimensional parameters:

$$\gamma = 10, \;\; \beta = 10, \;\; \overline{\omega} = 1, \;\; \text{Re} = 100, \;\; \delta = 0.1, \;\; \text{and} \;\; \phi = 0.005. \tag{5.4}$$

When studying the shear-thinning and Newtonian models, we assume $n = $ -0.5 and 0, respectively. Also, when using the Newtonian model we set $\overline{\mu} = 300\hat{\mu}$. The function $\dfrac{\mathbf{g}_j}{\mathrm{Re}}$ was chosen in such a way that it never attains a value less than one. This is because we wish to compare the shear-thinning effects to the chemical-thinning/thickening effects. To this end, let us define the *competition number* (CN) as the following:

$$\mathrm{CN} = \frac{\dfrac{\mathbf{g}_j(\varsigma)}{\mathrm{Re}}}{\left[1 + \delta \left(\frac{\partial \lambda}{\partial \epsilon}\right)^2\right]^{-n}}. \tag{5.5}$$

The numerator represents the chemical-thickening/thinning effects while the shear-thinning effects are shown in the denominator. This ratio will prove useful in analyzing the results.

C.   Solution Method

We were unable to obtain exact solutions to the equations (4.10) and (4.16), in general, and therefore they were solved numerically. Since numerical methods are employed one might expect errors, especially near $\epsilon = 0$, due to the singularities in the governing equations. Fortunately, a finite element algorithm has been developed [13] to handle such difficulties. We use this finite element method to reduce the system of partial differential equations to a system of ordinary differential equations in time at discrete spatial locations. More specifically, the method uses a piecewise non-linear Petrov-Galerkin method that is second-order accurate to discretize the space variable. The finite element method utilized differs from the regular Galerkin method since the shape functions for the trial solution are logarithmic and not equal to the weight functions. Once the system of ordinary differential equations is obtained, a variable order solver that uses difference formulas for the derivatives is used to reduce the system of ordinary differential equations to a system of algebraic equations. The algebraic equations are then solved using standard methods.

Accuracy in the spatial derivatives of the velocity are of particular importance since they appear in both the stress and the competition number. Cubic splines are used to approximate the velocity by interpolating between the discrete points at each time τ. Once the splines are calculated, the first derivatives are then easily obtained.

CHAPTER VI

RESULTS AND CONCLUSIONS[*]

If we restrict ourselves to steady flows we can find exact solutions to equations (4.10) and (4.16) by direct integration. These analytical solutions will help determine how the material parameters affect the state variables, and they will also aid in checking the qualitative behavior of the numerical solutions.

Let us assume that $\lambda(\epsilon)$, $\varsigma(\epsilon) \in \mathbf{C}^2[0, 1]$. We shall begin with the governing equation for the concentration since we can integrate it once and then apply the neumann conditions to find the concentration directly:

$$\frac{1}{\epsilon}\frac{d}{d\epsilon}\left[\epsilon\left(\frac{d\lambda}{d\epsilon}\right)^2\frac{d\varsigma}{d\epsilon}\right] = 0, \tag{6.1}$$

$$\epsilon\left(\frac{d\lambda}{d\epsilon}\right)^2\frac{d\varsigma}{d\epsilon} = \text{constant} = k_3. \tag{6.2}$$

Application of the second condition in equation (5.2) yields:

$$\varsigma(\epsilon) = \text{constant} = k_4 \tag{6.3}$$

where $0 \leqq k_4 \leqq 1$. The governing equation for the (steady) velocity is:

$$\frac{1}{\epsilon}\frac{d}{d\epsilon}\left\{\epsilon\mathbf{g}_j(\varsigma)\left[1 + \delta\left(\frac{d\lambda}{d\epsilon}\right)^2\right]^{-\frac{1}{2}}\frac{d\lambda}{d\epsilon}\right\} = -\gamma\text{Re}. \tag{6.4}$$

Direct integration results in the following equation:

$$\left[1 + \delta\left(\frac{d\lambda}{d\epsilon}\right)^2\right]^{-\frac{1}{2}}\frac{d\lambda}{d\epsilon} = -\frac{\gamma\text{Re}}{2\mathbf{g}_j(\varsigma)}\epsilon + \frac{k_5}{\mathbf{g}_j(\varsigma)\epsilon}. \tag{6.5}$$

Utilizing the above assumption of smoothness we can apply the first condition in equation (5.2) and after some algebra we arrive at the equation:

$$\frac{d\lambda}{d\epsilon} = -\frac{\gamma \mathrm{Re}\epsilon}{\left[4\mathrm{g}_j^2(\varsigma) - \delta\gamma^2\mathrm{Re}^2\epsilon^2\right]^{\frac{1}{2}}}. \tag{6.6}$$

Again, we can directly integrate this equation to obtain:

$$\lambda(\epsilon) = \frac{1}{\gamma\mathrm{Re}\delta}\left[4\mathrm{g}_j^2(\varsigma) - \delta\gamma^2\mathrm{Re}^2\epsilon^2\right]^{\frac{1}{2}} + k_6. \tag{6.7}$$

Finally, we apply the first boundary condition in equation (5.1) to obtain the particular solution:

$$\lambda(\epsilon) = \frac{1}{\gamma\mathrm{Re}\delta}\left\{\left[4\mathrm{g}_j^2(\varsigma) - \delta\gamma^2\mathrm{Re}^2\epsilon^2\right]^{\frac{1}{2}} - \left[4\mathrm{g}_j^2(\varsigma) - \delta\gamma^2\mathrm{Re}^2\right]^{\frac{1}{2}}\right\}. \tag{6.8}$$

