ON THE RHEOLOGY OF CONCENTRATED FIBER SUSPENSIONS

by

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B.E., Cooper Union, 1976
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Submitted to the Department of Chemical Engineering on April 27, 1981 in partial fulfillment of the requirements for the Degree of Doctor of Science

ABSTRACT

A rheological equation of state, interrelating the structural arrangement of the particles to the macroscopic properties, has been developed for a semi-concentrated suspension of fibers in a Newtonian liquid. The analysis is focused on a test fiber with the surrounding particles and the solvent represented by an effective medium. The drag force on the test particle is then approximated by a Stokes-Burgers model. The effective drag coefficient is estimated by equating the work required to move the test fiber in the effective continuum to the work needed to vacate the site occupied by the nearest neighbor in the structural model. Due to the uncertain initial location of the test fiber, a distribution function is utilized to track the trajectories of the collection of particles. For a rigid fiber in a homogeneous flow, the motion of the center of mass translates affinely with the bulk deformation, whereas the orientation of the fiber rotates affinely but without stretching. The calculations, based on this model, in a simple steady shear flow and in uniaxial and biaxial deformations demonstrate that the rheological properties depend strongly on the history of the flow. The strain is found to be a macroscopic representation of the changes in internal fiber orientation. The viscosity is initially very large due to the randomly dispersed fibers, but decreases as the particles are aligned toward the shearing planes. Transient normal stresses are exhibited as a result of the anisotropic distribution of the fibers. Experiments in shear flow confirm that the "zero-shear" viscosity is much greater than the "high-strain" or steady-state viscosity. In comparing the "zero-shear" viscosity data with the predicted values, the influence of the walls of the viscometer is modeled by subtracting the fraction of fibers that would poke through the rigid surfaces. In extensional flows, the model predicts that the steady-state Trouton viscosity is greater than the zero-strain elongational viscosity because the tension along a rigid fiber attains a maximum when the particle is oriented in the direction of the extension. In closing the governing equations for a suspension of deformable but inextensible fibers in a general flow field have been formulated. The solution to this problem is subject to future investigations.

Thesis Supervisor: Dr. Robert C. Armstrong

Title: Associate Professor of Chemical Engineering
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Finally, I have to thank Yuk-Ching who listened to my endless complaints, held my spirits high and helped me put together this thesis with her love and patience.
TO

MY PARENTS,

PHIL,

AND YUK-CHING.
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CHAPTER I
INTRODUCTION

Fiber reinforced composites is a versatile and attractive engineering material. In the automotive industry, for instance, fiber-filled polymer composites are being contemplated as substitutes for metals in the manufacturing of light weight end products without sacrificing much of the strength requirements. The ability to employ this family of reinforced materials relies on the proper control of the fiber alignment. The first step toward this undertaking is to determine the configuration of the particles as would be governed by the bulk deformation that occurred in the process. Based on this information the next task is to devise methods that would readjust particles into the desirable configuration.

This thesis is concerned with the first part of the problem, namely to predict the orientation of the particles and the suspension rheological properties in terms of the microstructure of the composite.

In this chapter we survey the industrial applications of fiber composites, identify the unusual behavior of this material, then formulate the objective of this work.

A. APPLICATION AND PROCESSING OF FIBER COMPOSITES

Short-fiber polymer composites are becoming an increas-
ingly important class of materials because of their potential in weight reduction and process flexibility. In light of the current striving to conserve fuel, this class of reinforced plastics is a particularly attractive material to the automotive industry. The two most widely used molding compounds for automotive applications are the glass fiber reinforced phenolics and polyesters. Both of these systems are thermostets.

The phenolic composites offer thermal stability. Accordingly they are utilized to make engine parts, exhaust systems, brake pistons, etc. Although the polyester systems are restricted to lower operating temperatures, they offer faster cure time and a relatively lower cost. Consequently they are used to fabricate car exteriors such as body panels and front-ends (Naitove, 1978).

The basic composition of the molding compounds includes a resin, fillers, glass fibers, a lubricant, a catalyst and other additives that are tailored to specific needs. A typical recipe of a glass fiber-polyester composite used to manufacture automotive exteriors is listed in Table (I-A-1). The role and properties of each ingredient are briefly described. The resin in the polyester composite contains a low molecular weight unsaturated polyester (\(M_w\) is approximately 1000) that has a relatively low viscosity ranging between 1 Pa.s to 3 Pa.s at room temperature (Burns, 1978). However in the heated mold the resin polymerizes by means of a free radical mechanism in the presence of a peroxide
<table>
<thead>
<tr>
<th>Ingredients</th>
<th>Composition (% by weight)</th>
</tr>
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<tbody>
<tr>
<td>Unsaturated polyester resin</td>
<td>34</td>
</tr>
<tr>
<td>Filler (CaCO₃)</td>
<td>37</td>
</tr>
<tr>
<td>Glass fiber</td>
<td>27</td>
</tr>
<tr>
<td>Catalyst</td>
<td>1</td>
</tr>
<tr>
<td>Lubricant</td>
<td>1</td>
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</tbody>
</table>

*Handbook of Reinforced Plastics (1964)
catalyst.

The filler is an inert material such as calcium carbonate. Its role is to increase the viscosity of the carrying fluid so as to lessen the degree of fiber segregation during the process. From an economic standpoint, it would also lower the cost of the molding compound.

The function of the glass fibers is to impart strength and rigidity to the molded product. They come in the form of a bundle of approximately 250 filaments held together by a sizing. Their lengths range from 0.3 cm to 2.5 cm. Shorter fiber composites are commonly processed by injection molding whereas the longer fibers are handled by compression molding.

Lubricants, in the form of a metal stearate or an organic phosphate, are included in small quantities to facilitate the removal of the molded part from the mold cavity.

The ingredients, described above, are mixed at room temperature, and at a very slow speed to minimize the amount of fiber degradation. The mixture is then processed by either compression molding or injection molding. The choice between these two competing processes would depend upon a trade-off between the kind of strength requirement in the molded product versus the production time (Bauer, 1976). In general, compression molded parts have higher impact strength whereas injection molded parts possess higher flexural strength because a significant portion of the glass fibers would be aligned by the flow field (Parker, 1977).

In compression molding the pre-metered material is hand-
placed directly in the mold cavity, and as the mold closes
the entire cavity is filled. The temperature in the mold is
then raised to the curing temperature. The chief advantage
in compression molding is the high strength obtained in the
product because an external load would be isotropically
dispersed among the more randomly oriented fibers. As a
consequence of the short transport distances in the mold
cavity, the likelihood of fiber-resin segregation is reduced,
and the probabilities of fiber breakage and fiber alignment
are minimized. However a number of drawbacks are often
encountered in compression molding. First, these tacky
materials have to be pre-measured, pre-weighed and cut into
the shape of the mold cavity before they are manually loaded
into the mold. Second, compression molding requires extended
cure times to allow adequate heat transfer from the mold to
the molding compound. Third, the excessive amount of flash
produced during molding is difficult to be trimmed off because
the material is reinforced with glass fibers. Therefore, the
processing cycle is long, the labor cost is increased, and
the flash, being a thermoset, cannot be reclaimed.

In the case of the injection molding process, a pre-
determined quantity of the molding compound is directly loaded
into the injection barrel from the mixing tank, thus elimin-
ating the need to handle the tacky material manually. Then
a plunger pushes the slurry forward through the nozzle, the
sprue bushing, past the gate, down the runner and into the
pre-heated mold cavity (Carmen, 1977). The fill time is on
the order of a few seconds whereas the cure time would be between 1 min. to 3 min. Since the ratio between the fill time to the cure time is small, curing of the molding compound in the flow stage is minimized. Consequently this highly complex problem can be decoupled into analyzing the fluid mechanics of the composite independently from the kinetics of this reinforced thermoset. After curing the mold is opened and the part is removed. Then the mold is closed, and while it is preheated for the next cycle, fresh material is introduced into the barrel as the plunger retracts. Therefore, injection molding is a highly automated process and offers the advantage of a shorter cycle time. The major drawback in this process is that the material would have to be transported over long and tortuous distances which would enhance the likelihood of fiber breakage and fiber segregation. Consequently shorter fibers are used instead. Furthermore a substantial degree of fiber alignment has been found to occur. As a result the mechanical properties of the end product are anisotropic.

Nevertheless injection molding has been a very attractive process, and its usefulness would gain greater appeal if the orientation of the fibers can be controlled. A number of methods may be contemplated to achieve this goal. Among these possibilities, the geometry of the mold cavity can be altered, thereby creating a flow field that would align the fibers into the desired configurations. Alternatively the local particle orientation may be changed by means of extern-
ally applied forces and moments.

Therefore a systematic approach to investigate this problem would begin by evaluating the effect of the flow field on the orientation of the suspended fibers. With this information, the desirability of the local particle orientation can be assessed from the nature of the local strength requirement. Thereafter the internal structure of the reinforcing particles may be adjusted locally through external means to conform with the mechanical properties of a conventional metallic part. The thrust of this investigation is aimed toward understanding the flow behavior of fiber suspensions. The next section provides a few preliminary observations into the unusual character of particles suspended in a viscous medium.
B. TRANSIENT RHEOLOGICAL BEHAVIOR

The material considered in this investigation consists of a mixture of fibers suspended in a viscous Newtonian liquid. The rheological properties of these fibrous dispersions have been reported to display transient behaviors (Mewis, 1979). Such changes are related to a rearrangement of the particles under a bulk deformation. However there are two types of transients that would need to be distinguished, a reversible phenomenon and an irreversible case.

The reversible phenomenon is termed thixotropic when the apparent viscosity decreases with time under shear, and the initial viscosity can be recovered subsequently as the flow is stopped. The opposite effect of the viscosity in increasing with time is known as rheoplexy. This reversible behavior is due to the re-establishment of weak inter-particle forces after the flow is discontinued. However the rheology of this class of suspensions, which contains sub-micron-sized fibers, will not be pursued in this thesis.

The fibers considered in this work are macroscopically visible, and typically range between 0.3 cm to 2.5 cm in length. Suspensions involving this class of fibers also display transient characteristics. However these time dependent effects are irreversible on the time scale of several years.

A qualitative set of shear experiments, shown in Figures (I-B-1) to (I-B-3), suggests that the suspension shear
viscosity is influenced by the structural distribution of the reinforcing particles. In each graph the relative viscosity is plotted versus the shear rate. The data in these figures are collected in a set of parallel plate viscometer at room temperature. The numerical values of these data are listed in Appendix 1.

The material, used in these experiments, is a suspension of 1.27 cm glass fibers dispersed in honey which is a Newtonian fluid. The concentration of fibers, shown in Figures (I-B-1) to (I-B-3) are respectively 15%, 10% and 5% by weight. Each of these graphs show two types of experiments. The darkened symbols represent data that were taken by placing the mixture between the plates of the viscometer. In this case the fibers are randomly oriented. The clear symbols represent data that were obtained by placing a monolayer of fibers between the plates. The results from each test showed that the suspension viscosity for the randomly dispersed fibers were greater than the results from which the fibers were placed near the plane of shear. These observations are intuitively expected because fibers that are not aligned in the shearing plane would form a three dimensional structure which would offer greater resistance to a shear deformation.

These results point out several unique properties of fiber suspensions. The suspension viscosity, measured at the same shear rate, can be significantly different when the internal structure of the particles has been rearranged.
Figure I-B-1  Plot of the relative viscosity versus the shear rate for a suspension containing 15% by weight of 1.27 cm glass fibers in honey
Figure I-B-2  Plot of the relative viscosity versus the shear rate for a suspension containing 10% by weight of 1.27 cm glass fibers in honey
Figure I-B-3  Plot of the relative viscosity versus the shear rate for a suspension containing 5% by weight of 1.27 cm glass fibers in honey
This phenomenon partially explains the vast disagreement of experimental results that are reported in the literature. The realignment of the fibers can also be achieved by allowing the flow to develop. Therefore, the suspension appears to exhibit transient behavior. This time-dependence is apparently governed by the interaction of bulk kinematics and fiber orientation.

The task is to describe this time-dependent phenomenon quantitatively, and to set forth methods for predicting a priori the rheological properties of the suspension, as well as the orientation distribution of the fibers.
C. RATIONALE

The purpose of using glass fiber reinforced plastics is to make strong parts. In addition, fine surface-finishing is often dictated by the product, such as in auto exteriors.

In order to ensure excellent mechanical and surface qualities in the product, the proper interplay between the molding compound formulation and the processing technique is essential. For instance, the mechanical behavior of fibrous composites is strongly influenced by the dimensions of the fiber, the fiber volume fraction, and in particular the fiber shape and the fiber orientation. The shape of the fiber determines whether a particle would fracture, and the orientation of the fiber dictates the ability of the composite to sustain external loads. These two important factors are determined during the transport of this material into the extremities of the mold cavity. Therefore, it would be advantageous to know a priori the state of the fibers so that one can decide on whether there is a need to alter the structure of the reinforcing particles.

To achieve this goal, it is necessary to understand the flow behavior of fiber suspensions, particularly in terms of the relation between the bulk deformation and the internal structure of the composite. To date, there is little agreement among the experimental data reported in the literature. Part of the reasons for these conflicting results are due to the coupling between the particle orientation and the bulk properties that are qualitatively dis-
played in Figures (I-B-1) to (I-B-3). In addition, there is also a lack of a structural rheological model that would describe this phenomenon.

Hence the general framework of this research is an attempt to understand the interrelationship between particle orientation and the rheological properties of the suspension.
D. SCOPE OF WORK

The objective of this research is to develop a rheological model capable of describing the rheological properties of a concentrated suspension of fibers in a Newtonian liquid. The problem is complicated by the dynamics of the particle configurations. Therefore a need arises to relate the macroscopic rheological properties to the instantaneous orientation distribution of the fibers. Ultimately it is hoped that the results from this investigation can then be adapted into a simulation package for evaluating the processability of a fiber reinforced composite.

The scope of this work is organized in the following way. In Chapter II the characterizations of concentrated fiber suspensions immersed in a Newtonian liquid are reviewed. In Chapter III the constitutive equation and the governing equation for the motion of the particle are formulated for the case of a suspension of rigid fibers in homogeneous flows. The solution to the particle motion and explicit forms of the stress tensor are given in Chapter IV. These results are illustrated in a variety of homogeneous flows in Chapter V. An attempt to consider the effect of solid boundaries on the rheological properties is provided in Chapter VI. Experimental data on the shear viscosity of the suspension are compared to the predicted values in Chapter VII. In Chapter VIII we formulate a model that would account for the case of deformable fibers in arbitrary flows.
CHAPTER II
LITERATURE REVIEW

The task of constructing a rheological model can be achieved in a number of ways. These methods are divided into experimental and theoretical schemes. This chapter surveys the current state of the art for characterizing the rheology of concentrated suspensions of fibers in a Newtonian liquid.

A. EXPERIMENTAL CHARACTERIZATIONS

The experimental approach is perhaps the most direct route to obtain rheological informations on an unknown specimen. However the determination of the suspension rheological properties is faced with a fundamental difficulty in that the dimensions of the particles are of the same order of magnitude as the characteristic length scale of the flow field in standard rheometers. Consequently the measured material functions, such as shear viscosity and normal stress coefficients, may not be intrinsic properties of the suspension. Nevertheless a multitude of data have been documented in the literature and summarized in review papers by Rutgers (1962), Brenner (1972), Jinescu (1974), Jeffrey and Acrivos (1976), and Markovitz and Berry (1978). The following summary is a concise account of the important findings in shear and extensional flows for a concentrated suspension of
rod-like particles. A brief overview of each experiment is presented in Table II-A-1.

Blakeney (1966) utilized a concentric-cylinder viscometer to investigate the shear flow properties of a suspension of nylon fibers in a tetrachloroethane-paraffin oil solution. Two sets of fibers were considered. The diameters were 16.9 and 43.1 microns with aspect ratios of 19.2 and 20.3 respectively. The viscosity measurements were made over a volume concentration range of 0 to 0.009, and at shear rates of 0.1 to 0.5 s\(^{-1}\). The experiment was allowed to proceed for approximately one-half hour in order to ensure that the data were collected at steady-state. For a volume concentration of fibers below \((d/l)^2\) i.e., dilute suspensions, the results agreed to within 2\% of Burgers' predictions (1938). Beyond the dilute limit, the suspension viscosity deviated substantially from Burgers' theory. However, the maximum relative viscosity, which corresponded to a fiber volume fraction of 0.009, was 1.055. Therefore, the viscosity of a non-dilute suspension does not seem to deviate considerably from the solvent viscosity.

Rosinger et al. (1974) used a cone and plate viscometer to measure the shear viscosity of a suspension containing asbestos fibers dispersed in water at room temperature. Two aqueous slurries were prepared. Each sample contains 1\% by weight of asbestos. In both of these batches the diameter of the fibers ranged between 20 - 50 nm. In one case 70\% of the fibers were 0.6 - 2.5 mm long whereas 69\% of the fibers were
Table II-A-1 Survey of rheological tests on concentrated fiber suspensions in a Newtonian liquid

<table>
<thead>
<tr>
<th>Author</th>
<th>Flow</th>
<th>Apparatus</th>
<th>Solvent</th>
<th>Fiber</th>
<th>l</th>
<th>l/d</th>
<th>$\phi_v$</th>
<th>Yield Stress</th>
<th>Power Law</th>
<th>Transient Behavior</th>
</tr>
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<tbody>
<tr>
<td>Blakeney</td>
<td>Shear</td>
<td>Concentric</td>
<td>Tetrachloro-</td>
<td>Nylon</td>
<td>16.9-</td>
<td>19.2-</td>
<td>0-</td>
<td></td>
<td>Yes</td>
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<tr>
<td>(1966)</td>
<td></td>
<td>cylinders</td>
<td>ethane-</td>
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<td>Paraffin</td>
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<tr>
<td>Rosinger et al.</td>
<td>Shear</td>
<td>Cone and plate</td>
<td>Water</td>
<td>Asbestos</td>
<td>0.6-</td>
<td>$\sim 10^4$</td>
<td>0.01</td>
<td>Yes</td>
<td>Yes</td>
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<td>(1974)</td>
<td></td>
<td></td>
<td>Asbestos</td>
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<td>Maschmeyers and Hill</td>
<td>Shear</td>
<td>Capillary</td>
<td>Silicone oil</td>
<td>Glass</td>
<td>0.025</td>
<td>20</td>
<td>0.15, No</td>
<td>Yes</td>
<td></td>
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<tr>
<td>(1977)</td>
<td></td>
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<tr>
<td>Tucker</td>
<td>Shear</td>
<td>Capillary</td>
<td>Water/glycerine</td>
<td>Milled</td>
<td>0.159-</td>
<td></td>
<td>0.025-</td>
<td>Yes</td>
<td></td>
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<tr>
<td>(1978)</td>
<td></td>
<td></td>
<td>glass</td>
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<tr>
<td>Horie and Pinder</td>
<td>Shear</td>
<td>Concentric</td>
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<td>Nylon</td>
<td>0.987</td>
<td>22.9-</td>
<td>0.04-</td>
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<tr>
<td>(1979)</td>
<td></td>
<td>cylinders</td>
<td>glycol-water-sodium chloride-dextran solution</td>
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<tr>
<td>Author</td>
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<td>Solvent</td>
<td>Fiber</td>
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<td>1/d</td>
<td>$\phi_v$</td>
<td>Yield Stress</td>
<td>Power Transient Stress Law Behavior</td>
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<tr>
<td>Kizior-Seyer (1974)</td>
<td>Extens-</td>
<td>Flow</td>
<td>Sugar</td>
<td>Rayon</td>
<td>15μm</td>
<td>340</td>
<td>0.001</td>
<td></td>
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<tr>
<td></td>
<td>ional</td>
<td>through an</td>
<td>solution</td>
<td>orifice</td>
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<tr>
<td>Weinberger-Goddard (1974)</td>
<td>Extens-</td>
<td>Mechanical</td>
<td>Silicone</td>
<td>Glass</td>
<td>200</td>
<td>57</td>
<td>0.0013</td>
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<td></td>
<td>ional</td>
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<td>apparatus</td>
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2.3 - 9.5 mm in the second lot. The results exhibited transient behavior. First, the shear viscosity decreased with increasing shear rates. However, when the shear rate was reduced, a larger stress was observed than at the same shear rate when it was being increased, thus producing a hysteresis. The hysteresis effect was smaller for the shorter fibers. A yield value was also observed from these tests. The yield values from the shorter fibers were lower. The conclusion from these experiments suggests that the addition of asbestos fibers in water produced non-Newtonian effects with a yield stress and transient characters. However, quantitative conclusions cannot be reached because of the substantial scatter in the data which might have resulted from the broad distribution of fiber lengths.

Maschmeyer and Hill (1977a-b) employed a capillary viscometer to determine the shear viscosity of suspensions containing 15% and 30% by volume of glass fibers in silicone oil. The mean fiber length was 0.025 cm, and the aspect ratio was 20. The study was based on a hypothesis such that the suspension would reach a limiting state beyond which continued mixing at the same conditions would not change their properties. To attain this limiting state, the slurry was required to pass through the extruder six times. The results indicated that wall effects are not significant nor are there any dependences on the capillary entrance angle and capillary diameter. The suspension viscosity increased with fiber concentration, but there was no observable yield stresses. The apparent viscosity
of the suspension is shear rate dependent, and this phenomenon is attributed to the small deviation from Newtonian behavior of the silicone oil.

