DEVELOPING NEW FITTED CLOSURE APPROXIMATIONS FOR
SHORT-FIBER REINFORCED POLYMER COMPOSITES

A Thesis presented to the Faculty
of the Graduate School at the
University of Missouri-Columbia

In Partial Fulfillment
of the Requirements for the Degree
Master of Science

by

MATTHEW MULLENS

Dr. Douglas Smith, Thesis Supervisor

JULY 2010
The undersigned, appointed by the dean of the Graduate School, have examined the thesis entitled

DEVELOPING NEW FITTED CLOSURE APPROXIMATIONS FOR
SHORT-FIBERREINFORCED POLYMER COMPOSITES

presented by Matthew Mullens,

a candidate for the degree of Master of Science,

and hereby certify that, in their opinion, it is worthy of acceptance.

________________________________________
Dr. Douglas Smith

________________________________________
Dr. J. K. Chen

________________________________________
Dr. Stephen Montgomery-Smith

________________________________________
Dr. David Jack
Acknowledgements

First and foremost, I would like to thank the Lord for giving me the academic talents that I possess that helped me to complete my studies. Also I would like to thank Him for giving me the strength and perseverance to continue my works, when things seemed to not always work out.

I would also like to thank my advisor Dr. Douglas Smith for all the work he has done with me, without his patience and encouragement things would have been infinitely more difficult. I would also like to thank Dr. Stephen Montgomery-Smith and Dr. David Jack for their continuous help whenever needed, they have also been patient with me and have taken the time to ensure I understand the concepts on which they have helped me.

Kyler Turner deserves special thanks because without his encouragement it is very possible that I would have never considered going back to school for my Master of Science. His experience and knowledge has been invaluable to me.

Another friend, Brad Snow, also deserves special thanks for helping me with all my many programming questions and issues that would occur throughout my master’s studies. I would also like to thank Dongdong Zhang, Roxana Martinez-Campuzano, and Najam Qadir for putting up with my ramblings and antics in our office for the past two years.

Most importantly of all, I would also like to thank my family, my mother and father, my brother, Brandon, my sisters, Dani and Sandy, for always believing in me and helping to provide me with the strength that I needed to complete my academic and professional goals.
List of Tables

Chapter 2

Table 2.1 Summary of Hinch and Leal closure approximations. ...................................................... 28
Table 2.2 Relationship between indices of contracted and tensor notation. ............................... 31

Chapter 3

Table 3.1 Summary of regression analysis on elliptic integral data set ordered from worst to best. ........................................................................................................................................ 63
Table 3.2 Summary of regression analysis of polynomials of order 4 from SPH data set........... 67
Table 3.3 Coefficients $C_{m(n)}^{(n)}$ of FFLAR4 closure.............................................................................. 70
Table 3.4 Coefficients $C_{m(n)}^{(n)}$ of LAR4 closure. .................................................................................... 71
Table 3.5 Coefficients $C_{m(n)}^{(n)}$ for LAR32 closure (below the separating line denotes denominator coefficients)......................................................................................................................... 72
Table 3.6 Error for select flows for various closures.............................................................................. 75
Table 3.7 Error for mixed flow for various closures. ............................................................................... 77
Table 3.8 Error for various closures for varying z-values of the center-gated disk..................... 83

Chapter 4

Table 4.1 Coefficients $C_{m(n)}^{(n)}$ for DAIJXX2 closure. ................................................................. 90
Table 4.2 Coefficients $C_{m(n)}^{(n)}$ for DAIJXX3 closure. ................................................................. 91
Table 4.3 Coefficients $C_{m(n)}^{(n)}$ for DAIJXX4 closure. ................................................................. 93
Table 4. 4 Coefficients $C_{m(n)}$ for DAIJX22 closure. ................................................................. 96
Table 4. 5 Error of DAIJPC closures for various flows................................................................. 103
Table 4. 6 Error of DAIJPC closures for varying z-values............................................................ 105
Table 4. 7 Error of DAIJNR closures for various flows................................................................. 113
Table 4. 8 Error of DAIJNR closures for varying z-values............................................................ 115
Table 4. 9 Normalization condition error results for various closures on selected flows.......... 117
# List of Figures

Chapter 2

Figure 2.1 Coordinate system defining the unit vector p. ......................................................... 9  
Figure 2.2 Eigenspace of all possible orientation states of the second order orientation tensor. 33  
Figure 2.3 Invariant space of all possible orientation states of second-order orientation tensor. 39  

Chapter 3

Figure 3.1 S vs. T space mapped into eigenspace........................................................................ 49  
Figure 3.2 Entire Eigenspace mapped to the eigenspace of first and second eigenvalues. .... 50  
Figure 3.3 Example of effect of robust regression over linear least squares regression.......... 57  
Figure 3.4 Data set chose for fitting created by elliptic integrals. ........................................ 62  
Figure 3.5 Different fourth-order tensor surfaces. ...................................................................... 64  
Figure 3.6 Unacceptable fit of selected closure surface due to Bisquare weighted regression.. 65  
Figure 3.7 Eigenspace created using spherical harmonics....................................................... 67  
Figure 3.8 Selected components of various closures for simple shear flow......................... 74  
Figure 3.9 Selected components from various closures for shear/stretch A flow. ................. 75  
Figure 3.10 Selected closures for given mixed flow component.............................................. 78  
Figure 3.11 Selected closures for given mixed flow component.............................................. 78  
Figure 3.12 Selected closures for given mixed flow components. .......................................... 79  
Figure 3.13 Selected closures for given mixed flow component.............................................. 79  
Figure 3.14 Selected components for various closures for center-gated disk, z=0.3............. 82  
Figure 3.15 Selected components for various closures of center-gated disk, z=0.7............. 82
Chapter 4

Figure 4.1 Selected PC closures for various components from simple shear .................................. 99
Figure 4.2 Selected PC closures for various components from shear/stretch a. ......................... 100
Figure 4.3 Selected PC closures for given mixed flow components. ........................................ 101
Figure 4.4 Selected PC closures for given mixed flow component. .......................................... 101
Figure 4.5 Selected PC closures for given mixed flow components. ........................................ 102
Figure 4.6 Selected PC closures for given mixed flow components. ........................................ 102
Figure 4.7 Selected components for various PC closures of center-gated disk, z=0.3. ............. 104
Figure 4.8 Selected components for various PC closures of center-gated disk, z=0.7. .......... 104
Figure 4.9 Selected NR closures for various components from simple shear. ......................... 109
Figure 4.10 Selected NR closures for various components from shear/stretch a. ...................... 109
Figure 4.11 Selected NR closures for given mixed flow component. ....................................... 110
Figure 4.12 Selected NR closures for given mixed flow component. ....................................... 111
Figure 4.13 Selected NR closures for given mixed flow component. ....................................... 111
Figure 4.14 Selected NR closures for given mixed flow component. ....................................... 112
Figure 4.15 Selected components for various NR closures of the center-gated disk, z=0.3. ... 114
Figure 4.16 Selected components for various NR closures of the center-gated disk, z=0.7. .... 114
Abstract

Short-fiber polymer composites are greatly used throughout the industry for many applications. The orientation state of the short-fibers within the matrix defines the material properties of the composite structure. It is necessary to develop accurate models and a complete understanding of fiber orientation. Material properties of the composite structure depend on the orientation state of the individual fibers inside of the polymer matrix. Calculating the exact orientation of each fiber is computationally expensive; to address this problem equations have been developed based on the orientation distribution of fibers inside the polymer matrix. A form of the distribution equation has been proposed where the orientation of the fibers is represented by a fourth-order tensor. These tensors capture the behavior of the fibers in a compact form. However, the time evolution equation requires that for each lower order tensor, you must make an approximation for the next higher even order tensor. These closure approximations have been a subject of research for many years. This work will explore many closures that have been used and revisit fitting methods and introduce new concepts in fitting, such as different regression types of the fitted polynomials. A new time derivative based closure will also be introduced which gives improved results and shows a need for more investigation of this type of closure.
Table of Contents

Acknowledgements ........................................................................................................ ii

List of Tables .................................................................................................................. iii

List of Figures ............................................................................................................... v

Abstract ....................................................................................................................... vii

Chapter 1. Introduction ................................................................................................. 1

Chapter 2. Fiber Orientation ......................................................................................... 7

  2.1 Modeling Fibers .................................................................................................... 8

  2.2 Distribution Function of Fibers .......................................................................... 10

    2.2.1 Non-Interacting Particle ............................................................................. 11

    2.2.2 Interacting Particles ................................................................................. 13

  2.3 Orientation Tensor Representation .................................................................... 15

    2.3.1 Folgar and Tucker Model ....................................................................... 15

    2.3.2 Other Models Related to the Folgar and Tucker Model ......................... 18

  2.4 Spherical Harmonics ......................................................................................... 20

  2.5 Fourth-Order Closure Approximations ............................................................. 21

    2.5.1 Linear Closure ...................................................................................... 22

    2.5.2 Quadratic Closure ............................................................................... 23
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5.3 Hybrid Closure</td>
<td>24</td>
</tr>
<tr>
<td>2.5.4 Hinch and Leal Closures</td>
<td>27</td>
</tr>
<tr>
<td>2.5.5 Eigenvalue Based Orthotropic Fitted Closure</td>
<td>29</td>
</tr>
<tr>
<td>2.5.6 Invariant Based Orthotropic Fitted Closure</td>
<td>36</td>
</tr>
<tr>
<td>2.6 Sixth-Order Closure Approximations</td>
<td>40</td>
</tr>
<tr>
<td>Chapter 3. Development of Fourth Order Fitted Closures</td>
<td>45</td>
</tr>
<tr>
<td>3.1 Acquiring the Data Set</td>
<td>46</td>
</tr>
<tr>
<td>3.1.3 Elliptic Integrals</td>
<td>47</td>
</tr>
<tr>
<td>3.1.4 On Data Sets</td>
<td>51</td>
</tr>
<tr>
<td>3.2 Fitting Data Sets</td>
<td>52</td>
</tr>
<tr>
<td>3.2.1 Equation Forms</td>
<td>53</td>
</tr>
<tr>
<td>3.2.2 Regression Techniques</td>
<td>56</td>
</tr>
<tr>
<td>3.3 Comparison of Fitting Forms</td>
<td>60</td>
</tr>
<tr>
<td>3.3.1 Elliptic Integrals</td>
<td>61</td>
</tr>
<tr>
<td>3.3.2 Spherical Harmonics</td>
<td>66</td>
</tr>
<tr>
<td>3.3.3 Performance of Fitted Closure Approximations</td>
<td>68</td>
</tr>
<tr>
<td>3.4 Summary of New Closure Fitting Techniques</td>
<td>84</td>
</tr>
<tr>
<td>Chapter 4. Development of Time Derivative Based Fourth Order Closure Approximations</td>
<td>86</td>
</tr>
<tr>
<td>4.1 Data Set and Fitting Procedure</td>
<td>87</td>
</tr>
<tr>
<td>4.2 Functional Forms</td>
<td>89</td>
</tr>
</tbody>
</table>
Chapter 1. Introduction

“Closure seems to be something rheologists would prefer to avoid. Here, the story of closure is told in such a way that one should enduringly forget any improper undertone of “uncontrolled approximation” or “necessary evil,” which might arise, for example, in reducing a diffusion equation in configuration space to moment equations. In its widest sense, closure is associated with the search for self-contained levels of description on which time-evolution equations can be formulated in a closed or autonomous form.[1]”

The type of closure that will be dealt with throughout this work is for short-fiber reinforced polymer composites. This type of composite material is widely used throughout industry today and will continue to be used due to its high strength to weight ratio. The closure problem becomes necessary when using an orientation tensor approach to simulate the fiber orientation of a given flow or injection molding process. When the fiber-orientation is known certain mechanical properties can be computed such as the stiffness tensor and the anisotropic coefficient of thermal expansion (see e.g. [2]). Given the fiber orientation, many useful properties may be computed for a given material. This work will discuss the background information that has lead to the closure approximation for short-fiber reinforced polymer composites and new approaches in creating closures.

Einstein’s work was perhaps the catalyst to which the study of fiber orientation became prominent. In his work on the motion of particles[3] he discusses the movement
of the particle due to molecular-kinetic theory and Brownian motion. However, in Einstein’s work he only considered spherical particles, it was not until Jeffrey[4] that the work was extended to an ellipsoidal particle. Jeffrey’s equation has been a topic of research for decades and is still widely discussed today. Jeffrey’s equation is only valid for very dilute suspensions and when the fiber-fiber interactions is not considered. Folgar and Tucker created a model that accounts for the fiber-fiber interactions using Jeffrey’s equation by including a phenomenological diffusion term[5]. Unfortunately, the model of Folgar and Tucker is not computationally feasible for complex flows because it can take days, even months for computations with the addition of the new diffusion term. There have been new methods of solving types of distributions, such as Montgomery-Smith et al.[6], in which they use a systematic approach involving spherical harmonics to numerically compute such distribution functions to machine precision with a reduced computational cost. The orientation tensor approach of Advani and Tucker[2] used moments of the distribution function to describe the fiber orientation. The evolution of the tensor equation dramatically reduces the computational time needed to predict fiber orientation even in complex flows such as the center-gated disk. However, there is a setback with the orientation tensor approach. The solution of any even-ordered orientation tensor equation requires the next the higher even-ordered orientation tensor. Because of this problem no closed form solution is possible, and thus the closure concept is introduced to approximate the higher-order tensor. The closure approximation takes the higher even-ordered orientation tensor and makes it a function of the lower even-
ordered orientation tensor. In this thesis, the fourth-order orientation tensor will be a function of the second order orientation tensor.

There have been many fourth-order closure approximations that have been developed over the past three decades. Initially, there was no robust closure that could be applied to all flows, rather certain closures for certain situations. The first closure in literature for the fiber orientation problem is the linear closure by Hand[7]. The linear closure was only valid for an isotropic distribution, that is if fibers are not randomly aligned the linear closure tends to under predict the alignment or show a non-physical oscillatory motion. Doi[8] and Lipscomb, et al.[9] introduced the quadratic closure, which is computed by the dyadic products of the second-order orientation tensor with itself. The quadratic closure is exact for perfectly aligned distributions and therefore performs well for uniaxial alignment states, but otherwise consistently over predicts alignment. Hinch and Leal[10] proposed many closure approximations, however they did not derive them explicitly, they derived them as products with the rate of deformation tensor. Two of the closures in Hinch and Leal’s work were actually the linear and quadratic closures. A hybrid closure was introduced by Advani and Tucker[2] that used the best attributes from the linear and quadratic closures and combined them with a scalar orientation factor. For isotropic distributions the scalar term would reduce quadratic terms to zero to recover the pure linear closure. Likewise, for highly aligned distributions the scalar term would send the linear terms are eliminated to recover the quadratic closure.
The natural closure of Verleye and Dupret[11] used the work of Lipscomb et al.[9] to define the closure. Verleye and Dupret found a general expression for the fourth-order orientation tensor based on the second-order orientation tensor by fitting analytical data. Unfortunately, their closure had singularity issues, but works well for dilute solutions.

The eigenvalue based orthotropic fitted closure of Cintra and Tucker[12] was defined by assuming the fourth-order orientation tensor had the same principle axes as the second-order orientation tensor. Under this assumption the fourth-order tensor was defined as a function of the eigenvalues of the second-order tensor. They used distribution function calculations to create the data in which they did there fitting. The Cintra and Tucker model was shown to have an oscillatory nature for small values of the interaction coefficient. Later, Chung and Kwon[13] produced a new eigenvalue based orthotropic fitted closure in which they used data over a variety of interaction coefficients and a higher degree polynomial to do there fitting. It was designed to be more accurate over a wide range of interaction coefficient unlike the Cintra and Tucker closure. Chung and Kwon[14] also introduced the invariant based orthotropic fitted closure. The invariant based orthotropic fitted closure is very similar to the natural closure in its functional form.

Jack and Smith[15-16] have made six order invariant based orthotropic fitted closures that are the most accurate to date. Jack et al.[17] and Qadir and Jack[18] have shown that using a neural network in the fitting procedure produces excellent results.
Also, Han and Im[19] defined new hybrid type closures using the orthotropic theory of Cintra and Tucker.

New ideas that are presented in this work consider the work of Cintra and Tucker[12] and investigate the type of different possibilities that can occur when changing certain steps of the fitting process. When creating a data set for fitting spherical harmonics and elliptic integral solutions are investigated as opposed to the distribution function calculations. Different orders of polynomials are used, and even rational polynomials are used for fitting. The fitting procedures that are used are no longer just the least squares regression, but also a bisquare weighted and least absolute residual regression. Finally the coefficient optimizations investigated are the traditional Levenberg-Marquardt and a trust region approach. The different combinations of these factors have many different results.

A new type of fitted closure is also introduced in this work. It is known as the time derivative based orthotropic fitted closure. It again uses the theory of Cintra and Tucker[12] but rather than using the eigenvalues alone for the fitting it uses the derivatives of the eigenvalues as well. When using these derivatives the evaluations of the closure become an implicit problem and must be solved using either a predictor-corrector or Newton-Raphson method. Many different polynomials were fitted for this approach, with a wide variety of results.

For all of the new methods and procedures that were produced, the measure of accuracy was based on comparing the second-order orientation tensor from the closure
method with the second-order orientation tensor calculated by spherical harmonics with the procedure as seen in [12]. Preliminary results for almost all new types of models fitted show that fourth-order closure approximations can still be improved. Some of these improvements may only be nominal, but as shown in this work some can also be large.
Chapter 2. Fiber Orientation

Composites have been used throughout industry on a wide variety of products, everything from the dashboard in a car to the blades on wind power turbines. One could not imagine the cost of producing a part, only to have it fail and lose large amounts of money due to inaccurate modeling, which is one of the many reasons accurate modeling of fiber distributions is necessary for design. Many models have been developed to accurately predict the evolution of fiber orientation distribution functions, some being more accurate than others. Knowledge of the fiber orientation is necessary to be able to compute mechanical and rheological properties including elastic stiffness, thermal conductivity and viscosity[2]. The initial methods that were used were computationally expensive and therefore were not practical in a design environment. The orientation tensor approach was developed to aid with computational time; however there were drawbacks in accuracy. This chapter shows how fiber modeling has evolved from Jeffrey’s model to some of the newest orientation tensor representations and explores all the most commonly used closure approximations.
2.1 Modeling Fibers

The idea of modeling rigid ellipsoidal particles has been explored by researchers for decades. Jeffrey’s equation[4] was perhaps the precursor to most all current fiber orientation models and is still being further researched to this day. Jeffrey’s equation is used to simulate the motion of a fiber in a Newtonian fluid, and assumes that the effects of surrounding fibers are neglected. Due to this assumption, Jeffrey’s equation is only valid for very dilute suspensions. The more concentrated the suspension becomes the volume fraction increases and as the volume fraction increases Jeffrey’s equation over predicts the true alignment of the fibers. In fact, Folgar and Tucker[5] have shown that Jeffrey’s equation was not valid for volume fractions greater than 0.1 %. This greatly limits the use of Jeffrey’s equation because for typical applications the volume fraction can exceed 30%[20].

The orientation of a single fiber can be described by a unit vector \( \mathbf{p} \) or alternatively by the angles \((\theta, \phi)\) that can be seen in Figure 2.1. The vector \( \mathbf{p} \) is written as a function of angles of \( \theta \) and \( \phi \) denoted as
The length of the vector is fixed to one, yielding

\[ p_i p_i = 1 \]  

(2.2)

where the classic Einstein summation conventions is implied, as it is throughout this thesis unless otherwise noted. Therefore, the set off all possible unit vectors would result in the unit sphere given as

\[ \int d\mathbf{p} = \int_0^{2\pi} \int_0^\pi \sin \theta d\theta d\phi \]  

(2.3)
Single fiber motion is described as a function $\mathbf{p}(\mathbf{p}, t)$ where $\dot{\mathbf{p}}$ is called the material time derivative. For the computation of $\dot{\mathbf{p}}$, one would need to solve initial condition problems for each individual fiber. This makes using single fibers to compute the needed information unrealistic; however this knowledge has been used to gain insight for fiber orientation purposes.