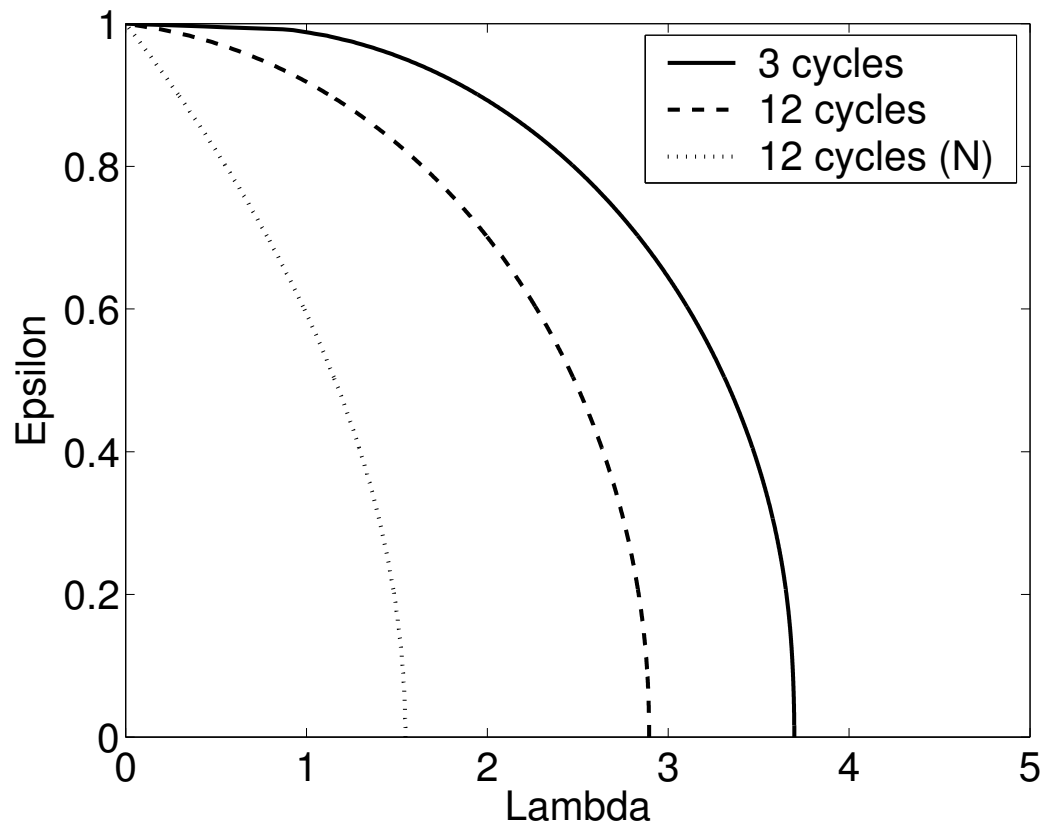A.   Shear-Thinning, Chemical-Thinning Fluid

Fig. 1. Velocity profiles at different times in the cycle for a shear-thinning, chemi-
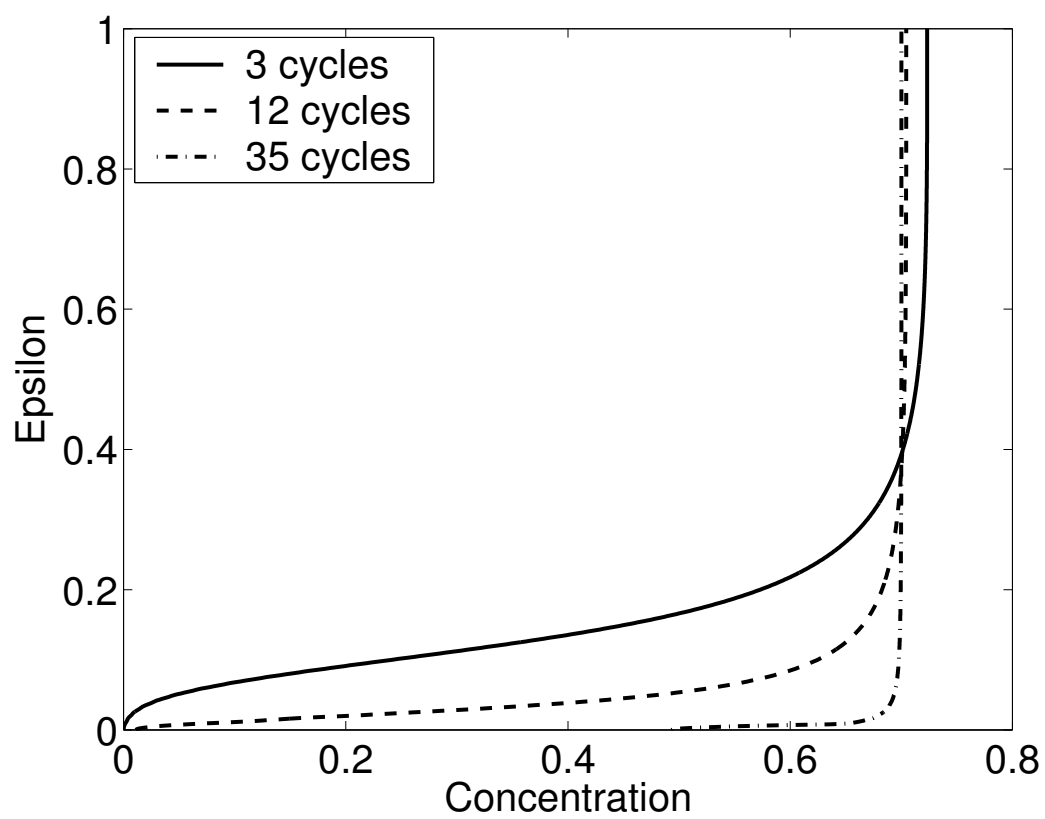   cal-thinning fluid and a Newtonian fluid (N).