Tucker (1978) investigated the shear viscosity of milled glass fibers in a water/glycerine mixture by means of a large bore capillary viscometer. The nominal fiber length ranged between 0.159 cm to 0.635 cm, and the volume fraction of solids varied between 2.5% to 12%. The suspension is shear thinning, and the degree of this effect increases with fiber length and fiber loading. Furthermore, the data can be fitted by a power law model for shear stress versus shear rate.

Horie and Pinder (1979) measured the viscosity of a suspension of nylon fibers in a polyethylene-glycol-water-sodium chloride-dextran solution at 30°C. The particle length ranged from 0.987 mm to 6.72 mm whereas the aspect ratio varied from 22.9 to 156. The volume fraction of solids varied from approximately 0.04 to 0.17. The shear flow experiment was carried out in a coaxial cylinder viscometer. The results show that the suspension viscosity decays with time. Secondly, the yield stress increases with particle concentration and particle aspect ratio. However, there is a maximum yield stress, after which the yield stress no longer depends on the loading and geometry of the particles. Subsequently, an empirical reaction-rate model is developed to fit the experimental data.

From these shear flow studies, the following qualitative agreements can be drawn. First, the bulk shear viscosity
of a concentrated suspension of fibers displays non-Newtonian behavior which can have power law and yield stress regions. Secondly, the suspension viscosity increases with fiber loading. Thirdly, each author suspects that fiber orientation, which results from the type of flow geometry, strongly influences the shearing properties of the suspension. At steady state the suspension viscosity is of the same order of magnitude as the solvent viscosity. However, the variables that will identify the effects of particle orientation are unknown. Therefore a stress-strain rate relation may not be sufficient to describe the complete rheological properties of the suspension.

The rheological properties of suspensions in extensional flows have been of considerable interests for fundamental analysis and for applied problems. Kizior and Seyer (1974) performed a series of converging flow experiments at room temperature using a suspension of rayon fibers in a Newtonian liquid. The dimensions of the fibers were 15 μm in length with an aspect ratio of 340. The volume fraction of solids was 0.001. The carrying liquid was a sugar solution. The experiment was carried out by forcing the suspension through an orifice. Thus, for a pre-set flow rate the jet thrust was measured by leaf springs mounted on the orifice plate. The result for the extensional viscosity of the suspension is an order of magnitude higher than the value of the pure Newtonian fluid. Although qualitative observations are made on a much more dilute suspension to indicate that the fibers are aligned
in the flow direction at the exit hole, there are some doubts as to whether the same particle configuration is attained for the concentrated suspension. Consequently the non-aligned fibers can significantly lower the value of the extensional viscosity.

Weinberger and Goddard (1974) used a mechanical spinning apparatus to generate an extensional flow. The test material consisted of glass fibers suspended in a silicone oil. The glass fibers measured 3.5 μm in diameter and 200 μm in length. The solid volume fraction was 1.3%. The principal features from their studies are that the suspension extensional viscosity is independent of the extension rate. Secondly, the tensile stress of the suspension is nearly ten-fold the value of the pure liquid. These authors have also reported that the zero-shear-rate viscosity for the same concentration of the fiber mixture is increased 10% over the solvent viscosity. Therefore, the suspension is probably in a transient state. Otherwise the extensional viscosity ought to be three times the shear viscosity at steady state.

The data from the extensional flows along with the results in the shear flows provide useful evidence that a suspension of fibers in a Newtonian liquid exhibits non-Newtonian behavior. The particle orientation is found to play an important role in both situations. For example, non-aligned fibers will produce a lower effective extensional viscosity. Consequently the data in the extensional flow experiments are not quantitatively conclusive because the
precise alignment of the fibers has not been verified. Therefore, the rheology of this class of materials will demand a careful inspection of the relation between the particle orientation and the bulk rheological properties.
B. CONTINUUM MODELS

A suspension is regarded as a continuous medium if the length of the particles is much smaller than the bulk characteristic length. This condition, although difficult to achieve experimentally, can be satisfied as long as the analysis is performed outside a boundary layer whose thickness is on the order of a particle length. The continuum approach consist of postulating certain features that the suspension would exhibit. However, these phenomena must conform with the conservation laws of physics.

The historical investigation was initiated by Einstein (1906) when he argued that the bulk rate of energy dissipation must be equal to the rate of work done by the motions of the suspended particles. This method was employed by Jeffery (1922) to estimate the shear viscosity of a dilute suspension of ellipsoids in a Newtonian solvent, and by Takserman-Krozer and Ziaibicki (1963b) to evaluate the extensional viscosity of the same suspension. However, this procedure would become extremely tedious for a concentrated suspension because of the need to compute the motion of each fiber strand. To overcome this difficulty, Ziegel (1970) claimed that the important energy-dissipating terms would involve the work to rotate all the unobstructed particles in the viscous medium, and the work required to disrupt agglomerates. Based on this assumption, Ziegel provided a semi-empirical model for the bulk shear viscosity of a concentrated suspension
containing prolate and oblate spheroids. The model predicted an infinite zero-shear viscosity which would account for the experimentally observed yield stress. However, the linear dependence of the relative viscosity on the solid volume fraction is indicative of a dilute suspension.

Another method to resolve the effective shear viscosity is by the successive addition of a small amount of fibers into a viscous medium. The prediction of the shear viscosity, from dilute theory was applied at each increment until the desired concentration of solids was attained. Brodnyan (1959) modified this idea to obtain the bulk shear viscosity of prolate ellipsoids with the assumption that the suspension behave as a Newtonian fluid.

An alternative concept of associating an anisotropic structure to a fluid containing elongated particles was formulated by Ericksen (1959, 1960). However, the theory excluded long range interactions. A director unit vector, \( \mathbf{n} \), was used to describe the micro-structure of the fluid. The stress tensor, \( \mathbf{\tau} \), was composed of tensorial products between the bulk deformation tensor, and the orientation vector. Then these relations must satisfy the requirement of material objectivity. With the assumption that the stress tensor depended linearly on the rate of deformation \( \dot{\mathbf{\tau}} \) and on the vorticity tensor \( \nabla \times \mathbf{u} \), Hand (1962) showed that the constitutive equation could be simplified to:

\[
\mathbf{\Pi} = (a_0 + a_1 \text{tr}(\mathbf{DD} \cdot \dot{\mathbf{n}})) \dot{\mathbf{n}} + (a_2 + a_3 \text{tr}(\mathbf{DD} \cdot \dot{\mathbf{n}})) \mathbf{DD} + a_4 \nabla \times \mathbf{u} + a_5 (\mathbf{DD} \cdot \nabla \times \dot{\mathbf{n}} + \nabla \times \dot{\mathbf{n}}) \cdot \mathbf{DD} \tag{II-B-1}
\]
where \( \Pi = \Pi + p\hat{v} \), \( p \) is the thermodynamic pressure, \( \hat{v} \) is an orientation vector, and the coefficients \( a_i \) are scalar functions of the invariants of \( pp \) only. In addition the governing equation for \( pp \) is:

\[
\frac{D}{Dt} pp = -\frac{1}{2}(w, pp) + \frac{1}{2}(pp, w) + b_0 \ddot{\hat{v}} + b_1 pp + b_2 \dot{\hat{v}}
\]

\[
+ b_3 \dot{\hat{v}} \cdot \dot{\hat{v}} + b_4 (pp, \dot{\hat{v}} + \dot{\hat{v}} \cdot pp)
\]

\[
+ b_5 (pp, \dddot{\hat{v}} + \dddot{\hat{v}} \cdot pp)
\]

(II-B-2)

where \( \frac{D}{Dt} \) is the substantial time derivative and the coefficients \( b_i \) are scalar polynomials of the invariants of \( pp \) and \( \ddot{\hat{v}} \).

Abhiraman and George (1980) employed this type of constitutive equations to compute the rheological properties in a simple shear flow and extensional flows. Duffy (1978, 1980a, b) also predicted the flow behaviors of anisotropic fluids. The calculations showed that under special circumstances, such as when the orientation pattern remained constant, the fluid would behave in a Newtonian fashion. Otherwise, the stresses would be time-dependent even when the bulk motion was steady.

The shortcoming of continuum mechanics in obtaining a rheological equation of state for fiber suspensions is perhaps its great generality. This method cannot furnish quantitative information on a material without recourse to an extensive experimental program. However, the proper experimental procedures are yet undetermined. Nevertheless the theory of anisotropic fluid does reveal an important aspect of a suspension. The stress tensor is not a simple function of the rate of deformation. Instead, the internal reorganization of
the particles produces a memory or a transient behavior. This effect requires a statement on the evolution of the microstructure.
C. STRUCTURAL MODELS

The structural approach provides a direct link between the microstructural properties and the macroscopic rheological behavior of a suspension. Therefore, the ambiguities encountered in the phenomenological models are avoided. Instead, the result from the structural study can be employed to identify the proper form of the continuum models. Furthermore the structural method offers an independent estimate of the suspension properties to be compared and contrasted with experimental data. However, the analysis is frequently hampered by mathematical complexities. The following section summarizes the theoretical methods used to formulate such a constitutive equation. An overview of these stress tensors is shown in Table II-C-1.

One of these methods is based on the kinetic theory of dumbbell molecules. A dumbbell contains two spherical beads that are separated by a rigid connector. The beads are free to rotate at each end. The connector which keeps the two beads at a fixed distance apart, does not interact with the solvent. A rigid fiber can be approximated by a straight array of beads that are closely spaced next to each other. This geometry facilitates the formulation of a constitutive equation that would account for the orientation of the suspended particle.

The kinetic theory of dumbbell suspensions has been modified by Doi and Edwards (1978a, b) to model a non-dilute suspension of rod-like molecules. Before discussing the work of Doi and Edwards, the important governing equations from the
Table II-C-1  Summary of structural models

<table>
<thead>
<tr>
<th>Author</th>
<th>Concentration</th>
<th>Particle Geometry</th>
<th>Stress Tensor</th>
</tr>
</thead>
</table>
| Kramers*           | Dilute          | Dumbbell          | $\mathbf{I} = -\eta_s \dot{\gamma} + \frac{\pi r l^2}{2} \kappa : \langle \mathbf{pppp} \rangle$  
                  |                 |                   | $- 3nkT \langle \mathbf{pp} \rangle + nkT \alpha$ |
| Giesekus*          | Dilute          | Dumbbell          | $\mathbf{I} = -\eta_s \dot{\gamma} + \frac{\pi r l^2}{4} \left( \frac{d}{dt} \langle \mathbf{pp} \rangle 
                  |                 |                   | $- \kappa \langle \mathbf{pp} \rangle - \langle \mathbf{pp} \rangle \kappa^\dagger \right)$ |
| Doi and Edwards    | Semi-concentrated | Rod             | $\mathbf{I} = -3nkT \langle \mathbf{pp} \rangle + nkT \alpha$ |

(1978) 

| Doi and Kuzuju     | Concentrated     | Rod               |                                                   |

(1980) 

| Batchelor          | Arbitrary        | Arbitrary         | $\mathbf{I} = -\eta_s \dot{\gamma} + \frac{1}{V} \sum_{\mathbf{m}} n_{\mathbf{m}} \cdot \mathbf{r} dA$ |

(1970) 

* Bird, Hassager, Armstrong, Curtiss (1977), Chapter 11
kinetic theory of a dilute suspension of dumbbells in a
Newtonian solvent will be outlined. The details on this
topic are presented by Bird, Warner and Evans (1971), Evans
(1975), and in a resourceful and authoritative text by Bird,
Hassager, Armstrong and Curtiss (1977). In this statistical
approach a macroscopic quantity, such as the bulk stress or
the bulk rate of deformation, represents a quantity that is
averaged over a number of events or experiments. The bulk
stress for such a dilute solution of rigid dumbbells consists
of contributions from the solvent, the intermolecular forces
which are divided into hydrodynamic and Brownian forces, and
the momentum carried by a typical particle. These respective
terms are mathematically expressed as:

\[ \mathbf{I} = -\eta_s \dot{\mathbf{Y}} - \frac{n k l^2}{2} \mathbf{<ppp>} - 3nkT \mathbf{<pp>} + nkT \dot{\phi} \]  (II-C-1)

where \( \eta_s \), \( n \), \( \zeta \), \( l \), \( k \), \( T \) are the solvent viscosity, the number
density, the Stokes' drag coefficient, the end-to-end separa-
tion of the dumbbell, Boltzmann's constant, and the absolute
temperature respectively. Equation (II-C-1) is the Kramers
expression for the stress tensor. Alternatively this equation
can be rewritten as:

\[ \mathbf{I} = -\eta_s \dot{\mathbf{Y}} + \frac{n k l^2}{4} (\mathbf{<pp>} - \zeta \mathbf{<pp>} - \mathbf{<pp>} \mathbf{<pp>} - \mathbf{<pp>} \mathbf{<pp>}) \]  (II-C-2)

Equation (II-C-2) is the Giesekus expression for the stress
tensor. The angular brackets in equations (II-C-1) and
(II-C-2) indicate that the variables are averaged with res-
pect to an orientation distribution function \( \psi(p,t) \). In
turn, this distribution function can be obtained by solving the following linear second order partial differential equation:

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial \mathbf{r}} \left( \left( \mathbf{F} - \mathbf{F} \cdot \mathbf{v} \right) \psi - \frac{2kT}{\xi^2} \frac{\partial \psi}{\partial \mathbf{r}} \right)$$  \hspace{1cm} (II-C-3)

The hydrodynamic contribution to the bulk stress, appearing in the second term of equation (II-C-1), is modeled by Stokes' law in which the drag force is given by the product of a drag coefficient and the relative velocity between the particle motion and the local solvent velocity. The stress tensor, given in equation (II-C-1), will also be valid for a string of equally spaced beads along a rigid rod, provided that the interactions between the beads are neglected. As the distance between the beads decreases, a string of beads will approach the shape of a rigid rod. In this analysis the dimensions of the particle are small compared to the characteristic length scale of the flow field. Consequently, on the microscopic level, the flow field is assumed to be homogeneous. Aubert and Tirrel (1979) have extended the analysis to nonhomogeneous flows by expanding the velocity field to the quadratic term. However, if the characteristic lengths of the particle and the flow field approach the same order of magnitude, then a Taylor expansion in the velocity field will not be useful because a large number of terms will be required in the series.

Doi and Edwards (1978b) have proposed a scheme that would extend the results from the dilute theory to a non-dilute concentration of rod-like molecules where the concentration
ranged from $1/l^3 < n < 1/dl^2$. In this concentration regime the rotational movement of a typical particle will be severely hindered by the presence of neighboring molecules. Consequently, the likelihood for a particle to tumble from end to end is negligibly small. These restrictions are introduced into the stress tensor, shown in equation (II-C-1), by two approximations. In the first of these two relations, the motion of the particle is assumed to follow the bulk deformation but is constrained by its own inextensibility. This statement is mathematically translated to:

$$\dot{\varepsilon} = \kappa \cdot \varepsilon - \kappa \varepsilon : \varepsilon$$  \hspace{2cm} (II-C-4)

Secondly, the rotational diffusivity of a test particle in a non-dilute solution is smaller than its diffusivity in a dilute medium (Kirkwood and Riseman, 1948) by a factor of $(nl^3)^2$. In essence, the time required for a test particle to rotate, by diffusion, to a position occupied by its nearest neighbor is equal to the time required for the adjacent particle to diffuse axially for a distance of approximately one particle length. Next, an order of magnitude analysis is performed to simplify the stress tensor expression. The first term in equation (II-C-1), which represents the solvent contribution, is ignored because the solution is not dilute. The second term is small compared to the third because of the limitation on the rotation of the test particle. Therefore, the bulk stress is reduced to:
\[ I = -3nkT<p_p> + nkT_0 \]  

(II-C-5)

The stress tensor in equation (II-C-5) along with the steady-state distribution function are solved numerically for the case of a simple steady shear flow by Doi and Edwards (1978b). However, the results presented by Doi and Edwards are not directly applicable to a concentrated suspension of macroscopic fibers because diffusion and Brownian processes will be insignificant. Nevertheless the idea of restricting the motion of a test particle, as means of extending the dilute theory into the non-dilute regions is physically appealing.

As the concentration of solids exceeds the value of \( n > 1/d^2 \), the suspension will behave like a solid. For concentrations ranging from \( 1/d^2 < n < 1/d^2 \), Doi and Kuzuu (1980) claim that the particles will bend. This mode of deformation will occur in a densely loaded system because segments from two adjacent particles cannot occupy the same location at the same time. The macroscopic energy dissipation is obtained from the microscopic free energies produced by each bent particle. Consequently the bulk engineering stress is calculated from the relative change of the total free energy with respect to the principal values of the deformation. In this analysis the orientation of the particles is not known precisely. Instead, Doi and Kuzuu (1980) presuppose that the particles are initially evenly distributed along the principal axes of deformation. The results indicate that the stress-strain relation is nonlinear even when the
deformation is small. Secondly, the stress-strain behavior produces a S-shaped curve which is unlike that of a rubbery material.

In circumventing the analysis of the various concentration regimes, Batchelor (1970) proposed a general constitutive equation for a suspension of particles immersed in a Newtonian liquid. The general theory can accommodate a non-uniform distribution of arbitrarily shaped and deformable particles in a force-free system. External couples are allowable. However, the following discussion only focuses on a suspension of rigid particles in which inertia terms could be neglected. The formulation for the macroscopic quantities are based on the volume averages of the microscopic variables. Consequently, the bulk rate of deformation is defined by:

$$\dot{\gamma} = \frac{1}{V} \int V_s \dot{\gamma}_s dV$$
$$= \frac{1}{V} \int V_s \dot{\gamma}_s dV + \frac{1}{V} \int_A V_s n dA$$  \hspace{1cm} (II-C-6)

where $V$ is the total volume of the suspension, $\dot{\gamma}_s$ is the local rate of deformation in the liquid phase, $V_s$ is the velocity of the solvent, and $n$ is a unit vector normal to the surface of the particle. In a similar manner, the bulk stress is obtained by a volume average of the local stresses. In the solid phase, volume integrals can be conveniently rewritten in terms of surface integrals by means of the divergence theorem. Therefore, the bulk stress is given by:
\[ I = -\eta_s \dot{\gamma} + \sum \int_{S} \Sigma_{s} \cdot \mathbf{n} r dA \]  

(II-C-7)

where \( \Sigma_s \) is the stress tensor of the solvent, \( \mathbf{r} \) is a vector to the surface of a particle from an arbitrary fixed coordinate system, and the summation is over the total number of suspended particles.

In general, the use of equation (II-C-7) to estimate the rheological properties of a non-dilute suspension is extremely difficult because the motion of each particle must be determined simultaneously. For a dilute suspension of ellipsoidal particles in a simple steady shear flow, Jeffery (1922) has shown that the particles will rotate in an orbit at a non-uniform rate. Batchelor (1970) makes use of this result to determine the shear stress for a dilute suspension of ellipsoids. For a concentrated suspension, the instantaneous orientation of each particle is often unknown. However, in the case of a pure straining flow, the steady state orientation of all the particles will be aligned in the direction of the streamlines. With the configurations of the particles known, Batchelor (1971) is able to calculate the stress field for a concentrated suspension of elongated particles in this class of flow fields.
D. PARTICLE ORIENTATION

In the preceding section the link between the particle orientation and the macroscopic rheological properties has been identified. This subject, concerning the motion of particles in a viscous medium, has been a continuing topic of interest in fluid mechanics. A comprehensive review of this problem has been provided by Leal (1980). To date, quantitative results are only obtainable for the case of isolated particles in simple flow fields. In concentrated suspensions and in complicated flow situations, the information is primarily based on experimental studies.

The early investigations on the motion of ellipsoidal particles are documented in Lamb's Hydrodynamics (1879), and in the works of Jeffery (1922) and Berry (1923). The analysis focused on a single particle, therefore, the results are restricted to dilute suspensions. The method consists of solving the velocity of the fluid that surrounds the particle. The inertia terms in the Navier-Stokes equation and the end-effects are neglected. The boundary conditions for this second order differential equation are the no-slip condition on the surface of the particle, and that the local fluid velocity approaches the bulk velocity at distances far away from the particle. The stresses on the surface of the particle are then obtained from the gradients of the velocity field. In the absence of external couples, the governing equation for the motion of an ellipsoid is:
\[ \dot{\mathbf{P}} = -\frac{1}{2} \mathbf{\omega} \cdot \mathbf{P} - \frac{(r_e^2 - 1)}{2(r_e^2 + 1)} (\dot{\mathbf{r}} \cdot \mathbf{P} - \dot{\mathbf{P}} : \ddot{\mathbf{P}}) \]  

Equation (II-D-1)

In a steady simple shear flow, Jeffery (1922) showed that an ellipsoid would rotate periodically in an orbit, but at a non-uniform rate. The shape of the elliptical orbit depends on the initial alignment of the particle. Trevelyan and Mason (1951), Mason and Manley (1956), Bartok and Mason (1957) have experimentally verified Jeffery's results by means of a concentric cylinder viscometer.

Anczurowski and Mason (1967 a, b, c), Okagawa and Mason (1973), Arp and Mason (1977) have demonstrated that Jeffery's results will not hold if the dilute limit is exceeded. Instead of maintaining a constant orbit, the particle will shift into a different one. This behavior is attributed to interactions in the form of hydrodynamic forces or two-body collisions.