2.2 Distribution Function of Fibers

Since the use of single fiber modeling is essentially unrealistic for practical applications, more practical solutions were developed. Fiber orientations are represented as statistical distributions. At a point in time, the fiber orientation state may be defined as a probability distribution function $\psi(\theta, \phi, t)$ such that the probability of finding a fiber between the angles of $\theta_i$ and $(\theta_i + d\theta)$ and also $\phi_i$ and $(\phi_i + d\phi)$, is given as (see [2])

$$P(\theta_i \leq \theta \leq \theta_i + d\theta, \phi_i \leq \phi \leq \phi_i + d\phi) = \psi(\theta_i, \phi_i) \sin \theta_i d\theta d\phi$$

(2.4)

There also exist a similar definition of the probability distribution function $\psi(\mathbf{p}, t)$, that determines the likelihood that a fiber is between $\mathbf{p}$ and $\mathbf{p} + d\mathbf{p}$ at a given time $t$. 

10
Since there are certain physical conditions that the function $\psi(p)$ must satisfy, it is not possible to distinguish between a fiber in the $(\theta, \phi)$ direction or the exact opposite $(\pi - \theta, \phi + \pi)$ direction. Which means $\psi(p)$ is periodic.

$$
\psi(\theta, \phi) = \psi(\pi - \theta, \pi + \phi) \\
\psi(p) = \psi(-p)
$$

(2.5)

The next constraint is known as the normalization constraint. This states that the probability of a fiber being oriented in some direction in space is one, which is written as

$$
\oint \psi(p) dp = \int_0^{2\pi} \int_0^\pi \psi(\theta, \phi) \sin \theta d\phi d\theta = 1
$$

(2.6)

Finally the third condition is known as the continuity condition. It states that if a given fibers is leaving one orientation state it must be entering another. Advani[21] states it as

$$
\frac{D\psi}{Dt} = -\frac{\partial}{\partial \theta} (\dot{\theta}\psi) - \frac{\partial}{\partial \phi} (\dot{\phi}\psi) \\
\frac{D\psi}{Dt} = -\frac{\partial}{\partial p} \left( \psi \frac{Dp}{Dt} \right)
$$

(2.7)

2.2.1 Non-Interacting Particle
In Jeffrey’s equation\[4\], the problem of the ellipsoid in a Newtonian fluid was solved under the assumption that the net forces and moments of the ellipsoid summed to zero. This means that the centroid of the ellipsoid moves with the motion of the bulk fluid. In terms of the time derivative of the unit vector $\mathbf{p}$, Jeffrey’s equation can be denoted \[21\]

$$\dot{\mathbf{p}} = -\frac{1}{2} \mathbf{\omega} \cdot \mathbf{p} + \frac{1}{2} \lambda (\dot{\mathbf{\gamma}} : \mathbf{p} - \mathbf{\gamma} : \mathbf{ppp})$$

(2.8)

or in index notation, \[21\]

$$\dot{p}_i = -\frac{1}{2} \omega_{ij} p_j + \frac{1}{2} \lambda (\dot{\gamma}_{ij} p_j - \gamma_{ij} p_k p_i p_k)$$

(2.9)

where $\mathbf{\omega}$ is the vorticity tensor, $\dot{\mathbf{\gamma}}$ is the strain rate tensor, and $\lambda$ is related to the aspect ratio of the ellipsoid each respectively given as

$$\dot{\gamma}_{ij} = \frac{\partial v_j}{\partial x_i} + \frac{\partial v_i}{\partial x_j}$$

(2.10)

$$\dot{\omega}_{ij} = \frac{\partial v_j}{\partial x_i} - \frac{\partial v_i}{\partial x_j}$$

(2.11)

$$\lambda = \frac{r_e^2 - 1}{r_e^2 + 1}$$

(2.12)

with velocity components $v_i$ written as
As stated previously in this chapter, Jeffrey’s equation is only valid for very dilute solutions. Therefore if actual fiber-fiber interactions exist, alignment is not possible. There are very few applications of this type of theory, but again the knowledge that is gained from this information gave insight to later developments.

2.2.2 Interacting Particles

Since Jeffrey’s equation is only valid for dilute suspensions, a different model is needed. Most practical applications are in the semi-dilute to concentrated suspension category. A model was introduced by Folgar and Tucker[5] based on the six following conditions [5]:

(1) The fibers are rigid cylinders, uniform in length and diameter.

(2) The fibers are sufficiently large that Brownian motion is negligible.

(3) The suspension is incompressible.
The matrix fluid is sufficiently viscous that particle inertia and particle buoyancy are negligible.

The centers of mass of the particles are randomly distributed.

There are no external forces or torques acting on the suspension.

Under these conditions the evolution for \( \dot{\psi} \) from Equation (2.8) becomes [22]

\[
\dot{\psi} = -\frac{1}{2} \omega \cdot p + \frac{1}{2} \lambda (\dot{\gamma} \cdot p - \dot{\gamma} : p p p) - \frac{D_r}{\psi} \frac{\partial \psi}{\partial p}
\]  

(2.14)

where \( D_r \) is a rotary diffusion term. Note that if \( D_r \) is set to zero, one would recover Jeffrey’s equation. Folgar and Tucker[5] set the \( D_r \) term to \( \gamma C_i \) where \( C_i \) is the coefficient of interaction which represents the random tendencies due to fiber-fiber interaction and \( \dot{\gamma} \) is the scalar magnitude of the strain rate tensor calculated as

\[
\dot{\gamma} = \sqrt{\frac{1}{2} \dot{\gamma}_x \dot{\gamma}_y}
\]  

(2.15)

The resulting equation for the fiber orientation distribution function is

\[
\frac{D\psi(\theta, \phi)}{Dt} = C_i \dot{\gamma} \frac{\partial^2 \psi}{\partial \theta^2} + \frac{C_i \dot{\gamma}}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial \psi}{\partial \theta} \left( C_i \dot{\gamma} \cos \theta \frac{\cos \theta}{\sin \theta} - \frac{\lambda - 1}{2} \kappa : \delta, \delta - \frac{\lambda + 1}{2} \kappa : \delta, \delta \right) \\
+ \frac{1}{\sin \theta} \frac{\partial \psi}{\partial \phi} \left( \frac{\lambda - 1}{2} \kappa : \delta, \delta - \frac{\lambda + 1}{2} \kappa : \delta, \delta + \psi (3 \lambda \kappa : \delta, \delta) \right)
\]  

(2.16)

Equation (2.16) is a combination of Equation (2.14) and a conservation equation for \( \psi(p) \). For flows with simple conditions, Equation (2.16) is a great tool, but for more
complex flows such as the center gated disk computation time is greatly increased. Depending on the coefficient of interaction, the numerical solution of Equation (2.16) can take on the order of months to reach steady state from an initially random condition [23].

2.3 Orientation Tensor Representation

Because of the immense computation effort that is needed to solve Equation (2.16), Advani and Tucker[2] developed an orientation tensor form to model the distribution of short fibers. Fiber orientations become computationally more efficient with the compact tensor form which retains the stochastic nature of the distribution function.

2.3.1 Folgar and Tucker Model

Orientation tensors are defined by forming dyadic products of the orientation vector $\mathbf{p}$ and then integrating the product of the tensors with the distribution function over all possible directions[21].
\[ a_{ij} = \int \psi(p) p_i p_j dp \]
\[ a_{ijkl} = \int \psi(p) p_i p_j p_k p_l dp \]
\[ a_{ij...} = \int \psi(p) p_i p_j ... dp \] (2.17)

Note that odd ordered tensors are of no interest because the integrals are zero due to the fact the distribution function is even. The tensors from Equation (2.17) are shown to be completely symmetric, that is \[2\]

\[ a_{ij} = a_{ji} \]
\[ a_{ijkl} = a_{jikl} = a_{kijl} = a_{lijk} = ... \]
\[ a_{ijklmn} = a_{jiklmn} = a_{kijlmn} = a_{lijkmn} = a_{mnlkij} = ... \] (2.18)

Furthermore, it can be shown that every higher order orientation tensor provides complete information about the lower order orientation tensors. That is using Equations (2.1) and (2.6) \[15\]

\[ a_{ij} = a_{ijpp} \]
\[ a_{ijkl} = a_{ijklqq} \] (2.19)

From the normalization condition in Equation (2.6) it can be shown that

\[ a_{ii} = 1 \] (2.20)

Also, using Equation (2.19) the normalization conditions for the fourth-order and sixth-order tensors are
\[
\begin{align*}
a_{ij} &= 1 \\
a_{ijkl} &= 1
\end{align*}
\] (2.21)

Taking into account the definition of orientation tensors of Equation (2.17) one could rewrite the evolution of the distribution function (Equation (2.16)) in terms orientation tensors as follows [22]

\[
\frac{Da_{ij}}{Dt} = -\frac{1}{2}(\omega_{ik}a_{kj} - a_{ik}\omega_{kj}) + \frac{1}{2} \lambda(\gamma_{ik}a_{kj} + a_{ik}\gamma_{kj} - 2\gamma_{kl}a_{ijkl}) + 2C_i\gamma_i(\delta_{ij} - 3a_{ij})
\] (2.22)

The orientation tensors are moments of the distribution function. There are a few advantages to using the orientation tensor representation. One of the most important and obvious is the fact that it is more compact, giving the same information with less computation. Along that line of thought, this means less computation time. Also, by imposing the normalization condition from Equation (2.20) and the symmetry conditions from Equation (2.19) the second-order orientation tensor and thus Equation (2.22) has five independent components of the nine components that make it. Likewise, the fourth-order orientation tensor has fourteen independent components of eighty-one.

The main disadvantage of using the orientation tensor approach is the fact that the fourth-order orientation tensor \(a_{ijkl}\) is a term in the evolution of the second-order orientation tensor \(a_{ij}\). Similarly, the equation for the evolution of the fourth-order orientation tensor \(a_{ijkl}\) depends on the sixth-order orientation tensor \(a_{ijklmn}\). Every evolution equation of an even ordered orientation tensor depends on the next higher even-
order orientation tensor. Due to this fact the closure approximation is introduced, which approximates the next higher even-order orientation tensor based on the lower order tensor. For example a closure approximation is used to write $a_{ijkl}$ based on $a_{ij}$ based on Equation (2.22).

### 2.3.2 Other Models Related to the Folgar and Tucker Model

There are other models besides the Folgar and Tucker model that use fourth-order closure approximations. Some of the models are identical except for the diffusion term, others are identical except for a scalar term. These models have been proposed since it has been shown that the kinetics of the Folgar and Tucker model are “perhaps two to ten times slower[24].”

The first of the different models to discuss here is the strain reduction factor (SRF) model[25]. This model uses a factor $\kappa<1$ that simply slows the kinematics of Equation(2.22). Unfortunately the SRF model is not objective.
The reduced-strain closure (RSC) model[24] was introduced to take the idea of slowing the kinematics of the SRF model and create an objective model. It uses the factor $\kappa<1$ from above but only applies it to a new term introduced to the Folgar and Tucker model, that creates fourth-order tensors from the eigenvalues and eigenvectors for a complete explanation of this model see [24].

The last model and one of the most recent models that has been proposed is known as the anisotropic rotary diffusion (ARD) model[26] which modifies the diffusion term in the Folgar and Tucker model. Instead of $D_r = \dot{\gamma}C_1$ as in Equation (2.22) to be used for the diffusion of the model a fitting procedure is introduced to the diffusion term. They used five parameters, three of which are fitted and two are set arbitrarily, to obtain results that match experimental data as closely as possible. There is also a proposed model called the ARD, RSC[26] model which adds the RSC term to slow the kinematics of the ARD model. There are other models that have been referenced in [26] as anisotropic models such as the Koch model and the Fan and Pan-Thien model, the reader is encouraged to explore this work for greater knowledge.
2.4 Spherical Harmonics

The spherical harmonics method used by Montgomery-Smith, *et al.* [6] was one of the more recent methods used in solving the fiber orientation problem. They have shown great success with the use of spherical harmonics on all of the fiber orientation distribution models above including the original Folgar and Tucker model, the Koch model, the RSC model, and the ARD model. In general they solve

\[
\frac{\partial}{\partial t} \Phi = F(x, y, z, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}) \Phi
\]  

(2.23)

which is defined on the unit sphere. In partial differential equations that are used to solve fiber orientation distributions are given as

\[
\frac{\partial \Phi}{\partial t} = \Delta \left( \frac{D p^h}{D t} \Phi(p) \right) + \Delta(D, \Phi)
\]  

(2.24)

Using the spherical harmonics approach, the solution is written similarly to a Fourier series such as

\[
\Phi(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \hat{\Phi}_l^m Y_l^m
\]  

(2.25)

where
\[
\hat{\Phi}_m^n = \int_{\phi=0}^{\pi} \int_{\theta=0}^{\pi} \Phi(\theta, \phi) \bar{Y}_m^m(\theta, \phi) \sin \theta \, d\phi \, d\theta
\]  

(2.26)

With some mathematical manipulation, a system of ordinary differential equations is obtained in the form

\[
\frac{\partial}{\partial t} \hat{\Phi}_m^n = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \epsilon_{l,m,n}^{m,m'} \hat{\Phi}_{m'}^{n'}
\]  

(2.27)

In summary, the approach converts a partial differential equation to a system of ordinary differential equations and avoids the closure problem. For conciseness, the author shall refer you to [6] for more information. Spherical harmonics are not the basis of research in this work, but the tools of spherical harmonics are implemented. Spherical harmonics obtain the accuracy of distribution function calculations (DFC), while only being nominally slower than the orientation tensor approach.

### 2.5 Fourth-Order Closure Approximations

The use of orientation tensor closure has been a topic of research for over 40 years. The improvements from early closures have clearly been seen, but it is evident that research
may be nearing the limit of accuracy that can be seen from a fourth-order closure. Early closures were derived as analytic expressions that were considered exact under the proper conditions for certain flows. With these early closures it was difficult to obtain robustness over a wide variety of flow fields and also with varying interaction coefficients, $C_I$. More recently fitted closures have been shown to be more accurate over a wide variety of flow fields.

There are several conditions that must be met when constructing a fourth-order closure approximation. A general form of a closure approximation for a fourth-order orientation tensor is written as a function of the second order orientation tensor,

$$ a_{ijkl} = f_{ijkl}(a_{mn}) $$

(2.28)

The goal of all fourth-order closures is to capture fourth-order information of the distribution function with second-order information.

### 2.5.1 Linear Closure

Hand[7] proposed that all of the possible products of the second-order orientation tensor $a_{ij}$ and the kronecker delta $\delta_{ij}$ be used to define $a_{ijkl}$. When applying the normalization
and symmetry requirements it can be shown that only the linear terms may be used, hence it is called the linear closure approximation \( \hat{a}_{ijkl} \). Which is written as [7]

\[
\hat{a}_{ijkl} = -\frac{1}{35} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \frac{1}{7} (a_{ij} \delta_{kl} + a_{ik} \delta_{jl} + a_{il} \delta_{jk} + a_{kl} \delta_{ij})
\]  

and is considered exact for isotropic distributions. For any other orientation distributions other than completely random the linear closures tends to under estimate the true alignment of the fibers when used with Equation (2.22). Another problem with solving for \( a_{ij} \) with the linear closure is that non-physical oscillatory behavior occurs as the fibers shift out of an isotropic distribution. It can be said that the linear closure is really only useful in perfectly random distributions.

### 2.5.2 Quadratic Closure

The quadratic closure was introduced by Doi[8]. This closure has the simplest form of all fourth-order closures, and is also one of the easiest to implement in programming. It is formed by taking the dyadic product of the second-order orientation tensor with itself. For uniaxial distributions the quadratic closure seems to perform well, and it is exact for
highly aligned distributions. Other distributions that vary from uniaxial can be predicted by this closure, however the quadratic closure overestimates the fiber alignment. The fourth order approximation for the quadratic closure \( \bar{a}_{ijkl} \) is [8]

\[
\bar{a}_{ijkl} = a_{ij} a_{kl}
\] (2.30)

The quadratic closure was constructed it has been used to accurately predict uniaxial and highly aligned distributions, but since most fiber suspensions are concentrated its usefulness is very limited. Another drawback from the quadratic closure is that it does not support all of the symmetries of the fourth order tensor, i.e., \( a_{ijkl} \neq a_{klji} \), however when used in the equation of change in the second order tensor it does preserve the symmetry of \( a_{ij} \). Also the quadratic closure has the same symmetries of an elasticity tensor, thus it is acceptable to use with rheological property predictions when used with a transversely isotropic elasticity tensor.

### 2.5.3 Hybrid Closure

The hybrid closure was first introduced by Advani and Tucker[2] in an attempt to make a more accurate closure over a wide array of flow distribution functions. The concept of
the closure was to take the best attributes of the linear closure, \( \hat{a}_{ijkl} \), and the quadratic closure, \( \bar{a}_{ijkl} \), and combine them. Since we know that the linear closure is exact for isotropic distributions, and similarly the quadratic closure is exact for highly aligned distributions, they used a scalar function so that these two qualities would still hold true for this closure. The scalar, \( f \), would vary between \( 0 < f < 1 \). For completely isotropic distributions the scalar measure would vanish for the linear closure term and becomes equal to one for highly aligned fiber, so this closure, \( \bar{a}_{ijkl} \), is given by the equation [2]

\[
\bar{a}_{ijkl} = (1 - f)\hat{a}_{ijkl} + f\bar{a}_{ijkl}
\]  

(2.31)

Over the entire range of flow distributions the hybrid closure worked very well at that time and still works relatively well to this date. The hybrid closure behaves much better than the linear or quadratic closures. Since the linear closure in Equation (2.29) tends to under predict alignment in distributions other than isotropic and the quadratic closure in Equation (2.30) tends to over predict the true alignment in distributions other than highly aligned the scalar term creates a more correct solution between the two inaccuracies. However, the hybrid closure still over predicts distributions between isotropic and perfect alignments because of the influence of the quadratic closure term.

There are a few different methods of calculating the scalar measure \( f \) of the orientation. Advani[21] proposed that the scalar measure must be independent of coordinate system and free from assumptions of the distribution function. The invariants
of the second-order orientation tensor fulfill these requirements and are applicable to form $f$. For example, $f$ can be computed as 

$$f = 1 - 3I_2$$  \hspace{1cm} (2.32)$$

or

$$f = 1 - 27I_3$$  \hspace{1cm} (2.33)$$

where $I_2$ and $I_3$ are respectively the 2\textsuperscript{nd} and 3\textsuperscript{rd} invariants of $a_{ij}$ given as

$$I_2 = \frac{1}{2}(a_{ij}a_{ji} - a_{ii}a_{jj})$$

$$I_3 = \frac{1}{6}(a_{ij}a_{jk}a_{kl} + a_{ji}a_{kj}a_{lk} - 3a_{ij}a_{jk}a_{li})$$  \hspace{1cm} (2.34)$$

From the normalization conditions mentioned previously it has been shown that $I_1 = a_{ii} = 1$. Another form that was proposed by Advani and Tucker[2] was to calculate $f$ in terms of $a_2$. 

$$f = \frac{3}{2}a_{ij}a_{ji} - \frac{1}{2}$$  \hspace{1cm} (2.35)$$

Every form of $f$ that has been given follow the criteria to create scalar measure as given for the hybrid closure, although it has been shown in numerical calculations that Equation (2.33) return the greatest accuracy.
2.5.4 Hinch and Leal Closures

In their study of suspensions of fiber-like particles, Hinch and Leal[10] derived a wide variety of closure approximations to deal with different flow distribution functions. They proposed exact closures for isotropic distributions (“weak flow” in their nomenclature) or for perfectly aligned fiber distributions (“strong flow”). They were combined to form a composite closure that would be exact in both limits, similar to the Advani and Tucker hybrid closure works. The Hinch and Leal closures did not derive explicit formulas for their $a_{ijkl}$, but instead derived expressions for $a_{ijkl} \tilde{Y}_{ijkl}$. Advani and Tucker[27] employed the Hinch and Leal closures and provided the explicit formulas for $a_{ijkl}$. The first three were known as W1 (weak flow 1), S1 (strong flow 1), and H&L 1 (Hinch and Leal Composite 1). The S1 closure approximation is identical to the quadratic closure.