Fig. 2. Concentration profiles at different times in the cycle for a shear-thinning, chemical-thinning fluid.
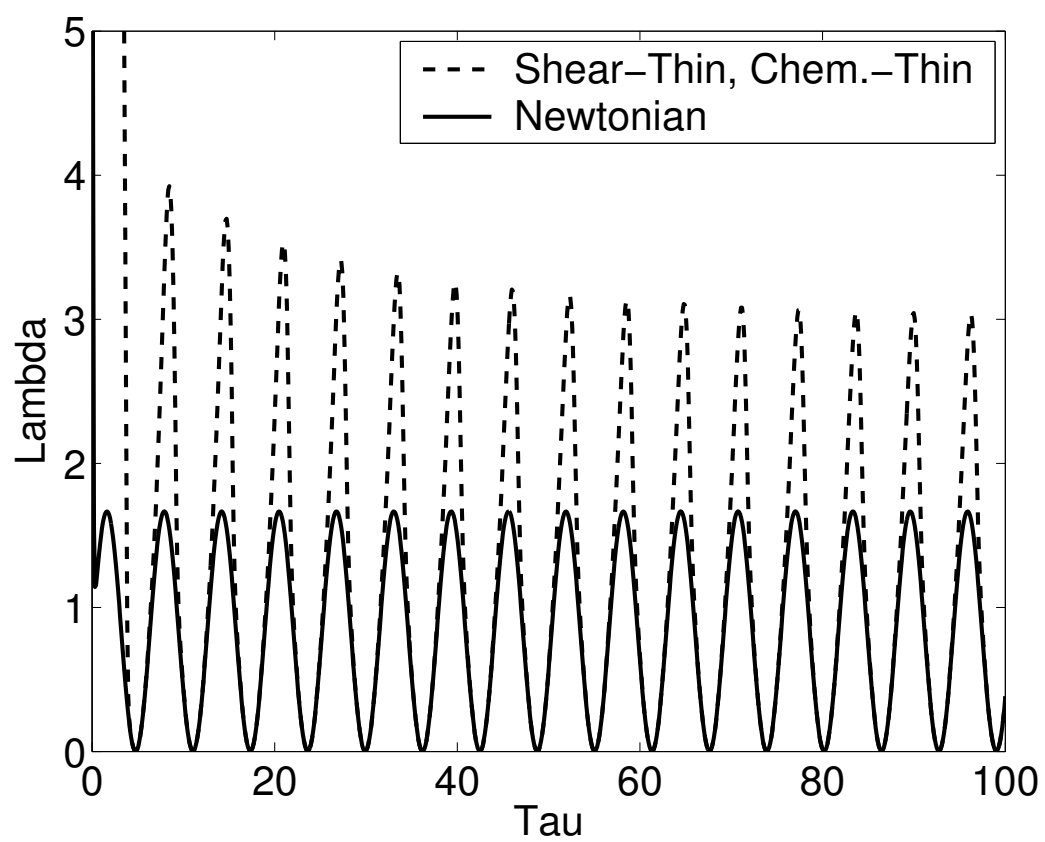
Fig. 3. Maximum velocity as a function of time for a shear-thinning, chemical-thin-
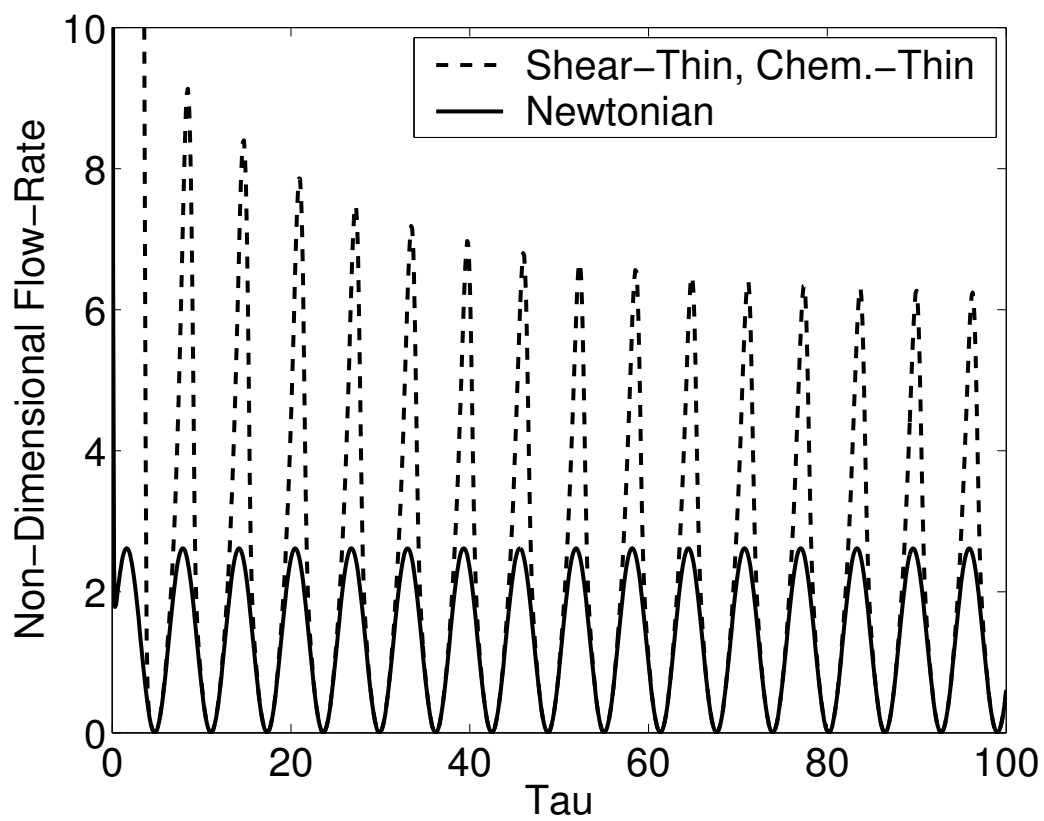ning fluid and a Newtonian fluid.