A similar analysis is carried out by Taksman-Krozer and Ziaabicki (1963a) for a solution containing ellipsoidal molecules in an extensional flow. The results indicate that the particles are aligned with the principal axis of extension.

The above experiments address a dilute suspension of fibers. When the concentration increases, accurate characterizations of the particle orientation are not always feasible. Nevertheless a number of qualitative observations and semi-empirical models have been documented.

As an example, Tadmor (1974) proposed a semi-quantitative model to describe the molecular orientation of injection molded products. The flow pattern into a rectangular cavity is divided into an advancing front, and a section behind the
front. The advancing front is modeled by a steady elongation flow, whereas a shearing flow follows behind this region. This combination of flows is able to qualitatively describe the molecular orientation of molded parts in which the particles are aligned in the direction of the streamlines near the surface, whereas in the core the particles are oriented perpendicular to the streamlines.

In other non-homogeneous flows, such as in flows through capillaries, Karnis, Goldsmith and Mason (1966), and Stankoi et al. (1968) observed that the velocity profile of the fiber suspension became more blunt and eventually flat, as the particle concentration increased. This behavior was attributed to particle interactions with other particles and with the wall of the capillary.

In converging circular channels, Bell (1969) reported that the velocity profile of a suspension containing 1/8 inch glass fibers at approximately 50% by volume in an epoxy resin is flat. Secondly, the fibers are not fully aligned with the flow. Instead, these particles are, on average, 30° relative to the flow direction. Furthermore, the orientation is independent on the flow rate, the convergence angle and the channel length. In addition, the influence of a non-Newtonian fluid on the suspension behavior is not clear.

Goetler (1970) also observed that fibers tend to be aligned in the flow axis in a converging flow. However, the preferred orientation is roughly 20° from the flow direction in tests using 40% by volume of 1/8 inch glass fibers.
Contrary to Bell's results (1969), Goetler found that the orientation depended on the extension rate, convergence angle, and the viscosity of the carrying fluid.

Lee and George (1978) carried out flow visualization studies on a suspension of glass fibers in an epoxy resin. The fiber length was 13 μm, and the concentration was 30% by weight. A small amount of steel fibers were included as tracers. The results indicate that the velocity profile is flat in a uniform capillary. In a converging channel that is followed by a straight circular tube, the velocity profile is flat at the entrance of the conic section, but progressively becomes parabolic towards the exit end of the tube.
CHAPTER III
MODELING OF RIGID FIBERS IN HOMOGENEOUS FLOWS

A suspension is a heterogeneous mixture of solid particles that are immersed in a liquid. This chapter begins by identifying three important concentration regimes in which the macroscopic properties of the suspension would exhibit very different behavior. The ensuing analysis is concerned with the middle regime which would encompass a variety of fiber reinforced composites.

The rheology for this type of material that is composed of rigid fibers suspended in a Newtonian liquid, is formulated from a structural approach. The governing equations for the stress tensor, the particle motion, and the distribution function along with their appropriate initial conditions are obtained for the case of homogeneous flows. The bulk stress is formulated by averaging the microscopic variables; the particle motion is derived by applying the conservation of angular momentum on a test particle; and the orientation distribution function is obtained by conserving system points in the configuration space. The consideration of the general problem involving inextensible particles in arbitrary flow fields will be discussed in Chapter VIII.

A. CONCENTRATION REGIMES

The rheological behavior of fiber suspensions is influenced by the amount and the orientation of the particles in the
system. In the dilute region, each fiber strand is free to rotate in all directions. As the number of fibers increases, the motion of each particle becomes restricted by the presence of neighboring particles. Consequently the mobility of each particle decreases as the number density of fibers increases.

To quantify the degree of crowding in the suspension, we introduce a variable, \( a_c \), which is the separation between a particle and its closest neighbor. For a random distribution of orientations with no concentration gradients, this distance has been related to the concentration of solids by Doi and Edwards (1978) in which:

\[
    a_c = \frac{1}{n l^2}
\]  \hspace{1cm} (III-A-1)

where \( n \) and \( l \) are respectively the number density and the particle length. Alternatively the quantity \( a_c \) can be rewritten in terms of the volume fraction of solids, \( \phi_v \):

\[
    a_c = \left( \frac{d}{l} \right)^2 \frac{1}{\phi_v}
\]  \hspace{1cm} (III-A-2)

In equations (III-A-1) and (III-A-2), numerical factors of order 1 have been neglected. Therefore, the approximate sign is used in place of the equal sign.

The study of the rheology of fiber suspensions is divided into three regions of solid concentrations. These regimes are listed in Table III-A-1, and the corresponding physical situations would be subsequently described.

1. **Dilute Region**

The dilute regime is defined to be the one in which the
<table>
<thead>
<tr>
<th>Regime</th>
<th>Concentration</th>
<th>Inter-particle spacing</th>
<th>Suspension behavior</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. Dilute</td>
<td>( n \leq \left( \frac{1}{l^3} \right) )</td>
<td>( a_c &gt; 1 )</td>
<td>Viscous</td>
</tr>
<tr>
<td></td>
<td>( \phi_v \leq \left( \frac{d}{l} \right)^2 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>II. Semi-</td>
<td>( \frac{1}{l^3} &lt; n &lt; \left( \frac{1}{dl^2} \right) )</td>
<td>( d &lt; a_c &lt; 1 )</td>
<td>Visco-elastic</td>
</tr>
<tr>
<td>concentrated</td>
<td>( \left( \frac{d}{l} \right)^2 &lt; \phi_v &lt; \left( \frac{d}{l} \right) )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>III. Concentrated</td>
<td>( \frac{1}{dl^2} &lt; n &lt; \left( \frac{1}{d^2 l} \right) )</td>
<td>( a_c &lt; d )</td>
<td>Solid</td>
</tr>
<tr>
<td></td>
<td>( \left( \frac{d}{l} \right) &lt; \phi_v &lt; 1 )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
spacing between a fiber and its nearest neighbor is at least a fiber length apart. Since $a_c > 1$, then the number density is given by $n < (1/l^3)$, or the volume fraction is $\phi_v < (d/l)^2$. In this region a fiber is free to rotate and tumble from end to end without interfering with the other particles. Therefore, the solid concentration that defines the dilute region can also be conceived as the ratio of the fiber volume to the volume of a sphere swept out by a rotating particle (Mason, 1950).

$$\phi_v = \frac{\text{actual volume}}{\text{effective volume}} = \frac{\frac{\pi d^2}{4} - 1}{\frac{4\pi}{3} \left(\frac{1}{2}\right)^3} = 1.5 \left(\frac{d}{l}\right)^2$$  (III-A-3)

Aside from a numerical factor of 1.5, which would be neglected, a suspension is dilute as long as the volume fraction of solids does not exceed the inverse of the square of the fiber aspect ratio.

The rheological properties of a dilute suspension would vary linearly with the solid concentration as can be seen from the bulk stress tensor (equation II-C-6) obtained by Batchelor (1970). In equation (II-C-6), the summation of surface integrals can be replaced by the total number of fibers in the suspension because each particle can be considered as an isolated fiber. Therefore, the stress tensor can be rewritten as:

$$\mathbf{I} = -\eta_s \left[ \dot{\mathbf{Y}} + n_j \dot{\mathbf{Y}}_s \cdot n \mathbf{d} \mathbf{A} \right]$$  (III-A-4)

Since the number density is small ($n < (1/l^3)$), the ratio of the second term to the first term on the right side of equation
(III-A-4) is approximately $d/l$. Consequently the contribution to the bulk properties from the particles cannot exceed the contribution from the solvent. Therefore, the suspension behavior is described as viscous.

In the dilute region, the motion of a fiber is governed by equation (II-D-1). This equation was obtained from a torque balance on a particle suspended in a viscous medium, and there was no external couple acting on the system. Case studies in a simple steady shear flow and in extensional flows were provided by Jeffery (1922) and Takserman-Krozer and Ziabicki (1963) respectively.

To summarize the dilute regime, the rheology of a suspension in this range of solid concentrations is fairly well understood both in terms of theoretical predictions (Brenner, 1972; Jinescu, 1974; Jeffrey and Acrivos, 1976) and experimental data (Rutgers, 1962; Markovitz and Berry, 1978) on the bulk properties, and the motion of particles in a viscous medium (Leal, 1980). However the reinforcement provided by a small quantity of fibers is commonly not sufficient for practical use.

2. Semi-concentrated Region

In the semi-concentrated region, the distance between a fiber and its nearest neighbor, in a randomly packed suspension, varies from a fiber length to a fiber diameter apart. The corresponding number density of fibers ranges from $(1/l^3) < n < (1/dl^2)$, whereas the volume fraction varies from $(d/l)^2 < \phi_v < (d/l)$. This
regime of concentration would cover a wide range of reinforced composites because of the considerable fraction of solids present in the system.

In this region the motion of a fiber is limited because of the presence of other particles. In particular particles cannot pass through each other. For these bundles of randomly dispersed fibers, the resistances to rotation and to motion perpendicular to the fiber major axis are much greater than the resistance to a displacement along the axial direction of the particle. Therefore, it is unlikely for a fiber to tumble from end to end (Doi and Edwards, 1978).

The rheological behavior of the suspension would depend strongly on the structural arrangement of the particles. For instance, the resistance to shear deformation for a suspension of randomly packed fibers would be much greater than the same loading of particles that are aligned near the shearing planes. Consequently, the bulk character of the suspension may appear like an effective viscous medium under certain conditions, but may behave like a solid under other circumstances. Therefore, the suspension is described as a visco-elastic material where the word elastic would be defined in Chapter V.

The rheological characterization of a semi-concentrated suspension of fibers are extremely difficult from both the experimental and theoretical approaches. The difficulties are primarily due to the dynamics of the particle orientation and its coupled effect on the hydrodynamic interactions between the fibers. The attempt to model the suspension in
this concentration regime is the subject of discussions in subsequent sections.

3. Concentrated region

The concentrated regime is one in which the distance between fibers is less than a fiber diameter apart. The number density and the volume fraction of solids that corresponds to this range of concentrations are respectively \((1/d^2) < n < (1/d^2)\) and \((d/l) < \phi_v < 1\). The upper limit for the volume fraction \(\phi_v = 1\) would be \(\phi_v = \pi/4\) if we have not disregarded coefficients of order 1. A volume fraction of \(\phi_v = \pi/4\) would correspond to the maximum packing limit for randomly distributed fibers.

In this densely populated system the relative motion between the particles and the solvent is minimal. Consequently, the entire suspension would deform like a solid. Since the deformation of the suspension requires the cooperative deformation of large numbers of fibers, the constitutive equation that would describe this type of deformation would be best approached from the theories of solid mechanics. The characterization of the bulk properties for these highly concentrated suspensions is beyond the scope of the present work.
E. STRESS TENSOR

The rheological model developed here addresses the semi-concentrated regime in which the concentration of solids ranges from \((1/l^3) < n < (1/dl^2)\). In such a heterogeneous system that contains numerous particles suspended in a liquid, the measurable or observable quantities are meaningful only in a statistical sense because the microscopic variables would differ from one experiment to the next one, even under the same macroscopic conditions. However, the uncertainty only lies in the initial configuration of the particles. As will be shown later, the problem is deterministic.

The bulk stress tensor can be constructed from the volume average approach suggested by Batchelor (1970), or from the kinetic theory of rod-like polymers (Bird, Hassager, Armstrong, and Curtiss, 1977). The corresponding results are identical. Each of these methods is described below.

1. Volume Average

A volume average is an approximation of an ensemble average. However, the volume average is a useful approximation because it can be readily related to physical situations. As discussed in Section (II-C), Batchelor formulated the macroscopic quantities from the volume averages of the microscopic variables. The bulk stress was given by:

\[
\mathbf{I} = -\eta_s \dot{\mathbf{X}} + \frac{1}{V} \int_{V} \mathbf{H}_s \cdot \mathbf{n} \mathbf{r} \mathbf{d}A
\] (III-B-1)

where \(\mathbf{I}\) is the non-equilibrium part of the stress tensor, \(\eta_s\) is the solvent viscosity, \(\dot{\mathbf{X}}\) is the bulk rate of deformation tensor,
V is the volume of the suspension, $\tau_s$ is the local stress in the solvent, $\hat{n}$ is an outwardly-directed unit vector that is perpendicular to the particle surface, $\mathbf{r}$ is a vector to the surface of a particle from an arbitrary coordinate system, and $dA$ is a surface element of the particle.

In a semi-concentrated suspension of fibers, equation (III-B-1) cannot be conveniently used to estimate the rheological properties of a suspension because of the need to evaluate the surface integrals. The surface integrals are coupled because the rate of deformation of the solvent on the surface of a fiber depends on the orientation of the particle, but it is also perturbed by the configuration of the surrounding fibers. In a dynamical situation, the particle orientations change with time, and therefore, a direct calculation of this set of surface integrals is nearly impossible.

To overcome the computational difficulties, Brinkman (1947, 1952) proposed that the interactions among the particles be modeled by a Darcy term. In essence the analysis is focused on a single particle, and the surrounding particles are represented by a porous medium. Freed and his coworkers (1978a, b, 1979) have also employed the mean field theory approach to consider the hydrodynamics of concentrated spherical suspensions and concentrated polymer solutions. Instead of having to evaluate the properties of the porous medium experimentally, Freed and his coworkers determined the effective medium through a self-consistent argument. The calculations are carried out in accordance to the multiple scattering method of Freed and
The approach that we take is to focus the analysis on a test fiber, shown in Figure (III-B-1), that is immersed in an effective medium. A summary of the assumptions used in the ensuing analysis is listed in Table (III-B-1). The fiber is a cylindrical particle. Therefore, a vector to a point on the center-line of the particle from an arbitrary coordinate system can be equivalently expressed by the center of mass \( \mathbf{r}_c \), the orientation and the arc length of the fiber. The particle orientation is described by a unit vector \( \mathbf{p} \) that points in the axial direction of the fiber. The arc length \( s \) is the distance from a reference point to any position along the major axis of the fiber. Since the position of the test fiber is to be representative of an average particle in the suspension, a distribution function \( \Psi(\mathbf{r}_c, \mathbf{p}, s, t) \) is introduced to follow the probability that the test particle has a specific configuration. Consequently, the original multi-particle problem has been converted into a single particle problem. The bulk stress is rewritten as:

\[
\mathbf{I} = -\eta_s \mathbf{\dot{x}} + \frac{1}{V} \int dV \mathbf{\Pi}_{\text{eff}} \cdot \mathbf{n} \Psi(\mathbf{r}_c, \mathbf{p}, s, t) d\mathbf{r}_c d\mathbf{p} dA \tag{III-B-2}
\]

where \( \mathbf{\Pi}_{\text{eff}} \) is the stress tensor that describes the effective medium. The integrals over all possible values of the center of mass and the particle orientation ensure that the test fiber has been accounted for. For a cylindrical particle, the surface element \( dA \) is given by the product of the circumference and the differential arc length \( ds \), \( dA = (\pi d) ds \).
Figure III-B-1  Schematic diagram of a test fiber immersed in an effective medium
Table (III-B-1) Summary of assumptions for the development of the stress tensor in homogeneous flows for a suspension of rigid fibers

1. The solvent is a Newtonian liquid.

2. The suspension is an incompressible fluid.

3. The fibers are rigid.

4. Brownian motion is neglected.

5. Inertia terms are neglected.

6. There are no external forces acting on the suspension.

7. There are no external couples acting on the suspension.

8. The interaction between a test fiber and the remaining particles is modeled by a test fiber immersed in an effective medium.

9. The drag force on the surface of a particle is modeled by a line force along the major axis of the fiber. This drag force is approximated by a Stokes-Burgers model.

10. The centers of mass of the particles are randomly distributed.
In equation (III-B-2), $\mathbf{F}_{\text{eff}} \cdot \mathbf{r} dA$ is a drag force on the surface of the particle. Instead of allowing the drag force to vary around the circumference of the fiber, we assume that this force is concentrated at the center of the particle cross-sectional area. Therefore, the total drag force on the particle is replaced by a line force along the axis of the fiber. Secondly the vector $\mathbf{r}$ is now a vector from an arbitrary fixed coordinate to a position on the center-line of the particle.

The term $(\mathbf{r} dA) \mathbf{F}_{\text{eff}} \cdot \mathbf{r}$ becomes the drag force per unit length. This quantity is approximated by a Stokes-Burgers model in which the drag force is the product of a drag coefficient $\zeta_{\text{eff}}$ and the relative velocity, $(\mathbf{v} - \dot{\mathbf{r}})$, between the effective medium and the test particle. With these modifications, the bulk stress becomes:

$$\mathbf{t} = -\eta \frac{d}{d} \frac{1}{2} \int_{V} \mathbf{F}_{\text{eff}} (\mathbf{v} - \dot{\mathbf{r}}) \mathbf{r} d\mathbf{r} d\mathbf{s}$$

(III-B-3)

Since the resistance to flow for a rod depends on the orientation of the particle with respect to the flow direction, the tensorial drag coefficient is given by:

$$\zeta_{\text{eff}} = \zeta_{\text{eff}} (2\mathbf{\hat{a}} - \mathbf{I})$$

(III-B-4)

where the magnitude of the drag coefficient $\zeta_{\text{eff}}$ depends on the concentration, the dimensions of the particle, and the proximity of the nearest neighbor; and $\mathbf{\hat{a}}$ is the unit tensor.

In this section we are only considering the case of rigid fibers in homogeneous flows. For this class of flows, the bulk stress and the bulk rate of strain are independent of
position in the physical space. In such case the velocity of the effective medium can be rewritten as:

\[ \dot{\mathbf{y}} = \mathbf{x} \cdot \mathbf{r} \]  

(III-B-5)

where \( \mathbf{x} = (\nabla \mathbf{y})^T \). Secondly, the orientation vector \( \mathbf{p} \) is only a function of time because the fiber is rigid. Consequently, the distribution function can be decomposed into contributions from the center of mass and the orientation vector.

\[ \psi(r_c, \mathbf{p}, s, t) = n(r_c, t) \psi(p, t) \]  

(III-B-6)

where \( n \) is the number density, and \( \psi \) is the orientation distribution function.

The next step is to recast the relative motion between the particle and the effective medium in terms of a rotational part and a translational part. To do so, the vector \( \mathbf{r} \) can be written as:

\[ \mathbf{r} = r_c + s \mathbf{p} \]  

(III-B-7)

and,

\[ \dot{\mathbf{r}} = \dot{r}_c + s \dot{\mathbf{p}} \]  

(III-B-8)

By substituting these relations into equation (III-B-3), the bulk stress tensor becomes:

\[ \mathbf{\Pi} = -\eta_s \dot{\mathbf{y}} - \frac{1}{VI} \left[ \frac{1}{2} \int \zeta_{\text{eff}} \cdot ((\mathbf{k} \cdot \dot{\mathbf{r}}_c - \mathbf{r}_c) (\mathbf{r}_c + s \mathbf{p}) + s(\mathbf{k} \cdot \dot{\mathbf{p}} - \dot{\mathbf{p}}) \mathbf{r}_c + s^2(\mathbf{k} \cdot \dot{\mathbf{p}} - \dot{\mathbf{p}}) \mathbf{r}_c \cdot \mathbf{r}_c \psi(p, t) d\mathbf{r}_c dp ds \right] \]  

(III-B-9)

The vector \((\mathbf{k} \cdot \mathbf{r}_c - \mathbf{r}_c)\) represents the translation of the particle, whereas the vector \((\mathbf{k} \cdot \dot{\mathbf{p}} - \dot{\mathbf{p}})\) describes the rotation of the fiber.
To determine the relative motion between the center of mass of the particle and the effective medium, the conservation of linear momentum is used. For a suspension of rigid fibers in a homogeneous flow field which is not under the influence of an external force and in which Brownian motion is negligible, a force balance at the center of mass of the particle reveals that:

\[(\mathbf{\xi} \cdot \dot{\mathbf{r}}_c - \ddot{\mathbf{r}}_c) = 0\]  

(III-B-10)

The condition to ignore Brownian motion can be satisfied by making the product of the particle volume, the viscosity of the effective medium, and the rate of deformation sufficiently large, or by making the temperature sufficiently small (Leal and Hinch, 1971). Such criteria are usually fulfilled for the type of fibers and the range of solid concentrations considered in this work.

In order to further simplify equation (III-B-9) we employ three identities:

1) \(\int \mathbf{r}_c \, d\mathbf{r}_c = 0\)  

(III-B-11)

2) \(\int d\mathbf{r}_c = V\)  

(III-B-12)

3) \(\rho \cdot \ddot{\mathbf{u}} = 0\)  

(III-B-13)

In the first relation, the vector \(\mathbf{r}_c\) is integrated over all spatial values. Since for each vector there is always an opposite one, then the net contribution is zero. The second relation is simply a definition of the volume of the suspension. The last relation is obtained by recalling that the fibers are rigid or inextensible.
For a suspension where the centers of mass of the particles are randomly dispersed, the concentration gradient of the centers of mass is equal to zero. In such case the number density, \( n \), is a constant.

By inserting these assumptions and identities into equation (III-B-9), and after integrating along the axis of the fiber, the bulk stress is reduced to:

\[
\mathbf{\tau} = -n s \mathbf{\dot{y}} - \frac{n l^2}{12} \int \zeta_{\text{eff}} \cdot (\mathbf{\dot{y}} \cdot \mathbf{\dot{y}} - \mathbf{y} \mathbf{y}) \psi d\mathbf{y} \tag{III-B-14}
\]

The bulk stress tensor is not complete until the quantities \( \mathbf{\dot{y}}, \psi \), and \( \zeta_{\text{eff}} \) are specified. These quantities are respectively described in sections (III-C), (III-D) and (III-E).