Another set of closure approximations were also derived by Hinch and Leal, which were not only accurate for isotropic and highly aligned orientation distributions but also very accurate for large and small values of $C_I$. These advanced closures were defined with asymptotically derived approximations from the steady-state solutions of both weak and strong flows. These solutions were also used to construct a new composite closure based on their two asymptotic approximations designated as S2, W2, and H&L2. The W2 closure approximation is identical to the linear closure. A general equation for all of their derived closures is written as
\[ a_{ijkl} = \beta_1(\delta_i \delta_k) + \beta_2(\delta_i \delta_l + \delta_j \delta_k) + \beta_3(\delta_j \delta_k + a_{ij} \delta_{kl}) \\
+ \beta_4(a_{ik} \delta_l + a_{il} \delta_k + a_{ji} \delta_k + a_{ji} \delta_l) + \beta_5(a_{ij} a_{kl}) + \beta_6(a_{ik} a_{jl} + a_{il} a_{jk}) \\
+ \beta_7(a_{im} a_{nj} a_{mn} a_{nl}) + \beta_8(\delta_{ij} a_{km} a_{kl} + a_{nm} a_{mj} \delta_{kl}) \]  

(2.36)

These new closures were more accurate than the previous closures they derived and all of
the closures can be summarized in Table 2.1 below.

<table>
<thead>
<tr>
<th>Term</th>
<th>Approximation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \beta_1 )</td>
</tr>
<tr>
<td>W1 (isotropic)</td>
<td>( \frac{1}{15} )</td>
</tr>
<tr>
<td>W2 (linear)</td>
<td>( -\frac{1}{35} )</td>
</tr>
<tr>
<td>S1 (quadratic)</td>
<td>...</td>
</tr>
<tr>
<td>S2 (strong flow)</td>
<td>...</td>
</tr>
<tr>
<td>H&amp;L1</td>
<td>...</td>
</tr>
<tr>
<td>H&amp;L2</td>
<td>( \frac{26\alpha}{315} )</td>
</tr>
</tbody>
</table>

\[ \alpha = \exp \left[ \frac{2(1 - 3a_{ij} a_{ji})}{1 - a_{ij} a_{ji}} \right] \]
2.5.5 Eigenvalue Based Orthotropic Fitted Closure

Cintra and Tucker[12], created the Eigenvalue Based Orthotropic Fitted (EBOF) closure, which involved a fitting process to define the fourth-order orientation tensor. The EBOF closure is based on the assumption that the principle axes of the second-order orientation tensor also define the planes of orthotropic material symmetry of the fourth-order orientation tensor. Under this assumption, the fourth-order orientation tensor can be written in terms of the second-order orientation tensors principle components. Calculating the fourth-order tensor was done by fitting a polynomial to the eigenvalues of the second-order orientation tensor. Cintra and Tucker used a complete second-order polynomial for fitting based on DFC data. Cintra and Tucker fit five flow distributions all of which had a $C_i$ of $10^{-2}$, this closure is known as ORF. Cintra and Tucker and later Chung and Kwon[13] showed that the ORF closure suffered from non-physical oscillations for simple shear in flows with coefficients of interaction between $10^{-3}$ and $10^{-4}$, so they proposed their own EBOF closure as a solution to the problem. Cintra and Tucker later corrected this problem, by creating the ORL closure[12] which fit data with coefficient of interaction of $10^{-3}$. Chung and Kwon[13] created a closure known as the ORW closure, which used ten flows with the coefficients of interaction between $10^{-2}$ and $10^{-4}$. The ORW closure performed well, so Chung and Kwon introduced a new closure using a complete third order polynomial to fit the same data as ORW. Chung and Kwon
found that fitting a third order polynomial did give more accurate results while higher orders did not significantly improve their results, this closure they called ORW3[13]. Wetzel[28] and Verweyst[29] generated their data from Carlson elliptic integrals and assumed that the coefficient of interaction was zero. Using these integrals Wetzel and Verweyst were able to homogenously populate the eigenspace and fit their fourth order polynomials. Verweyst’s[29] ORT closure is still commonly used today. Wetzel was only involved with research related to fiber orientation, but his idea is what Verweyst used to make his closure. Wetzel also proposed fitting rational polynomials[30], no such work for our fiber orientation problem has been published and later you may read about results on fitting Rational Ellipsoidal (RE) closures.

Using the assumption that the fourth-order orientation tensor is orthotropic, we know that the planes of material symmetry of the fourth-order tensor are the same as the principle directions defined by the second-order tensor. Using the notation in Cintra and Tucker[12] all eighty-one components of the fourth-order tensor can be contracted to a $6 \times 6$ matrix, using certain rules about the indices of $a_{ijkl}$ and of our new matrix $A_{mn}$ which is denoted as

$$A_{mn} = a_{ijkl}$$

(2.37)
This contracted notation is commonly used to represent fourth-order tensors, where double indices are replaced by single number, the relations are given in Table 2.2 below

Table 2.2 Relationship between indices of contracted and tensor notation.

<table>
<thead>
<tr>
<th>Contracted Notation</th>
<th>Tensor Notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m$ or $n$</td>
<td>$ij$ or $kl$</td>
</tr>
<tr>
<td>1</td>
<td>11</td>
</tr>
<tr>
<td>2</td>
<td>22</td>
</tr>
<tr>
<td>3</td>
<td>33</td>
</tr>
<tr>
<td>4</td>
<td>23 or 32</td>
</tr>
<tr>
<td>5</td>
<td>31 or 13</td>
</tr>
<tr>
<td>6</td>
<td>12 or 21</td>
</tr>
</tbody>
</table>

For all EBOF closures there are certain relations that apply. Due to the symmetry of the second-order orientation tensor, we know that $a_{ij}$ possesses three orthogonal eigenvectors and three corresponding eigenvalues. If $a_{ij}$ is diagonalized it becomes a matrix of the form

$$A_{mn} = \begin{bmatrix} \bar{A}_{11} & \bar{A}_{12} & \bar{A}_{13} & 0 & 0 & 0 \\ \bar{A}_{21} & \bar{A}_{22} & \bar{A}_{23} & 0 & 0 & 0 \\ \bar{A}_{31} & \bar{A}_{32} & \bar{A}_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{A}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \bar{A}_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & \bar{A}_{66} \end{bmatrix}$$  (2.38)
where $a_{(1)}$, $a_{(2)}$, and $a_{(3)}$ are the eigenvalues. The trace of a matrix is an invariant yielding

$$a_{(1)} + a_{(2)} + a_{(3)} = 1$$

therefore only two eigenvalues are independent. Next we must choose the number of eigenvalues such that

$$a_{(1)} \geq a_{(2)} \geq a_{(3)}$$

then, all possible orientation states will fall inside the UBT triangle as shown

$$a_{ij} = \begin{bmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{bmatrix} = \begin{bmatrix} a_{(1)} & 0 & 0 \\ 0 & a_{(2)} & 0 \\ 0 & 0 & a_{(3)} \end{bmatrix}$$
where U, B, and T correspond to uniaxial, biaxial, and triaxial orientation states respectively. Uniaxial orientation is when all the fibers are aligned in a single direction. Biaxial orientation is described as the fibers being evenly divided between two perpendicular axes, this can be thought of as in plane. Triaxial or isotropic orientation is when the fibers are evenly divided among all three axes.

EBOF closures are written in a form such that they are functions of the second order orientation tensors first and second eigenvalues $a_{(1)}$ and $a_{(2)}$, respectively. That is

$$\overline{A}_{mn} = f_{mn}(a_{(1)}, a_{(2)})$$  \hspace{1cm} (2.42)
There are nine independent components of $\overline{A}_{mn}$ that are to be approximated, but it can be shown that the off-diagonal terms are functions of the diagonal terms as shown below

$$A_{12} = A_{66}, \quad A_{23} = A_{44}, \quad A_{13} = A_{55} \quad (2.43)$$

This makes six independent variables remaining in Equation (2.38), which are the terms along the diagonal. The final relation takes into account the relation between the second and fourth-order orientation tensor components, it solves the system of equations

$$\begin{align*}
A_{11} + A_{66} + A_{55} &= a_{11} \\
A_{66} + A_{22} + A_{44} &= a_{22} \\
A_{55} + A_{44} + A_{33} &= a_{33}
\end{align*} \quad (2.44)$$

so that now there are only three independent variables remaining. Cintra and Tucker[12] chose to fit the $\overline{A}_{11}$, $\overline{A}_{22}$, and $\overline{A}_{33}$. There closure had eighteen coefficients and fit the second degree polynomial

$$A_{mn}^{\text{Closure}} = C_{m(1)} + C_{m(2)}a_{(1)} + C_{m(3)}[a_{(1)}]^2 + C_{m(4)}a_{(2)} + C_{m(5)}[a_{(2)}]^2 + C_{m(6)}a_{(1)}a_{(2)} \quad (2.45)$$

$m = 1, 6; \text{no sum on } m$

Chung and Kwon’s ORW3 closure had thirty coefficients and Verweyst’s ORT had forty-five coefficients. These fitted closure showed significant improvement over previous closure approximations. Cintra and Tucker outlined their procedure in six steps which are as follows[12]:

34
(1) Select a set of flow fields that will generate a wide variety of orientation states.

(2) For each individual flow field select an initial condition, which is chosen to be isotropic for orthotropic closures and integrate $\psi(p)$ from Equation

(3) Select a representative time step and compute the exact orientation tensors $a_{ij}$ and $a_{ijkl}$.

(4) Compute the eigenvalues and the eigenvectors of the exact second-order orientation tensor.

(5) Rotate the exact fourth-order orientation tensor into the principle axes of the second-order orientation tensor to find the values of $\tilde{A}_{mn}$.

(6) For each independent component of $\tilde{A}_{mn}$, collect all values and create a function of $a_{(1)}$ and $a_{(2)}$. Use a least squares fitting process to create the best approximation to fit each independent $\tilde{A}_{mn}$.

For Cintra and Tucker’s ORF, five flow fields were chosen and implemented in the fitting procedure. The five flows were simple shear, uniaxial elongation, biaxial elongation, and two shear/stretching flows all flows used the value of $\lambda=1$ and a $C_1 = 0.01$.

The final step of fitting the closure is using a cost function to minimize the coefficients. The cost function simultaneously compares and minimizes the exact fourth-
order orientation tensor with the calculated tensor values from the closure. The function to be minimized is

\[ x^2 = \sum_{i=1}^{\text{NDATA}} \sum_{m=1}^{6} \left( \overline{A}_{mm}^{\text{exact}} - \overline{A}_{mm}^{\text{closure}} \right)^2 \]

(2.46)

where \( \overline{A}_{mm}^{\text{exact}} \) is the exact fourth-order component from the integrations of \( \psi(p) \) and \( \overline{A}_{mm}^{\text{closure}} \) is the fourth-order closure approximation. The summation from 1 to 6 accounts for the six independent variables from Equation (2.38) and NDATA represents the number of discrete data points from the distribution function.

2.5.6 Invariant Based Orthotropic Fitted Closure

An invariant-based orthotropic fitted (IBOF) closure[14] could be considered as a hybrid between the natural closure of Verleye and Dupret[11] and the form of EBOF closures that were discussed previously in this work. As in all other closures IBOF closures relate the structural components of the second-order orientation tensor to the fourth-order
orientation tensor. However, with IBOF closure they use the invariants of the second-order orientation tensor to create their formula for their fitting procedure.

If the fiber-fiber interaction is neglected, Lipscomb[9] showed that an exact one-to-one correspondence existed between the second-order orientation tensor and the fourth-order orientation tensor. With the use of this theory, Verleye and Dupret[11] created the natural (NAT) closure when the fiber-fiber interaction is completely neglected. In their closure they created an expression for $a_{ijkl}$ in terms of $a_{ij}$ and $\delta_{ij}$, by fitting data calculated from analytical solutions where the fiber-fiber interaction was neglected. The NAT closure had many good qualities to build off of, but it did suffer from problems of singularities within the matrix.

Chung and Kwon realized the elegance of the NAT closure and EBOF closures. They sought to create a closure as accurate as EBOF closures, but with less computational time and none of the singularity issues of the NAT closure. They investigated the performance of their closure with accuracy as well as computational time.

In their work principal invariants are adopted as the fitting variable rather than the eigenvalues. They chose the invariants since they can easily be computed in any coordinate system and it eliminates the need to do a coordinate transformation for any of the tensor components. Chung and Kwon started with the most general expression for the full fourth-order orientation tensor and used the Cayley-Hamiltonian theorem to derive the expression
\begin{equation}
\alpha_{ijkl} = \beta_1 S(\delta_{ij} \delta_{kl}) + \beta_2 S(\delta_{ij} \alpha_{kl}) + \beta_3 S(\alpha_{ij} \alpha_{kl}) + \beta_4 S(\alpha_{k\alpha m} \alpha_{ml}) + \beta_5 S(\alpha_{ijkl} \alpha_{km} \alpha_{ml}) + \beta_6 S(\alpha_{k\alpha m} \alpha_{km} \alpha_{ml})
\tag{2.47}
\end{equation}

where the operator $S$ indicates the symmetric part of its argument and is denoted as

\begin{equation}
S(T_{ijkl}) = \frac{1}{24} (T_{ijkl} + T_{jikl} + T_{ijkl} + T_{jikl} + 20 \text{ terms})
\tag{2.48}
\end{equation}

Similarly to EBOF closures, IBOF closures fit the six $\beta$ coefficients as functions of the second and third invariants $II$ and $III$, which are known as

\begin{align*}
II &= a_{(1)} a_{(2)} + a_{(2)} a_{(3)} + a_{(1)} a_{(3)} \\
III &= a_{(1)} a_{(2)} a_{(3)}
\end{align*}

\tag{2.49}

where $a_{(i)}$ are the eigenvalues of $a_{ij}$. Using the symmetry and normalization conditions, it can be shown that there are only three independent $\beta$ coefficients of the six in Equation (2.47). The equations for $\beta_1$, $\beta_2$, and $\beta_3$ were written as functions of the $\beta_3$, $\beta_4$, and $\beta_6$ and the equations are

\begin{align*}
\beta_1 &= \frac{3}{5} \left[ -\frac{1}{7} + \frac{1}{5} \beta_3 \left( \frac{1}{7} + \frac{4}{3} II + \frac{8}{3} III \right) - \beta_4 \left( \frac{1}{5} - \frac{8}{15} II - \frac{14}{15} III \right) \\
&\quad - \beta_6 \left( \frac{1}{35} - \frac{24}{105} III - \frac{4}{35} II + \frac{16}{15} III + \frac{8}{35} II^2 \right) \right] \\
\beta_2 &= \frac{6}{7} \left[ 1 - \frac{1}{5} \beta_3 (1 + 4II) + \frac{7}{5} \beta_4 \left( \frac{1}{6} - II \right) - \beta_6 \left( \frac{1}{5} + \frac{2}{3} III + \frac{4}{5} II - \frac{8}{5} II^2 \right) \right] \\
\beta_3 &= \frac{4}{5} \beta_3 - \frac{7}{5} \beta_4 - \frac{6}{5} \beta_6 \left( 1 - \frac{4}{3} II \right)
\end{align*}

\tag{2.50}
Analogous to EBOF eigenspace as seen in Figure 2.3, there is an equivalent invariant space to which all the second and third invariant values can be mapped and is shown below.

![Invariant space of all possible orientation states of second-order orientation tensor.](image)

The final equation that was fit was a complete fifth order polynomial written as a function of the second and third invariants, there are 63 coefficients in all and the function is of the form

\[
\beta_i = a(i,1) + a(i,2)I + a(i,3)I^2 + a(i,4)III + a(i,5)III^2 + a(i,6)II\ III + a(i,7)II^2\ III + a(i,8)II\ III^2 + a(i,9)III^3 + a(i,10)III^3 + a(i,11)II^3\ III + a(i,12)II^2\ III^2 + a(i,13)II\ III^3 + a(i,14)II^4 + a(i,15)III^4 + a(i,16)II^4\ III + a(i,17)II^3\ III^2 + a(i,18)II^2\ III^3 + a(i,19)II\ III^4 + a(i,20)II^5 + a(i,21)III^5 \ (i = 3, 4, 6)
\]
where \( a(i, j) \) are all possible coefficients of the polynomial.

The fitting procedure that was employed is the exact same as in EBOF closures. They would take the exact answers from DFC calculations and perform a least squares type fit. After the least squares fit, Chung and Kwon even used the exact same cost function which is Equation (2.46). The IBOF of Chung and Kwon was found to be computationally superior to EBOF closures, as the IBOF closure performed 40% faster than the fifth-order EBOF they fitted. This is due to the fact that with IBOF closures there are no fourth-order tensor rotations. They also showed how increasing the order in polynomials was insignificant to overall CPU calculation time.

2.6 Sixth-Order Closure Approximations

The idea that came behind the development of sixth-order closure approximations was simple, the higher-order the closure, the more orientation information could be recorded, hence more accurate results. However, Advani and Tucker[2] suggested that there is no need for a sixth-order closure, as all information of merit was already contained in fourth
order closures. For almost every fourth-order closure a corresponding sixth-order closure has been developed. These closures are the linear, quadratic, hybrid, eigenvalue-based orthotropic fitted, and invariant-based orthotropic fitted. Unfortunately, literature does not cover information over sixth-order closures as it does over fourth-order closures. Also it is difficult to find published computational results for some of these closures. The IBOF sixth-order closure of Jack and Smith[15] is the most accurate of any fourth or sixth order closure to date.

The form of the typical sixth-order closure is given as a function of the fourth-order orientation tensor, $a_{ijkl}$, the second-order orientation tensor, $a_{ij}$, or of a combination of the two different order tensors. For the use of a sixth-order closure you use the fourth-order evolution equation which is given as

$$\frac{Da_{ijkl}}{Dt} = -\frac{1}{2}(\omega_{im}a_{mjkl} - a_{ijkm}\omega_{ml} + \omega_{jm}a_{iklm} - a_{ijlm}\omega_{mk})$$

$$+ \frac{1}{2}\lambda(\dot{\gamma}_{im}a_{iklm} + \dot{\gamma}_{jm}a_{iklm} + \dot{\gamma}_{lm}a_{ijkm} + \dot{\gamma}_{im}a_{ijkm} - 4\dot{\gamma}_{mn}a_{ijklmn})$$

$$+ C_{ij}\dot{\gamma}[ -20a_{ijkl} + 2(a_{ij}\delta_{kl} + a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{jk}\delta_{il} + a_{jl}\delta_{ik} + a_{ki}\delta_{lj}) ]$$

(2.52)

A sixth-order linear closure $\hat{a}_{ijklmn}$ was derived similarly to the way Hand’s fourth order linear closure was. This sixth-order closure incorporates all the same symmetry arguments as used in the fourth order linear closure. This closure, given as[2]
\[ \tilde{a}_{ijklmn} = \frac{1}{693}[\delta_{ij} \delta_{jk} \delta_{mn} + ... + (15 \text{ total terms})] \]

\[ -\frac{1}{99}[a_{ijk} \delta_{mn} + ... + (45 \text{ total terms})] \]

\[ +\frac{1}{11}[a_{ijkl} \delta_{mn} + ... + (15 \text{ total terms})] \]  

(2.53)

was shown to only be accurate in randomly oriented distribution functions. As with the fourth-order linear closure in Section 2.5, the sixth-order linear closure suffers from non-physical solutions and only being useful in isotropic orientation states.

The sixth-order quadratic closure, \( \tilde{a}_{ijklmn} \), was developed by Altan[31]. It is analogous to Doi’s[8] fourth-order quadratic closure. Altan only investigated its use with dilute suspensions and non-interacting particles. The form of the sixth-order quadratic closure is rather simple and is given as

\[ \tilde{a}_{ijklmn} = a_{ijkl} a_{mapp} \]  

(2.54)

As suspected, the sixth-order quadratic closure yields exact solutions to highly aligned distributions just as the fourth-order quadratic closure does. For other distributions the sixth-order quadratic closure consistently over predicts the alignment of the fiber distribution.