Fig. 4. Flow-rate as a function of time for a shear-thinning, chemical-thinning fluid and a Newtonian fluid.
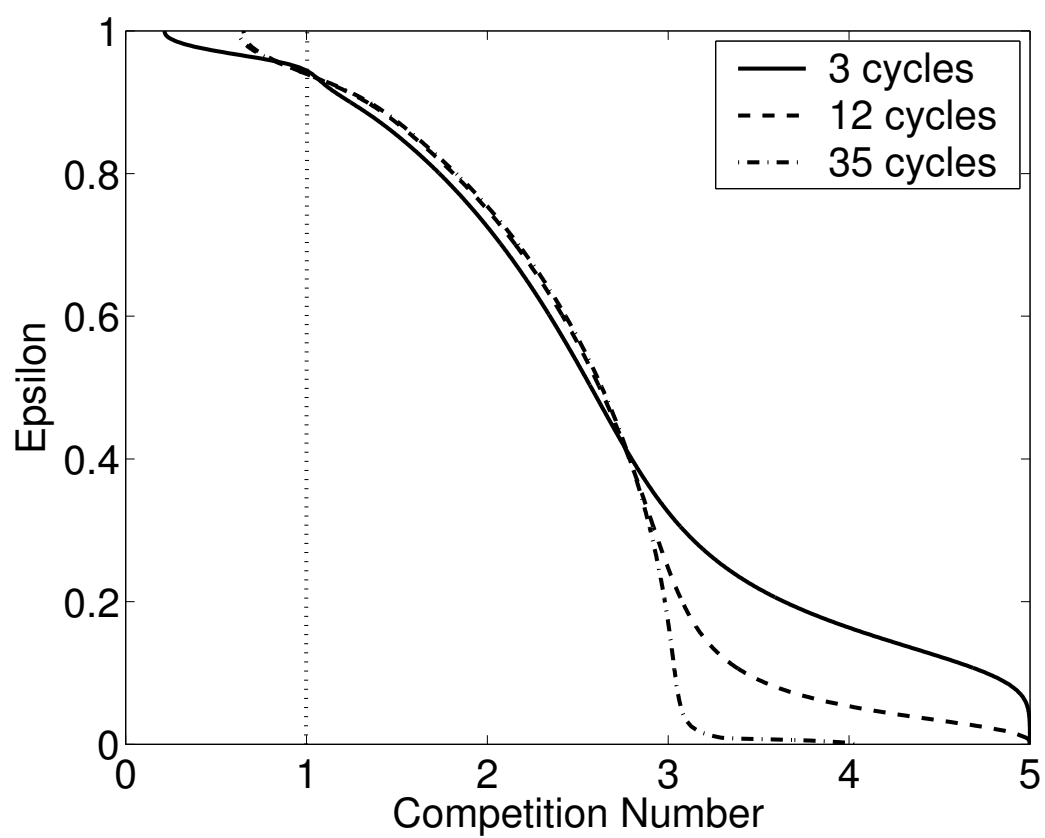
Fig. 5. Competition number at different times in the cycle for a shear-thinning, chemical-thinning fluid.
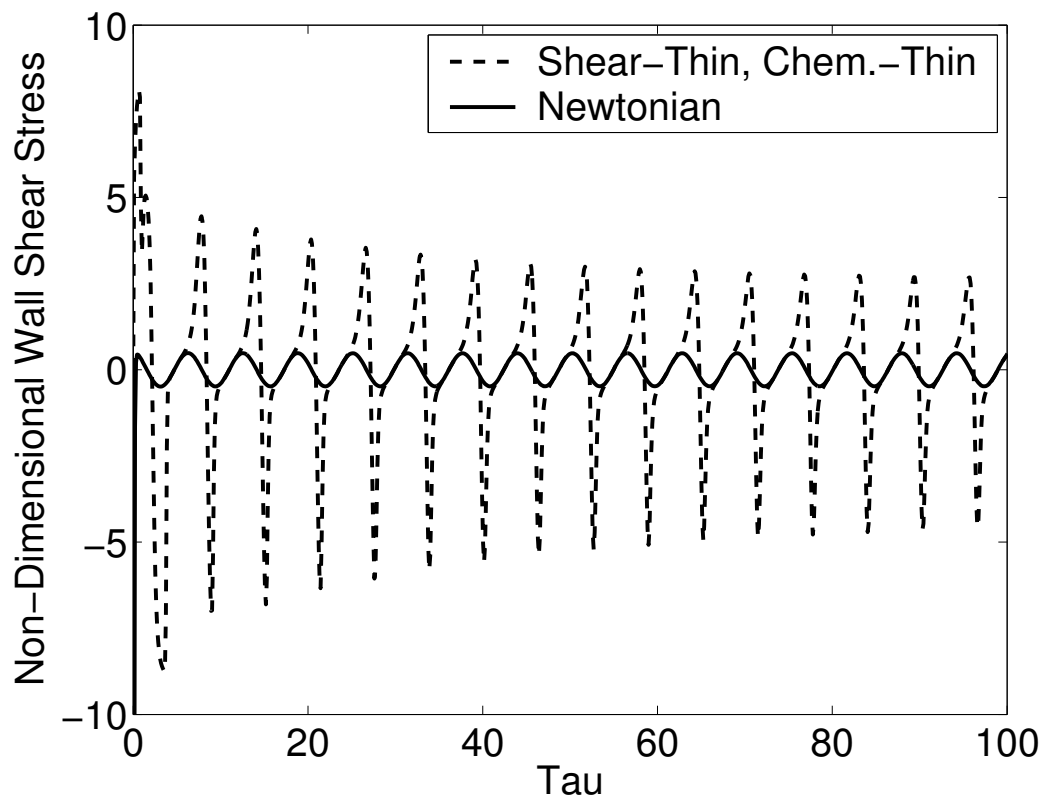
Fig. 6. Illustration of the shear stress at the wall for a shear-thinning, chemical-thin-
ning fluid and a Newtonian fluid.