2. Kinetic Theory

The kinetic theory approach is a statistical mechanical treatment of the average process to obtain the macroscopic quantities. An elaborate derivation of the bulk stress for a polymer solution of arbitrary concentrations has been presented by Bird, Hassager, Armstrong, and Curtiss (1977).

In general the bulk stress can be expressed as:

\[
\mathbf{\tau} = \mathbf{\tau}_k + \mathbf{\tau}_p + \mathbf{\tau}_{ss} + \mathbf{\tau}_{sp+ps} + \mathbf{\tau}_{pp} \tag{III-B-15}
\]

where \( \mathbf{\tau}_k \) reflects the momenta carried by the motion of the solvent and the polymer molecules; \( \mathbf{\tau}_p \) is from the intramolecular forces in the polymer chain; \( \mathbf{\tau}_{ss}, \mathbf{\tau}_{sp+ps}, \) and \( \mathbf{\tau}_{pp} \) are intermolecular interactions between solvent and solvent molecules, solvent and polymer molecules, polymer and polymer molecules.
However, if the analysis is focused on an isolated particle which can be any kind of bead-rod-spring model, then the constitutive equation is reduced to:

\[ \mathbf{I} = -\eta_s \mathbf{\dot{\psi}} - n_2 \sum_{\nu=1}^{N} F_{\nu}(Q, t) dQ \]  

(III-B-16)

In equation (III-B-16), \( \nu \) is a label for a bead; \( N \) is the total number of beads; \( \mathbf{R}_{\nu} \) is the vector from bead \( \nu \) to the center of mass of the whole particle; \( \mathbf{F}_{\nu} \) is the average force from the solvent molecules to bead \( \nu \), and \( Q \) is the set of internal coordinates which give the configuration of the polymer chain.

To extend the result from the dilute theory to a semi-concentrated suspension of rigid fibers in homogeneous flows, the following modifications are introduced. First, the rigid rod is approximated by a string of beads in which each bead is free to rotate. In this case the total number of beads is given by:

\[ N = \frac{l}{\Delta s} \]  

(III-B-17)

where \( l \) is the length of the fiber, and \( \Delta s \) is the center-to-center distance between two adjacent beads.

\[ \Delta s = |\mathbf{R}_{\nu+1} - \mathbf{R}_{\nu}| \]  

(III-B-18)

Here, the vector \( \mathbf{R}_{\nu} \) can be rewritten as \( s \mathbf{p} \) where \( s \) is the arc length to bead \( \nu \) from the center of mass, and \( \mathbf{p} \) is co-linear with \( \mathbf{R}_{\nu} \). Secondly, the drag force over the entire fiber is approximated by the sum of drag forces on each bead. However, each bead does not experience the full Stokes drag because it is shielded by its neighbors. Consequently, the tensorial
drag coefficient in the Stokes-Burgers model is utilized to account for the partial "shielding" effect. Thirdly, the interactions between the particles are modeled by a test fiber in an effective medium. Consequently the drag force on the test fiber is the product of an effective drag coefficient and the relative velocity between the effective medium and the particle.

In equation (III-B-16) the drag force on bead \( v \) is given by:

\[
F = \zeta_{\text{eff}} \cdot (v - \ddot{r}) \frac{\Delta s}{l}
\]

\[
= \zeta_{\text{eff}} \cdot \left[ (\kappa \cdot \Gamma_c - \dot{\zeta}_c) + s(\kappa \cdot \ddot{p} - \dot{\zeta}_c) \right] \frac{\Delta s}{l}
\]

\[
= s\zeta_{\text{eff}} \cdot (\kappa \cdot \ddot{p}) \frac{\Delta s}{l}
\]  

(III-B-19)

where the quantity \( \zeta_{\text{eff}} \cdot (v - \ddot{r}) \) is the drag force on a cylindrical rod of length \( l \).

By substituting these modifications into equation (III-B-16) we obtain:

\[
I = -n_s \dot{\gamma} - n \sum_{v=1}^{N} \int_{-l/2}^{l/2} s^2 \zeta_{\text{eff}} \cdot (\kappa \cdot \ddot{p} - \dot{\zeta}_c) \frac{\Delta s \psi(p,t)}{l} dp
\]

(III-B-20)

In the limit that \( N \) approaches infinity, or \( \frac{\Delta s}{l} \) approaches zero, then equation (III-B-20) is the Riemann sum of the integral

\[
I = -n_s \dot{\gamma} - n \int_{-l/2}^{l/2} s^2 \zeta_{\text{eff}} \cdot (\kappa \cdot \ddot{p} - \dot{\zeta}_c) \frac{\Delta s \psi dp}{l}
\]

\[
= -n_s \dot{\gamma} - \frac{n l^2}{12} \int \zeta_{\text{eff}} \cdot (\kappa \cdot \ddot{p} - \dot{\zeta}_c) \psi dp
\]

(III-B-21)
This result is identical to equation (III-B-14) which is the bulk stress developed by the volume average method.
C. EQUATION OF MOTION

The equation of motion is the governing equation that describes the evolution of the unit vector \( \mathbf{p} \). As shown in Figure (III-B-1), the unit vector \( \mathbf{p} \) indicates the orientation of a test fiber. Because the particle is rigid, the fiber cannot deform. Consequently, the configuration of the fiber can be given by two components of \( \mathbf{p} \) instead of requiring three independent variables. A convenient choice of an orthogonal coordinate system would be a spherical coordinate system. The vector \( \mathbf{p} \) can then be labeled by the spherical angles \( (\theta, \phi) \).

In addition, the rate of change of the director vector, \( \dot{\mathbf{p}} \), needs to be expressed in terms of \( \mathbf{p} \). This relation is then substituted into the stress tensor in equation (III-B-14) so that the integration over all possible configurations can be performed.

In the previous section the conservation of linear momentum has been applied to determine the translation of the particle. In order to describe the rotation of the particle, the conservation of angular momentum is invoked. Since the momentum balance can be applied anywhere in the system, a convenient location would be at the center of mass with the moment arm being directed along the fiber axis. With the inertia term neglected,

\[
Q = \int_{-\frac{1}{2}}^{\frac{1}{2}} \mathbf{sp} \times \mathbf{z}_{\text{eff}} \cdot (\mathbf{v} - \dot{\mathbf{r}}) \, ds
\]
\[
= \int_{-1/2}^{1/2} s^2 \mathbf{p} \times \left[ \mathbf{z}_{\text{eff}} \cdot (\mathbf{k} \cdot \mathbf{p} - \dot{\mathbf{p}}) \right] ds
\]  \quad (III-C-1)

Since the unit vector \( \mathbf{p} \) is independent of \( s \):

\[
0 = \mathbf{p} \times \left[ \mathbf{z}_{\text{eff}} \cdot (\mathbf{k} \cdot \mathbf{p} - \dot{\mathbf{p}}) \right] \quad (III-C-2)
\]

In order for equation (III-C-2) to hold, the vector \( \mathbf{z}_{\text{eff}} \cdot (\mathbf{k} \cdot \mathbf{p} - \dot{\mathbf{p}}) \) is either the zero vector, or it is co-linear with \( \mathbf{p} \). The first case is the trivial situation in which there is no relative motion between the fiber and the effective medium. Therefore, this case is of no interest. When \( \mathbf{z}_{\text{eff}} \cdot (\mathbf{k} \cdot \mathbf{p} - \dot{\mathbf{p}}) \) is co-linear with \( \mathbf{p} \) then:

\[
2\mathbf{k} \cdot \mathbf{p} - 2\dot{\mathbf{p}} - \mathbf{k} : \mathbf{ppp} = f(t) \mathbf{p} \quad (III-C-3)
\]

where \( f(t) \) can be a scalar function of time. Since the fiber is inextensible, the function \( f(t) \) can be rewritten in terms of \( \mathbf{k} \) and \( \mathbf{p} \) by performing a scalar product between equation (III-C-3) and \( \mathbf{p} \).

\[
f(t) = \mathbf{k} : \mathbf{pp} \quad (III-C-4)
\]

Consequently, the rate of change of \( \mathbf{p} \) is given by:

\[
\dot{\mathbf{p}} = \mathbf{k} \cdot \mathbf{p} - \mathbf{k} : \mathbf{ppp} \quad (III-C-5)
\]

This equation will be solved in section (IV-A) along with the initial condition of \( \mathbf{p} = \mathbf{P}_0 \).

An alternative method to arrive at the same result is illustrated in Figure (III-C-1). Here, a force balance is performed on a segment of the fiber. The hydrodynamic force is balanced by a tension \( F \) which is directed along the fiber axis.
Effective medium

$F_{\text{hydrodynamic}} = \int \mathbf{s}_{\text{eff}} \cdot (\mathbf{v} - \mathbf{v}) ds$

Figure III-C-1 A free body diagram of a rigid fiber
\[ F = F_p \]
\[ = \int \zeta_{\text{eff}} \cdot \left( \mathbf{v} - \mathbf{v}_i \right) ds \]
\[ = \zeta_{\text{eff}} \cdot (\mathbf{k} \cdot \mathbf{p} - \mathbf{v}_i) \int ds \]

By employing the condition of inextensibility, we can again arrive at the same result for \( \mathbf{v}_i \) which is given in equation (III-C-5).

The governing equation for the evolution of the unit vector \( \mathbf{v}_i \) can be physically interpreted in the following way. The orientation of the fiber follows the bulk deformation with the exception that the particle cannot stretch. In equation (III-C-5), \( \mathbf{k} \cdot \mathbf{p} \) represents the component of the bulk deformation of a fluid element which is coincident with the fiber. The term \( \mathbf{k} \cdot \mathbf{ppp} \) is the stretching component of \( \mathbf{k} \cdot \mathbf{p} \). Consequently the fiber rotates but cannot stretch, and its motion is mathematically expressed in equation (III-C-5). With this result, the stress tensor becomes:

\[ \mathbf{I} = -\eta_s \frac{\mathbf{v}_i}{s} - \frac{\eta_1}{12} \int \zeta_{\text{eff}} \mathbf{k} \cdot \mathbf{ppp} \psi dp \]

(III-C-7)
D. DISTRIBUTION FUNCTION

The orientation distribution function $ψ(p,t)$ describes the probability that a fiber would be oriented somewhere in the range of $p$ to $p + dp$ at time $t$. The governing equation for the evolution of $ψ$ is a conservation statement in which a fiber cannot be created nor destroyed. Instead, when a particle leaves one orientation, it must appear in another one. Hence the rate of change of $ψ$ is given by the divergence of the orientation flux.

$$\frac{∂ψ}{∂t} = -\frac{∂}{∂p} \cdot (pψ)$$

(III-D-1)

Equation (III-D-1) is the same as the equation of continuity in fluid mechanics when the orientation distribution function is replaced by the mass density. For this reason equation (III-D-1) is also referred to as the equation of continuity. Another common name for equation (III-D-1) is the Fokker-Planck equation.

In equation (III-D-1) the rate of change of the orientation vector, $\dot{p}$ was given by equation (III-C-5). Using this result, equation (III-D-1) can be rewritten as:

$$\frac{∂ψ}{∂t} = -\frac{∂}{∂p} \cdot [(κ \cdot p - κ \cdot \dot{p} \cdot p)ψ]$$

(III-D-2)

If the fibers are initially randomly dispersed, then the initial orientation distribution function is a constant. In order to normalize $ψ$ to unity, this constant is set equal to $1/4π$. Physically, this value corresponds to a point located
on the surface of a unit sphere.

Equation (III-D-2) is analogous to the diffusion equation in the kinetic theory of polymer solutions. The difference being that equation (III-D-2) does not contain the diffusion term which would account for Brownian motions. For this problem, the particles are simply convected by the bulk flow. Therefore, equation (III-D-2) should perhaps be called the convection equation. The solution for the orientation distribution function is provided in section (IV-B).
E. EFFECTIVE DRAG COEFFICIENT

The effective drag coefficient is a measure of the particle-particle interactions in a semi-concentrated suspension. In this analysis we are seeking the order of magnitude of $\zeta_{\text{eff}}$. Consequently terms of order 1 are neglected. This quantity is estimated by comparing the work required to move a test particle in two corresponding situations. As diagramed in Figure (III-E-1), a test particle is immersed in an effective medium in the continuum model, whereas the same test particle is shown with its nearest neighbor in the structural approach. Long range effects are neglected in the following argument.

When a suspension is deformed, the particles are rearranged. In the course of these internal motions, the interactions between particles are dominated by fibers that are separated by a distance $a_c$, where $a_c$ is the distance between a particle and its nearest neighbor. In the continuum model (Figure III-E-1), the work required to displace a test fiber over a distance $a_c$ for a given period $\Delta t$ is given by the product of the effective drag coefficient, the relative velocity between the particle and the mean field, and the displacement.

$$W = \zeta_{\text{eff}} \frac{a_c}{\Delta t}$$  \hspace{1cm} (III-E-1)

In the structural model (Figure III-E-1), when the test fiber moves over a distance $a_c$, the nearest neighbor has to move out of its original position in order to prevent a head-
Continuum model

Effective medium

Test fiber

\[ W = \zeta_{\text{eff}} \left( \frac{a_c}{\Delta t} \right) a_c \]

Structural model

Nearest neighbor

Test fiber

\[ W = \zeta \left( \frac{l}{\Delta t} \right) l \]

Figure III-E-1 Estimate of the effective drag coefficient
on collision. We are assuming that in the semi-concentrated region, the spacing between particles is sufficiently large to avoid solid-solid contacts. Instead, all interactions are transmitted in the form of hydrodynamic forces. In this case the neighboring particle is displaced along its axis by a distance of approximately a fiber length for the same time interval $\Delta t$. The work required to execute this motion would then be:

$$W \sim \zeta \left( \frac{1}{\Delta t} \right)$$  \hspace{1cm} (III-E-2)

where $\zeta$ is the drag coefficient of a fiber in a Newtonian liquid. Hence the effective drag coefficient is determined by setting equation (III-E-1) equal to equation (III-E-2).

$$\zeta_{\text{eff}} = \zeta \left( \frac{1}{a_c} \right)^2$$  \hspace{1cm} (III-E-3)

The inter-particle distance $a_c$ has been given in equation (III-A-1) for the case of a random distribution of particles. Substituting this value into equation (III-E-3) we obtain:

$$\zeta_{\text{eff}} = \zeta (nl^3)^2$$  \hspace{1cm} (III-E-4)

The drag coefficient of a cylinder in a Newtonian liquid has been investigated by Burgers (1938), Broersma (1960), Cox (1965), Tillett (1970). If terms of order 1 are neglected, then this quantity is approximated by the product of the solvent viscosity and the length of the particle. Therefore, the effective drag coefficient can be rewritten as:

$$\zeta_{\text{eff}} \sim \eta_s (nl^3)^2$$  \hspace{1cm} (III-E-5)
With this result, the stress tensor becomes:

\[ \mathbf{I} = -\eta_s \mathbf{\ddot{X}} - \eta_s (\frac{nl_1^2}{12}) \mathbf{\int X: PPP \psi dp} \quad (\text{III-E-6}) \]
F. POTENTIAL DIFFICULTIES

The effective drag coefficient has been estimated on the assumption that the separation between particles is much less than the distance over which hydrodynamic disturbances are important. To assess the validity of the physics used to evaluate \( \zeta_{\text{eff}} \), we shall first inspect each of these length scales.

The characteristic length scale for hydrodynamic disturbance is a measure of the farthest particle that can interfere with the test fiber. This dimension is denoted by \( a_h \). In general \( a_h \) varies with the orientation of the particles, and therefore depends on the history of the flow field. For a random distribution of fibers, \( a_h \) is on the order of a fiber diameter because all the particles are aligned along the streamlines (Batchelor, 1971). However, the precise dependence of \( a_h \) on the orientation of the particles, or on the history of the flow is not known.

A second quantity that varies with the history of the flow is the separation between the nearest neighboring particles which has been denoted by \( a_c \). Doi and Edwards (1978) have determined that the transient behavior of \( a_c \) is given by:

\[
a_c = \left( 2n 1^2 \int |\mathbf{p} \times \mathbf{p}'| \psi(\mathbf{p}', t) d\mathbf{p}' \right)^{-1} \tag{III-F-1}
\]

where \( \mathbf{p}' \) is the unit vector that describes the configuration of the nearest neighbor, \( \psi(\mathbf{p}', t) \) is the probability of locating an adjacent particle with orientation \( \mathbf{p}' \), and \( |\mathbf{p} \times \mathbf{p}'| \) is the sine
of the angle between the unit vectors $\mathbf{p}$ and $\mathbf{p}'$. If all the particles are randomly distributed then $\psi(\mathbf{p}', t) = \frac{1}{4\pi}$, and $a_c$ is given by:

$$a_c = \frac{2}{\pi} \frac{(1)}{n!^2} \sim \frac{1}{n!^2}$$  \hspace{1cm} (III-F-2)

Earlier in this chapter the value of $a_c$ for a random distribution of fibers has been employed to distinguish three concentration regimes in which the suspension would exhibit different rheological behaviors. In this section we reconsider these limits by incorporating the length scale $a_h$, and point out the complexity of including $a_h$ in the analysis. These concentration regimes are listed in Table (III-F-1).

The dilute regime is the region in which the separation between particles is greater than the length scale of the hydrodynamic disturbance. Consequently, a suspension may be non-dilute at the start of an experiment due to the random orientation of the particles, but may end up as a dilute suspension when steady-state is attained, or when all the particles are aligned into a steady configuration. Because of this fact, Batchelor(1971) was able to calculate the stress generated in a non-dilute suspension of elongated particles in a straining flow at steady state by multiplying the stress contribution from one particle by the total number of particles.

When the separation between particles is less than the length scale of the hydrodynamic disturbance, then two possibilities may occur; either $a_c < d$ or $d < a_c < a_h$. The case of $a_c < d$ corresponds to the concentrated regime which is not pursued in
Table III-F-1  Summary of the concentration regimes and the associated constitutive equations

<table>
<thead>
<tr>
<th>Regime</th>
<th>Particle spacing</th>
<th>Constitutive equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilute</td>
<td>$a_c &gt; a_n$</td>
<td>$\xi = -\eta_s \dot{\gamma} - \frac{n l^2}{12} \zeta \psi \rho \psi dp$</td>
</tr>
<tr>
<td>Semi-concentrated</td>
<td>$d &lt; a_c &lt; a_n$</td>
<td>$\xi = -\eta_s \dot{\gamma} - \frac{n l^2}{12} \zeta_{eff} \psi \rho \psi dp$</td>
</tr>
<tr>
<td>Concentrated</td>
<td>$d &gt; a_c$</td>
<td></td>
</tr>
</tbody>
</table>
this work.

The scaling argument presented in Section (III-E) for obtaining $\zeta_{\text{eff}}$ is directed toward the case of $d < a_c < a_h$. In general the length scales $a_c$ and $a_h$ are functions of the particle orientation, with $a_c$ given by equation (III-F-1), and $a_h$ bound between $d$ and $l$. Consequently, the effective drag coefficient, $\zeta_{\text{eff}}$, that appears in the bulk stress (equation III-C-7) also depends on the orientation of the particle. Although the transient behavior of $\zeta_{\text{eff}}$ can be included by inserting $a_c$ in equation (III-F-1) into $\zeta_{\text{eff}}$ in equation (III-E-3), the transition region from a non-dilute to a dilute suspension is unclear because of the uncertainty in $a_h$. The physics employed in estimating $\zeta_{\text{eff}}$ in a non-dilute suspension (Section III-E) is invalid for a dilute suspension because there is no longer any interactions between adjacent particles in the later case.

In spite of this difficulty, the values of $a_c$ and $a_h$ are known for a random distribution of fibers in which $a_c \sim \frac{1}{n l^2}$ and $a_h \sim l$. Furthermore the semi-concentrated regime defined in Table (III-A-1) ensures that $d < a_c < a_h$. These results for $a_c$ and $a_h$ coupled with the estimate of $\zeta_{\text{eff}}$ in Section (III-E) then lead to the constitutive equation that is shown in equation (III-E-6). Therefore, the error in utilizing the stress tensor in equation (III-E-6) to estimate the rheological properties of the suspension may increase as the system tends toward steady-state. However, this error is minimized in flow fields where the solid contribution to the bulk
stress (the second term on the right hand side of equation III-C-7) vanishes at steady-state. In other words, if the effective drag force on a test fiber decreases as the particle approaches a steady configuration then the errors made in estimating the effective drag coefficient would be minimized. An example of such a flow situation is a simple steady shear flow, whereas an extensional flow is a counterexample. Each of these flow fields will be investigated in Chapter V.
CHAPTER IV
RHEOLOGICAL EQUATION OF STATE

In the preceding chapter the rheological equation of state has been established for a semi-concentrated suspension of fibers in homogeneous flows. Before this constitutive equation can be employed to predict rheological properties, there is a need to evaluate the particle motion and the orientation distribution function. The solutions to these quantities are presented in this chapter. The bulk stress, developed from the structural approach, is then related to various continuum models.