The combination of the of both the sixth-order linear and quadratic closure through a scalar measure \( f \) as mentioned in Equations (2.32),(2.33), and (2.35). The result was the sixth-order hybrid closure, \( \tilde{a}_{ijklmn} \). Advani[21] derived this closure; however
he did not provide any calculations to show its performance and behavior. The sixth-order hybrid closure is of the form

\[ \tilde{\alpha}_{ijklmn} = (1 - f)\hat{\alpha}_{ijklmn} + f\tilde{\alpha}_{ijklmn} \]  (2.55)

The theory was to again take the best attributes of the sixth-order linear and the sixth-order quadratic closures. It should be mentioned that because of the non-physical behavior of the sixth-order linear closure, the sixth-order quadratic closure yields more accurate solutions to transient behavior over the sixth-order hybrid closures.

The final two sixth-order closure approximations that will be discussed are the sixth-order EBOF and IBOF. Jack and Smith[15-16] have created both an EBOF and IBOF sixth-order closure. The EBOF fitting procedure is similar in process to how a fourth-order EBOF would be fitted. However, to get the exact second-order orientation tensor from Equation (2.52) they would have to use the relation as stated in Equation (2.19). Once the second-order orientation was calculated, one would then compute the eigenvalues and eigenvectors from \( a_{ij} \). Using the second-order eigenvectors, the fourth and sixth-order orientation tensors are then rotated in the principle frame. Then the fitting procedure outlined in Section 2.5.5 was applied to four arbitrarily chosen independent variables of the ten possible that remained. They chose to use the same complete second-order polynomial as Cintra and Tucker[12]. The cost function for minimization that was used was only slightly different from that of the form in Equation(2.46). The IBOF was also very similar to the fitting in Section 2.5.5; however
the number of $\beta$ parameters from Section 2.5.6 changes from six to ten for a sixth-order closure. Of the 10 $\beta$ parameters, three of them are chosen to be solved for in terms of the remaining seven. It is of note that Jack and Smith[15] chose to use $\beta_1$, $\beta_2$, and $\beta_3$ to solve for so that singularities are avoided. They chose to fit each of the remaining $\beta_i$ parameters to a third-order complete polynomial. For conciseness, a full discussion of their work will not presented, but their work has shown great promise with sixth-order closure approximations.
Chapter 3. Development of Fourth Order Fitted Closures

One goal of this research is to develop a new fourth-order closure approximation that is more accurate than current fourth-order approximations, equally accurate as current fourth-order closure approximations but computationally faster, or a combination of better accuracy and faster computational time. The basis of the investigations follows the ideas of Cintra and Tucker[12] which is discussed in Section 2.5.5. Their procedure for fitting a fourth-order closure was followed in the most basic way and investigations following their procedure, but with more current methods, give improved results. These new methods include:

- Created data from calculations other than DFC, such as using spherical harmonics or elliptic integrals.
- Using different fitting equations such as rational polynomials.
- Using different regression techniques other than a least squares procedure including least absolute residual.

Through some of these techniques or a combination of all of the above techniques improvements have been made.
Three ways were investigated to acquire different data sets. There is the standard DFC calculation that has been considered the benchmark calculation to acquire exact values for over a decade now. Also, the spherical harmonic method[6] was investigated, which is a newer method and is significantly faster than the DFC method and has been shown to be accurate. Carlson elliptic integrals[32] are the final method that was investigated and in the three methods considered here, gives the most robustly accurate results.

In this thesis the DFC and spherical harmonic method are used in a similar manner to compute solutions to the fiber orientation distribution function $\psi$. Spherical harmonics can produce exact answers with less computation than that required in DFC calculations. Using spherical harmonics and DFC as the fitting data, does have advantages when compared to elliptic integral calculations. DFC and spherical harmonics are both capable of incorporating data over a range of coefficients of interaction, where as elliptic integrals ignore rotary diffusion. DFC and the spherical harmonic method must rotate all of the data into the principle frame of the second order orientation tensor. Then after rotation it may be necessary to take away certain data points to populate the UBT triangle as desired.
3.1.3 Elliptic Integrals

Elliptic integrals were originally used in connection with the problem of giving the arc length of an ellipse. They later became useful for expressing a variety of rational functions. For our fiber problem, the eigenvalues of the second-order orientation tensor, as well as all fourth-order orientation tensor components can be written in the contracted notation used by Cintra and Tucker[12] and can be solved using elliptic integrals of the Carlson type[33]. The fourth-order orientation tensor is already in the principle frame when solved for using Carlson elliptic integrals. Elliptic integrals assume that $C_l = 0$.

There are only two independent components of $a_{ij}$, therefore elliptic integrals can be used to solve for the exact values of $a_{(1)}$ and $a_{(2)}$, then obtain $a_{(3)}$ from Equation (2.40). Likewise, as given in Section 2.5.5, an orthotropic closure is only required to compute values of $\overline{A}_{11}$, $\overline{A}_{22}$, and $\overline{A}_{33}$. The calculation of all of the above exact answers are similar to the method in which Verweyst[29] used to create his ORT closure. Verweyst got his idea for populating the eigenspace from Wetzel, who used elliptic integrals to create a fourth-order area tensor over an ellipsoid using Cintra and Tucker’s fitting procedure with constraints imposed at the corners and edges of the UBT triangle. To obtain the exact solutions for the eigenvalues the following formulae are used [33]
\[ a_{(1)} = \frac{1}{2} \int_0^\infty \frac{ds}{(b_1 + s)^{3/2} \sqrt{(b_2 + s)} \sqrt{(b_3 + s)}} \]
\[ a_{(2)} = \frac{1}{2} \int_0^\infty \frac{ds}{\sqrt{(b_1 + s)} \sqrt{(b_2 + s)^{3/2} \sqrt{(b_3 + s)}}} \]
\[ a_{(3)} = \frac{1}{2} \int_0^\infty \frac{ds}{\sqrt{(b_1 + s)} \sqrt{(b_2 + s)} \sqrt{(b_3 + s)^{3/2}}} \]

(3.1)

and the exact solutions for the necessary fourth-order orientation tensor components are computed as [33]

\[ \tilde{A}_{11} = \frac{3}{4} \int_0^\infty \frac{sds}{(b_1 + s)^{5/2} \sqrt{(b_2 + s)} \sqrt{(b_3 + s)}} \]
\[ \tilde{A}_{22} = \frac{3}{4} \int_0^\infty \frac{sds}{\sqrt{(b_1 + s)} (b_2 + s)^{3/2} \sqrt{(b_3 + s)}} \]
\[ \tilde{A}_{33} = \frac{3}{4} \int_0^\infty \frac{sds}{\sqrt{(b_1 + s)} \sqrt{(b_2 + s)} (b_3 + s)^{3/2}} \]

(3.2)

where \( b_1, b_2, \) and \( b_3 \) are mapping functions of a symmetric point mesh grid on the \( s-t \) plane to the \( a_{(1)}-a_{(2)} \) plane given as

\[ b_1 = e^{s+t} \]
\[ b_2 = e^{s-t} \]
\[ b_3 = e^{-2s} \]

(3.3)

it can be seen in Figure 3.1 below shows that using Equations (3.1) and (3.3) provides a mapping that is one-to-one and onto.
Figure 3. S vs. T space mapped into eigenspace.

The mapping in Equations (3.1) and (3.3) is for the entire $a_{(1)} - a_{(2)}$ eigenspace, for fitting using these integrals we are only interested in the space represented in Figure 2.2 and 3.2. After mapping over into the eigenspace the data set must be sorted according to Equation (2.41) only then will the desired result be achieved and look as shown in Figure 3.2.
The elliptic integrals do not homogenously populate the UBT triangle. When sorted, certain data points will become duplicates. There are exactly 169 data points in each side of Figure 3.2 so duplicates would be discarded if that is desired. If equally spaced data points are desired, a dense point mesh could be generated, followed with a radial filtering routine on the data points to sort the points into UBT triangle. It should be noted that once sorted, some fourth order tensor components change labels due to symmetries. For examples, the $A_{ij}$ components in the triangle below the UBT triangle in Figure 3.2, are actually the $A_{22}$ component when sorted to inside the UBT triangle.
3.1.4 On Data Sets

The data set that is attained to produce fits is very significant to the overall outcome of how accurate your fit will be. It has been shown in this thesis that data sets can be obtained in three ways, through DFC, through spherical harmonics, and using elliptic integrals. If using DFC or spherical harmonics be sure to select a wide range of flow fields with varying coefficient of interaction, this should help eliminate all non-physical behavior of the final fit. Perhaps one of the best set of flow fields chosen was by Jack and Smith[15], which uses fourteen flows and populates the UBT triangle very well. Experimentation with data sets is important, for instance if the transient part of the flows is desired to be more accurate populating the transients with more data points can be done. Cintra and Tucker[12] stated that their data sets used “different ending times were chosen for each flow so as to cover the transient period and include the final steady state without over emphasizing the steady state results”. In his PhD thesis, Wetzel[28] tested a variety of corner and edge conditions along the UBT triangle, he found certain constraints imposed around the edges and corners provided more accurate results in a problem that was different, but related to, fiber orientation. Also, Wetzel[28] mentions that rather than adding constraints to the edges and corners, more data points can be added around those regions to get more exact answers, the latter is the fitting approach used in this thesis.
Verweyst used Wetzel’s method for his ORT closure which is now the most widely used ORT closure in the fiber orientation calculation.

### 3.2 Fitting Data Sets

To date fitted closure approximations have employed complete second through fifth order polynomials such as EBOF or IBOF closures. The fiber orientation problem seems to use many different polynomials expansions, Cintra and Tucker[12] originally fit a complete second-order, Chung and Kwon[13] fit a complete third-order, and Verweyst[29] used a complete fourth-order polynomial, all using the EBOF procedure. Chung and Kwon[14] later used a complete fifth-order polynomial to fit their IBOF closure. Wetzel[28, 30] used rational polynomials to fit his closures. The only type of fit that can be found in literature is a “least squares-type fitting procedure”[12]. It seems that literature only mentions this type of fitting, as it is a commonly used method. There are other possible types of fitting procedures that can be employed for fiber orientation, but it seems that none have been investigated.
As mentioned above the only type of polynomial that has been fitted in fiber orientation closure approximations have been complete second through fifth-order polynomials. In this research, investigations using both incomplete polynomials and fitting rational polynomials were performed.

The typical form of a complete polynomial uses an expansion of the \( a_{(1)} \) and \( a_{(2)} \) terms to the same degree in the exponent. The fourth-order polynomial of this can be seen below

\[
\overline{A}_{nm} = C_{(m)1} + C_{(m)2}a_{(2)} + C_{(m)3}a_{(1)} + C_{(m)4}a_{(1)}a_{(2)} + C_{(m)5}a_{(1)}^2 + C_{(m)6}a_{(2)}^2 \\
+ C_{(m)7}a_{(2)}^2 + C_{(m)8}a_{(1)}a_{(2)}^2 + C_{(m)9}a_{(1)}^3 + C_{(m)10}a_{(2)}^3 + C_{(m)11}a_{(1)}a_{(2)}^2 \\
+ C_{(m)12}a_{(1)}^3 + C_{(m)13}a_{(1)}^2a_{(2)} + C_{(m)14}a_{(1)}^4 + C_{(m)15}a_{(2)}^4
\]  
(3.4)

no sum on \( m \)

The first six terms of Equation (3.4) is the second order polynomial that Cintra and Tucker[12] used and the first ten terms are the polynomial that Chung and Kwon[13] employed. There has been great success with accurately representing the distribution function with these types of polynomials.

Another type of polynomial for fitting that was investigated in this thesis was an incomplete polynomial, \textit{i.e.} one where the final polynomial form of the fitting function
has the highest power exponent degree of the $a_{(1)}$ and $a_{(2)}$ terms not equal. One example is when the $a_{(1)}$ term remains linear and the $a_{(2)}$ term is raised to the third order, \textit{i.e.}

\[
\overline{A}_{mn} = C_{(m)1} + C_{(m)2}a_{(1)} + C_{(m)3}a_{(2)} + C_{(m)4}a_{(1)}^2a_{(2)} + C_{(m)5}a_{(2)}^2 \\
+C_{(m)6}a_{(1)}a_{(2)}^2 + C_{(m)7}a_{(2)}^3
\]  

(3.5)

Fitting orientation data using Equation (3.5) and related equations does give relatively accurate results. However, it was found that fitting an incomplete polynomial would be less accurate than fitting a complete polynomial matching the highest degree in the exponent of $a_{(1)}$ or $a_{(2)}$. Thus no further investigation of incomplete polynomial functions will be presented.

The final type of fitting function to be considered is a rational polynomial. An example of a rational function is a complete third-order polynomial divided by a complete second-order polynomial. According to Wetzel, “greater functional flexibility is possible by fitting a rational polynomial function[28]”, so this type of polynomial is included in this work. The general form of a rational polynomial used here is
\[ \overline{A}_{mn} = \frac{P(a_{(1)}, a_{(2)})}{Q(a_{(1)}, a_{(2)})} \]

\[ P(a_{(1)}, a_{(2)}) = C_{(m)1} + C_{(m)2}a_{(1)} + C_{(m)3}a_{(2)} + C_{(m)4}a_{(1)}^2 + \]
\[ + C_{(m)5}a_{(1)}^3 + C_{(m)6}a_{(2)}^2 + C_{(m)7}a_{(1)}a_{(2)} + C_{(m)8}a_{(1)}^2a_{(2)} + \]
\[ + C_{(m)9}a_{(1)}^3 + C_{(m)10}a_{(2)}^3 + \ldots \] (3.6)

\[ Q(a_{(1)}, a_{(2)}) = 1 + C_{(m)0}a_{(1)} + C_{(m)n+1}a_{(2)} + C_{(m)n+2}a_{(1)}a_{(2)} + \]
\[ + C_{(m)n+3}a_{(1)}^2 + C_{(m)n+5}a_{(2)}^2 + \ldots \]

It is necessary to fix the first term in the \( Q \) to one to ensure that the solution will be unique, and also so that the asymptotic behavior of the function will not affect the critical region of the fitted surface. Wetzel[28] showed that a third-order polynomial \( P \) over a second-order polynomial \( Q \) was almost twice as accurate as a fifth order polynomial, so fitting functions of this type shows great promise for fiber orientation closure approximation.

Fitting functions in the form of polynomials is all that has been done in literature thus far for fiber orientation. It is important to realize that even though polynomials have been found to give good results, other types of equations could work just as well or better. For instance possibly fitting a sine curve with a large period could work, or maybe an exponential function. Also, not all fitting techniques are alike, so fitting a higher degree polynomial does not always mean that it will be more accurate.
3.2.2 Regression Techniques

As stated above at this point in literature, the only type of regression technique used to define a fitted closure approximation is a least squares regression which has been shown to give great accuracy with the results. In statistical terms a regression is performed with two independent variables, \( a_{(1)} \) and \( a_{(2)} \), and one response variable, \( A_{mn} \), to get the desired results for a closure approximation. Two other types of regression are presented in this work. The least absolute residuals (LAR) regression, minimizes the absolute value of the residuals[34]. The bisquare iteratively reweighted least squares (BIS) regression, reweights the data set values so that outlying cases take on less weight in the overall regression[35]. Both LAR and BIS regression methods are considered robust regression techniques, which mean that these methods attempt to reduce the influence of outlying data in an effort to make a better fit for most cases. Since the pure least squares regression has been used extensively for fitting closure approximations[12-14, 16, 23, 28-30] it will not be discussed here. Figure 3.3 below shows an example of how well robust fitting works. As one can see there are two outlying data points on
Figure 3.3 Example of effect of robust regression over linear least squares regression.

Figure 3.3, least squares is greatly affected by the two data points, A and B, while the robust fitting curve appears to give a better fit to the rest of the data set excluding A and B. The robust technique above is the BIS method; other examples can be seen in [34]. Even though this is a two dimensional fit, the techniques work analogously in three dimensions.

In texts[35], LAR is known by other names such as least absolute deviations (LAD) or the minimum $L_1$-norm regression. The LAR regression estimator may not give unique solutions, but has many benefits that the least squares estimator does not. LAR regression is one of the most widely used robust regression techniques. This
technique is insensitive to both outlying data as well as inadequacies of the model that is
being fitted. Since the surface is fit to minimize absolute residuals rather than squared
differences extreme values have less influence on the overall fit. The only difference in
the actual fitting technique is the cost function. Rather than the cost function in Equation
(2.46), the cost function becomes

\[ \chi = \sum_{i=1}^{N_{\text{DATA}}} \sum_{m=1}^{3} | \overline{A}_{nm}^{\text{exact}} - \overline{A}_{nm}^{\text{closure}} | \]  

(3.7)

If a non-homogenous data set is used, then LAR regression will return accurate results
regardless to the fact that the overall data set may, for example, be weighted towards
steady state. Thus, one could save the computational time of radial filtering the data set.
For the LAR method, an accurate initial guess of the coefficients can be obtained through
a least squares regression.

BIS regression is used in robust regression to give less influence to outliers by
assigning weights that vary inversely according to the size of the residual. Data points
that are near the plane get full weight, while points that get further from the plain receive
less weight. Extreme outliers are assigned a zero weight. The weights are revised
iteratively. It is called the bisquare iteratively reweighted regression because the bisquare
function assigns the weights given by [35]

\[ w = \begin{cases} 
1 - \left( \frac{u}{4.685} \right)^2 & |u| \leq 4.685 \\
0 & |u| > 4.685 
\end{cases} \]  

(3.8)
where

\[ u_i = \frac{e_i}{MAD} \]

\[ MAD = \frac{1}{0.6745} \text{median}[|e_i - \text{median}(e_i)|] \]

where \( e_i \) are the residuals measured from the current iteration. The method for iteratively updating the weights in the least squares robust regression are as follows [35]:

1. Choose a weight function for weighting each data point. In this work the weight function is given in Equations (3.8) and (3.9).

2. Obtain starting weights for each data point. For bisquare weighting a weight of one is given to each data point.

3. Use the starting weights in weighted least squares and obtain residuals, \( e_i \), from the fitted function. An initial guess is needed for the unknown coefficients, typically the results from an LAR regression is sufficient.

4. Use the residuals in step 3 to obtain revised weights.

5. Continue the iterations until desired convergence is obtained.

Convergence can be defined by many different criteria such as whether the residuals, weights, or the fitted coefficients do not change between iterations. Data point homogeneity is more important when using the BIS method since fitting a solution can be bias toward a dense region of points. Thus, the BIS method may discard data points of
interest because those points may be in a region that does not have a high point density relative to other regions. In most cases, the BIS method is preferred over the LAR regression because it minimizes the effect of outliers while optimizing the fit in a least squares manner. However, for this use the BIS method may not yield normalized results. One issue with the BIS regression is that it may discard data points, if this happens each individual fourth-order tensor component, may actually be fit to different data sets.

With the generation of exact data, every data may be desirable for fitting. Robust regression techniques do account for almost all data points just certain points more than others. The focus of these techniques is to account for most of the data points to get the best overall representation.

### 3.3 Comparison of Fitting Forms

Many different closure approximations were formed in order to investigate a variety of techniques used in fitting and to yield the most accurate closure. Data was generated
using elliptic integrals and spherical harmonics calculation methods. The results are illustrated below.

### 3.3.1 Elliptic Integrals

In order to have an accurate representation of how different regression techniques and functions forms can affect the overall fit, 15 different fits were chosen to illustrate the different results that can occur with these techniques. For this example the same data set was used for all the resulting fits. The elliptic integrals in Equations (3.1) and (3.2) were used to generate this data set as shown in Figure 3.4 below.
The only variables that will be different in this series of fits are the type of function used, the regression used, and the coefficient optimization used. The best results for polynomials with a least-squares fit was using a Levenberg-Marquardt[36] optimization routine on the coefficients, all other regression techniques gave best results when using a trust-region algorithm[36] approach to their optimization.