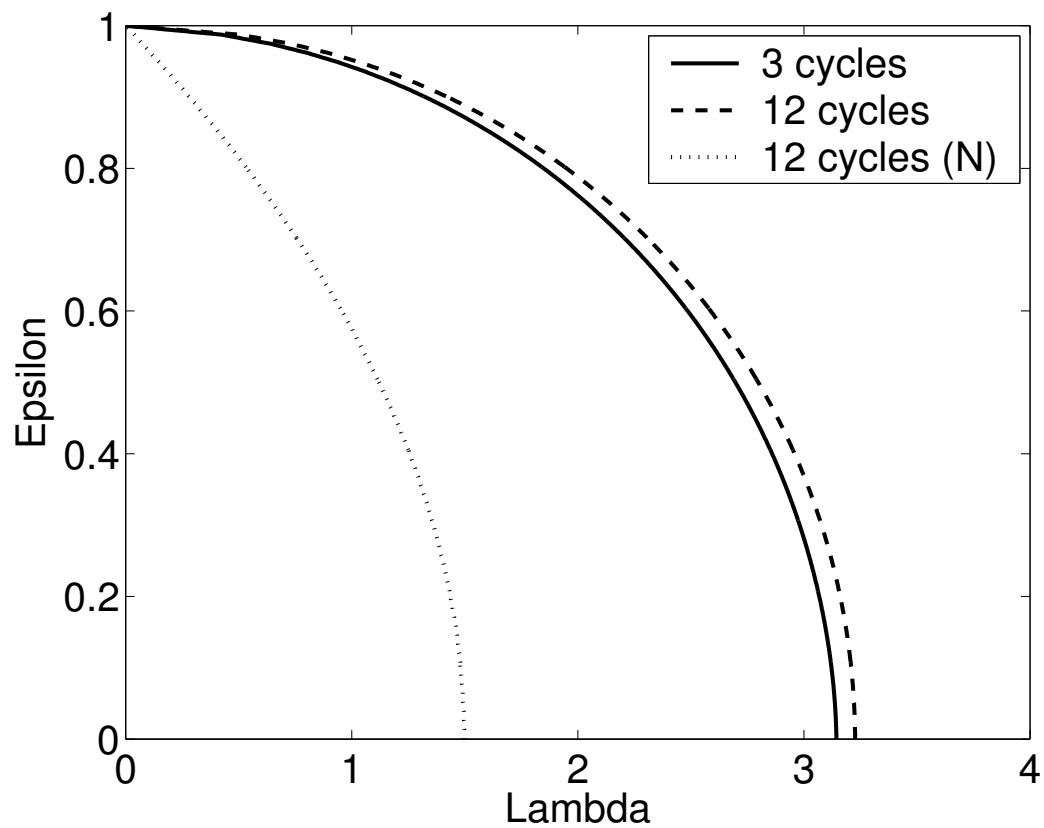B.   Shear-Thinning, Chemical-Thickening Fluid

Fig. 7. Velocity profiles at different times in the cycle for a shear-thinning, chemi-
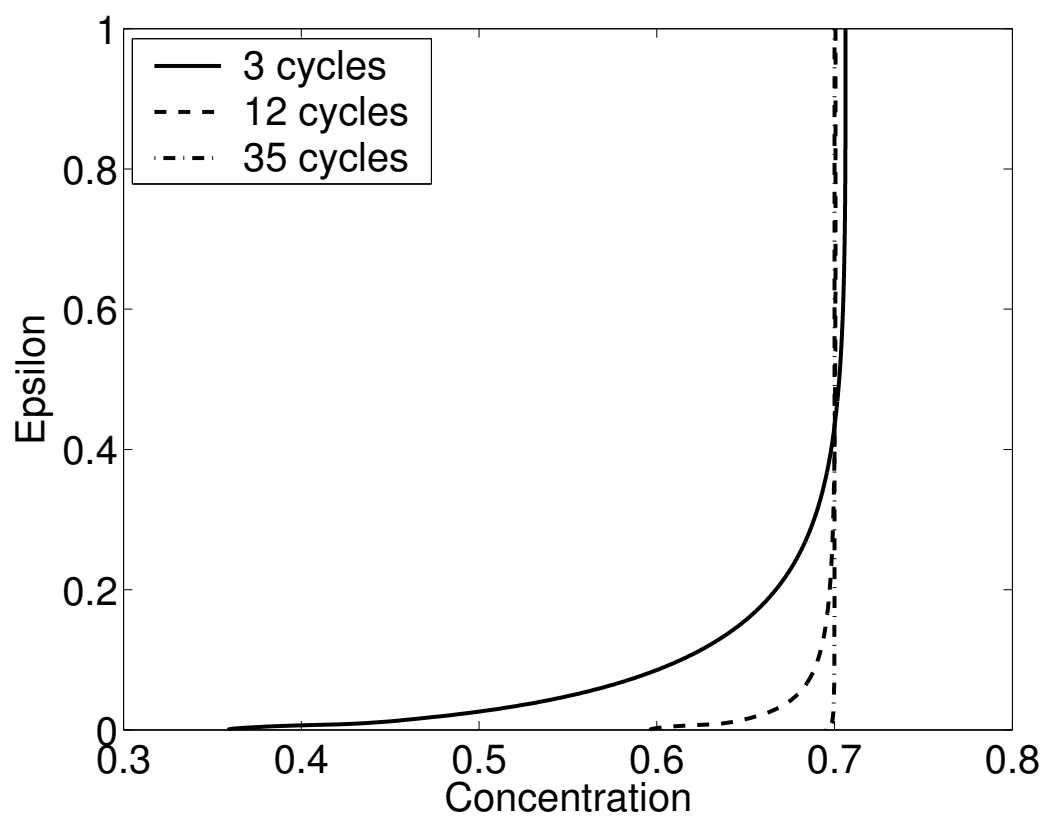cal-thickening fluid and a Newtonian fluid (N).

Fig. 8. Concentration profiles at different times in the cycle for a shear-thinning, chemical-thickening fluid.

Fig. 9. Maximum velocity as a function of time for a shear-thinning, chemical-thickening fluid and a Newtonian fluid.

Fig. 10. Flow-rate as a function of time for a shear-thinning, chemical-thickening fluid and a Newtonian fluid.