A. SOLUTION TO THE EQUATION OF MOTION

The equation of motion describes the kinematics of a test particle that is immersed in an effective medium. The governing equation has been obtained in Section (III-D); from which the rate of change of the orientation vector is given by:

$$ \dot{p} = \kappa \cdot p - \kappa : \mathbf{PP} $$  \hspace{1cm} (IV-A-1)

with the initial condition,

$$ t = 0, \quad p = p_0 $$  \hspace{1cm} (IV-A-2)

where $p_0$ is the initial orientation of a fiber. Before presenting the solution to this system of first order non-linear equations, which is prerequisite toward the calculation of the orientation distribution function, a brief review of the
displacement and the strain functions is given here. The
details on this subject are discussed in Chapter 9 of Bird,

1. Displacement and strain functions in homogeneous flows

The bulk deformation of a fluid can be completely
characterized in terms of displacement functions. These
functions relate the position of a material point at the
present time, \( \mathbf{x} \), with respect to its location at the start of
the flow, \( \mathbf{x}' \). Therefore, the entire history of the flow
field is contained in the displacement function which can be
formally expressed as:

\[
\mathbf{x} = \mathbf{x}(\mathbf{x}', t)
\]  \hspace{1cm} (IV-A-1)

It is generally assumed that equation (IV-A-1) can be inverted
so that the displacement function \( \mathbf{x}' \) can be written in terms
of the vector \( \mathbf{x} \).

The relative displacement of a material point from its
initial location defines the strain tensor \( \mathbf{E} \). In cartesian
coordinates the components of \( \mathbf{E} \) are given by:

\[
E_{ij} = \frac{\partial x_i}{\partial x'_j}
\]  \hspace{1cm} (IV-A-2)

In a homogeneous flow the displacement function varies
linearly with the fixed spatial coordinates. Consequently
the strain tensor is independent of position, but it can be
time dependent. At the start of the flow, \( \mathbf{x} = \mathbf{x}' \), hence the
strain tensor \( \mathbf{E} \) is equal to the unit tensor \( \mathbb{I} \).
The inverse of the strain tensor $\mathbb{E}$ is another strain tensor $\mathbb{A}$. The components of $\mathbb{A}$ are:

$$\Delta_{ij} = \frac{\partial x_i}{\partial x_j}$$  \hspace{1cm} (IV-A-3)

Before returning to the solution of the orientation vector, we list a few useful properties of the strain tensors $\mathbb{E}$ and $\mathbb{A}$.

a) Properties of a tensor and its inverse

$$\mathbb{E} \cdot \mathbb{A} = \mathbb{A} \cdot \mathbb{E} = \mathbb{1}$$ \hspace{1cm} (IV-A-4)

where $\mathbb{1}$ is the unit tensor.

b) The determinant of the strain tensors for an incompressible fluid.

$$\det(\mathbb{E}) = \det(\mathbb{A}) = 1$$ \hspace{1cm} (IV-A-5)

c) The time derivative of $\mathbb{E}$

$$\frac{\partial \mathbb{E}}{\partial t} = \frac{\partial}{\partial t} \frac{\partial x_i}{\partial x_j}$$

$$= \frac{\partial}{\partial x_j} \frac{\partial x_i}{\partial t}$$

$$= \frac{\partial x_k}{\partial x_j} \frac{\partial}{\partial x_k} \frac{\partial x_i}{\partial t}$$

$$= (\frac{\partial}{\partial x_i} \frac{\partial x_k}{\partial t}) \frac{\partial x_k}{\partial x_j}$$

$$= \{\nabla \mathbf{v}\}^T \cdot \mathbb{E}$$

$$= \mathbb{K} \cdot \mathbb{E}$$ \hspace{1cm} (IV-A-6)

Based on the results in equations (IV-A-4) and (IV-A-6), the time derivative of $\mathbb{A}$ is:

$$\frac{\partial \mathbb{A}}{\partial t} = -\mathbb{A} \cdot \mathbb{K}$$ \hspace{1cm} (IV-A-7)
The transpose of the time derivatives of the strain tensors \( E \) and \( \dot{A} \) can be readily written down by recalling that the transpose of a product is \((A \cdot E)^\dagger = E^\dagger \cdot A^\dagger\).

With the above relations, the displacement functions in a homogeneous flow can be determined. For this type of flow, the bulk velocity \( \dot{X} \) can be expressed as:

\[
\dot{X} = \frac{\partial}{\partial t} X = \dot{E} \cdot X \tag{IV-A-8}
\]

with,

\[
X = X' \quad \text{at } t = 0 \tag{IV-A-9}
\]

The displacement function \( X \) is then evaluated by taking advantage of the result in equation (IV-A-6).

\[
X = E \cdot X' \tag{IV-A-10}
\]

The relations developed in this section will be frequently referred to in the rest of this chapter.

2. The orientation vector \( \rho \)

The solution to equation (IV-A-1) with the initial condition provided in equation (IV-A-2) can be arrived in a number of ways. Perhaps the easiest approach to solve this problem is to relate equation (IV-A-1) to the physical situation which it is describing. As indicated in Section (III-D), equation (IV-1) says that the test fiber moves affinely except that the fiber cannot stretch. In order for the unit vector \( \rho \) to deform affinely, the direction of \( \rho \) is given by \( E \cdot \rho_0 \) according to the result in equation (IV-A-10). But in order simultaneously to preserve the length of the unit
vector \( \mathbf{p} \), the vector \( \mathbf{E} \cdot \mathbf{p}_0 \) is normalized to unity. Therefore, we postulate that the solution of equation (IV-A-1) is:

\[
P = \frac{\mathbf{E} \cdot \mathbf{p}_0}{(\mathbf{E}^T \cdot \mathbf{E} \cdot \mathbf{p}_0 \mathbf{p}_0)^{\frac{3}{2}}} \quad \text{(IV-A-11)}
\]

where the denominator is the length of the vector \( \mathbf{E} \cdot \mathbf{p}_0 \).

To verify this result, equation (IV-A-11) is substituted back into the governing equation and the initial condition. First, the time derivative of \( p \) given by equation (IV-A-11) leads to:

\[
\frac{\partial \mathbf{p}}{\partial t} = \frac{1}{(\mathbf{E}^T \cdot \mathbf{E} \cdot \mathbf{p}_0 \mathbf{p}_0)^{\frac{3}{2}}} \mathbf{E} \cdot \mathbf{p}_0 - \frac{1}{(\mathbf{E}^T \cdot \mathbf{E} \cdot \mathbf{p}_0 \mathbf{p}_0)^{\frac{3}{2}}} \mathbf{E} : (\mathbf{E} \cdot \mathbf{p}_0)(\mathbf{E} \cdot \mathbf{p}_0)(\mathbf{E} \cdot \mathbf{p}_0)
\]

\[
= \mathbf{E} \cdot \mathbf{p} - \mathbf{E} : \mathbf{p} \mathbf{p} \mathbf{p} \quad \text{(IV-A-12)}
\]

Hence, the solution to \( \mathbf{p} \) in equation (IV-A-11) satisfies its governing equation. Next, we consider the initial condition. At \( t = 0 \), the strain tensor \( \mathbf{E} \) equals to the unit tensor \( \mathbf{I} \).

This result leads to \( \mathbf{p} = \mathbf{p}_0 \). Therefore, equation (IV-A-11) is a solution for the orientation vector \( \mathbf{p} \) because it satisfies both the governing equation and the initial condition.

In the next chapter, the orientation of the particles in various homogeneous flows will be illustrated by means of equation (IV-A-11).
B. SOLUTION TO THE ORIENTATION DISTRIBUTION FUNCTION

The orientation distribution function $\psi(p, t)$ describes the probability that a fiber is aligned in the range of the vectors $p$ to $p + dp$ at time $t$. The governing equation is obtained in Section (III-B) in which:

$$\frac{\partial \psi}{\partial t} = -\frac{\partial}{\partial p} \cdot \left( \kappa \cdot p - \kappa : \dot{p} p \right) \quad (IV-B-1)$$

and,

$$\psi = \frac{1}{4\pi} \quad \text{at } t = 0 \quad (IV-B-2)$$

The techniques to solve this first-order partial differential equation can be found in standard references (Hildebrand, 1976; Aris and Amundson, 1973). In this section we present two methods to obtain the solution of $\psi(p, t)$. The first approach employs the method of characteristics whereas the second one is based on physical deductions.

1. Method of characteristics

The procedure to solve a first order partial differential equation by the method of characteristics is to reduce the partial differential equation into a system of ordinary differential equations. The set of ordinary differential equations are the characteristic equations, and their solutions define the characteristic curves. For the problem considered in this section, the governing equation (equation IV-B-1) can be rewritten as:
\[
\frac{\partial \psi}{\partial t} + (\kappa \cdot \mathbf{p} - \kappa \cdot \mathbf{PP}) \cdot \frac{\partial \psi}{\partial \mathbf{p}} = 3(\kappa \cdot \mathbf{pp}) \psi
\]

(IV-B-3)

The formal solution to equation (IV-B-3) can be expressed as:

\[
G(\mathbf{p}, t, \psi) = \psi(\mathbf{p}, t) - \psi = 0
\]

(IV-B-4)

After differentiating equation (IV-B-4) with respect to \(t\), and matching the result with equation (IV-B-3) the following set of ordinary differential equations are obtained.

\[
\frac{d}{dt} \psi = 3(\kappa \cdot \mathbf{pp}) \psi
\]

(IV-B-5)

\[
\frac{d}{dt} \mathbf{p} = \kappa \cdot \mathbf{p} - \kappa \cdot \mathbf{PP}
\]

(IV-B-6)

with the initial conditions,

\[
\psi = \frac{1}{4\pi} \quad \text{at} \quad t = 0
\]

(IV-B-7)

\[
\mathbf{p} = \mathbf{p}_0 \quad \text{at} \quad t = 0
\]

(IV-B-8)

Equation (IV-B-6) is readily recognized as the equation of motion for which the solution has been obtained in Section (IV-A).

\[
\mathbf{p} = \frac{\mathbf{E} \cdot \mathbf{p}_0}{(\mathbf{E} \cdot \mathbf{E} \cdot \mathbf{p}_0 \cdot \mathbf{p}_0)^{\frac{3}{2}}}
\]

(IV-B-9)

This result is substituted into equation (IV-B-5) to give:

\[
\frac{d\psi}{dt} = 3\kappa \cdot (\mathbf{E} \cdot \mathbf{p}_0)(\mathbf{E} \cdot \mathbf{p}_0) \psi
\]

(IV-B-10)

Using equation (IV-A-6) for the time derivative of \(\mathbf{E}\), equation (IV-B-10) is converted to:
\[ d(\ln \psi) = -3d(\ln (\mathbf{E}^\top \mathbf{E} : \mathbf{P} \mathbf{P}_0)^{3/2}) \quad (\text{IV-B-11}) \]

along with the initial condition that

\[ \psi = \frac{1}{4\pi}, \quad \mathbf{E} = \mathbf{0} \quad \text{at } t = 0 \quad (\text{IV-B-12}) \]

Equation (IV-B-11) is then integrated to give:

\[ \psi = \frac{1}{4\pi} (\mathbf{E}_0^\top \mathbf{E}_0 : \mathbf{P} \mathbf{P}_0)^{3/2} \quad (\text{IV-B-13}) \]

Thus far we have proceeded to solve the characteristic equations. The crucial step in the method of characteristics is to be able to convert \( \mathbf{P}_0 \) back to \( \mathbf{P} \) in equation (IV-B-13) because the orientation distribution function depends on \( \mathbf{P} \) and \( t \). This step can be carried out by inserting the strain tensor \( \mathbf{A} \), which is the inverse of \( \mathbf{E}_0 \), into equation (IV-B-9). Then,

\[ \mathbf{E}_0^\top \mathbf{E}_0 : \mathbf{P} \mathbf{P}_0 = (\mathbf{A}_0^\top \mathbf{A}_0 : \mathbf{P} \mathbf{P})^{-1} \quad (\text{IV-B-14}) \]

Therefore, the solution to the orientation distribution function is given by:

\[ \psi(\mathbf{P}, t) = \frac{1}{4\pi} (\mathbf{A}_0^\top \mathbf{A}_0 : \mathbf{P} \mathbf{P})^{-3/2} \quad (\text{IV-B-15}) \]

Equation (IV-B-15) is verified in Appendix 2. Prior to substituting this result into the stress tensor, we shall discuss a different approach to determine the orientation distribution function from physical deduction.

2. An alternative solution

The idea behind this solution scheme is to assess the nature of the forces that act on the particles. In this
system, the dimensions of the fibers are sufficiently large so that Brownian motion would be negligible. The analysis presented in this work has been focused on a test fiber with the interactions between particles modeled by an effective medium. Therefore, in the absence of an external force, the motion of the test fiber is solely determined by the hydrodynamic force from the effective medium. In this case the kinematics of the test fiber is deterministic which means that the path of the particle is unique once the initial orientation of the test fiber is specified.

Since there is no uncertainty in the motion of the particle, the purpose of the orientation distribution function is to follow the trajectory of a fiber from its initial orientation to a configuration at a later time \( t \). Therefore, the orientation distribution function can be specified by a Dirac delta function.

\[
\psi(p, t) = \frac{1}{4\pi} \delta(p - b(p_0, t)) dp_0 \quad (IV-B-16)
\]

In equation (IV-B-16), the unit vector \( b \) specifies the instantaneous orientation of a test fiber. If the fibers in the suspension are initially randomly distributed, then the initial orientation of each fiber is arbitrary. In order to ensure that all fibers have been accounted for, the Dirac delta function is integrated over all possible initial configurations \( p_0 \). The factor of \( \frac{1}{4\pi} \) in equation (IV-B-16) is to normalize \( \psi \) to unity.

To determine the motion of the test fiber, which in this
case is characterized by the unit vector $\mathbf{b}(\mathbf{p}_0,t)$, the equation of motion is once again used. The trajectory is given by equation (IV-A-11). Consequently, the orientation distribution function can be expressed as:

$$\psi(\mathbf{p},t) = \frac{1}{4\pi} \delta(\mathbf{p} - \frac{\mathbf{E} \cdot \mathbf{p}_0}{(\mathbf{E}^\top \mathbf{E} : \mathbf{p}_0 \mathbf{p}_0)^{\frac{1}{2}}}) d\mathbf{p}_0$$  (IV-B-17)

The result shown in equation (IV-B-17) is the solution to the governing equation for $\psi$ (equation IV-B-1) by the method of Green's function. Although this solution (equation IV-B-17) may not seem to appear like the one shown in equation (IV-B-15), the equivalence of these two results will be shown in the next section.

3. Equivalent forms of $\psi(\mathbf{p},t)$

The objective of this section is to demonstrate that the results for the orientation distribution function presented in equations (IV-B-15) and (IV-B-17) are identical. Beginning with equation (IV-B-16), the plan is to convert the integration variable from $d\mathbf{p}_0$ to $d\mathbf{b}$. This transformation can be carried out by evaluating the Jacobian, $J$, of the vectors $\mathbf{p}_0$ and $\mathbf{b}$ because

$$d\mathbf{p}_0 = J d\mathbf{b}$$  (IV-B-18)

To illustrate the procedure for calculating the Jacobian, spherical coordinates are used for simplicity. The components of the unit vector $\mathbf{b}$ are denoted by $(\theta, \phi)$, and the components

* For details, see chapter 3 of Aris(1962).
of \( \mathbf{p}_0 \) are \((\theta_0, \phi_0)\). These spherical angles are shown in Figure (III-B-1). Furthermore, we define a triad of orthonormal vectors \((\mathbf{b}, \mathbf{\delta}_{\theta_0}, \mathbf{\delta}_{\phi_0})\) and a second triad of orthonormal vectors \((\mathbf{p}_0, \mathbf{\delta}_{\theta_0}, \mathbf{\delta}_{\phi_0})\). Any second order tensor can be spanned by this set of basis vectors. For example, the components of the strain tensor \( \mathbf{\Delta} \) are:

\[
\mathbf{\Delta} = \begin{bmatrix}
\mathbf{\Delta} : \mathbf{b} \mathbf{p}_0 & \mathbf{\Delta} : \mathbf{b} \mathbf{\delta}_{\theta_0} & \mathbf{\Delta} : \mathbf{b} \mathbf{\delta}_{\phi_0} \\
\mathbf{\Delta} : \mathbf{\delta}_{\theta_0} \mathbf{p}_0 & \mathbf{\Delta} : \mathbf{\delta}_{\theta_0} \mathbf{\delta}_{\theta_0} & \mathbf{\Delta} : \mathbf{\delta}_{\theta_0} \mathbf{\delta}_{\phi_0} \\
\mathbf{\Delta} : \mathbf{\delta}_{\phi_0} \mathbf{p}_0 & \mathbf{\Delta} : \mathbf{\delta}_{\phi_0} \mathbf{\delta}_{\theta_0} & \mathbf{\Delta} : \mathbf{\delta}_{\phi_0} \mathbf{\delta}_{\phi_0}
\end{bmatrix} \quad (IV-B-19)
\]

Having established the coordinate system, the Jacobian of this problem is defined by:

\[
J = \frac{\sin \theta_0}{\sin \theta} \left( \frac{\partial \theta_0}{\partial \theta} \frac{\partial \phi}{\partial \phi} - \frac{\partial \theta_0}{\partial \phi} \frac{\partial \theta}{\partial \phi} \right) \quad (IV-B-20)
\]

In order to determine the partial derivatives which appear in equation (IV-B-20), we shall express the unit vector \( \mathbf{p}_0 \) in terms of \( \mathbf{b} \) by means of equations (IV-A-11) and (IV-A-14).

\[
\mathbf{p}_0 = \frac{\mathbf{\Delta} : \mathbf{b}}{(\mathbf{\Delta}^\top \mathbf{\Delta} : \mathbf{b} \mathbf{b})^{\frac{1}{2}}} \quad (IV-B-21)
\]

At this juncture several useful relations can be obtained from (IV-B-21) by noting that \((\mathbf{p}_0 \cdot \mathbf{p}_0) = 1\), and \((\mathbf{p}_0 \cdot \mathbf{\delta}_{\theta_0}) = (\mathbf{p}_0 \cdot \mathbf{\delta}_{\phi_0}) = 0\). Hence,

\[
(\mathbf{\Delta}^\top \mathbf{\Delta} : \mathbf{b} \mathbf{b})^{\frac{1}{2}} = \mathbf{\Delta} : \mathbf{b} \mathbf{p}_0 \quad (IV-B-22)
\]

\[
(\mathbf{\Delta} : \mathbf{b} \mathbf{\delta}_{\theta_0}) = 0 \quad (IV-B-23)
\]

and,

\[
(\mathbf{\Delta} : \mathbf{b} \mathbf{\delta}_{\phi_0}) = 0 \quad (IV-B-24)
\]

To calculate the partial derivatives in the Jacobian, we
employ equation (IV-B-21) to construct a null vector
\( \mathbf{H}(\theta, \phi, \theta_o, \phi_o) \) which is given by:
\[
\mathbf{H}(\theta, \phi, \theta_o, \phi_o) = \mathbf{p} - \frac{\mathbf{A} \cdot \mathbf{b}}{(\mathbf{A}^\top \mathbf{A} : \mathbf{b} b^2)^{1/2}} = 0 \quad \text{(IV-B-25)}
\]

From equation (IV-B-25) the following relations are derived by applying the chain rule:
\[
\frac{\partial H}{\partial \theta} + \frac{\partial H(\partial \theta_\theta)}{\partial \theta_\theta} + \frac{\partial H(\partial \theta_\phi)}{\partial \theta_\phi} = 0 \quad \text{(IV-B-26)}
\]
and,
\[
\frac{\partial H}{\partial \phi} + \frac{\partial H(\partial \phi_\theta)}{\partial \phi_\theta} + \frac{\partial H(\partial \phi_\phi)}{\partial \phi_\phi} = 0 \quad \text{(IV-B-27)}
\]

The partial derivatives of \( H \) with respect to the independent variables \( \theta, \phi, \theta_o, \phi_o \) would require the derivatives of the unit vectors. A convenient list of these relations is shown in Table IV-B-1. With these properties equations (IV-B-26) and (IV-B-27) become:
\[
\frac{\partial H}{\partial \theta} + \delta_{\theta_\theta} \frac{\partial H(\partial \theta_\theta)}{\partial \theta_\theta} + (\sin \theta_o) \delta_{\theta_\phi} \frac{\partial H(\partial \phi_\phi)}{\partial \theta_\phi} = 0 \quad \text{(IV-B-28)}
\]
and,
\[
\frac{\partial H}{\partial \phi} + \delta_{\phi_\theta} \frac{\partial H(\partial \phi_\theta)}{\partial \phi_\theta} + (\sin \theta_o) \delta_{\phi_\phi} \frac{\partial H(\partial \phi_\phi)}{\partial \phi_\phi} = 0 \quad \text{(IV-B-29)}
\]

The partial derivatives in the Jacobian can be readily identified from equation (IV-B-28) and equation (IV-B-29).
\[
\frac{\partial \theta_\theta}{\partial \theta} = -\delta_{\theta_\theta} \frac{\partial H}{\partial \theta} = (\mathbf{A}^\top \mathbf{A} : \mathbf{b} b^2)^{-1/2} (\mathbf{A} : \delta_{\theta} \delta_{\theta_\theta}) \quad \text{(IV-B-30)}
\]
Table IV-B-1  The derivatives of the unit vectors

\[ \frac{\partial \hat{b}}{\partial \theta} = \delta \theta \]
\[ \frac{\partial \hat{b}}{\partial \phi} = \sin \theta \delta \phi \]

\[ \frac{\partial \delta \theta}{\partial \theta} = -b \]
\[ \frac{\partial \delta \theta}{\partial \phi} = \cos \theta \delta \phi \]

\[ \frac{\partial \delta \phi}{\partial \theta} = 0 \]
\[ \frac{\partial \delta \phi}{\partial \phi} = -\sin \theta \hat{b} - \cos \theta \delta \theta \]
\[
\frac{\partial \phi_o}{\partial \theta} = -\frac{1}{\sin \theta_o} \frac{\delta \phi_o}{\delta \theta} \cdot \frac{\partial H}{\partial \theta} \\
= \frac{1}{\sin \theta_o} (\Delta^\dagger \Delta : \mathbf{b} \mathbf{b})^{-\frac{1}{2}} (\Delta : \delta \phi_o \delta \phi_o) \\
(IV-B-31)
\]

\[
\frac{\partial \theta_o}{\partial \phi} = -\frac{\delta \theta_o}{\delta \phi} \cdot \frac{\partial H}{\partial \phi} \\
= (\sin \theta)(\Delta^\dagger \Delta : \mathbf{b} \mathbf{b})^{-\frac{1}{2}} (\Delta : \delta \phi_o \delta \phi_o) \\
(IV-B-32)
\]

\[
\frac{\partial \phi_o}{\partial \phi} = -\frac{1}{\sin \theta_o} \frac{\delta \phi_o}{\delta \phi} \cdot \frac{\partial H}{\partial \phi} \\
= \frac{\sin \theta}{\sin \theta_o} (\Delta^\dagger \Delta : \mathbf{b} \mathbf{b})^{-\frac{1}{2}} (\Delta : \delta \phi_o \delta \phi_o) \\
(IV-B-33)
\]

With these results the Jacobian is given by:

\[
J = (\Delta^\dagger \Delta : \mathbf{b} \mathbf{b})^{-1} ((\Delta : \delta \phi_o \delta \phi_o) (\Delta : \delta \phi_o \delta \phi_o)) - (\Delta : \delta \phi_o \delta \phi_o) (\Delta : \delta \phi_o \delta \phi_o)) \\
= (\Delta^\dagger \Delta : \mathbf{b} \mathbf{b})^{-3/2} (\Delta : \mathbf{b} \mathbf{b} \delta \phi_o \delta \phi_o) (\Delta : \delta \phi_o \delta \phi_o) - \\
(\Delta : \delta \phi_o \delta \phi_o) (\Delta : \delta \phi_o \delta \phi_o)) \\
= (\Delta^\dagger \Delta : \mathbf{b} \mathbf{b})^{-3/2} (\text{det} \Delta) \\
(IV-B-34)
\]

The last line is obtained by means of the relations given from equation (IV-B-22) to equation (IV-B-24). For an incompressible fluid the determinant of the strain tensor \( \Delta \) is unity.