The measure of the fits was done using statistical details such as the correlation coefficient (R-square)[35], sum of squared errors (SSE)[35], and the root mean square error (RMSE)[35] that the fit provided. Table 3.1 below shows all details.
Table 3.1 Summary of regression analysis on elliptic integral data set ordered from worst to best.

<table>
<thead>
<tr>
<th>Regression Type</th>
<th>Polynomial Order</th>
<th>SSE</th>
<th>R-Square</th>
<th>RMSE</th>
<th>COEFF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Least Squares</td>
<td>3</td>
<td>8.59E-05</td>
<td>0.99996736</td>
<td>0.00018186</td>
<td>30</td>
</tr>
<tr>
<td>BIS</td>
<td>3</td>
<td>3.73E-05</td>
<td>0.99998526</td>
<td>0.00011553</td>
<td>30</td>
</tr>
<tr>
<td>Least Squares</td>
<td>4</td>
<td>2.56E-05</td>
<td>0.99999023</td>
<td>0.00009800</td>
<td>45</td>
</tr>
<tr>
<td>Least Squares</td>
<td>5</td>
<td>9.30E-06</td>
<td>0.99999648</td>
<td>0.00005892</td>
<td>63</td>
</tr>
<tr>
<td>BIS</td>
<td>4</td>
<td>8.46E-06</td>
<td>0.99999700</td>
<td>0.00005552</td>
<td>45</td>
</tr>
<tr>
<td>LAR</td>
<td>3</td>
<td>4.64E-06</td>
<td>0.99999822</td>
<td>0.00004211</td>
<td>30</td>
</tr>
<tr>
<td>BIS</td>
<td>5</td>
<td>4.83E-06</td>
<td>0.99999785</td>
<td>0.00004123</td>
<td>63</td>
</tr>
<tr>
<td>LAR</td>
<td>4</td>
<td>2.67E-06</td>
<td>0.99999898</td>
<td>0.00003164</td>
<td>45</td>
</tr>
<tr>
<td>LAR</td>
<td>5</td>
<td>1.76E-06</td>
<td>0.99999932</td>
<td>0.00002556</td>
<td>63</td>
</tr>
<tr>
<td>Least Squares</td>
<td>3rd/2nd</td>
<td>9.10E-07</td>
<td>0.99999965</td>
<td>0.00002014</td>
<td>45</td>
</tr>
<tr>
<td>BIS</td>
<td>3rd/2nd</td>
<td>5.35E-07</td>
<td>0.99999979</td>
<td>0.00001442</td>
<td>45</td>
</tr>
<tr>
<td>Least Squares</td>
<td>4th/2nd</td>
<td>2.64E-07</td>
<td>0.99999989</td>
<td>0.00001103</td>
<td>60</td>
</tr>
<tr>
<td>LAR</td>
<td>3rd/2nd</td>
<td>1.08E-07</td>
<td>0.99999995</td>
<td>0.00000685</td>
<td>45</td>
</tr>
<tr>
<td>BIS</td>
<td>4th/2nd</td>
<td>1.04E-07</td>
<td>0.99999996</td>
<td>0.00000620</td>
<td>60</td>
</tr>
<tr>
<td>LAR</td>
<td>4th/2nd</td>
<td>3.90E-08</td>
<td>0.99999998</td>
<td>0.00000384</td>
<td>60</td>
</tr>
</tbody>
</table>

It can be seen in the table that the LAR regression type with a rational polynomial yields the best results. It is interesting to see that a 3rd order LAR fit gave better results than a 5th order least-squares fit and a 4th order BIS fit. This result clearly shows how an LAR regression is ideal for the fiber orientation problem. Another fact that the table shows is that using a rational polynomial does give drastically better results. For instance, a 3rd/2nd order polynomial of the least squares type is more than twice as accurate as a 5th order polynomial of the least squares type. The same goes for both BIS and LAR regressions. There are however some problems with the BIS regression type. Due to the way the BIS regression works the higher order the polynomial the more nonphysical the results
become. If one thinks about fitting each fourth order tensor component individually it is the same as fitting a surface. The ideal surface is smooth and triangular due to what our fitting region is, each of the three surfaces are shown in Figure 3.5.

![Figure 3.5 Different fourth-order tensor surfaces.](image)

The data in Figure 3.5 are exact data points. In the plot of $A_{mm}$ (bottom right) it is shown that some of the edges are “connected.” With the BIS method, some higher order polynomials trail off from certain regions as shown in Figure 3.6.
Figure 3.6 Unacceptable fit of selected closure surface due to Bisquare weighted regression.

This BIS fifth-order complete polynomial fit would not be acceptable due to the surface not following the data points in the upper left corner producing nonphysical results and may not necessarily be normalized.
3.3.2 Spherical Harmonics

Spherical Harmonics, as stated above were also used to create data sets from various flow field simulations. One data set that was created was the original Cintra and Tucker[12] flow fields for the ORF closure. Fourteen flows from Jack and Smith[15] were also used to generate spherical harmonic data. The results for the most accurate polynomials based on the regression type and polynomial were analogous to the above Table 3.1. The data set was created using a fourth order Runge-Kutta method with step-size of 1e-4 with spherical harmonics of order 250. Once the data was obtained and rotated into the principal axes of the second-order orientation tensor, a radial filter was performed to each flow field in order to obtain a total of 514 data points as shown in Figure 3.7.
Even though the data set is not homogenously populated, it still gives desirable results and populates the UBT triangle very well. Since later in this work fourth order polynomials will be evaluated in terms of error calculations only fourth-order polynomial fitting statistics will be shown.

Table 3.2 Summary of regression analysis of polynomials of order 4 from SPH data set.

<table>
<thead>
<tr>
<th>Regression Type</th>
<th>Polynomial Order</th>
<th>SSE</th>
<th>R-Square</th>
<th>RMSE</th>
<th>COEFF</th>
</tr>
</thead>
<tbody>
<tr>
<td>LAR</td>
<td>4</td>
<td>4.02E-04</td>
<td>0.999948375</td>
<td>0.00081637</td>
<td>45</td>
</tr>
<tr>
<td>BIS</td>
<td>4</td>
<td>4.88E-04</td>
<td>0.999912649</td>
<td>0.00093718</td>
<td>45</td>
</tr>
<tr>
<td>Least Squares</td>
<td>4</td>
<td>0.001346617</td>
<td>0.999827265</td>
<td>0.00149336</td>
<td>45</td>
</tr>
</tbody>
</table>
Again the LAR is the best, also with this data set a least squares is a whole order of magnitude worse than LAR or BIS.

3.3.3 Performance of Fitted Closure Approximations

Another way to accurately assess the accuracy of a closure approximation is to compare the solution based on $a_{ij}$ obtained from Equations (2.16) and (2.22). In this work the author chooses to use the error tensor defined by Cintra and Tucker[12] which is just one way to quantitatively evaluate the error of a closure approximation. That is, define $e_{ij}$ to be the difference between the exact second-order orientation tensor and the second-order orientation tensor from the closure approximations,

$$e_{ij} = a_{ij}^{spherical} - a_{ij}^{closure}$$

(3.10)

Once the error matrix is calculated use the equation
to obtain the scalar magnitude of the error matrix. Next, the average error over the entire flow was calculated with the following equation.

\[
e = \sqrt{\frac{1}{2}e_je_{ji}}
\]

\[(3.11)\]

Next, the average error over the entire flow was calculated with the following equation.

\[
Average \ Error = \frac{1}{t_{end} - t_0} \int_{t_0}^{t_{end}} e(t)dt
\]

\[(3.12)\]

The five Cintra and Tucker flows, the mixed flow[12, 28], and nine different center-gated disk flows were used to test the accuracy of each closure. Four different fitted closures were used to obtain error results. Verweyst’s ORT closure was used as a comparison of the closures, which uses a fourth order polynomial for fitting \(A_{mm}\) in Equation (3.4). Other closures chosen were fits from the above Tables 3.1 and 3.2. Two are both fourth-order polynomials, one is chosen from the using flow fields to create the closure FFLAR4 where FF denotes flow field, LAR denotes regression type and 4 is polynomial order. The second is LAR4, where no character in front of regression type assumes elliptic integrals for fitting. The third closure approximation is a rational polynomial LAR32, where 32 stands for 3\textsuperscript{rd} order / 2\textsuperscript{nd} order polynomial. LAR32 was chosen because a 3\textsuperscript{rd} order/ 2\textsuperscript{nd} order polynomial has the same amount of coefficients as a 4\textsuperscript{th} order polynomial. The coefficients for FFLAR4 according to Equation (3.4) appear in Table 3.3.
Table 3.3 Coefficients $C_{mn}$ of FFLAR4 closure.

<table>
<thead>
<tr>
<th>n</th>
<th>m=1</th>
<th>m=2</th>
<th>m=3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.678225884</td>
<td>0.748226727</td>
<td>3.167356369</td>
</tr>
<tr>
<td>2</td>
<td>-3.834359034</td>
<td>-4.249612053</td>
<td>-13.2882664</td>
</tr>
<tr>
<td>3</td>
<td>-2.664862865</td>
<td>-2.987266447</td>
<td>-11.68017933</td>
</tr>
<tr>
<td>4</td>
<td>14.20996267</td>
<td>14.93820941</td>
<td>43.70060768</td>
</tr>
<tr>
<td>5</td>
<td>9.746185193</td>
<td>8.641488072</td>
<td>23.78843134</td>
</tr>
<tr>
<td>6</td>
<td>2.700369681</td>
<td>5.974489008</td>
<td>17.38312143</td>
</tr>
<tr>
<td>7</td>
<td>-22.4472527</td>
<td>-21.75721716</td>
<td>-58.354308</td>
</tr>
<tr>
<td>8</td>
<td>-13.07864964</td>
<td>-15.79867632</td>
<td>-49.51370564</td>
</tr>
<tr>
<td>9</td>
<td>-8.013024236</td>
<td>-7.521216405</td>
<td>-19.95905461</td>
</tr>
<tr>
<td>10</td>
<td>-0.125467689</td>
<td>-3.616551654</td>
<td>-11.7552593</td>
</tr>
<tr>
<td>11</td>
<td>12.68948457</td>
<td>12.64035267</td>
<td>35.42535413</td>
</tr>
<tr>
<td>12</td>
<td>10.56324841</td>
<td>10.22218578</td>
<td>25.84431792</td>
</tr>
<tr>
<td>13</td>
<td>2.487386515</td>
<td>4.788201652</td>
<td>18.22644393</td>
</tr>
<tr>
<td>14</td>
<td>2.417857515</td>
<td>2.376441613</td>
<td>6.291273472</td>
</tr>
<tr>
<td>15</td>
<td>-0.328195677</td>
<td>1.056519961</td>
<td>2.925785795</td>
</tr>
</tbody>
</table>

The coefficients for LAR4 are given in Table 3.4
Table 3. 4 Coefficients $C_{mn}$ of LAR4 closure.

<table>
<thead>
<tr>
<th>n</th>
<th>$m=1$</th>
<th>$m=2$</th>
<th>$m=3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.813175172</td>
<td>1.768619587</td>
<td>4.525066937</td>
</tr>
<tr>
<td>3</td>
<td>-4.659333003</td>
<td>-6.484058476</td>
<td>-17.65017809</td>
</tr>
<tr>
<td>4</td>
<td>14.747639777</td>
<td>28.90593675</td>
<td>61.54397954</td>
</tr>
<tr>
<td>5</td>
<td>6.329870878</td>
<td>19.9869947</td>
<td>33.90123961</td>
</tr>
<tr>
<td>6</td>
<td>9.739797775</td>
<td>10.75996301</td>
<td>28.46735597</td>
</tr>
<tr>
<td>7</td>
<td>-15.92224091</td>
<td>-40.4923871</td>
<td>-76.73863881</td>
</tr>
<tr>
<td>8</td>
<td>-20.8185719</td>
<td>-27.4422175</td>
<td>-68.97758329</td>
</tr>
<tr>
<td>9</td>
<td>-4.216519964</td>
<td>-17.71540927</td>
<td>-27.7680827</td>
</tr>
<tr>
<td>10</td>
<td>-8.993993112</td>
<td>-7.230748101</td>
<td>-22.39903613</td>
</tr>
<tr>
<td>11</td>
<td>11.47097452</td>
<td>19.72963124</td>
<td>43.87513563</td>
</tr>
<tr>
<td>12</td>
<td>5.834142985</td>
<td>18.70904748</td>
<td>32.48067994</td>
</tr>
<tr>
<td>13</td>
<td>9.874209286</td>
<td>8.882877701</td>
<td>26.92832021</td>
</tr>
<tr>
<td>14</td>
<td>1.138888034</td>
<td>5.785725498</td>
<td>8.600822308</td>
</tr>
<tr>
<td>15</td>
<td>3.100457733</td>
<td>2.224834058</td>
<td>7.101978254</td>
</tr>
</tbody>
</table>

and for closure approximation LAR32 the coefficients appear in Table 3.5
Table 3. 5 Coefficients $C_{\text{m,n}}$ for LAR32 closure (below the separating line denotes denominator coefficients).

<table>
<thead>
<tr>
<th>n</th>
<th>m=1</th>
<th>m=2</th>
<th>m=3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.087602233</td>
<td>0.156805152</td>
<td>1.072423739</td>
</tr>
<tr>
<td>2</td>
<td>0.02820555</td>
<td>-0.577818864</td>
<td>-2.803554028</td>
</tr>
<tr>
<td>3</td>
<td>-0.426784335</td>
<td>-0.51428092</td>
<td>-2.661576129</td>
</tr>
<tr>
<td>4</td>
<td>0.876469059</td>
<td>2.132305029</td>
<td>4.566728489</td>
</tr>
<tr>
<td>5</td>
<td>1.27467711</td>
<td>0.684250887</td>
<td>2.389379765</td>
</tr>
<tr>
<td>6</td>
<td>0.602031647</td>
<td>3.454835266</td>
<td>2.097523143</td>
</tr>
<tr>
<td>7</td>
<td>-1.918931146</td>
<td>-1.61412261</td>
<td>-1.904704744</td>
</tr>
<tr>
<td>8</td>
<td>-0.934291306</td>
<td>-4.005261132</td>
<td>-1.754978355</td>
</tr>
<tr>
<td>9</td>
<td>-1.066583115</td>
<td>-0.263237143</td>
<td>-0.65824893</td>
</tr>
<tr>
<td>10</td>
<td>-0.262854903</td>
<td>-2.228133231</td>
<td>-0.508282668</td>
</tr>
<tr>
<td>11</td>
<td>-0.244001948</td>
<td>0.365652907</td>
<td>-1.068512526</td>
</tr>
<tr>
<td>12</td>
<td>-0.574150861</td>
<td>1.385725477</td>
<td>-0.771356469</td>
</tr>
<tr>
<td>13</td>
<td>-0.895226091</td>
<td>-2.866357848</td>
<td>0.206908269</td>
</tr>
<tr>
<td>14</td>
<td>-0.432097367</td>
<td>-1.359687152</td>
<td>0.067386858</td>
</tr>
<tr>
<td>15</td>
<td>-0.462709527</td>
<td>-1.518996192</td>
<td>-0.248999874</td>
</tr>
</tbody>
</table>

where the rational polynomial used for the data is given as the equation
\[ \bar{A}_{nm} = \frac{P(a_{1(1)}, a_{2(1)})}{Q(a_{1(1)}, a_{2(1)})} \]

\[ P(a_{1(1)}, a_{2(1)}) = C_{(m)1} + C_{(m)2}a_{1(1)} + C_{(m)3}a_{1(1)}a_{2(1)} + C_{(m)4}a_{1(1)}a_{2(2)} + C_{(m)5}a_{1(1)}^2 + C_{(m)6}a_{2(2)} + C_{(m)7}a_{1(2)}a_{2(2)} + C_{(m)8}a_{1(1)}a_{2(2)}^2 + C_{(m)9}a_{1(1)}^3 + C_{(m)10}a_{1(2)}^3 \]  

\[ Q(a_{1(1)}, a_{2(1)}) = 1 + C_{(m)1}a_{1(1)} + C_{(m)2}a_{1(2)} + C_{(m)3}a_{1(1)}a_{2(2)} + C_{(m)4}a_{1(1)}^2 + C_{(m)5}a_{1(2)}^2 \]

Each of these closures was tested against flows generated with the spherical harmonics method of order 250. Unless stated otherwise all flows were performed starting with the random orientation initial condition, \( \lambda = 1 \) and \( C_I = 0.01 \).

It can be seen in the figure below that for simple shear flow ORT, LAR4, and LAR32 all seem to have only the slightest of differences as they appear to be the same line in the figure. FFLAR4 has noticeable improvements to the final steady state, however it does seem to overshoot the transient of \( a_{11} \) more than the other three closures.

It can also be seen that in the \( a_{12} \) component that FFLAR4 follows the spherical harmonics (SPH) line more accurately for the entire duration of the flow. This might be expected since all the closures ORT, LAR4, and LAR32 used elliptic integrals (i.e. \( C_I = 0 \)) to generate the fitting data, and FFLAR used fitting data generated from the spherical harmonic solution of \( \psi \).
Figure 3.8 Selected components of various closures for simple shear flow.

For the flow known as shear/stretch A, the figure again shows that FFLAR4 has large improvements for the all shown components and seems to be exact for steady state. ORT, LAR4, and LAR32 appear as the same line, however one can barely see that LAR4 is nominally better than ORT and LAR32.
Figure 3.9 Selected components from various closures for shear/stretch A flow.

Table 3.6 Error for select flows for various closures.

<table>
<thead>
<tr>
<th>Flow</th>
<th>ORT</th>
<th>FFLAR4</th>
<th>LAR4</th>
<th>LAR32</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple Shear</td>
<td>0.0362</td>
<td>0.0264</td>
<td>0.0360</td>
<td>0.0362</td>
</tr>
<tr>
<td>Biaxial Elongation</td>
<td>0.0020</td>
<td>0.0028</td>
<td>0.0023</td>
<td>0.0022</td>
</tr>
<tr>
<td>Uniaxial Elongation</td>
<td>0.0179</td>
<td>0.0114</td>
<td>0.0178</td>
<td>0.0178</td>
</tr>
<tr>
<td>Shear/Stretch A</td>
<td>0.0292</td>
<td>0.0152</td>
<td>0.0285</td>
<td>0.0283</td>
</tr>
<tr>
<td>Shear/Stretch B</td>
<td>0.0242</td>
<td>0.0189</td>
<td>0.0242</td>
<td>0.0242</td>
</tr>
<tr>
<td>Ave All Flows</td>
<td>0.0219</td>
<td>0.0149</td>
<td>0.0218</td>
<td>0.0217</td>
</tr>
</tbody>
</table>
The FFLAR4 closure is the most accurate closure in all case except for biaxial elongation, however it is only 0.0007 different from the best closure in that flow, ORT. It seems that between ORT, LAR4, and LAR32 which closure is best behind the FFLAR4 closure changes, with all of them usually being the same to the third decimal point. Overall FFLAR4 is approximately 1.5 times better than the other flows, this is not only because of using a LAR regression, but also because the flow fields used in fitting FFLAR4 are very similar to the ones that were tested. LAR32 is next best overall, closely followed by LAR4 with an average difference of only 0.00004. Of all the closures ORT was the least accurate, behind LAR4 only 0.0001. Since the data set for ORT and LAR4 and LAR32 are so similar the main difference in the numbers is due to using the LAR regression.

Next the mixed flow was tested. This is a combined flow that uses three different flows for ten seconds each. Each part of the flow does not reach steady state, and what are the final conditions for one flow are the initial conditions for the next flow. This combination provides a means to see if a large error at the end of one flow, significantly affects the results during the next flow. The first flow is simple shear, then switches to a shearing/stretching flow, and ends with a shearing/strong stretching flow in different directions than the previous shear stretching flow. The velocity gradient tensor for each of these flows are
The FFLAR4 closure again is the best closure overall. However, the next best closure is LAR4, then ORT, then LAR32; all closures being within about 0.01 of each other. Error calculations are given in Table 3.7.