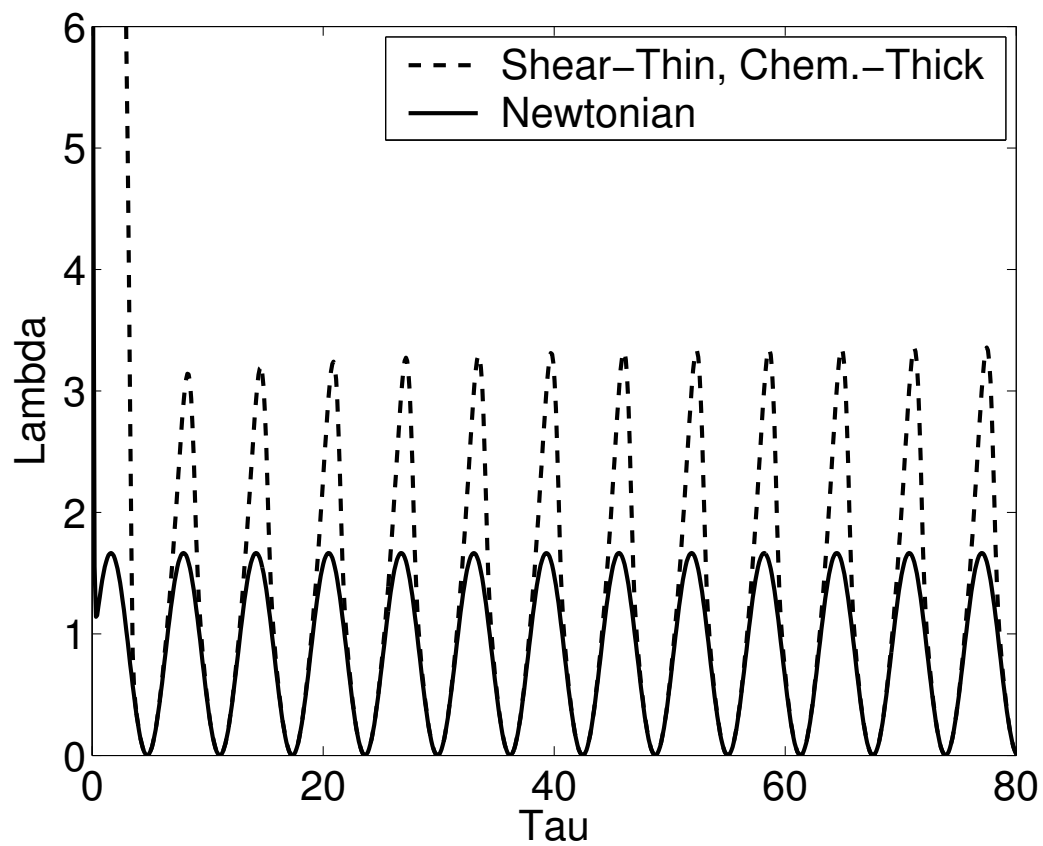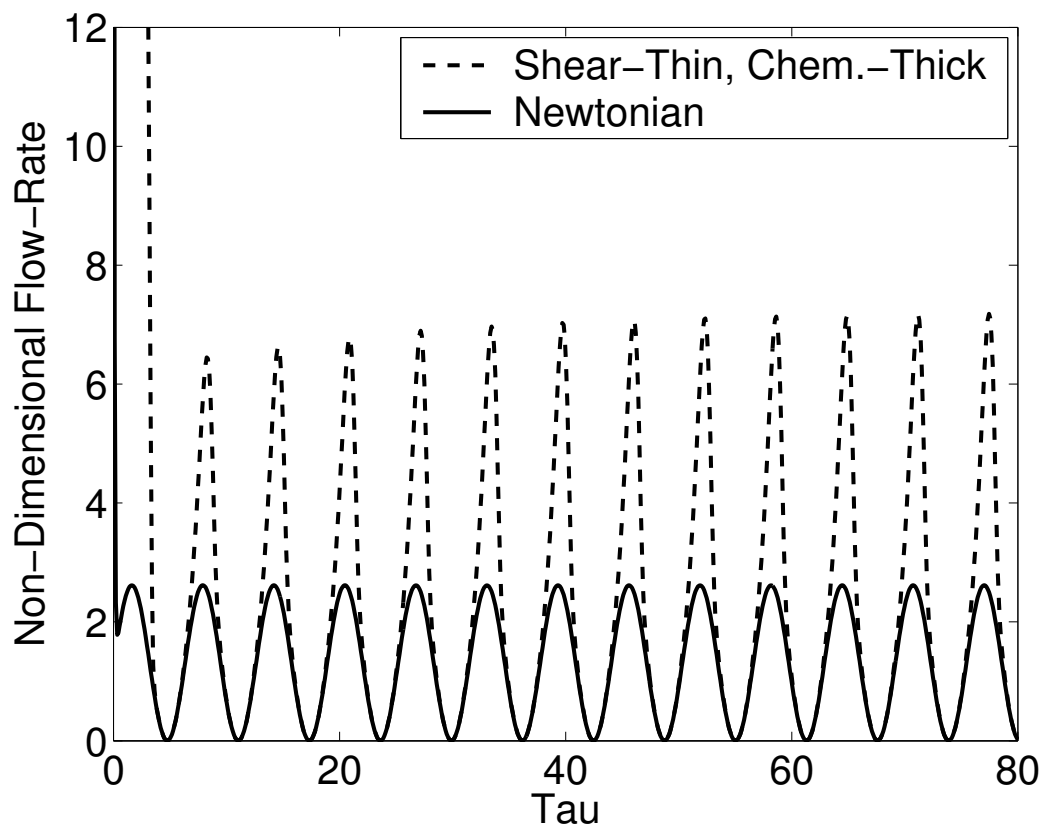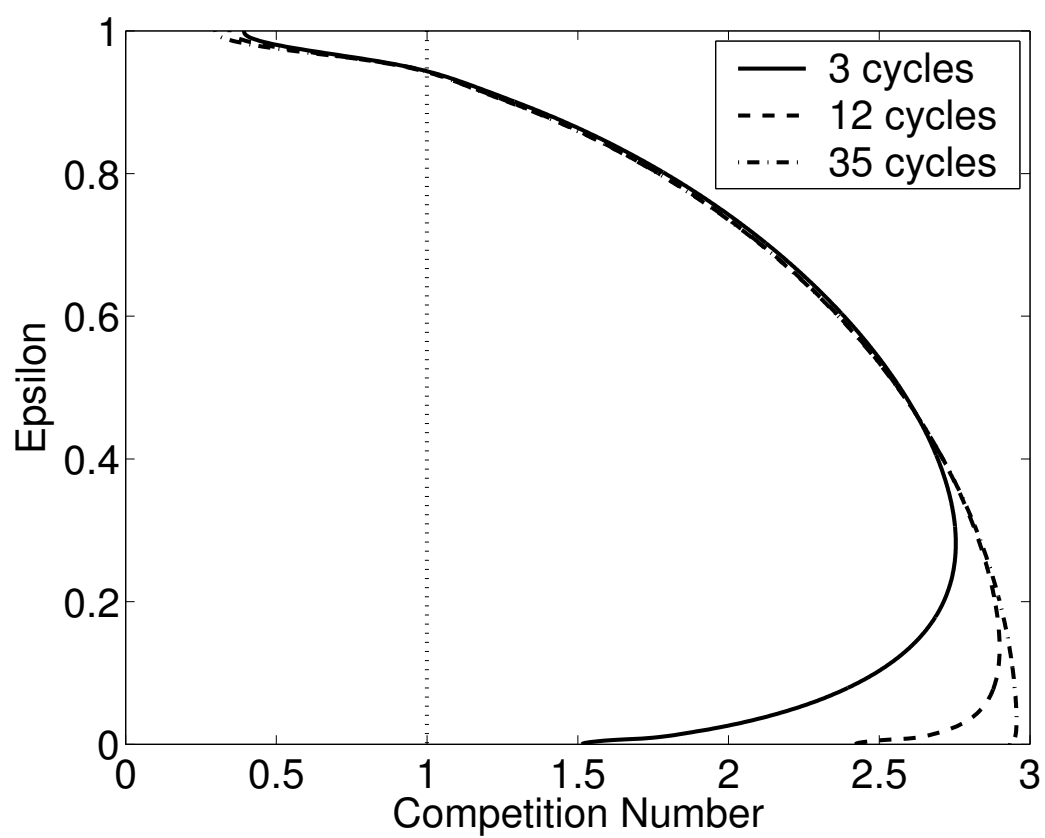Fig. 11. Competition number at different times in the cycle for a shear-thinning, chemical-thickening fluid.
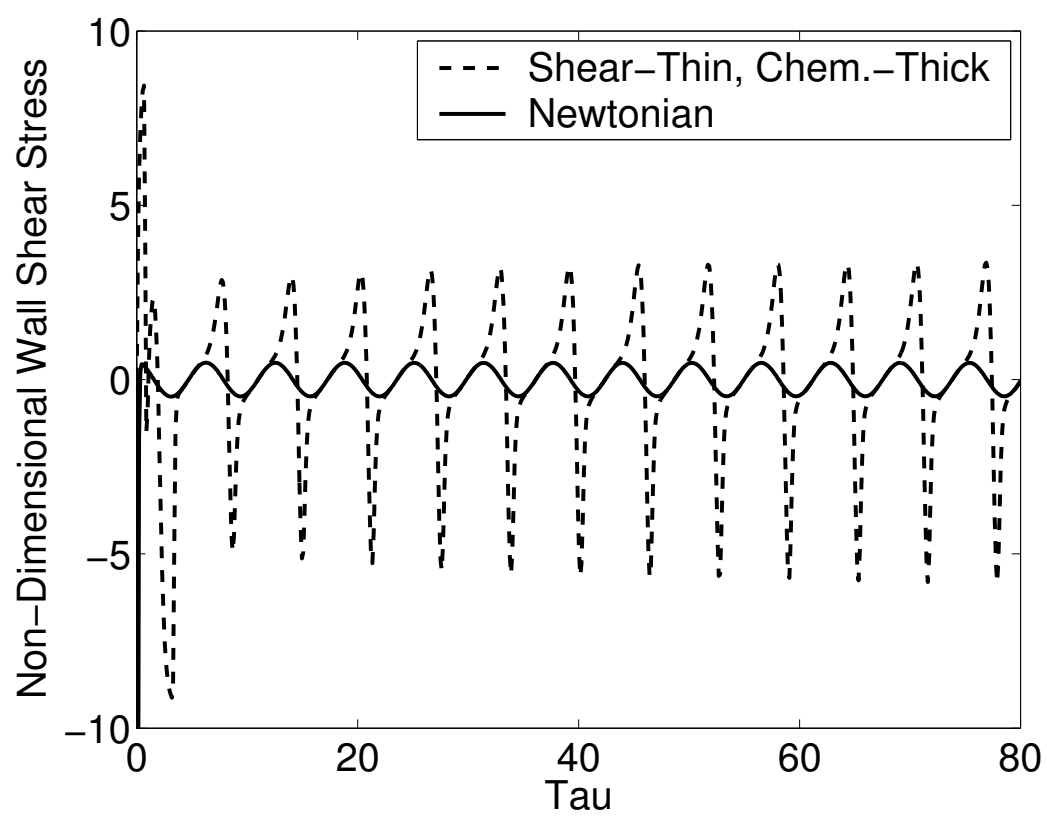
Fig. 12. Illustration of the shear stress at the wall for a shear-thinning, chemical-thickening fluid and a Newtonian fluid.