At last the transformation for the integration variable is complete.

\[
d\phi_o = (\Delta^\dagger \Delta : \mathbf{b} \mathbf{b})^{-3/2} d\mathbf{b} \\
(IV-B-35)
\]

Inserting equation (IV-B-35) into equation (IV-B-16), the orientation distribution function is given by:

\[
\psi(p, t) = \frac{1}{4\pi} \int (\Delta^\dagger \Delta : \mathbf{b} \mathbf{b})^{-3/2} \delta(p - \mathbf{b}) d\mathbf{b}
\]
\[
\frac{1}{4\pi} (\Delta^+ \Delta : \mathbf{p} \mathbf{p})^{-3/2}
\]  

Hence, the result for \( \psi(\mathbf{p}, t) \) in equation (IV-B-16) is identical to the one obtained by the method of characteristics (equation IV-B-15).

In retrospect the two approaches for determining the orientation distribution function can be geometrically envisioned in the following way. The method of characteristics describes the transition of a flat surface that converges into a straight line with time. The points on this "funnel-shaped" surface correspond to the probability of locating a particle that is pointed in the direction \( \mathbf{p} \) at time \( t \).

In the second method we follow the trajectory of a fiber that has an initial orientation \( \mathbf{p}_0 \). Then we sum up the contribution from each possible \( \mathbf{p}_0 \) weighted by the fraction of fibers with that value. The locus of the weighted sum of all these trajectories then maps out the "funnel-shaped" surface described by the method of characteristics.
C. CONSTITUTIVE EQUATIONS

The stress tensor for a suspension of rigid fibers in homogeneous flows has been established in Section (III-D). The result, shown in equation (III-D-7), requires a separate equation to determine the orientation distribution equation. This quantity has been evaluated in the last section. Therefore, the remaining task is to substitute the orientation distribution function into the expression for the stress tensor, and obtain a single expression for the constitutive equation.

In this section, we shall first present the various equivalent forms of the constitutive equation as derived from the structural approach. Then, we shall identify these results with some continuum models. From this comparison, the coefficients in the corresponding continuum models can be related to the microstructural properties of the suspension.

1. Structural Models

In this section the equivalent forms of the constitutive equation, derived from the structural approach are summarized. The first one is obtained by inserting the orientation distribution function arrived from the method of characteristics (equation IV-B-15) into equation (III-D-7). Hence,

\[ \mathbf{I} = -\eta_{s} \dot{\gamma} - \eta_{s} (\mathbf{n} \mathbf{l}^{3})^{3} \frac{\mathbf{P}_{\mathbf{R}}}{12} \int \frac{\mathbf{P}_{\mathbf{R}}}{4\pi \left( \mathbf{A}^+ \cdot \mathbf{A}^{+BD} \right)^{3/2}} \, dp \]  

(IV-C-1)

Alternatively we can use equation (IV-B-17) for the orientation distribution function to arrive at:
\[
\mathbf{I} = \mathbf{\dot{\sigma}} - \eta \mathbf{\ddot{\sigma}} - \eta_s \frac{(n_l^3)}{2} \mathbf{K} : \left[ \left( \mathbf{E} \cdot \mathbf{p} \right) \left( \mathbf{E} \cdot \mathbf{p} \right) \left( \mathbf{E} \cdot \mathbf{p} \right) \right] \frac{\mathbf{d} \rho_0}{4\pi (\mathbf{E} \cdot \mathbf{p} \cdot \mathbf{p} \cdot \mathbf{p})^2}
\]

(IV-C-2)

Equation (IV-C-1) and equation (IV-C-2) are two identical representations of the stress tensor. These equations are referred to as the Kramers expression for the stress tensor. Alternatively the Kramers expression for the stress tensor can be transformed into the Giesekus expression for the stress tensor by noting that:

\[
\frac{d}{dt} \langle \mathbf{p} \mathbf{p} \rangle = \mathbf{K} \cdot \langle \mathbf{p} \mathbf{p} \rangle + \langle \mathbf{p} \mathbf{p} \rangle \mathbf{K}^T - 2\mathbf{K} : \langle \mathbf{p} \mathbf{p} \mathbf{p} \rangle
\]

(IV-C-3)

where the angular brackets mean that the quantity inside the brackets is averaged with respect to the orientation distribution function, \( \langle \mathbf{p} \mathbf{p} \rangle = \int \mathbf{p} \mathbf{p} \psi \mathbf{d} \rho \). The derivation of equation (IV-C-3) can be found in chapter 11 of Bird, Hassager, Armstrong and Curtiss (1977).

By means of the relation in equation (IV-C-3), the stress tensors in equations (IV-C-1) and (IV-C-2) can be rewritten as:

\[
\mathbf{I} = \mathbf{\dot{\sigma}} + \frac{\eta}{24} \left( \begin{array}{c} \mathbf{p} \mathbf{p} \mathbf{p} \\ \mathbf{d} \mathbf{d} \mathbf{d} \end{array} \right) \mathbf{K} : \left[ \left( \mathbf{E} \cdot \mathbf{p} \right) \left( \mathbf{E} \cdot \mathbf{p} \right) \left( \mathbf{E} \cdot \mathbf{p} \right) \right] \frac{\mathbf{d} \rho_0}{4\pi (\mathbf{E} \cdot \mathbf{p} \cdot \mathbf{p} \cdot \mathbf{p})^{3/2}}
\]

(IV-C-4)

and,

\[
\mathbf{I} = \mathbf{\dot{\sigma}} + \frac{\eta}{24} \left( \begin{array}{c} \mathbf{p} \mathbf{p} \mathbf{p} \\ \mathbf{d} \mathbf{d} \mathbf{d} \end{array} \right) \mathbf{K} : \left[ \left( \mathbf{E} \cdot \mathbf{p} \right) \left( \mathbf{E} \cdot \mathbf{p} \right) \right] \frac{\mathbf{d} \rho_0}{4\pi (\mathbf{E} \cdot \mathbf{p} \cdot \mathbf{p} \cdot \mathbf{p})^{3/2}}
\]

(IV-C-5)
The stress tensors, shown in equations (IV-C-4) and (IV-C-5), are referred to as the Giesekus form of the stress tensor.

In summary the equivalent forms of the stress tensor, obtained from the structural approach, are given in equation (IV-C-1) to equation (IV-C-4). The right-hand side in each of these equations contains two terms. The first one represents the contribution from the solvent to the bulk stress. The second term reflects the internal structure and the amount of solids in the suspension. A comparison between these two groups indicates that the second term can be orders of magnitude greater than the contribution from the solvent depending on the type of flows and on the microstructural properties of the particles. These calculations will be illustrated in the next chapter as part of characterizing the rheological properties of a suspension of rigid fibers in a number of homogeneous flows.

2. Continuum models

In this section, the constitutive equation derived from the structural approach is related to models developed from continuum mechanics. The models to be compared are the theory of anisotropic fluids (Hand, 1962), the Oldroyd 4-constant model, and a constitutive equation described by Curtiss and Bird (1980).

a) Ericksen-Hand model

The model proposed by Ericksen (1960) and Hand (1962) for an anisotropic fluid has been summarized in section (II-B).
The contribution to the bulk stress from the microstructure is characterized by a director vector $\mathbf{p}$, as shown in equation (II-B-1). The rate of change of the director vector is described by equation (II-B-2). In order to make the connection between the results of Ericksen and Hand and our structural model, the result in equation (IV-C-2) is rewritten to reflect the contribution from an arbitrary particle.

$$\mathbf{I}^b(p_0, t) = -\eta S \mathbf{v} - \eta S(\mathbf{n} \mathbf{l}^3)^3 \kappa : \mathbf{b} \mathbf{b} \mathbf{b}$$

(IV-C-6)

where $\mathbf{I}^b$ is the bulk stress if we follow the evolution of a single particle. In equation (IV-C-2) we have subsequently averaged over all possible trajectories because of the mixture of initial orientations. Therefore, the bulk stress written in terms of $\mathbf{I}^b$ is given by:

$$\mathbf{I} = \int \mathbf{I}^b(p_0, t) dp_0$$

(IV-C-7)

The expression governing the rate of change of $\mathbf{b} \mathbf{b}$ is obtained by modifying the equation of motion (equation III-D-5) to:

$$\frac{d}{dt} \mathbf{b} \mathbf{b} = \mathbf{k} : \mathbf{b} \mathbf{b} + \mathbf{b} \mathbf{b} : \mathbf{k} \mathbf{k}^\top - 2 \mathbf{k} : \mathbf{b} \mathbf{b} \mathbf{b}$$

(IV-C-8)

In equation (IV-C-8), $\mathbf{b}$ is a unit vector as in equation (III-C-5). Consequently the trace of this equation yields:

$$\mathbf{k} : \mathbf{b} \mathbf{b} = \frac{1}{2} \text{tr}(\mathbf{b} \mathbf{b} \mathbf{v})$$

(IV-C-9)

In this chapter we have determined the solution to the motion of the particle (equation IV-A-11). Therefore, the solution to equation (IV-C-8) is simply,
\[ \mathbf{b}_b = \frac{(\mathbf{e} \cdot \mathbf{p}_o) (\mathbf{e} \cdot \mathbf{p}_o)}{(\mathbf{e}^T \cdot \mathbf{e} \cdot \mathbf{p}_o \cdot \mathbf{p}_o)} \]  

(IV-C-10)

With these results, the previously undetermined coefficients appearing in the model of Ericksen and Hand are identified by comparing equation (IV-C-6) to equation (II-B-1) and equation (IV-C-8) to equation (II-B-2). These coefficients are given by:

\[ a_0 = p \]  

(IV-C-11)

\[ a_1 = a_2 = a_5 = 0 \]  

(IV-C-12)

\[ a_3 = -\eta_s \frac{(n_1^3)^3}{24} \]  

(IV-C-13)

\[ a_4 = -\eta_s \]  

(IV-C-14)

\[ b_0 = b_2 = b_3 = b_5 = 0 \]  

(IV-C-15)

\[ b_1 = -2(\xi : \mathbf{b}_b) \]  

(IV-C-16)

\[ b_4 = \frac{1}{2} \]  

(IV-C-17)

These results are consistent with the claims made by Hand (1962) that the coefficients \( a_i \) may be scalar invariants of the tensor \( \mathbf{b}_b \) only, whereas the coefficients \( b_i \) may be scalar invariants of the tensors \( \mathbf{b}_b \) and \( \mathbf{b}_b \).

b) Oldroyd 4-constant model

The structural model shown in either equation (IV-C-2) or equation (IV-C-5) can be rewritten in terms of a differential Oldroyd model in which the coefficients are expressed by the invariants of the stress tensor \( \mathbf{I}^b \). The stress tensor \( \mathbf{I}^b \) has been defined in equation (IV-C-6), its equivalent form is
given by:

\[ \mathbf{I}^b(p_0, t) = -\eta_s \dot{\mathbf{y}} + \eta_s (n_{13}^3)^3 \{ \mathbf{b} \} \]  

(IV-C-18)

where the codeformational time derivative is defined by:

\[ \mathbf{A}(1) = \frac{D}{Dt} \mathbf{A} - \mathbf{\kappa} \cdot \mathbf{A} - \mathbf{A} \cdot \mathbf{\kappa}^\top \]  

(IV-C-19)

with the recurrence formula,

\[ \mathbf{A}(n+1) = \frac{D}{Dt} \mathbf{A}(n) - \mathbf{\kappa} \cdot \mathbf{A}(n) - \mathbf{A}(n) \cdot \mathbf{\kappa}^\top \]  

(IV-C-20)

The plan is to express the tensor \( \mathbf{b} \) in terms of the invariants of \( \mathbf{I}^b \), and substitute this result into equation (IV-C-18) to eliminate \( \mathbf{b} \). The first step is to take the trace of equation (IV-C-6), and to note that for an incompressible fluid \( \text{tr}(\dot{\mathbf{y}}) = 0 \). Hence,

\[ \text{tr} \mathbf{I}^b = -\eta_s (n_{13}^3)^3 \kappa : \mathbf{b} \]  

(IV-C-21)

The structural tensor \( \mathbf{b} \) is obtained by substituting equation (IV-C-21) back into equation (IV-C-6):

\[ \mathbf{b} = \frac{1}{\text{tr} \mathbf{I}^b} (\mathbf{I}^b + \eta_s \dot{\mathbf{y}}) \]  

(IV-C-22)

Next, the result in equation (IV-C-22) is inserted into equation (IV-C-18) to yield:

\[ \mathbf{I}^b(p_0, t) = -\eta_s \dot{\mathbf{y}} + \eta_s (n_{13}^3)^3 \{ \frac{1}{\text{tr} \mathbf{I}^b} (\mathbf{I}^b + \eta_s \dot{\mathbf{y}}) \} \]  

(IV-C-23)

and the bulk stress is obtained from equation (IV-C-7).

It is interesting to note that the stress tensor \( \mathbf{I}^b \) has the appearance of a "4-constant Oldroyd" differential model (Bird, Armstrong, and Hassager, 1977) with the exception that
the coefficients are not constants, but are functions of $\text{tr}^{b}$. This empirical model is given by:

$$\dot{\text{I}}^{b} + \lambda_{1} \dot{\text{I}}_{(1)}^{b} + \frac{1}{2} \mu_{s} (\text{tr}^{b}) \dot{\text{Y}} = -\eta_{0} (\dot{\text{Y}} + \lambda_{2} \dot{\text{Y}}_{(1)})$$ (IV-C-24)

The coefficients in equation (IV-C-24) are determined by comparing with equation (IV-C-23).

$$\mu_{0} = 0$$ (IV-C-25)

$$\eta_{0} = \eta_{s}$$ (IV-C-26)

$$\lambda_{1} = \lambda_{2} = -\eta_{s} (n_{l}^{1})^{3} \left[ 4 + \frac{\eta_{s} (n_{l}^{1})^{3}}{3 (\text{tr}^{b})} \frac{d (\text{tr}^{b})}{dt} \right]^{-1}$$ (IV-C-27)

c) An equivalent model

The bulk stress shown in equation (IV-C-1) has been related to a continuum model that involves the invariants of a strain tensor $\gamma^{(0)}$ by Curtiss and Bird(1980). The strain tensor $\gamma^{(0)}$ is defined by:

$$\gamma^{(0)} = \Delta^{+} \Delta - \delta$$ (IV-C-28)

The equivalent continuum model of the bulk stress is given in Table (IV-C-1) in which $\gamma^{(0)}^{2} = \gamma^{(0)} \gamma^{(0)}$, and the coefficients, $\beta_{i}$, are complicated functions of the invariants of the strain tensor $\gamma^{(0)}$ that have been determined by Curtiss and Bird(1980).

The above relation shows that a seemingly complicated continuum model may be converted to a simpler structural model.
Table (IV-C-1) An equivalent continuum model

\[ T = -n_s \dot{Y} - n_s \frac{(n-1)^3}{12} \{ \beta_0 \dot{\gamma} + \beta_1 \{ \dot{\gamma} \gamma(0) \gamma(0) + \gamma(0) \dot{\gamma} \gamma(0) \} \right. \\
+ \beta_2 \{ \frac{1}{2} \dot{\gamma} \gamma(0) \dot{\gamma} \gamma(0) + \frac{1}{2} \gamma(0) \dot{\gamma} \gamma(0) \} \right. \\
+ \beta_3 \{ \dot{\gamma} \dot{\gamma}(0) + \dot{\gamma}(0) \dot{\gamma} + \frac{1}{2} \dot{\gamma} \gamma(0) \} \right. \\
+ \beta_4 \{ \dot{\gamma} \dot{\gamma}(0) \dot{\gamma} + \frac{1}{2} \gamma(0) \dot{\gamma} \gamma(0) \} \\
+ \beta_5 \{ \gamma(0) \dot{\gamma} \dot{\gamma}(0) \dot{\gamma} + \frac{1}{2} \gamma(0) \dot{\gamma} \gamma(0) \} \right. \\
+ \frac{1}{2} \gamma(0) \dot{\gamma} \gamma(0) \dot{\gamma} \gamma(0) \} \} \]
CHAPTER V

ILLUSTRATIVE HOMOGENEOUS FLOWS

The general solutions for the rheological equation of state, developed in the preceding chapter, are utilized to characterize the rheological properties of a suspension of rigid fibers in homogeneous flows. The flow fields that have been selected for the purpose of elucidating the interrelationship between the particle orientation and the bulk properties of the suspension are summarized in Table (V-A-1). In each case the kinematics of the fiber is described, and the corresponding rheological properties are evaluated. The predicted results are then compared to the appropriate experimental data documented in the literature.

A. TYPE OF FLOWS INVESTIGATED

The types of homogeneous flows studied in this chapter are: a simple steady shear flow, an uniaxial extensional flow, and a biaxial extensional flow. The cartesian coordinate system used to specify the bulk velocity field is shown in Figure (III-B-1). In this section the bulk kinematics of each flow is described. A convenient summary of this information is presented in Tables (V-A-1) and (V-A-2).