Table 3.7 Error for mixed flow for various closures.

<table>
<thead>
<tr>
<th>Flow</th>
<th>ORT</th>
<th>FFLAR4</th>
<th>LAR4</th>
<th>LAR32</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed Flow</td>
<td>0.0309</td>
<td>0.0222</td>
<td>0.0305</td>
<td>0.0314</td>
</tr>
</tbody>
</table>

Four individual components are given below in a graphical representation which appear in Figures 3.10-3.13.
Figure 3. 10 Selected closures for given mixed flow component.

Figure 3. 11 Selected closures for given mixed flow component.
Figure 3.12 Selected closures for given mixed flow components.

Figure 3.13 Selected closures for given mixed flow component.
It is very difficult to see the subtle differences between the closure approximations of the $a_{11}$ component of Figure 3.10 and the $a_{22}$ component of Figure 3.11. The $a_{12}$ (Figure 3.12) and $a_{23}$ (Figure 3.13) components have a better representation as to why the FFLAR4 is a better closure in this case.

The final type of flow, which is a non-homogenous flow, is the center gated disk. This type of flow is commonly seen in injection molding processes. The center-gated disk is an important test problem in the modeling of fiber orientation in injection molding[12].

In the case of an isothermal, Newtonian fluid the velocity field in a center-gated disk is

$$v_r = \frac{3Q}{8\pi rb} \left(1 - \frac{z^2}{b^2}\right), \quad v_\theta = v_z = 0$$

where $Q$ is the volume flow rate, the total gap thickness is $2b$, and $z=0$ lies at the midplane between the wall. The solution for this problem uses the lubrication approximation and is only valid for $r \gg b$. In this case only the kinematics of Equation (3.17) will be considered for the test case. Changing the coordinates to a Cartesian system where $(r, \theta, z)$ correspond to $(x, y, z)$ axes you would obtain the velocity gradient tensor of
The radius in the center-gated disk is time dependent, therefore if Equation (3.17) is integrated, one is able to obtain the position of a particle as a function of time. Assuming an initial time of $t = 0$, an initial radius, $r_0$, and a constant $z$, the radial position is given by the equation

$$r^2 = r_0^2 + \frac{3Qt}{4\pi b} \left( 1 - \frac{z^2}{b^2} \right)$$

(3.19)

As for all other test cases, numerical solutions were carried out for nine different values of $z$ from 0.1 to 0.9. For all test cases of the center-gated disk, $Q = 10$, $b = 1$, $C_T = 0.01$, and $r_0 = 1$. 

\[
\frac{\partial v_i}{\partial x_j} = \frac{3Q}{8\pi rb} \begin{bmatrix}
-\frac{1}{r} & 0 & -\frac{2b}{z^2} \\
0 & 1 & \frac{1}{r} \left( 1 - \frac{z^2}{b^2} \right) \\
0 & 0 & 0
\end{bmatrix}
\] (3.18)
Figure 3. 14 Selected components for various closures for center-gated disk, \( z=0.3 \).

Figure 3. 15 Selected components for various closures of center-gated disk, \( z=0.7 \).
Results for the evolution of the center-gated disk for $z/b = 0.3$ and $z/b = 0.7$ are graphed in Figure 3.14 and 3.15 above. For Figure 3.14 it is hard to differentiate all the different closure approximations as they are all extremely close to the exact solutions. Figure 3.15 shows quite well again how the FFLAR4 closure approximation dominates in accuracy for this flow. For this flow, FFLAR4 is almost twice as accurate as all the other closure approximations, with ORT being the least accurate and still giving very desirable results.

All results for the nine different $z$ values can be seen in Table 3.8 below.

Table 3.8 Error for various closures for varying $z$-values of the center-gated disk.

<table>
<thead>
<tr>
<th>$z$</th>
<th>ORT</th>
<th>FFLAR4</th>
<th>LAR4</th>
<th>LAR32</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.0154</td>
<td>0.0029</td>
<td>0.0152</td>
<td>0.0153</td>
</tr>
<tr>
<td>0.2</td>
<td>0.0054</td>
<td>0.0096</td>
<td>0.0058</td>
<td>0.0060</td>
</tr>
<tr>
<td>0.3</td>
<td>0.0078</td>
<td>0.0058</td>
<td>0.0070</td>
<td>0.0068</td>
</tr>
<tr>
<td>0.4</td>
<td>0.0181</td>
<td>0.0072</td>
<td>0.0183</td>
<td>0.0181</td>
</tr>
<tr>
<td>0.5</td>
<td>0.0286</td>
<td>0.0132</td>
<td>0.0287</td>
<td>0.0287</td>
</tr>
<tr>
<td>0.6</td>
<td>0.0362</td>
<td>0.0180</td>
<td>0.0360</td>
<td>0.0361</td>
</tr>
<tr>
<td>0.7</td>
<td>0.0413</td>
<td>0.0221</td>
<td>0.0403</td>
<td>0.0407</td>
</tr>
<tr>
<td>0.8</td>
<td>0.0433</td>
<td>0.0247</td>
<td>0.0425</td>
<td>0.0429</td>
</tr>
<tr>
<td>0.9</td>
<td>0.0433</td>
<td>0.0266</td>
<td>0.0429</td>
<td>0.0434</td>
</tr>
<tr>
<td>AVE</td>
<td>0.0266</td>
<td>0.0145</td>
<td>0.0263</td>
<td>0.0264</td>
</tr>
</tbody>
</table>
3.4 Summary of New Closure Fitting Techniques

It is easy to see that changing the regression technique can help the fit of the data. The robust regression methods presented have statistically shown that they are superior to a general least squares fitting technique. The LAR regression has the most significant effect on obtaining desired fits, with the exact same data set it was shown that using LAR over least squares could result in an order of magnitude improvement in RMSE. The BIS regression did greatly increase accuracy of fitting; however it did produce unrealistic as well as non-objective results. More investigation should be done to be able to fully utilize the advantages that the BIS regression technique. Polynomial form was also shown to help with creating more accurate fits, as suspected the rational polynomials did increase accuracy of fits. The rational polynomial is extremely better according to the statistical data, however there were limitations in fitting using robust techniques and the actual error calculations were did not show a large difference. Obtaining convergence to minimize the polynomial coefficients was sometimes not possible, as in the case of fitting and LAR or BIS 4\textsuperscript{th} order / 3\textsuperscript{rd} order polynomial, however the least squares type fit of this polynomial was easily obtainable. Also, using robust fitting methods with a 4\textsuperscript{th} order / 2\textsuperscript{nd} order polynomial while possible, took over 250,000 iterations to converge. The rational polynomials did require more computation time, but it would be considered negligible. In this work, these techniques were merely investigated. More in-depth analysis of these procedures could produce much greater results than those shown here.
The three closures tested here were all better than the ORT closure, LAR4 and LAR32 only marginally, but the FFLAR4 was almost twice as accurate in most flows tested. FFLAR4 could be adopted and used, when looking for more promising results in flows with a $C_r$ around 0.01.
Closures have now been around for four decades. It seems that since the creation of EBOF and IBOF closures that very few attempts have been made to create a new type of closure. Jack et al.[17] and Qadir and Jack[18] have created neural network based closures and Han and Im[19] have made different hybrid type closures. In this chapter a new type of closure is developed, it will use the derivative terms of the Advani-Tucker evolution equation to aid in the fitting process. Because of the use of the derivative terms, Equation (2.22) becomes an implicit problem to solve; two methods will be discussed on solving this problem.
4.1 Data Set and Fitting Procedure

The data set that will be used in this fitting procedure will be the same data set used in fitting the FFLAR4 closure mentioned in Chapter 3, which are the 14 flows used in Jack and Smith[15]. The data set must be obtained using flow fields, therefore the spherical harmonics method is used to compute exact \( a_{ij} \), \( a_{ijkl} \), and \( \frac{da_{ij}}{dt} \). Elliptic integrals are not usable in this case since there is not an explicit form for computing the components of \( \frac{da_{ij}}{dt} \). When evolving each flow and collecting the data, one must obtain the exact answers for \( \frac{da_{ij}}{dt} \) as well as \( a_{ij} \) and \( a_{ijkl} \).

The next step is to create a functional form and do a least squares type fitting procedure. Least squares regression is what will be used in this work. Since the purpose of this thesis is initial investigation, other fitting techniques such as the LAR or BIS method will not be used. With the goal of objectivity in mind, we will use the time derivatives of the eigenvalues. To obtain the derivatives of the eigenvalues, a relation was used to relate \( \frac{da_{ij}}{dt} \) with \( \frac{d\lambda}{dt} \). The relation that was used was based on a paper by Smith and Siddhi[37], that incorporated the eigenvector normalization conditions for
design sensitivity analysis. From this paper, an equation was developed that takes the general eigenproblem, that is

$$[A - \lambda_i I] \Phi_i = 0$$  \hspace{1cm} (4.1)

where $A$ is our $a_{ij}$, $\lambda_i$ is the $i$-th eigenvalue and $\Phi_i$ is the $i$-th eigenvector. After differentiation and algebraic manipulation it can be shown that

$$\frac{d\lambda_i}{dt} = \frac{1}{\Phi_i^T \Phi_i} \Phi_i^T \frac{da_{ij}}{dt} \Phi_i$$  \hspace{1cm} (4.2)

Where the eigenvectors are normalized such that $\Phi_i^T \Phi_i = 1$, Equation (4.2) is reduced to

$$\frac{d\lambda_i}{dt} = \Phi_i^T \frac{da_{ij}}{dt} \Phi_i$$  \hspace{1cm} (4.3)

For fitting purposes, only the first 2 diagonal values of $\frac{d\lambda_1}{dt}$ and $\frac{d\lambda_2}{dt}$ where used because it is known that

$$\frac{d\lambda_1}{dt} + \frac{d\lambda_2}{dt} + \frac{d\lambda_3}{dt} = 0$$  \hspace{1cm} (4.4)

It should be noted that the first 2 values are chosen arbitrarily.
4.2 Functional Forms

The idea behind the form of polynomial was to start out with a simple polynomial structure such as Equation (2.45) and simply add terms using the derivative components. This was quickly found to not be the optimal way of producing an accurate fit, so other terms were investigated.

In all fits that were produced only two of the derivative terms were used as previously mentioned. Many different forms were tested and in the end only five different functions were chosen. All functions started with a second to fourth degree polynomial, with some combination of derivative terms added. The first form that was considered uses a complete second degree polynomial with derivative terms written as

\[
A_{\text{m1}}^{\text{Closure}} = C_{m(1)} + C_{m(2)}a_1 + C_{m(3)}[a_1]^2 + C_{m(4)}a_2 + C_{m(5)}[a_2]^2 + C_{m(6)}a_1a_2 + C_{m(7)}[da_1] + C_{m(8)}[da_2] + C_{m(9)}[da_1]a_1 + C_{m(10)}[da_1][a_1]^2 + C_{m(11)}[da_1][a_2] + C_{m(12)}[da_2] + C_{m(13)}[da_1][a_2] + C_{m(14)}[da_2]a_1 + C_{m(15)}[da_2][a_1]^2 + C_{m(16)}[da_2][a_2] + C_{m(17)}[da_2][a_2]^2 + C_{m(18)}[da_2][a_1][a_2] \tag{4.5}
\]

with coefficients given in Table 4.1 where \( da_1 \) and \( da_2 \) are respectively \( \frac{d\lambda}{dt} \) and \( \frac{d\lambda_2}{dt} \) from above.
Table 4.1 Coefficients $C_{mn}$ for DAIJXX2 closure.

<table>
<thead>
<tr>
<th>n</th>
<th>$m=1$</th>
<th>$m=2$</th>
<th>$m=3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.002216928</td>
<td>0.056020908</td>
<td>1.158024526</td>
</tr>
<tr>
<td>2</td>
<td>0.364348919</td>
<td>-0.303284895</td>
<td>-2.035984917</td>
</tr>
<tr>
<td>3</td>
<td>0.624817577</td>
<td>0.241621517</td>
<td>0.876957639</td>
</tr>
<tr>
<td>4</td>
<td>-0.064742597</td>
<td>0.332242419</td>
<td>-1.930375827</td>
</tr>
<tr>
<td>5</td>
<td>0.04273325</td>
<td>0.606214167</td>
<td>0.765676548</td>
</tr>
<tr>
<td>6</td>
<td>0.216007079</td>
<td>0.365264797</td>
<td>1.643223602</td>
</tr>
<tr>
<td>7</td>
<td>0.385001059</td>
<td>0.242887307</td>
<td>-0.083755056</td>
</tr>
<tr>
<td>8</td>
<td>-0.415235294</td>
<td>-0.322369392</td>
<td>-0.116988058</td>
</tr>
<tr>
<td>9</td>
<td>-0.280036828</td>
<td>-0.075852987</td>
<td>0.469809732</td>
</tr>
<tr>
<td>10</td>
<td>0.053557286</td>
<td>-0.082205089</td>
<td>-0.321410371</td>
</tr>
<tr>
<td>11</td>
<td>-1.639960381</td>
<td>-1.164706487</td>
<td>-0.06852575</td>
</tr>
<tr>
<td>12</td>
<td>1.438042067</td>
<td>1.117928016</td>
<td>0.437866058</td>
</tr>
<tr>
<td>13</td>
<td>0.803338256</td>
<td>0.496729271</td>
<td>-0.577794117</td>
</tr>
<tr>
<td>14</td>
<td>1.819258317</td>
<td>1.363404874</td>
<td>0.452280396</td>
</tr>
<tr>
<td>15</td>
<td>-1.191372366</td>
<td>-0.934784834</td>
<td>-0.245383464</td>
</tr>
<tr>
<td>16</td>
<td>0.320508742</td>
<td>0.307628697</td>
<td>0.229682793</td>
</tr>
<tr>
<td>17</td>
<td>0.30835978</td>
<td>0.148454476</td>
<td>0.050843451</td>
</tr>
<tr>
<td>18</td>
<td>-1.807741638</td>
<td>-1.335084108</td>
<td>-0.803797426</td>
</tr>
</tbody>
</table>

The next equation used for fitting is very similar to the previous equation, however it uses a third order polynomial in $\frac{da_{ij}}{dt}$ as.
\[ A^{\text{Closure}}_{mn} = C_{m(1)} + C_{m(2)} a_{1} + C_{m(3)} \left[ a_{1} \right]^2 + C_{m(4)} a_{2} + C_{m(5)} \left[ a_{2} \right]^2 + C_{m(6)} a_{1} a_{2} \\
+ C_{m(7)} \left[ a_{1} \right]^2 a_{2} + C_{m(8)} a_{1} \left[ a_{2} \right]^2 + C_{m(9)} \left[ a_{1} \right]^3 + C_{m(10)} \left[ a_{2} \right]^3 \\
+ C_{m(11)} \left[ d_{a_{1}} \right] + C_{m(12)} \left[ d_{a_{2}} \right] + C_{m(13)} \left[ d_{a_{1}} \right] a_{1} + C_{m(14)} \left[ d_{a_{1}} \right] a_{2} \\
+ C_{m(15)} \left[ d_{a_{1}} \right] a_{2} + C_{m(16)} \left[ d_{a_{1}} \right] \left[ a_{2} \right]^2 + C_{m(17)} \left[ d_{a_{1}} \right] a_{1} a_{2} \\
+ C_{m(18)} \left[ d_{a_{1}} \right] \left[ a_{1} \right]^2 a_{2} + C_{m(19)} \left[ d_{a_{1}} \right] a_{1} \left[ a_{2} \right]^2 + C_{m(20)} \left[ d_{a_{1}} \right] \left[ a_{1} \right]^3 \quad (4.6) \\
+ C_{m(21)} \left[ d_{a_{1}} \right] \left[ a_{2} \right]^3 + C_{m(22)} \left[ d_{a_{2}} \right] a_{1} + C_{m(23)} \left[ d_{a_{2}} \right] \left[ a_{1} \right]^2 \\
+ C_{m(24)} \left[ d_{a_{2}} \right] a_{2} + C_{m(25)} \left[ d_{a_{2}} \right] \left[ a_{2} \right]^2 + C_{m(26)} \left[ d_{a_{2}} \right] a_{1} a_{2} \\
+ C_{m(27)} \left[ d_{a_{2}} \right] \left[ a_{1} \right]^2 a_{2} + C_{m(28)} \left[ d_{a_{2}} \right] a_{1} \left[ a_{2} \right]^2 \\
+ C_{m(29)} \left[ d_{a_{2}} \right] \left[ a_{1} \right]^3 + C_{m(30)} \left[ d_{a_{2}} \right] \left[ a_{2} \right]^3 \]

There are a total of ninety coefficients to create a closure approximation, it does seem lengthy, but as stated early this work is for investigation purposes so speed is not an important concern. The coefficients for Equation (4.6) appear in Table 4.2.

**Table 4.2 Coefficients \( C_{mn} \) for DAIJXX3 closure.**

<table>
<thead>
<tr>
<th>n</th>
<th>m=1</th>
<th>m=2</th>
<th>m=3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.274771771</td>
<td>-0.509210023</td>
<td>0.345141149</td>
</tr>
<tr>
<td>2</td>
<td>0.541930244</td>
<td>1.286746167</td>
<td>0.787088327</td>
</tr>
<tr>
<td>3</td>
<td>0.876860533</td>
<td>-1.275495165</td>
<td>-2.442763614</td>
</tr>
<tr>
<td>4</td>
<td>2.128729297</td>
<td>3.060553452</td>
<td>1.40765895</td>
</tr>
<tr>
<td>5</td>
<td>-5.061992559</td>
<td>-3.683240071</td>
<td>-4.116298099</td>
</tr>
<tr>
<td>6</td>
<td>-1.548719429</td>
<td>-4.699661791</td>
<td>-5.569125022</td>
</tr>
<tr>
<td>7</td>
<td>-0.210809012</td>
<td>2.345223378</td>
<td>3.996101013</td>
</tr>
<tr>
<td>8</td>
<td>3.124345563</td>
<td>4.104427587</td>
<td>5.023742488</td>
</tr>
<tr>
<td>9</td>
<td>-0.1515064</td>
<td>0.492945222</td>
<td>1.309727508</td>
</tr>
<tr>
<td>10</td>
<td>3.21999836</td>
<td>2.051727881</td>
<td>2.373804199</td>
</tr>
</tbody>
</table>
A fourth order polynomial in $\frac{da_{ij}}{dt}$ was also considered that was created in the manner of Equations (4.5) and (4.6). The coefficients appear in Table 4.3 and the equation is given as