C.   Discussion of Results

Equations (6.3) and (6.8) represent steady solutions to the system of partial differential equations (4.10) and (4.16), respectively. The solution (6.8) exhibits a 'parabolic-type' profile reminiscent of the Newtonian profile, however, note that $4\mathrm{g}_j^2(\varsigma) \geqq \gamma^2\mathrm{Re}^2\delta$ must be satisfied for all ς or else a real solution is not possible. If this is the case, one must conclude that solution does not exist. However, for the functions $\mathrm{g}_j(\varsigma)$ and parameter values chosen the solution (6.8) is valid. As stated previously, it is possible that other C^2 solutions or even solutions with less smoothness exist. One should expect the result (6.3) as the boundary and symmetry conditions for the concentration are both Neumann.

Let us now analyze the results for the shear-thinning, chemical-thinning fluid. In this case, both the shear-index and the function $\mathrm{g}_2(\varsigma)$ contribute to the thinning. Figure 2 shows the concentration of the reactant increases, as time increases, in a region about 0.4 units from the the center-line while the concentration of the reactant contained in the remaining portion of the cross-section is approximately constant. Since the fluid chemically-thins, this causes the viscosity of the fluid to decrease. Therefore, the center-line velocity decreases to a lower-bound as depicted in figures 1 and 3. At first, this might seem strange that a decrease in viscosity leads to a decrease in maximum velocity. However, a careful consideration of the situation convinces one that the result is not counter-intuitive, rather what one should expect. For example, consider the flow of an incompressible fluid in a diverging pipe. Balance of mass requires that the center-line velocity downstream be smaller than the center-line velocity upstream. This is just the case we have here, except in our case there is no notion of a geographic upstream or downstream. For us, the 'downstream' is the increase in concentration, as time

increases, which in turn causes the fluid to thin (as time increases). Note that after 35 cycles the concentration approaches a constant value just as the steady solution (6.3) predicts. The chemical-thinning of the fluid also causes the flow-rate to decrease, as shown in figure 4, which seems unusual since one would expect the flow-rate of the chemical-thinning fluid to increase. This anomaly is contributed to the aforementioned behavior of the velocity of the fluid. A plot of the profiles for the competition number (CN) in figure 5 reveals that the chemical-thinning effects are dominant except for a small layer approximately 0.1 unit thick near the wall. Here, the effects due to shear-thinning are the most important, but become less important as time increases. Naturally, one would question what effect this has on the wall shear-stress. In figure 6 we plot the wall shear-stress for both the shear-thinning fluid and the Newtonian fluid. The wall shear-stress associated with the shear-thinning fluid is approximately 5 times that of the Newtonian fluid.