1. Simple steady shear

In a simple steady shear flow the components of the bulk velocity are given by:
<table>
<thead>
<tr>
<th>Flow fields</th>
<th>Velocity components, $v_i$</th>
<th>Velocity gradient tensor $\kappa = (\nabla v)^T$</th>
<th>Rheological properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shear flow</td>
<td>$v_x = \gamma y$</td>
<td>$\kappa = \begin{bmatrix} 0 &amp; \gamma &amp; 0 \ 0 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 \end{bmatrix}$</td>
<td>$\eta^+, \psi_1^+, \psi_2^+$</td>
</tr>
<tr>
<td></td>
<td>$v_y = 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$v_z = 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\dot{\gamma} = 0, t &lt; 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\dot{\gamma} = \dot{\gamma}, t \geq 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniaxial extensional flow</td>
<td>$v_x = -\frac{1}{2} \dot{\varepsilon} x$</td>
<td>$\kappa = \begin{bmatrix} -\frac{1}{2} \dot{\varepsilon} &amp; 0 &amp; 0 \ 0 &amp; -\frac{1}{2} \dot{\varepsilon} &amp; 0 \ 0 &amp; 0 &amp; \dot{\varepsilon} \end{bmatrix}$</td>
<td>$\tilde{\eta}^+$</td>
</tr>
<tr>
<td></td>
<td>$v_y = -\frac{1}{2} \dot{\varepsilon} y$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$v_z = \dot{\varepsilon} z$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\dot{\varepsilon} = 0$ for $t \leq 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Biaxial extensional flow</td>
<td>$v_x = \frac{1}{2} \dot{\varepsilon} x$</td>
<td>$\kappa = \begin{bmatrix} \frac{1}{2} \dot{\varepsilon} &amp; 0 &amp; 0 \ 0 &amp; \frac{1}{2} \dot{\varepsilon} &amp; 0 \ 0 &amp; 0 &amp; -\varepsilon \end{bmatrix}$</td>
<td>$\tilde{\eta}^+$</td>
</tr>
<tr>
<td></td>
<td>$v_y = \frac{1}{2} \dot{\varepsilon} y$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$v_z = -\varepsilon z$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\dot{\varepsilon} = 0$ for $t \leq 0$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table V-A-2  The bulk displacement function and the bulk strain tensors for the type of flows investigated

<table>
<thead>
<tr>
<th>Flow fields</th>
<th>Displacement function</th>
<th>Strain tensor $\mathbf{E}$</th>
<th>Strain tensor $\mathbf{A}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shear flow</td>
<td>$x = x' + \gamma y$</td>
<td>$\mathbf{E} = \begin{bmatrix} 1 &amp; \gamma &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{bmatrix}$</td>
<td>$\mathbf{A} = \begin{bmatrix} 1 - \gamma &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{bmatrix}$</td>
</tr>
<tr>
<td></td>
<td>$y = y'$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$z = z'$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniaxial extensional flow</td>
<td>$x = x'\exp(-\frac{1}{2}\varepsilon)$</td>
<td>$\mathbf{E} = \begin{bmatrix} e^{-\varepsilon/2} &amp; 0 &amp; 0 \ 0 &amp; e^{-\varepsilon/2} &amp; 0 \ 0 &amp; 0 &amp; e^{\varepsilon} \end{bmatrix}$</td>
<td>$\mathbf{A} = \begin{bmatrix} e^{\varepsilon/2} &amp; 0 &amp; 0 \ 0 &amp; e^{\varepsilon/2} &amp; 0 \ 0 &amp; 0 &amp; e^{-\varepsilon} \end{bmatrix}$</td>
</tr>
<tr>
<td></td>
<td>$y = y'\exp(-\frac{1}{2}\varepsilon)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$z = z'\exp(\varepsilon)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Biaxial extensional flow</td>
<td>$x = x'\exp(\frac{1}{2}\varepsilon)$</td>
<td>$\mathbf{E} = \begin{bmatrix} e^{\varepsilon/2} &amp; 0 &amp; 0 \ 0 &amp; e^{\varepsilon/2} &amp; 0 \ 0 &amp; 0 &amp; e^{-\varepsilon} \end{bmatrix}$</td>
<td>$\mathbf{A} = \begin{bmatrix} e^{-\varepsilon/2} &amp; 0 &amp; 0 \ 0 &amp; e^{-\varepsilon/2} &amp; 0 \ 0 &amp; 0 &amp; e^{\varepsilon} \end{bmatrix}$</td>
</tr>
<tr>
<td></td>
<td>$y = y'\exp(\frac{1}{2}\varepsilon)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$z = z'\exp(-\varepsilon)$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
\[ v_x = \dot{\gamma} y \] (V-A-1)
\[ v_y = 0 \] (V-A-2)
\[ v_z = 0 \] (V-A-3)

where the shear rate \( \dot{\gamma} \) is a positive constant. From this set of relations the velocity gradient tensor is constructed according to \( \kappa_{ij} = \frac{\partial v_i}{\partial x_j} \)

\[
\kappa = \begin{bmatrix}
0 & \dot{\gamma} & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\] (V-A-4)

Secondly, the displacement functions can be readily obtained by integrating the components of the velocity field from \( t = 0 \) to \( t = t \). Consequently,

\[ x = x' + \gamma y \] (V-A-5)
\[ y = y' \] (V-A-6)
\[ z = z' \] (V-A-7)

where \( x_i' \) is the position of a fluid particle at \( t = 0 \), and \( \gamma \) is the product of the shear rate and the elapsed time \( (\gamma = \dot{\gamma}(t - 0)) \). From the displacement functions the strain tensors \( \mathbf{E} \) and \( \mathbf{A} \) are evaluated according to their respective definitions in equations (IV-A-2) and (IV-A-3). Hence,

\[
\mathbf{E} = \begin{bmatrix}
1 & \gamma & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\] (V-A-8)

and,
\[
\Delta = \begin{bmatrix}
1 & -\gamma & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix} \tag{V-A-9}
\]

The bulk rheological properties of interest for this flow are listed in Table (V-A-1). These material functions may be transient properties, and therefore they are denoted by a super-scripted plus sign. The bulk shear viscosity \(\eta^+\) is defined by:

\[
\eta^+ = -\tau_{yx}/\dot{\gamma} \tag{V-A-10}
\]

The bulk primary normal stress coefficient \(\psi_1^+\) is given by:

\[
\psi_1^+ = - (\tau_{xx} - \tau_{yy})/\dot{\gamma}^2 \tag{V-A-11}
\]

and the bulk secondary normal stress coefficient \(\psi_2^+\) is described by:

\[
\psi_2^+ = - (\tau_{yy} - \tau_{zz})/\dot{\gamma}^2 \tag{V-A-12}
\]

The velocity gradient tensor and the strain tensors described here complete the requirements to determine the particle motion, the orientation distribution function and the bulk rheological properties in a simple steady shear flow. These calculations are carried out in Section (V-B).

2. Uniaxial and biaxial extensional flows

In an uniaxial extensional flow the components of the bulk velocity are given by:

\[
v_x = -\frac{1}{2} \dot{\varepsilon} \tag{V-A-13}
\]

\[
v_y = -\frac{1}{2} \dot{\varepsilon} y \tag{V-A-14}
\]

\[
v_z = \dot{\varepsilon} z \tag{V-A-15}
\]
where the extension rate $\dot{\varepsilon}$ is a positive constant for this flow field. From the prescribed velocity field, the velocity gradient tensor is given by:

$$\gamma = \begin{pmatrix} -\frac{1}{2}\dot{\varepsilon} & 0 & 0 \\ 0 & -\frac{1}{2}\dot{\varepsilon} & 0 \\ 0 & 0 & \dot{\varepsilon} \end{pmatrix} \quad (V-A-16)$$

The displacement functions are obtained by integrating the components of the velocity field from $t = 0$ to $t = t$.

$$x = x'\exp(-\frac{3}{2}\varepsilon) \quad (V-A-17)$$

$$y = y'\exp(-\frac{3}{2}\varepsilon) \quad (V-A-18)$$

$$z = z'\exp(\varepsilon) \quad (V-A-19)$$

where the Hencky strain $\varepsilon$ is the product of the extensional rate and the duration of the flow field ($\varepsilon = \dot{\varepsilon}(t - 0)$). From the displacement functions the strain tensors $\mathbb{E}$ and $\Delta$ are evaluated.

$$\mathbb{E} = \begin{pmatrix} \exp(-\varepsilon/2) & 0 & 0 \\ 0 & \exp(-\varepsilon/2) & 0 \\ 0 & 0 & \exp(\varepsilon) \end{pmatrix} \quad (V-A-20)$$

and,

$$\Delta = \begin{pmatrix} \exp(\varepsilon/2) & 0 & 0 \\ 0 & \exp(\varepsilon/2) & 0 \\ 0 & 0 & \exp(\dot{\varepsilon}) \end{pmatrix} \quad (V-A-21)$$

The rheological property of interest in an extensional flow is the Trouton viscosity, or the extensional viscosity, or the elongational viscosity which is defined by:
This material function and the orientation of the particle for this type of flow are determined in Section (V-C).

In the case of a biaxial extensional flow, the equations that describe the kinematics of the bulk deformation are similar to those of the uniaxial extensional flow except that \( \dot{\varepsilon} \) is replaced by \(-\dot{\varepsilon}\). Therefore, the velocity gradient tensor and the strain tensors are:

\[
K = \begin{pmatrix}
\frac{3}{2} \dot{\varepsilon} & 0 & 0 \\
0 & \frac{1}{2} \dot{\varepsilon} & 0 \\
0 & 0 & -\dot{\varepsilon}
\end{pmatrix}
\quad (V-A-23)
\]

\[
M = \begin{pmatrix}
\frac{e^{\varepsilon/2}}{2} & 0 & 0 \\
0 & \frac{e^{\varepsilon/2}}{2} & 0 \\
0 & 0 & e^{-\varepsilon}
\end{pmatrix}
\quad (V-A-24)
\]

and,

\[
A = \begin{pmatrix}
\frac{e^{-\varepsilon/2}}{2} & 0 & 0 \\
0 & \frac{e^{-\varepsilon/2}}{2} & 0 \\
0 & 0 & e^{\varepsilon}
\end{pmatrix}
\quad (V-A-25)
\]

The motion of the particle and the behavior of the stress field for this flow are discussed in Section (V-D).
B. SIMPLE STEADY SHEAR FLOW

The results describing the motion of a test fiber and the bulk rheological properties for the start-up of a simple steady shear flow are presented in this section.

1. Particle kinematics

The general solution to the motion of a test particle in homogeneous flows has been provided in equation (IV-A-11) where:

\[ \mathbf{p} = \frac{\mathbf{E} \cdot \mathbf{p}_0}{(\mathbf{E}^T \cdot \mathbf{E} : \mathbf{p}_0 \mathbf{p}_0)^{\frac{1}{2}}} \]  

(V-B-1)

The strain tensor \( \mathbf{E} \) for a simple steady shear flow is shown in Table (V-A-2). Consequently \( \mathbf{p} \) can be directly evaluated:

\[ \mathbf{p} = (\gamma^2 \sin^2 \theta_0 \sin^2 \phi_0 + \gamma \sin^2 \theta_0 \sin 2 \phi_0 + 1)^{-\frac{1}{2}} \left( (\sin \theta_0 \cos \phi_0 + \gamma \sin \theta_0 \sin \phi_0) \hat{\mathbf{e}}_x + (\sin \theta_0 \sin \phi_0) \hat{\mathbf{e}}_y + (\cos \theta_0) \hat{\mathbf{e}}_z \right) \]  

(V-B-2)

where \( \theta_0 \) and \( \phi_0 \) indicate the initial configuration of the test fiber, and \( \hat{\mathbf{e}}_i \) are the orthonormal vectors of the coordinate system that describe the bulk deformation. Since the orientation vector \( \mathbf{p} \) can be resolved into:

\[ \mathbf{p} = \sin \theta \cos \phi \hat{\mathbf{e}}_x + \sin \theta \sin \phi \hat{\mathbf{e}}_y + \cos \theta \hat{\mathbf{e}}_z \]  

(V-B-3)

Equations (V-B-2) and (V-B-3) then lead to the following relations between \( (\theta, \phi) \) and \( (\theta_0, \phi_0) \):

\[ \theta = \tan^{-1} \left( \tan \theta_0 (\gamma^2 \sin^2 \phi_0 + 2 \gamma \sin \phi_0 \cos \phi_0 + 1)^{\frac{1}{2}} \right) \]  

(V-B-4)

\[ \phi = \tan^{-1} \left( \frac{1}{\cot \phi_0 + \gamma} \right) \]  

(V-B-5)
Alternatively, the displacement functions \( (\theta, \phi) \) can be inverted to give:

\[
\theta_0 = \tan^{-1} \left( \tan \theta \left( \gamma^2 \sin^2 \phi - 2 \gamma \sin \phi \cos \phi + 1 \right)^{\frac{1}{2}} \right) \quad (V-B-6)
\]

\[
\phi_0 = \tan^{-1} \left( \frac{1}{\cot \phi - \gamma} \right) \quad (V-B-7)
\]

The motion of a test fiber is described by the results in equations (V-B-4) and (V-B-5). At the start of the flow \( (\gamma = 0) \), the orientation of the particle \( (\theta, \phi) \) is given by \( (\theta_0, \phi_0) \). As the flow develops or as \( \gamma \) increases, the fibers are aligned toward the flow direction \( (\theta = \frac{\pi}{2}, \phi = 0) \), except for the special cases in which the particles are initially located in the plane of shear. In the situations where \( (\theta_0 = 0, \phi_0) \) and \( (\theta_0, \phi_0 = 0) \), the particles would remain permanently in those positions. Consequently, it may be concluded that a simple steady shear flow will eventually orient the suspended particles into the shearing planes, and the rate of alignment varies algebraically with the duration of the bulk deformation.

The results in equations (V-B-4) and (V-B-5) show that the rate of rotation of the test fiber toward the plane of shear is non-uniform. The rate of rotation is greater when the major axis of the fiber is aligned perpendicular to the streamline. Thereafter the test fiber slows down, and asymptotically approaches the plane of shear at large strain. This behavior is identical to the orbits calculated by Jeffery (1922) for the case of particles with an infinite aspect ratio. This agreement is expected because the effect-
ive hydrodynamic force acting on the test particle has been replaced by a line force along the center-line of the fiber.

2. Rheological properties

The rheological properties that characterize the behavior of the suspension in shear flows have been tabulated in Table (V-A-1). These material functions can be estimated from the bulk stress tensor in either equation (IV-C-1) or equation (IV-C-2). In this section the bulk shear viscosity, the bulk primary and secondary normal stress coefficients are evaluated by employing Simpson's rule to integrate the appropriate components of the stress tensor in equation (IV-C-1). The quantities to be integrated are listed below.

a) Dimensionless bulk shear viscosity

\[
\frac{12}{(n_1^3)^3} \left( \frac{\eta^+}{\eta_s} \right) = \frac{2\pi}{0} \int_0^\pi \sin^5 \theta \sin^2 2\theta \, d\theta d\phi
\]

\[
0 \int_0^{16\pi} (\gamma \sin^2 \theta \sin^2 \phi - \gamma \sin^2 \theta \sin^2 2\phi + 1)^{3/2}
\]

(V-B-8)

b) Dimensionless bulk primary normal stress coefficient

\[
\frac{12}{(n_1^3)^3} \gamma^+ 1 = \frac{2\pi}{0} \int_0^\pi \sin^5 \theta \sin^4 \theta \sin^4 \phi \, d\theta d\phi
\]

\[
0 \int_0^{16\pi} (\gamma \sin^2 \theta \sin^2 \phi - \gamma \sin^2 \theta \sin^2 2\phi + 1)^{3/2}
\]

(V-B-9)

c) Dimensionless bulk secondary normal stress coefficient

\[
\frac{12}{(n_1^3)^3} \gamma^+ 2 = \frac{2\pi}{0} \int_0^\pi \sin^5 \theta \sin 2\phi (\sin^2 \phi - \cot^2 \theta) \, d\theta d\phi
\]

\[
0 \int_0^{8\pi} (\gamma \sin^2 \theta \sin^2 \phi - \gamma \sin^2 \theta \sin^2 2\phi + 1)^{3/2}
\]

(V-B-10)

The computer program to determine each of these integrals as functions of the shear strain is shown in Appendix 3, and
the results are depicted in Figures (V-B-1) to (V-B-5).

The dimensionless bulk shear viscosity is shown in Figure (V-B-1). At the inception of the shear flow \((\gamma=0^+)\), the rheological equation of state for the suspension can be obtained from equation (IV-C-1):

\[
\mathcal{I} = -\eta_s \left[ 1 + \frac{(nl^3)^3}{180} \right] \gamma 
\]  \hspace{1cm} (V-E-11)

This result indicates that the suspension behaves as a highly viscous Newtonian fluid with a bulk-zero-shear-relative viscosity that equals to:

\[
\frac{\eta^+}{\eta_s} = 1 + \frac{(nl^3)^3}{180} \hspace{1cm} (V-B-12)
\]

In this region, the particles are randomly oriented. Therefore, the bulk resistance to a shear deformation can be significantly greater than the resistance of an unfilled system. Bulk shear viscosity data for a suspension of randomly dispersed fibers have not been reported in the literature. In Chapter VII we compare the predicted shear viscosity with the measured values near the start of the shear flow.

As the flow develops, the test fiber acquires a preferred orientation which is governed by the hydrodynamic couple. As shown in Figures (V-B-1) and (V-B-2), the bulk shear viscosity then displays a shear overshoot. This behavior is the result of fibers accumulation near the principal axes of the strain rate at the beginning of the experiment. For this problem the x-axis of the principal coordinates of the strain rate is
Figure V-B-1  Plot of the dimensionless bulk shear viscosity versus the shear strain
Figure V-B-2  Log-log plot of the dimensionless bulk shear viscosity versus the shear strain
Figure V-B-3  Plot of the dimensionless bulk primary normal stress coefficient versus the shear strain.
Figure V-B-4  Plot of the dimensionless bulk secondary normal stress coefficient versus the shear strain
Figure V-B-5  Ratio of the primary normal stress difference to the shear stress versus the shear strain as a function of the solid concentration
rotated counter-clockwise at an angle of $\pi/4$ with respect to the direction of the shear flow. When the test fiber is aligned in this direction, the particle experiences an extensional deformation which tends to pull apart the fiber. Consequently the tension in the fiber reaches a maximum. This result leads to a slightly higher resistance to the bulk shear deformation as indicated by the hump in Figures (V-B-1) and (V-B-2).

Once the fiber passes by the principal axis of the strain rate, the tension along the particle decreases progressively because the particle is heading toward the plane of shear. Subsequently, the bulk shear viscosity decreases exponentially with the shear strain as indicated by the power-law-like dependence of the dimensionless bulk shear viscosity on the shear strain in Figure (V-B-2).

At sufficiently large strain, typically when $\gamma$ is greater than 10, the tension along the test fiber is almost removed. In this region, the particle is near the plane of shear, and hence the contribution to the bulk stress from the suspended fibers becomes negligible. As a result the character of the suspension is dominated by the solvent which is a Newtonian fluid. In the limit of infinite strain, the suspension viscosity is identical to the solvent viscosity. This result is supported by the experimental shear viscosity data reported by Blakeney (1966) in which the relative bulk viscosity is less than 1.06. In order to ensure that the data were collected at steady state, the experiment was allowed to proceed for
half an hour at shear rates that ranged between 0.1 to 0.5 s\(^{-1}\) in a Couette viscometer. The materials tested by Flakeney have been summarized in Chapter II. In Chapter VII we compare our experimental data with the predictions in the large strain region.

The dimensionless primary and secondary normal stress coefficients are shown in Figures (V-B-3) and (V-B-4) respectively. When \(\gamma=0^+\), the particles are randomly oriented. Therefore, the net effect of the normal components of the drag force on the fiber that are summed over all possible configurations is zero. As a result, the normal stress coefficients are zero at \(\gamma=0^+\). As the flow develops, the test fiber acquires a preferential direction which would produce a net contribution to normal forces in the suspension. These results are illustrated by the transient normal stress coefficients in Figures (V-B-3) and (V-B-4). At large strain, the normal stresses vanish as the tension along the particle is removed. Therefore, the normal stress coefficients in Figures (V-B-3) and (V-B-4) approach zero as \(\gamma\) increases.

The ratio of the primary normal stress difference to the shear stress is shown in Figure (V-B-5) as a function of the amount of solids in the suspension. In Figure (V-B-5) the group \(\dot{\gamma}\psi_1^+/\eta^+\) is plotted versus \(\gamma\), and the concentration of fibers is represented by \((n \text{l}^2)^3/12\). The results indicate that the ratio of \(\dot{\gamma}\psi_1^+/\eta^+\) increases with the concentration of solids in the suspension at a fixed strain \(\gamma\). An increase in \(\dot{\gamma}\psi_1^+/\eta^+\) means that the suspension would tend to exert a greater
normal force in the y-direction. Therefore, a greater clamp force is required to prevent the suspension from expanding in the normal direction to the flow field.

In this section we have taken a case study of the behavior of the bulk stress in a simple steady shear flow. The calculations show that the resistance of the composite to the bulk deformation is initially much higher than the resistance of the unfilled system. Hence, the suspension appears to be very viscous (but Newtonian) initially because of the random structure of the particles. As the flow progresses, normal stresses appear because the test fiber acquires a preferential orientation. The normal stresses then disappear at large strain because the tension on the fiber is completely removed. In this region the suspension behaves as if the particles are not present. Because the model predicts the presence of normal stresses, the suspension has been described earlier as a visco-elastic material. However, there is no elastic energy stored in the system. If the flow is stopped then the orientation of the particles is frozen at that instant because of the absence of Brownian forces that would restore the particles to their initial configurations. Consequently, this model predicts that the bulk stress would relax instantaneously to zero as the flow field is turned off.

In this study we have also observed that the contributions to the bulk stress from the solid particles and the solvent exchange roles as the suspension reaches steady-state. Steady-state is attained when all the particles have been
aligned into the plane of shear.

For this type of flow where the contribution from the particles vanishes at steady-state, the errors involved in estimating the effective drag coefficient from the initial random orientation distribution is not very severe because the drag force along the test fiber becomes less and less important as the flow develops. Consequently, the bulk stress tensor in equation (IV-C-1) predicts correctly to within an order of magnitude the zero-shear strain properties, and the infinite shear strain properties. The intermediate strain predictions may be improved by allowing the spacing between adjacent particles to vary with the history of the flow. This investigation will be explored in the future.
C. UNIAXIAL EXTENSIONAL FLOW

1. Particle kinematics

The bulk kinematics of an uniaxial extensional flow have been described in Section (V-A). By substituting the strain tensor \( \mathbb{E} \) listed in Table (V-A-2) into equation (IV-A-11), the motion of the test fiber is given by:

\[
p = (e^{-\varepsilon \sin^2 \theta_0} + e^{2\varepsilon \cos^2 \theta_0})^{-\frac{1}{2}} \left( e^{-\varepsilon/2 \sin \theta_0 \cos \theta_0 \delta_x} + e^{-\varepsilon/2 \sin \theta_0 \sin \theta_0 \delta_y} + e^{\varepsilon \cos \theta_0 \delta_z} \right) \quad (V-C-1)
\]

Similar to the development in the previous section, the particle motion can be alternatively expressed as:

\[
\theta = \tan^{-1} \left( \tan \theta_0 e^{-\frac{3}{2} \varepsilon} \right) \quad (V-C-2)
\]

\[
\phi = \phi_0 \quad (V-C-3)
\]

where \((\theta_0, \phi_0)\) is the initial orientation of the test fiber, and \(\varepsilon = \dot{\varepsilon} t\).