<table>
<thead>
<tr>
<th></th>
<th>1.11039052</th>
<th>0.078687706</th>
<th>3.963818648</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>-1.299014816</td>
<td>0.070126699</td>
<td>-3.242027514</td>
</tr>
<tr>
<td>13</td>
<td>-1.650274932</td>
<td>0.059849914</td>
<td>-10.23002498</td>
</tr>
<tr>
<td>14</td>
<td>1.681328202</td>
<td>0.457206949</td>
<td>9.359271294</td>
</tr>
<tr>
<td>15</td>
<td>-7.587884357</td>
<td>-1.218675286</td>
<td>-18.94110709</td>
</tr>
<tr>
<td>16</td>
<td>15.25309295</td>
<td>3.768736299</td>
<td>26.43825295</td>
</tr>
<tr>
<td>17</td>
<td>7.898692077</td>
<td>-0.081353463</td>
<td>34.55997633</td>
</tr>
<tr>
<td>18</td>
<td>-1.019502244</td>
<td>0.866412631</td>
<td>-16.39361465</td>
</tr>
<tr>
<td>19</td>
<td>-14.46116316</td>
<td>-3.548519507</td>
<td>-26.37442013</td>
</tr>
<tr>
<td>20</td>
<td>-0.916924536</td>
<td>-0.491981988</td>
<td>-3.005741144</td>
</tr>
<tr>
<td>21</td>
<td>-4.939800052</td>
<td>-0.953297446</td>
<td>-9.77171617</td>
</tr>
<tr>
<td>22</td>
<td>-2.003231055</td>
<td>-4.473351314</td>
<td>14.29645404</td>
</tr>
<tr>
<td>23</td>
<td>12.67738067</td>
<td>11.01074973</td>
<td>-17.3696658</td>
</tr>
<tr>
<td>24</td>
<td>12.95301659</td>
<td>4.995565495</td>
<td>9.571729001</td>
</tr>
<tr>
<td>25</td>
<td>-25.26089616</td>
<td>-12.30227794</td>
<td>-9.844768623</td>
</tr>
<tr>
<td>26</td>
<td>-17.55873294</td>
<td>-2.840659899</td>
<td>-30.52776413</td>
</tr>
<tr>
<td>27</td>
<td>0.770680473</td>
<td>-4.052325637</td>
<td>19.47667862</td>
</tr>
<tr>
<td>28</td>
<td>17.80185189</td>
<td>7.190785577</td>
<td>15.19407831</td>
</tr>
<tr>
<td>29</td>
<td>-9.131116831</td>
<td>-6.503249647</td>
<td>6.417603398</td>
</tr>
<tr>
<td>30</td>
<td>17.53585703</td>
<td>9.182890989</td>
<td>4.865593612</td>
</tr>
</tbody>
</table>
\[
\begin{align*}
A_{mm}^{\text{Closure}} &= C_{(m)} + C_{(m)2}a_{(1)} + C_{(m)4}a_{(1)}a_{(2)} + C_{(m)5}a_{(1)}^2 + C_{(m)6}a_{(2)}^2 \\
&+ C_{(m)7}a_{(1)}^2a_{(2)} + C_{(m)8}a_{(1)}a_{(2)}^2 + C_{(m)10}a_{(1)}^3 + C_{(m)11}a_{(1)}a_{(2)}^2 \\
&+ C_{(m)12}a_{(1)}^3a_{(2)} + C_{(m)13}a_{(1)}a_{(2)}^3 + C_{(m)14}a_{(1)}^4 + C_{(m)15}a_{(2)}^4 \\
&+ C_{(m)16}da_{(1)} + C_{(m)17}da_{(2)} + C_{(m)18}a_{(1)}[da_{(1)}] + C_{(m)19}a_{(2)}[da_{(1)}] \\
&+ C_{(m)20}a_{(1)}a_{(2)}[da_{(1)}] + C_{(m)21}a_{(1)}^2[da_{(1)}] + C_{(m)22}a_{(2)}^2[da_{(1)}] \\
&+ C_{(m)23}a_{(1)}^3a_{(2)}[da_{(1)}] + C_{(m)24}a_{(1)}a_{(2)}^2[da_{(1)}] + C_{(m)25}a_{(1)}^4[da_{(1)}] \\
&+ C_{(m)26}a_{(1)}^3[da_{(1)}] + C_{(m)27}a_{(2)}^2a_{(1)}^2[da_{(1)}] + C_{(m)28}a_{(1)}a_{(2)}^3[da_{(1)}] \\
&+ C_{(m)29}a_{(1)}a_{(2)}^3[da_{(1)}] + C_{(m)30}a_{(1)}^4[da_{(1)}] + C_{(m)31}a_{(2)}^4[da_{(1)}] \\
&+ C_{(m)32}a_{(1)}[da_{(2)}] + C_{(m)33}a_{(2)}[da_{(2)}] + C_{(m)34}a_{(1)}a_{(2)}[da_{(2)}] \\
&+ C_{(m)35}a_{(2)}[da_{(2)}] + C_{(m)36}a_{(1)}^2[da_{(2)}] + C_{(m)37}a_{(2)}^2[da_{(2)}] \\
&+ C_{(m)38}a_{(2)}a_{(1)}^2[da_{(2)}] + C_{(m)39}a_{(1)}^3[da_{(2)}] + C_{(m)40}a_{(1)}a_{(2)}^3[da_{(2)}] \\
&+ C_{(m)41}a_{(1)}a_{(2)}^3[da_{(2)}] + C_{(m)42}a_{(1)}^3[da_{(2)}] + C_{(m)43}a_{(1)}a_{(2)}^3[da_{(2)}] + C_{(m)44}a_{(1)}^4[da_{(2)}] + C_{(m)45}a_{(2)}^4[da_{(2)}] \\
&+ C_{(m)46}da_{(2)}[da_{(2)}] + C_{(m)47}da_{(1)}[da_{(2)}] + C_{(m)48}a_{(1)}a_{(2)}[da_{(2)}] \\
&+ C_{(m)49}a_{(1)}^2[da_{(2)}] + C_{(m)50}a_{(1)}a_{(2)}^2[da_{(2)}] + C_{(m)51}a_{(1)}^3[da_{(2)}] \\
&+ C_{(m)52}a_{(1)}a_{(2)}^3[da_{(2)}] + C_{(m)53}a_{(1)}^4[da_{(2)}] + C_{(m)54}a_{(2)}^4[da_{(2)}].
\end{align*}
\] (4.7)

Table 4.3 Coefficients $C_{mn}$ for DAIJXX4 closure.

<table>
<thead>
<tr>
<th>n</th>
<th>m=1</th>
<th>m=2</th>
<th>m=3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.78016967</td>
<td>4.482507191</td>
<td>6.020372893</td>
</tr>
<tr>
<td>2</td>
<td>-18.60768629</td>
<td>-16.24275647</td>
<td>-22.27042844</td>
</tr>
<tr>
<td>3</td>
<td>-29.08535143</td>
<td>-29.12598658</td>
<td>-31.92680563</td>
</tr>
<tr>
<td>4</td>
<td>91.61980157</td>
<td>83.06649595</td>
<td>91.30769124</td>
</tr>
<tr>
<td>5</td>
<td>27.92546481</td>
<td>21.3313079</td>
<td>34.96425589</td>
</tr>
<tr>
<td>6</td>
<td>60.75371441</td>
<td>70.04673937</td>
<td>69.80771367</td>
</tr>
<tr>
<td>7</td>
<td>-90.56389431</td>
<td>-76.79432472</td>
<td>-94.0952894</td>
</tr>
<tr>
<td>8</td>
<td>-138.4856177</td>
<td>-132.9503544</td>
<td>-136.9454991</td>
</tr>
<tr>
<td>9</td>
<td>-17.14216946</td>
<td>-12.03132563</td>
<td>-27.1194933</td>
</tr>
</tbody>
</table>

93
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>-49.64491331</td>
<td>-69.62091502</td>
<td>-67.57799467</td>
</tr>
<tr>
<td>11</td>
<td>73.83778091</td>
<td>63.90802759</td>
<td>69.98016148</td>
</tr>
<tr>
<td>12</td>
<td>28.46804146</td>
<td>23.44385714</td>
<td>34.65077872</td>
</tr>
<tr>
<td>13</td>
<td>61.72118402</td>
<td>66.79908765</td>
<td>67.87712577</td>
</tr>
<tr>
<td>14</td>
<td>4.037934895</td>
<td>2.455456217</td>
<td>8.40575532</td>
</tr>
<tr>
<td>15</td>
<td>13.48093907</td>
<td>25.65998336</td>
<td>23.4732906</td>
</tr>
<tr>
<td>16</td>
<td>-1.46734286</td>
<td>4.26065028</td>
<td>-45.42998415</td>
</tr>
<tr>
<td>17</td>
<td>-2.250180648</td>
<td>-10.22387077</td>
<td>40.88798286</td>
</tr>
<tr>
<td>18</td>
<td>9.111855125</td>
<td>-20.63120247</td>
<td>164.3802578</td>
</tr>
<tr>
<td>19</td>
<td>-10.51003831</td>
<td>-26.09074166</td>
<td>274.0666583</td>
</tr>
<tr>
<td>20</td>
<td>19.58222023</td>
<td>106.9552249</td>
<td>-775.982273</td>
</tr>
<tr>
<td>21</td>
<td>-26.43418193</td>
<td>28.56608249</td>
<td>-223.6401011</td>
</tr>
<tr>
<td>22</td>
<td>74.4480004</td>
<td>56.83150832</td>
<td>-573.5679466</td>
</tr>
<tr>
<td>23</td>
<td>10.56420887</td>
<td>-119.9523343</td>
<td>740.4818283</td>
</tr>
<tr>
<td>24</td>
<td>-143.1764865</td>
<td>-163.3937235</td>
<td>1106.754032</td>
</tr>
<tr>
<td>25</td>
<td>33.41080126</td>
<td>-11.49888687</td>
<td>136.8945115</td>
</tr>
<tr>
<td>26</td>
<td>-116.8760842</td>
<td>-56.45429888</td>
<td>503.9412494</td>
</tr>
<tr>
<td>27</td>
<td>33.63901849</td>
<td>84.66011481</td>
<td>-545.0600689</td>
</tr>
<tr>
<td>28</td>
<td>-17.88018811</td>
<td>40.67557227</td>
<td>-239.3641505</td>
</tr>
<tr>
<td>29</td>
<td>163.8932803</td>
<td>105.3041192</td>
<td>-486.8153679</td>
</tr>
<tr>
<td>30</td>
<td>-14.36650949</td>
<td>-0.61412044</td>
<td>-32.08509103</td>
</tr>
<tr>
<td>31</td>
<td>31.18410181</td>
<td>9.074011335</td>
<td>-160.4196262</td>
</tr>
<tr>
<td>32</td>
<td>1.90914177</td>
<td>46.93696159</td>
<td>-244.0794163</td>
</tr>
<tr>
<td>33</td>
<td>34.7392285</td>
<td>59.07535488</td>
<td>-151.9481046</td>
</tr>
</tbody>
</table>
The last of the polynomial forms to be investigated is one in which the eigenvalues and the eigenvalue derivatives compose 2 second-order polynomials, shown as follows

\[ A_{mn}^{\text{Closure}} = C_{m(1)} + C_{m(2)}a_{(1)} + C_{m(3)}[a_{(1)}]^2 + C_{m(4)}a_{(2)} + C_{m(5)}[a_{(2)}]^2 + C_{m(6)}a_{(1)}a_{(2)} \\
+ C_{m(7)}[da_{(1)}] + C_{m(8)}[da_{(1)}]^2 + C_{m(9)}[da_{(2)}] + C_{m(10)}[da_{(2)}]^2 + C_{m(11)}[da_{(1)}][da_{(2)}] \]  

(4.8)

with coefficients in Table 4.4.
<table>
<thead>
<tr>
<th>n</th>
<th>m=1</th>
<th>m=2</th>
<th>m=3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.111985397</td>
<td>0.122381169</td>
<td>1.235666103</td>
</tr>
<tr>
<td>2</td>
<td>0.297821663</td>
<td>-0.346909076</td>
<td>-2.091018254</td>
</tr>
<tr>
<td>3</td>
<td>0.581224705</td>
<td>0.219222957</td>
<td>0.853610395</td>
</tr>
<tr>
<td>4</td>
<td>-0.561920228</td>
<td>0.035168641</td>
<td>-2.267251152</td>
</tr>
<tr>
<td>5</td>
<td>0.46151302</td>
<td>0.858572614</td>
<td>1.043943562</td>
</tr>
<tr>
<td>6</td>
<td>0.538380844</td>
<td>0.557282594</td>
<td>1.865927247</td>
</tr>
<tr>
<td>7</td>
<td>0.001835719</td>
<td>0.001510103</td>
<td>0.001987622</td>
</tr>
<tr>
<td>8</td>
<td>-0.001242723</td>
<td>-0.000915877</td>
<td>-0.000907292</td>
</tr>
<tr>
<td>9</td>
<td>0.002189737</td>
<td>0.001806014</td>
<td>0.002469553</td>
</tr>
<tr>
<td>10</td>
<td>-0.002418697</td>
<td>-0.000568662</td>
<td>-0.003281907</td>
</tr>
<tr>
<td>11</td>
<td>0.002286616</td>
<td>0.001398278</td>
<td>2.63723E-05</td>
</tr>
</tbody>
</table>

As shown by the table, the coefficients for the terms that are purely for the derivatives do not have as much weight as the terms that are for the eigenvalues alone. It is because of this fit that further investigation of polynomials of this type was not completed. Also it should be noted that when fitting the fourth order components, each component was fit separately so normalization is not guaranteed. This will be further discussed in the results of the DAIJNR closures.
4.3 Methods of Implementation

Since the fiber orientation tensor evolution equation becomes an implicit problem when the closure includes derivatives terms, a calculation procedure must be implemented to account for this. Two such ways are used here: the predictor-corrector (PC) method and also a Newton-Raphson (NR) type method. Each of these methods produce desirable results, in the end the PC method is quicker but not necessarily as accurate overall.

4.3.1 Predictor-Corrector Method

The predictor-corrector method is perhaps one of the easiest ways to see if your derivative closure fit will work. What is meant by the PC method is that we will predict the $da_{ij}$ values using a current closure, in this case the FFLAR4 closure, then correct the PC derivative closures with the FFLAR4 $\frac{da}{dt}$ results. In order to do the PC method the
The evolution equation must be evaluated twice, first with FFLAR4 closure, then with a PC closure. This is a fixed-point iteration method with one iteration. The time-step must be fixed to do this, to ensure the derivative values for the “corrector” part of the closure are correct.

The main program that was written by the author was made to call a closure file, and input into that closure file the $a_{ij}$ matrix. Since now a $\frac{da_{ij}}{dt}$ matrix is needed to input to use the PC method, the author created a file that only input the $a_{ij}$ values and inside that file it called the predictor closure (FFLAR4) and stored the $\frac{da_{ij}}{dt}$ values at the current time step. It also did the corrector step in that file, by calling the corrector PC derivative closure after the initial $\frac{da_{ij}}{dt}$ values were solved for and outputting the new values for $a_{ijkl}$.

There were four different predictor-corrector derivative closures investigated. The first was DAIJPC2, this uses the second-order type polynomial as seen in Equation (4.5). The naming convention here is DAIJ to imply it is a derivative based closure, PC to show the method (NR will be shown later), and 2 to give the polynomial type. DAIJPC3 will use Equation (4.6), and DAIJPC4 will use Table 4.3 as the coefficients for that polynomial. DAIJPC22 is denoted 22 because of the second-order eigenvalue polynomial added to a second-order eigenvalue derivative polynomial, use Equation (4.8)

As in chapter three above all the same error test and results will be shown for these four polynomials. In most of the graphs only the DAIJPCX polynomials will be shown, but in
the tables the FFLAR4 results will be shown as well, FFLAR4 was chosen here because it was, on average, the best closure approximation.

The graphical results for simple shear given in Figure 4.1 are quite interesting. It seems that all fits are acceptable fits. One of the main observation that can be made is that the time it takes for the closure to reach steady state is increased, this is due to the fact the derivative terms scale the polynomial. Another interesting observation is that for the $a_{11}$ component it seems the DAIJPC3 is best, but is seems to be the opposite in the $a_{12}$ component.

![Figure 4.1 Selected PC closures for various components from simple shear.](image-url)
Figure 4.2 shows that in shear/stretch A the $a_{12}$ components all seem to be the same. The $a_{11}$ and $a_{33}$ seem very close in the initial part of the flow then all the $a_{ij}$ components for the closures slowly spread away from each other. The mixed flow results are also desirable, except for the third phase of the $a_{11}$ (Figure 4.3), $a_{22}$ (Figure 4.5), and $a_{23}$ (Figure 4.6) components. Some of the closures as shown below seem to deviate from the curve more than the others. Figure 4.4 shows accurate results throughout the flow for the $a_{12}$ component.
Figure 4.3 Selected PC closures for given mixed flow components.

Figure 4.4 Selected PC closures for given mixed flow component.
Figure 4.5 Selected PC closures for given mixed flow components.

Figure 4.6 Selected PC closures for given mixed flow components.
Table 4.5 below summarizes all the calculated error per flow as well as giving an average error. Here the error calculation is the same as stated in Chapter 3.

Table 4.5 Error of DAIJPC closures for various flows.

<table>
<thead>
<tr>
<th>Flow</th>
<th>FFLAR4</th>
<th>DAIJPC2</th>
<th>DAIJPC3</th>
<th>DAIJPC4</th>
<th>DAIJPC22</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed</td>
<td>0.0222</td>
<td>0.0253</td>
<td>0.0294</td>
<td>0.0315</td>
<td>0.0238</td>
</tr>
<tr>
<td>Simple Shear</td>
<td>0.0264</td>
<td>0.0263</td>
<td>0.0265</td>
<td>0.0283</td>
<td>0.0302</td>
</tr>
<tr>
<td>Biaxial Elongation</td>
<td>0.0028</td>
<td>0.0064</td>
<td>0.0009</td>
<td>0.0006</td>
<td>0.0008</td>
</tr>
<tr>
<td>Uniaxial Elongation</td>
<td>0.0114</td>
<td>0.0442</td>
<td>0.0204</td>
<td>0.0177</td>
<td>0.0044</td>
</tr>
<tr>
<td>Shear/Stretch A</td>
<td>0.0152</td>
<td>0.0256</td>
<td>0.0182</td>
<td>0.0145</td>
<td>0.0184</td>
</tr>
<tr>
<td>Shear/Stretch B</td>
<td>0.0189</td>
<td>0.0171</td>
<td>0.0172</td>
<td>0.0167</td>
<td>0.0154</td>
</tr>
<tr>
<td>Ave All Flows</td>
<td>0.0161</td>
<td>0.0242</td>
<td>0.0188</td>
<td>0.0182</td>
<td>0.0155</td>
</tr>
</tbody>
</table>

It seems that only one closure was more accurate than the FFLAR4 closure. This is due to the fact that in the 2 elongation flows, the DAIJPC22 closure was superior to all other closures. It behaved well for all other results, but it was not necessarily the best. DAIJPC2 was the only closure that performed worse than ORT, which is not shown in the above table but results for ORT can be seen in Table 3.6 and 3.7.

As with all new closure approximations the center-gated disk problem was also tested. Just as in Chapter 3, nine different flows with $z$-values varying from 0.1 – 0.9 were tested. The results are quite accurate as well. Figure 4.7 is for a $z$ value of 0.3, and Figure 4.8 is for a $z$ value of 0.7.
Figure 4. 7 Selected components for various PC closures of center-gated disk, z=0.3.

Figure 4. 8 Selected components for various PC closures of center-gated disk, z=0.7.

104
Table 4. 6 Error of DAIJPC closures for varying z-values.

<table>
<thead>
<tr>
<th>Z-Value</th>
<th>FFLAR4</th>
<th>DAIJPC2</th>
<th>DAIJPC3</th>
<th>DAIJPC4</th>
<th>DAIJPC22</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.0029</td>
<td>0.0037</td>
<td>0.0042</td>
<td>0.0062</td>
<td>0.0042</td>
</tr>
<tr>
<td>0.2</td>
<td>0.0096</td>
<td>0.0085</td>
<td>0.0064</td>
<td>0.0076</td>
<td>0.0123</td>
</tr>
<tr>
<td>0.3</td>
<td>0.0058</td>
<td>0.0068</td>
<td>0.0050</td>
<td>0.0073</td>
<td>0.0083</td>
</tr>
<tr>
<td>0.4</td>
<td>0.0072</td>
<td>0.0146</td>
<td>0.0079</td>
<td>0.0079</td>
<td>0.0097</td>
</tr>
<tr>
<td>0.5</td>
<td>0.0132</td>
<td>0.0230</td>
<td>0.0154</td>
<td>0.0109</td>
<td>0.0175</td>
</tr>
<tr>
<td>0.6</td>
<td>0.0180</td>
<td>0.0271</td>
<td>0.0213</td>
<td>0.0163</td>
<td>0.0244</td>
</tr>
<tr>
<td>0.7</td>
<td>0.0221</td>
<td>0.0281</td>
<td>0.0244</td>
<td>0.0221</td>
<td>0.0287</td>
</tr>
<tr>
<td>0.8</td>
<td>0.0247</td>
<td>0.0275</td>
<td>0.0247</td>
<td>0.0262</td>
<td>0.0318</td>
</tr>
<tr>
<td>0.9</td>
<td>0.0266</td>
<td>0.0262</td>
<td>0.0234</td>
<td>0.0286</td>
<td>0.0336</td>
</tr>
<tr>
<td>AVE</td>
<td>0.0145</td>
<td>0.0184</td>
<td>0.0147</td>
<td>0.0148</td>
<td>0.0189</td>
</tr>
</tbody>
</table>

None of the DAIJPCX closures in Table 4.6 are more accurate than the FFLAR4 closures in this case. It is interesting to see that what was the best closure, DAIJPC22, on average for the homogenous and mixed flows, is now the worst closure for the nonhomogenous center-gated disk. In this case, all closure approximations were better than the ORT closure in Table 3.8.
4.3.2 Newton-Raphson Method

The Newton-Raphson method is used in this work to solve the implicit function for \( \frac{da_{ij}}{dt} \).