We shall now analyze the numerical results from the shear-thinning, chemical-thickening fluid. The results for the velocity, in this case, are similar to those for an incompressible fluid flowing in a converging pipe. As the pipe converges, there is less space through which the fluid can flow, and consequently the center-line velocity increases. Once again, the concentration of the fluid near the center-line increases as depicted in figure 8. However, in this case, the fluid is chemically-thickening, and therefore the viscosity increases in this region. This causes the center-line (maximum) velocity to increase just as in the case of the converging pipe. This is shown in the plots of the velocity in figures 7 and 9. Note that the velocity for the shear-thinning fluid is approximately twice that for the Newtonian fluid, and yet again, the velocity appears to have a limiting value except in this case it is an upper-bound. This phenomenon is also illustrated by plotting the flow-rate in figure 10. The CN profiles for the chemical-thickening fluid, depicted in

figure 11, show that the shear-thinning effects are still dominant near the boundary. We again plot the wall shear stress in figure 12. As stated previously, the CN for the chemical-thinning fluid shows the shear-thinning effects become less important as time increases, and therefore the wall shear-stress decreases. For the chemical-thickening fluid, however, the CN shows that the shear-thinning effects become more and more dominant, as time increases, at the wall and hence the wall shear-stress increases. Also note that the velocity and concentration, in the case of the chemical-thickening fluid, reach a steady state value more quickly than the velocity and concentration from the chemical-thinning fluid. This suggests that the chemical-thickening process takes less time. This seems contradictory since one would expect the interplay between the thickening and thinning to take longer as they are opposing effects. Note the center-line CN for the chemical-thinning fluid, depicted in figure 5, is initially 5, while the initial, center-line CN for the chemical-thickening fluid is approximately 1.5, and the CN for both the chemical-thinning and chemical-thickening fluid tends to a steady-state value of 3 along the center-line. Thus, the chemical-thinning process takes longer since the initial conditions, which determine the initial CN, are closer to the steady-state values for the chemical-thickening fluid.

REFERENCES

[1] A. Kuharsky and A. Fogelson, Surface-Mediated Control of Blood Coagulation: The Role of Binding Site Densities and Platelet Deposition. *Biophysical Journal*. **80** (3) 1050-1074 (2001).

[2] A. Mohan, K.R. Rajagopal, and K. Rajagopal, A Model Incorporating some of the Mechanical and Biochemical Factors Underlying Clot Formation and Dissolution in Flowing Blood. *Journal of Theoretical Medicine*. **5** (3-4) 183-218 (2003).

[3] C. Truesdell, Sulle Basi Della Termomeccanica I. *Rendiconti Lincei*. **8** (22) 22-38 (1957).

[4] C. Truesdell, Sulle Basi Della Termomeccanica II. *Rendiconti Lincei*. **8** (22) 158-166 (1957).

[5] I. Samohyl, *Rational Thermodynamics of Chemically-Reacting Mixtures*, Academia, Prague (1982).

[6] K.R. Rajagopal and L. Tao, *Mechanics of Mixtures*, *Series on Advances in Mathematics for Applied Sciences*, World Scientific, Vol. 35, (1995).

[7] R.S. Rivlin and J.L. Ericksen, Stress-Deformation Relations for Isotropic Materials. *Journal of Rational Mechanics and Analysis*. **4** (3) 323-425 (1955).

[8] C. Truesdell and W. Noll, *The Non-Linear Field Theories of Mechanics, Fliigge's Handbuch der Physik, I11/3*, Springer, Berlin (1965).

[9] P.J. Carreau, D. De Kee and R.J. Chhabra, *Rheology of Polymeric Systems: Principles and Applications*, Hanser/Gardner Publications, Inc., Cincinnati, OH (1997).

[10] J. Malek, J. Necas, M. Rokyta, and M. Ruzicka, *Weak and Measure-Valued Solutions to Evolutionary PDEs*, Chapman and Hall, London (1996).

[11] J. Malek, K.R. Rajagopal, and M. Ruzicka, Existence and Regularity of Solutions and the Stability of the Rest State for Fluids with Shear Dependent Viscosity. M^3AS. **5** 789-812 (1995).

[12] K.R. Rajagopal and A. Srinivasa, A Thermodynamic Framework for Rate Type Fluid Models. *Journal of Non-Newtonian Fluid Mechanics*. **88** 207-227 (2000).

[13] R. Skeel and M. Berzins, A Method for the Spatial Discretization of Parabolic Equations in One Space Variable. *SIAM Journal on Scientific and Statistical Computing*. **11** (1) 1-32 (1990).

[14] G.G. Stokes, On the Theories of Internal Friction of Fluids in Motion and of the Equilibrium and Motion of Elastic Solids. *Trans. Cambridge Society*. **8** 287-305 (1845).

VITA

Ronald Craig Bridges, II

230A Engineering/Physics, College Station, Texas 77843-3123

- **Texas A & M University**—College Station, TX

  Master of Science in Mechanical Engineering

    – GPA: 3.9 (overall)

    – Graduation Date: May 2007

- **Texas A & M University**—College Station, TX

  Bachelor of Science in Mechanical Engineering

    – GPA: 3.8 (ME major)

    – Graduation Date: May 2005

The typist for this thesis was Ronald Craig Bridges, II.