Since the Jacobian is difficult and changes with closure form, we evaluate it with a forward finite difference approximation method. To this end, Equation (2.22) is rearranged to obtain

\[
F_y = \frac{Da_{ij}}{Dt} \left[ -\frac{1}{2} (\omega_k a_{kj} - a_{ik} \omega_k) + \frac{1}{2} \lambda (\dot{\gamma}_a a_{kj} + a_{ik} \dot{\gamma}_k - 2 \dot{\gamma}_k a_{ij} + 2 C \dot{\gamma}_i (\delta_{ij} - 3 a_{ij}) \right] \tag{4.9}
\]

Where we note that the derivative based closure approximations are now function of \( \frac{da_{ij}}{dt} \). Following the convention of Cintra and Tucker[12] in Table 2.2 it is assigned that

\[
\begin{bmatrix} F_{11} \\ F_{22} \\ F_{33} \\ F_{23} \\ F_{13} \\ F_{12} \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \\ F_6 \end{bmatrix} \tag{4.10}
\]
where each function $F_i$ is used to calculate the Jacobian. It should be noted that if the
relation as given in Equation (4.4) were used only five $F_i$ components are needed. Using
a similar relation as Equation (4.10) the $\frac{da_{ij}}{dt}$ components are written

$$
\begin{bmatrix}
\frac{da_{11}}{dt} \\
\frac{da_{22}}{dt} \\
\frac{da_{33}}{dt} \\
\frac{da_{12}}{dt} \\
\frac{da_{13}}{dt} \\
\frac{da_{12}}{dt}
\end{bmatrix}
= 
\begin{bmatrix}
\frac{da_1}{dt} \\
\frac{da_2}{dt} \\
\frac{da_4}{dt} \\
\frac{da_4}{dt} \\
\frac{da_5}{dt} \\
\frac{da_6}{dt}
\end{bmatrix}
$$

(4.11)

The Jacobian used is defined as

$$
J_{ij} = \frac{\partial F_j}{\partial da_i} = 
\begin{bmatrix}
\frac{\partial F_1}{\partial da_1} & \frac{\partial F_1}{\partial da_2} & \frac{\partial F_1}{\partial da_3} & \frac{\partial F_1}{\partial da_4} & \frac{\partial F_1}{\partial da_5} & \frac{\partial F_1}{\partial da_6} \\
\frac{\partial F_2}{\partial da_1} & \frac{\partial F_2}{\partial da_2} & \frac{\partial F_2}{\partial da_3} & \frac{\partial F_2}{\partial da_4} & \frac{\partial F_2}{\partial da_5} & \frac{\partial F_2}{\partial da_6} \\
\frac{\partial F_3}{\partial da_1} & \frac{\partial F_3}{\partial da_2} & \frac{\partial F_3}{\partial da_3} & \frac{\partial F_3}{\partial da_4} & \frac{\partial F_3}{\partial da_5} & \frac{\partial F_3}{\partial da_6} \\
\frac{\partial F_4}{\partial da_1} & \frac{\partial F_4}{\partial da_2} & \frac{\partial F_4}{\partial da_3} & \frac{\partial F_4}{\partial da_4} & \frac{\partial F_4}{\partial da_5} & \frac{\partial F_4}{\partial da_6} \\
\frac{\partial F_5}{\partial da_1} & \frac{\partial F_5}{\partial da_2} & \frac{\partial F_5}{\partial da_3} & \frac{\partial F_5}{\partial da_4} & \frac{\partial F_5}{\partial da_5} & \frac{\partial F_5}{\partial da_6} \\
\frac{\partial F_6}{\partial da_1} & \frac{\partial F_6}{\partial da_2} & \frac{\partial F_6}{\partial da_3} & \frac{\partial F_6}{\partial da_4} & \frac{\partial F_6}{\partial da_5} & \frac{\partial F_6}{\partial da_6}
\end{bmatrix}
$$

(4.12)
where the Jacobian was calculated with a forward finite difference

\[
J_{ij} = \frac{\partial F_i}{\partial da_j} = \frac{F_i(da_j + \Delta da_j) - F_i(da_j)}{\Delta da_j}
\]

(4.13)

with a perturbation of 1e-10. The simplest form of the update equation of \( F_i \) would be given as

\[
F_i^{\text{new}} = F_i^{\text{old}} + \Delta F_i^{\text{old}}
\]

(4.14)

where the \( \Delta F_i^{\text{old}} = -J^{-1}_{ij}F_i^{\text{old}} \).

All results for the DAIJNRX closure approximations are analogous to the DAIJPCX closure approximation, except the NR class is more accurate. When the flows that were tested were all evolved, all converged to within 1e-6 of zero with a maximum two iterations per time step, most only required one iteration. The initial guess for the first time step that was used 0 for all \( \frac{da_{ij}}{dt} \). The following time steps initial guesses were the converged \( \frac{da_{ij}}{dt} \) from the previous time step. In all the flows that were tested, this was acceptable initial guess criteria. For the five Cintra and Tucker flows and the mixed flow the results are as follows:
Figure 4.9 Selected NR closures for various components from simple shear.

Figure 4.10 Selected NR closures for various components from shear/stretch a.
The simple shear flow in Figure 4.9 still overshoots at the transient of the $a_{11}$ component of the flow, but the steady state is greatly improved. The polynomial order has a great effect on the accuracy as shown in Figures 4.9 and 4.10. For shear/stretch A (Figure 4.10) the graphical results appear to be the same as the DAIJPCX approximations in Figure 4.2.

![Graph showing mixed flow component](image)

**Figure 4.11 Selected NR closures for given mixed flow component.**
Figure 4. 12 Selected NR closures for given mixed flow component.

Figure 4. 13 Selected NR closures for given mixed flow component.
The mixed flow results in Figure 4.11 through 4.14 are more accurate than the DAIJPCX results as well. This is extremely noticeable in the third phase of the flow, the DAIJNRX closure approximations follow the final part of the flow more closely. The NR method solved the problem of the deviation that occurred in this part of the flow when using the PC method. The quantitative results are in Table 4.7 as follows.
Table 4.7 Error of DAIJNR closures for various flows.

<table>
<thead>
<tr>
<th>Flow</th>
<th>ORT</th>
<th>DAIJNR2</th>
<th>DAIJNR3</th>
<th>DAIJNR4</th>
<th>DAIJNR22</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed</td>
<td>0.0222</td>
<td>0.0234</td>
<td>0.0227</td>
<td>0.0220</td>
<td>0.0236</td>
</tr>
<tr>
<td>Simple Shear</td>
<td>0.0264</td>
<td>0.0259</td>
<td>0.0241</td>
<td>0.0262</td>
<td>0.0301</td>
</tr>
<tr>
<td>Biaxial Elongation</td>
<td>0.0028</td>
<td>0.0064</td>
<td>0.0007</td>
<td>0.0004</td>
<td>0.0008</td>
</tr>
<tr>
<td>Uniaxial Elongation</td>
<td>0.0114</td>
<td>0.0032</td>
<td>0.0061</td>
<td>0.0054</td>
<td>0.0044</td>
</tr>
<tr>
<td>Shear/Stretch A</td>
<td>0.0152</td>
<td>0.0254</td>
<td>0.0175</td>
<td>0.0144</td>
<td>0.0185</td>
</tr>
<tr>
<td>Shear/Stretch B</td>
<td>0.0189</td>
<td>0.0159</td>
<td>0.0125</td>
<td>0.0147</td>
<td>0.0154</td>
</tr>
<tr>
<td>Ave All Flows</td>
<td>0.0161</td>
<td>0.0167</td>
<td>0.0139</td>
<td>0.0138</td>
<td>0.0154</td>
</tr>
</tbody>
</table>

Again all flows are more accurate than the ORT closure. Using the NR method all closures except DAIJNR2 are more accurate than the FFLAR4 closure. DAIJNR3 and DAIJNR4 are almost twice as accurate as ORT. These closures just like the PC method closures are again very accurate in the elongational flows.

The results for the center-gated disk flows were quite satisfying as well. However, there were some unexpected findings.
Figure 4. 15 Selected components for various NR closures of the center-gated disk, $z=0.3$.

Figure 4. 16 Selected components for various NR closures of the center-gated disk, $z=0.7$. 
Table 4.8 Error of DAIJNR closures for varying z-values.

<table>
<thead>
<tr>
<th>Z-Value</th>
<th>FFLAR4</th>
<th>DAIJNR2</th>
<th>DAIJNR3</th>
<th>DAIJNR4</th>
<th>DAIJNR22</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.0029</td>
<td>0.0054</td>
<td>0.0060</td>
<td>0.0064</td>
<td>0.0044</td>
</tr>
<tr>
<td>0.2</td>
<td>0.0096</td>
<td>0.0062</td>
<td>0.0058</td>
<td>0.0078</td>
<td>0.0121</td>
</tr>
<tr>
<td>0.3</td>
<td>0.0058</td>
<td>0.0058</td>
<td>0.0047</td>
<td>0.0077</td>
<td>0.0081</td>
</tr>
<tr>
<td>0.4</td>
<td>0.0072</td>
<td>0.0154</td>
<td>0.0080</td>
<td>0.0076</td>
<td>0.0096</td>
</tr>
<tr>
<td>0.5</td>
<td>0.0132</td>
<td>0.0235</td>
<td>0.0154</td>
<td>0.0106</td>
<td>0.0176</td>
</tr>
<tr>
<td>0.6</td>
<td>0.0180</td>
<td>0.0273</td>
<td>0.0214</td>
<td>0.0157</td>
<td>0.0245</td>
</tr>
<tr>
<td>0.7</td>
<td>0.0221</td>
<td>0.0283</td>
<td>0.0245</td>
<td>0.0221</td>
<td>0.0287</td>
</tr>
<tr>
<td>0.8</td>
<td>0.0247</td>
<td>0.0276</td>
<td>0.0247</td>
<td>0.0262</td>
<td>0.0318</td>
</tr>
<tr>
<td>0.9</td>
<td>0.0266</td>
<td>0.0262</td>
<td>0.0233</td>
<td>0.0285</td>
<td>0.0335</td>
</tr>
<tr>
<td>AVE</td>
<td>0.0145</td>
<td>0.0184</td>
<td>0.0149</td>
<td>0.0147</td>
<td>0.0189</td>
</tr>
</tbody>
</table>

Figure 4.15 is for a z value of 0.3, and Figure 4.16 is for a z value of 0.7. Table 4.8 shows the error calculations for the center-gated disk. One of the unexpected findings is that the DAIJNRX closures are only very slightly more accurate than the corresponding DAIJPCX closure. Another unexpected finding is that the DAIJNR2 closure was actually less accurate than the DAIJPC2 closure, which seems extremely counterintuitive.

As discussed previously in this section the way that the least squares regression was performed does not necessarily guarantee the normalization condition as given in Equations (2.19) and (2.21). Each fourth-order tensor component was fit separately. Cintra and Tucker claim that “functions fit in this way will not necessarily satisfy normalization conditions[12].” Other closures have been produced that do not satisfy all
requirements of closures given in Equations (2.18)-(2.21). The quadratic closure does not satisfy the symmetry conditions[2], and by extension the hybrid closure would not either. “Note that a closure approximation does not need to satisfy the symmetry and normalization requirement[12].” Advani and Tucker[27] showed that only the symmetry of the elasticity tensor and a weaker normalization condition were required. Jack et al.[17] created a neural network based closure that was not objective. As shown above, there are closures in literature that do not maintain all stated requirements that are accepted and even widely used.

In all flows tested the normalization condition is maintained with numerical error. This was done by testing the normalization condition of Equation (2.19) by setting the right hand side of the equation to zero, that is

\[ e_{ij}^n = a_{ij} - a_{ipp} \]  \hspace{1cm} (4.15)

was tested. Each individual tensor component of \( e_{ij}^n \) was tested and it was found that no individual tensor component was greater than \( 1^{-15} \) and likewise for the magnitude. While normalization was not imposed, for flows test it was maintained. Error on the \( 1^{-15} \) scale could simply be due to the numerical method being used to solve the Equation (2.22). The magnitude of \( e_{ij}^n \) was also calculated and is given as

\[ e^n = \sqrt{\frac{1}{2} e_{ij}^n e_{ji}^n} \]  \hspace{1cm} (4.16)
similar to Section 3.3.3 the average error over the entire flow was also calculated as

\[ \text{Average Normalization Error} = \frac{1}{t_{\text{end}}} \int_{0}^{t_{\text{end}}} e^n(t) dt \]  \hspace{1cm} (4.17)

The table below summarizes the results of the findings, the ORT closure of Verweyst[29] is also shown as a comparison to a well known closure.

Table 4.9 Normalization condition error results for various closures on selected flows.

<table>
<thead>
<tr>
<th>Flow</th>
<th>ORT</th>
<th>DAIJR2</th>
<th>DAIJR3</th>
<th>DAIJR4</th>
<th>DAIJR22</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed</td>
<td>8.14E-16</td>
<td>5.47E-16</td>
<td>7.51E-16</td>
<td>6.16E-16</td>
<td>9.17E-16</td>
</tr>
<tr>
<td>Simple Shear</td>
<td>2.44E-16</td>
<td>1.39E-16</td>
<td>2.55E-16</td>
<td>4.73E-16</td>
<td>2.86E-16</td>
</tr>
<tr>
<td>Biaxial Elongation</td>
<td>9.29E-16</td>
<td>1.49E-16</td>
<td>5.06E-16</td>
<td>3.52E-16</td>
<td>7.57E-16</td>
</tr>
<tr>
<td>Uniaxial Elongation</td>
<td>3.50E-16</td>
<td>2.58E-16</td>
<td>6.99E-16</td>
<td>8.31E-16</td>
<td>7.54E-16</td>
</tr>
<tr>
<td>Shear/Stretch A</td>
<td>1.97E-16</td>
<td>8.41E-16</td>
<td>8.91E-16</td>
<td>5.85E-16</td>
<td>3.80E-16</td>
</tr>
<tr>
<td>Shear/Stretch B</td>
<td>2.51E-16</td>
<td>2.54E-16</td>
<td>9.59E-16</td>
<td>5.50E-16</td>
<td>5.68E-16</td>
</tr>
<tr>
<td>Ave All Flows</td>
<td>4.64E-16</td>
<td>3.65E-16</td>
<td>6.77E-16</td>
<td>5.68E-16</td>
<td>6.10E-16</td>
</tr>
</tbody>
</table>

The results show that the error is negligible. The DAIJR2 closure is more accurate than the ORT closure in normalization error. The DAIJR3, DAIJR4, and DAIJR22 closures are accurate enough that the normalization criteria are fulfilled.
4.4 Summary of Derivative Closures

As shown above a new class of closures is introduced. The time based derivative closure approximation creates a closure that is not only a function of $a_y$, but also of $\frac{da_y}{dt}$. The investigation done in this work should be considered as a starting point to begin research into this type of closure. There has been no attempt to optimize computational time, or to work on any other types of fitting procedures that could potentially create better results. The PC method is a great way to quickly test a fit that was made. One drawback of this method is that it seems that one may be compounding error with error. That is the predictor closure that is used will already have some error, therefore the corrector error might be larger. This seemed to be the case with homogenous flows such as simple shear and shear/stretch A. It was also the case for the mixed flow as well. The center-gated disk was different though, barely having any difference from the results based on the NR method and in the comparison of DAIJNR2 and DAIJPC2 the PC closure was more accurate. This could be due to the fact the predictor closure, FFLAR4, is already extremely accurate for the center gated disk. All calculations were performed with a value of $G=1$. Other values of $G$ were not investigated, however if there were any problems with a normalization to $G$, dividing all derivative terms by $G$ would resolve the issue. One thing that is lacking with the use of DAIJ closures is computational
efficiency, since for either type (NR or PC) there must be at least two iterations per time step. There is no feasible way to make them faster than current fourth-order closure approximations, thus making them more accurate should be the first basis for later work and time optimization should come later.
Chapter 5. Conclusions

Short-fiber reinforced polymer composites will continue to be used throughout industry. One of the main reasons for this is due to their high strength to weight ratios. Even though large amounts of research have been put into this project by numerous authors, the problem is still not fully understood but work continues to improve the accuracy of calculations and knowledge of the researchers involved. The distribution of the short-fibers is used to approximate the material properties. However, the calculation of this distribution is still very difficult because of the complexity and time involved in computing the fiber orientation distribution.

There are a few methods that have been proposed to compute the orientation of the fibers. One of the first methods was to use the evolution of the probability distribution function of the fiber, but this is very computationally expensive. Another method is the evolution of the orientation tensor; this method greatly reduces computational time and is very accurate. The last method, which is very recent is using spherical harmonics to compute the evolution. This method is also fast computationally and gives accurate answers as well, however the orientation tensor method is still faster.

As seen throughout this work, the use of the orientation tensor was investigated. The problem with using the orientation tensor approach is that the evolution of the
second-order orientation requires knowledge of the fourth order orientation tensor, which is why the closure approximation has been introduced. The analytical closures such as the linear, quadratic, hybrid and all the Hinch and Leal closures have been used previously with acceptable results depending on the flows that were being used. The fitted closures of Cintra and Tucker, Chung and Kwon, and Verweyst have greatly increased the accuracy of how the closure is measured, and the ORT closure is among the most commonly used closures to date.

Two new methods of fitting closures have been investigated in this work. The first is revisiting the Cintra and Tucker EBOF procedure and taking each component involved with the fitting procedure and assessing the use of other methods in an attempt to produce better results. The second was to add derivative terms to the polynomial that was to be regressed, this made the problem implicit and a root finding method was used to obtain final answers.

The first method was done in a number of different ways. In Cintra and Tucker they outlined three main steps to create an EBOF closure. The first was to select your data set for fitting. Elliptic integrals and spherical harmonics were used in this work; DFC calculations have been used in the past. Cintra and Tucker proposed using a wide variety of flow fields with varying $C_I$. While desirable results have been produced with varying $C_I$, a closure for each individual $C_I$ could produce better results. The next step is to rotate the data into the principle frame of the second-order orientation tensor. This is only required for spherical harmonics and DFC calculations, elliptic integrals generate
data that is already in the principle frame. The final step was to use a fitting procedure to obtain an approximation and then optimize the coefficients of the fits produced. For the fitting procedure the LAR, BIS and least squares fitting methods were used. The LAR seemed to produce the most desirable results. The coefficient optimization that was used was either Levenberg-Marquardt or trust region methods. The polynomials used were of varying order complete polynomials as well as rational polynomials. Not all possible permutations of the variations have been made to produce the widest range in EBOF closure procedures; however the results given do show variety and promise to this type of work.

The second method uses a derivative term in the regression polynomials. It becomes an implicit problem with this calculation, but gives better results than the ORT closure. A predictor-corrector method and a Newton-Raphson method were used to address the problem. The only closure approximation that was consistently more accurate than these types of closures was the FFLAR4 closure, which was also developed in this work. The only short coming with this type of closure is that the computational time required will always be more than a closure that does not have a derivative term. More work should be done in this area not only in optimization of accuracy, but also computational time.

Fourth order closures have been investigated throughout this work. Literature seems to be lacking on new works of fourth-order closures, thus it can be inferred that there is not much more that can be done to produce better results. Two new methods
were used to produce new closure approximations with very desirable results. Each method was shown to be more accurate than the ORT closure. This work shows further investigation into this type of work is needed and that perhaps even more accurate closures can be found.
REFERENCES