The results in equations (V-C-2) and (V-C-3) show that \((\theta, \phi) = (\theta_0, \phi_0)\) at the inception of the extensional flow. As the flow progresses, \(\theta\) tends toward \(0\) whereas \(\phi\) remains constant at \(\phi_0\). These values indicate that each particle rotates toward the direction of the extension \((z\text{-axis})\) at a fixed initial azimuthal angle \(\phi_0\). Consequently, particles are oriented in the direction of the extensional flow, and the rate of alignment varies exponentially with the duration of the flow. Therefore, particles can be aligned much faster in an extensional flow than in a shear flow.

2. Rheological properties
The rheological property that characterizes an extensional flow is the Trouton viscosity which has been defined in equation (V-A-22). The dimensionless form of this quantity is obtained by evaluating the following integral by Simpson's rule:

\[
\frac{12}{(n_1^n)} \left( \frac{n^n}{\eta_s} - 3 \right) = \int_0^2 \frac{(2 - 3 \sin^2 \theta)(\cos^2 \theta - \sin^2 \theta \cos^2 \phi) \sin \theta d \theta d \phi}{8 \pi (e^{\varepsilon \sin^2 \theta} + e^{-2 \varepsilon \cos^2 \theta})^{3/2}}
\]

(V-C-4)

The computer program to evaluate the integral in equation (V-C-4) for a range of strain values is tabulated in Appendix 4. The results are also shown in Figure (V-C-1) in which the dimensionless extensional viscosity is plotted versus the Hencky strain \( \varepsilon \).

At the start of the flow (\( \varepsilon = 0 \)), the integral in equation (V-C-4) can be evaluated analytically. The resulting dimensionless extensional viscosity is:

\[
\frac{12}{(n_1^n)} \left( \frac{n^n}{\eta_s} - 3 \right) = 0.2
\]

(V-C-5)

As the particle progressively aligns with the streamline, the tension along the fiber increases because the particle is rigid. When the particle is perfectly aligned in the direction of the streamline, then the suspension has reached steady-state in which case the dimensionless extensional viscosity approaches an asymptotic value of one. At this point, the resistance to the bulk deformation is the greatest since the particle is aligned with the principal strain-rate axis.

This model predicts that the contribution from the
Figure V-C-1 Plot of the dimensionless Trouton viscosity versus the Hencky strain in an uniaxial extensional flow
suspended particles to the bulk stress becomes dominant as the system tends toward steady-state. In the model, the kinematics of the test particle has been properly accounted for because the governing equation for the particle motion is derived from a torque balance. Consequently, the portion of the hydrodynamic force along the fiber which describes the relative motion of the test particle in the effective medium has been correctly formulated. However, the estimate of the effective drag coefficient presented in Section (III-5) worsens as the suspension deviates from the state of a randomly dispersed suspension of fibers. As shown below the steady-state result will overestimate the experimental values of Kizior and Seyer (1974), and Weinberger and Goddard (1974). The source of a severe over-estimate of the bulk properties lies in the time-dependent length scales discussed in Section (III-F). As the flow develops, the distance between adjacent fibers increases for a fixed load of solids. Simultaneously the hydrodynamic length scale decreases. Therefore, the suspension becomes dilute when the separation between neighboring fibers exceeds the hydrodynamic length scale. The details of this transient variation in length scales are subject to future investigations.

To illustrate the error produced by an incorrect estimate of the effective drag coefficient, the predicted steady-state value obtained from equation (V-C-4) is compared to the experimental data of Kizior and Seyer (1974), and Weinberger and Goddard (1974). These experiments have been described in
Section (II-A).

In the work of Kizior and Seyer (1974), the volume fraction of solids was 0.001, the length of the fiber was 15 \( \mu \text{m} \), and the aspect ratio was 340. If the particles were randomly oriented then the suspension would be categorized in the semi-concentrated regime (Table III-A-1). The data were collected near steady-state, and the reported extensional viscosity was an order of magnitude greater than the solvent viscosity,

\[
\frac{\overline{n}}{\eta_s} = 10 \tag{V-C-6}
\]

If we had used the steady-state value of equation (V-C-4) as an estimate, then:

\[
\frac{\overline{n}}{\eta_s} = 10^5 \tag{V-C-7}
\]

As anticipated, a severe over-estimate is observed here. However, for a suspension of perfectly aligned fibers, the spacing between particles is approximately:

\[
a_c = (nl)^{-\frac{1}{2}} \tag{V-C-8}
\]

and the hydrodynamic length scale, \( a_h \), is of the same magnitude as the diameter of the fiber. For this experiment,

\[
a_c = 10a_h \tag{V-C-9}
\]

Hence the suspension is dilute in the sense that hydrodynamic interactions between particles are negligible. Consequently, the value of \( a_c \) in equation (V-C-8) cannot be inserted back into equation (III-E-3) to arrive at a new estimate of the effective drag coefficient because the physical argument
employed in Section (III-E) is only applicable when $a_c < a_h$.

Since the suspension is dilute, $\zeta$ should be used instead of $\zeta_{\text{eff}}$. The resulting constitutive equation for the dilute regime is shown in Table (III-F-1). With this constitutive equation, the estimated relative extensional viscosity is approximately equal to 15. This result is in good agreement with the measured value.

In the experimental work of Weinberger and Goddard (1974), the fiber dimensions were 3.5 μm in diameter and 200 μm in length. The solid concentration was 1.3% by volume. If the particles were randomly distributed, then the suspension would again be categorized in the semi-concentrated regime. Similar to the previous situation, the reported relative extensional viscosity at steady-state was 10, whereas the estimated value based on equation (V-C-4) is $10^8$. However, the suspension tested by Weinberger and Goddard is actually dilute because

$$a_c = 6a_h \quad \text{(V-C-10)}$$

This result suggests that $\zeta$ should be used in place of $\zeta_{\text{eff}}$. In such case the estimated relative extensional viscosity is 7.5. The later predicted value agrees closely with the experimental data.

In both of these investigations, the suspension examined were dilute, and the particle orientation was known at steady-state. Consequently, the volume averaged stress developed by Batchelor can be used to calculate the rheological properties of the suspension under this set of conditions. This computation has been worked out by Batchelor (1971), and the predicted
results are in close agreement with the experimental data.

In summarizing this case study, we have observed that there are two competing mechanisms to the bulk rheological behavior. First, the tension along the fiber increases as the flow continues. This phenomenon then leads to an increase in the resistance to the bulk deformation. However, the distance between particles increases simultaneously. This later effect reduces the hydrodynamic interactions between the fibers, and hence lowers the resistance to the bulk deformation. Consequently, if the effective drag coefficient is estimated on the basis of a suspension of randomly dispersed fibers, then the error produced in predicting the bulk properties will magnify as the flow develops. In order to correctly describe the physics of the problem, there is a need to assess the transient behavior of the hydrodynamic length scale since the transient property of the separation between nearest neighbors is known (equation III-F-1). This area is subject to future investigation.
D. BIAXIAL EXTENSIONAL FLOW

1. Particle kinematics

The motion of a test fiber in a biaxial extensional flow is determined by inserting the bulk kinematics of this flow (Table V-A-2) into equation (IV-A-11). The results are similar to those obtained from the uniaxial extensional flow except that $\varepsilon$ is replaced by $-\varepsilon$. Hence, the orbits of the test particle are described by:

$$\theta = \tan^{-1}(\tan\theta_0 e^{3\varepsilon/2})$$  \hspace{1cm} (V-D-1)

$$\phi = \phi_0$$  \hspace{1cm} (V-D-2)

When $\varepsilon = 0$, the initial configuration of the test particle is given by $(\theta_0, \phi_0)$. At large strain, $\theta$ approaches $\pi/2$ while $\phi$ remains constant at $\phi_0$. These results indicate that particles are oriented in directions perpendicular to the direction of compression which is the z-axis. Consequently, the particles are eventually aligned in the x-y plane. The only exception occurs when $\theta_0 = 0$. In this case the fiber remains in this position for all time because there is no moment arm to rotate this fiber into the x-y plane.

2. Rheological properties

The dimensionless extensional viscosity that characterizes the behavior of a suspension of fibers in a biaxial extensional flow is determined by evaluating the following integral by means of Simpson's rule.

$$\frac{12}{n_1^2 n_2^2 n_3} (\ddot{\eta} - 3) = \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} \frac{(2-3\sin^2 \theta)(\sin^2 \theta \cos^2 \phi - \cos^2 \phi) \sin \theta \sin \phi \sin \phi}{8\pi (e^{-\varepsilon \sin^2 \theta} + e^{2\varepsilon \cos^2 \theta})^{3/2}} d\phi d\theta d\phi$$  \hspace{1cm} (V-D-3)
The computer program to calculate this integral is presented in Appendix 4. The data are then plotted in Figure (V-D-1).

At the initiation of the flow ($\varepsilon = 0^+$), the integral in equation (V-D-3) can be directly calculated.

\[
\frac{12}{(n^3)^3(\eta_s^+)} - 3 = 0.2 \quad \text{(V-D-4)}
\]

At large strain, the dimensionless extensional viscosity increases to an asymptotic value of 0.25. When steady-state is reached, the test fiber experiences a maximum tension because the fibers align with the principal direction of straining. Consequently, the resistance to the bulk flow increases. However, the separation between nearest fibers also increases as the particles become perfectly aligned. This effect tends to lower the bulk resistance to deformation. Similar to the preceding flow, the error in estimating the effective drag coefficient will be amplified as the suspension approaches steady-state.
Figure V-D-1  Plot of the dimensionless Trouton viscosity versus the Hencky strain in a biaxial extensional flow
CHAPTER VI
WALL EFFECTS

The purpose of this chapter is to establish a transition from the ideal cases developed previously to more realistic flow situations. Two approximate methods are considered to account for the presence of rigid boundaries in a simple steady shear flow. In the first method, the initial fraction of fibers that would poke through the walls is subtracted out of the contribution to the bulk stress from the particles. This model, however, does not provide the detailed kinematics of fibers in a confined environment. Consequently, a particle tracking method is proposed to describe the trajectories of certain particles that would encounter the walls in the course of their paths toward the plane of shear. In closing this chapter, a general formulation of the wall-problem in homogeneous flows is presented.

A. RENORMALIZATION OF THE DISTRIBUTION FUNCTION

1. Description of the problem

In this analysis we consider the problem of a test fiber that is confined between two rigid walls moving in opposite directions. The center of mass of the test particle is assumed to be located half-way between the solid surfaces. This situation is sketched out in Figure (VI-A-1) where the separation between the walls is denoted by \( h \). The degree of confinement is then characterized by an angle \( \theta \), where,
Figure VI-A-1  Schematic drawing of a fiber that is confined between two rigid walls
\[ \theta_w = \cos^{-1} \frac{h}{l} \]  
(VI-A-1)

When \( \theta = \theta_w \), the tip of the test fiber just touches the surface of the wall. Consequently, \( \theta \) ranges between \( \theta_w \) and \( (\pi - \theta_w) \), and the shaded areas represent regions in which particles cannot exist. If \( h \) is greater than \( l \), then the motion of the test fiber is not constrained.

The bulk velocity field for the simple steady shear flow shown in Figure (IV-A-1) is described by:

\[ v_x = 0 \]  
(VI-A-2)

\[ v_y = \gamma z \]  
(VI-A-3)

\[ v_z = 0 \]  
(VI-A-4)

Subsequently, the bulk kinematical expressions can be obtained from a coordinate transformation of the results listed in Tables (V-A-1) and (V-A-2). In Chapter V the bulk shear deformation was occurring in the \( x-y \) plane, whereas here the shear flow is developing in the \( y-z \) plane. Consequently, the velocity gradient tensor that is associated with the velocity field prescribed in equations (VI-A-2) to (VI-A-4) is:

\[
\mathbf{\xi} = \begin{bmatrix}
0 & 0 & 0 \\
0 & \gamma & 0 \\
0 & 0 & 0
\end{bmatrix}
\]  
(VI-A-5)

and the deformation tensor \( \mathbf{\Delta} \) is:

\[
\mathbf{\Delta} = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & -\gamma \\
0 & 0 & 1
\end{bmatrix}
\]  
(VI-A-6)
With the above strain tensor, the orientation distribution function is determined from equation (IV-E-15),
\[ \psi(\theta, \phi, \gamma) = \frac{1}{4\pi} (\gamma^2 \cos^2 \theta - \gamma \sin 2\theta \sin \phi + 1)^{-3/2} \]  
(VI-A-7)
where the strain \( \gamma = \dot{\gamma} t \).

2. Modeling of the wall effect

The wall effect is modeled on the assumption that the center of mass of suspended particles are located halfway between the bounds of the wall. Therefore, the shaded areas in Figure (VI-A-1) represent regions which the particles are prohibited from occupying. Consequently, the second term on the right-hand side of the bulk stress in equation (IV-C-1), which represents the contribution from the solids, needs to be modified. Instead of integrating over all particle configurations, the integral is restricted to the following limits:
\[ \theta_w \leq \theta \leq (\pi - \theta_w), \text{ and } 0 \leq \phi \leq 2\pi. \]
In addition, the orientation distribution function needs to be renormalized so that all fibers can be located in the constrained area. The renormalized distribution function is then given by:
\[ \psi(\theta, \phi, \gamma) = \frac{1}{\int_0^{2\pi} \int_{\theta_w}^{\pi-\theta_w} (\gamma^2 \cos^2 \theta - \gamma \sin 2\theta \sin \phi + 1)^{-3/2} \sin \theta d\theta d\phi} \]  
(VI-A-8)

The dimensionless rheological properties are obtained by inserting equation (VI-A-8) into the appropriate components of the bulk stress in equation (IV-C-1).

a) The dimensionless shear viscosity
\[
\frac{12}{(nl^3)^3} (\frac{\eta_s}{\eta} - 1) = \int_0^{2\pi} \int_0^{\pi} \int_0^{\pi - \theta_w} (\cos^2 \theta \sin^2 \theta \sin^2 \phi) \psi \sin \theta \sin \phi \, d\theta d\phi
\]  

(VI-A-9)

b) The dimensionless primary normal stress coefficient

\[
\frac{12}{(nl^3)^3} \psi_{w1} = \int_0^{2\pi} \int_0^{\pi} \int_0^{\pi - \theta_w} \cos \theta \sin \theta \sin \phi (\sin^2 \theta \sin^2 \phi - \cos^2 \phi) \psi \sin \theta \sin \phi \, d\theta d\phi
\]  

(VI-A-10)

c) The dimensionless secondary normal stress coefficient

\[
\frac{12}{(nl^3)^3} \psi_{w2} = \int_0^{2\pi} \int_0^{\pi} \int_0^{\pi - \theta_w} \cos \theta \sin \theta \sin \phi (\cos^2 \phi - \sin^2 \theta \cos^2 \phi) \sin \theta \sin \phi \, d\theta d\phi
\]  

(VI-A-11)

In the above integrals, \( \psi \) is given in equation (VI-A-8).

These integrals are then evaluated numerically by Simpson's rule with \( \theta_w \) as a parameter that ranges from 0.1(\( \pi \)/2) to 0.9(\( \pi \)/2). The case of \( \theta_w = 0 \) corresponds to a suspension that is not confined. These results have been discussed in Section (V-B). When \( \theta_w = \pi/2 \), the surfaces of the wall just touch each other. Hence, the test particle is aligned in the plane of shear and would have no influence on the bulk properties of the suspension.

The computer program to evaluate the integrals in equations (VI-A-9) to (VI-A-11) are tabulated in Appendix 3. The results of the dimensionless shear viscosity are illustrated in Figures (VI-A-2) to (VI-A-10), the results for the dimensionless primary normal stress coefficient are shown in Figures (VI-A-11) to (VI-A-19), and the results for the
$\theta_w = 0.1(\pi/2)$

Figure VI-A-2 Comparison of the dimensionless bulk shear viscosity versus the shear strain in the confined and unconfined situations. The wall effect is modeled by the renormalization method.
Figure VI-A-3  Same as in Figure VI-A-2
\[ \theta_w = 0.3(\pi/2) \]

- confined
- unconfined

Figure VI-A-4 Same as in Figure VI-A-2
\[ \theta_w = 0.4(\pi/2) \]

Figure VI-A-5  Same as in Figure VI-A-2
\[ \theta_w = 0.5(\pi/2) \]

- confined
- unconfined

**Figure VI-A-6** Same as in Figure VI-A-2
\[ \theta_w = 0.6(\pi/2) \]

+ confined
- unconfined

Figure VI-A-7 Same as in Figure VI-A-2
Figure VI-A-8 Same as in Figure VI-A-2
$\theta_w = 0.8(\pi/2)$

+ confined
- unconfined

Figure VI-A-9  Same as in Figure VI-A-2
$\theta_w = 0.9(\pi/2)$

- confined
- unconfined

Figure VI-A-10  Same as in Figure VI-A-2
Figure VI-A-11 Comparison of the dimensionless bulk primary normal stress coefficient versus the shear strain in the confined and unconfined situations. The wall effect is modeled by the renormalization method.
\[ \theta_w = 0.2(\pi/2) \]

Figure VI-A-12 Same as in Figure VI-A-11
$\theta_w = 0.3(\pi/2)$

Figure VI-A-13  Same as in Figure VI-A-11
\[ \theta_w = 0.4(\pi/2) \]

+ confined
- unconfined

**Figure VI-A-14** Same as in Figure (VI-A-11)
\[ \theta_w = 0.5(\pi/2) \]

- confined
- unconfined

Figure VI-A-15  Same as in Figure VI-A-11
Figure VI-A-16  Same as in Figure VI-A-11
\[ \theta_w = 0.7(\pi/2) \]

- confined
- unconfined

**Figure VI-A-17** Same as in Figure VI-A-11
\[ \theta_w = 0.8(\pi/2) \]

+ confined
- unconfined

Figure VI-A-18  Same as in Figure VI-A-11
\[ \theta_w = 0.9(\pi/2) \]

- confined
- unconfined

Figure VI-A-19  Same as in Figure VI-A-11
dimensionless secondary normal stress coefficient are displayed in Figures (VI-A-20) to (VI-A-28). In each graph the plus sign (+) represents the bulk property of a confined suspension whereas the solid line is the corresponding result in the unconfined situation.

3. Discussion

The results of the dimensionless shear viscosity, shown in Figures (VI-A-2) to (VI-A-10), indicate that the walls will orient the particles closer to the plane of shear before the shear flow commences. Therefore when \( \theta_w \) is small, the zero-shear viscosity should be higher than the corresponding value in the unconfined case because a fraction of the particles is initially aligned near the principal axis of the rate of strain tensor. This behavior is shown in Figures (VI-A-2) to (VI-A-4) in which the zero-shear viscosity increases as the separation between the wall decreases. However the highest increment does not occur at \( \theta_w = \frac{\pi}{4} \) because the bulk viscosity is averaged over all available configurations. To determine where the maximum zero-shear viscosity occurs, equation (VI-A-9) is integrated analytically at the inception of the shear flow to give:

\[
\frac{12}{(nl^3)^3} \left( \frac{\eta_b}{\eta_s} - 1 \right) = \frac{1}{10} \left( \sin^2 \theta_w \cos^2 \theta_w + \frac{2}{3} \cos^2 \theta_w \right) \quad (VI-A-12)
\]

From equation (VI-A-12), the optima of the dimensionless zero-shear viscosity take place when \( \theta_w = 0 \) and \( \theta_w = 0.1339\pi \). The case of \( \theta_w = 0 \) corresponds to the unconfined situation. When \( \theta_w = 0.1339\pi \), the dimensionless zero-shear viscosity attains
Figure VI-A-20 Comparison of the dimensionless bulk secondary normal stress coefficient versus the shear strain in the confined and unconfined situations. The wall effect is modeled by the renormalization method.
Figure VI-A-21  Same as in Figure VI-A-20
\( \theta_w = 0.3(\pi/2) \)

+ confined
- unconfined

Figure VI-A-22  Same as in Figure VI-A-20
\( \theta_w = 0.4(\pi/2) \)

- confined
- unconfined

Figure VI-A-23  Same as in Figure VI-A-20
Figure VI-A-24  Same as in Figure VI-A-20
\[ \theta_w = 0.6 \left( \frac{\pi}{2} \right) \]

+ confined
- unconfined

Figure VI-A-25 Same as in Figure VI-A-20
$\theta_w = 0.7(\pi/2)$

+ confined
- unconfined

Figure VI-A-26  Same as in Figure VI-A-20
\[ \theta_w = 0.8(\pi/2) \]

- confined
- unconfined

Figure VI-A-27  Same as in Figure VI-A-20
$\theta_w = 0.9(\pi/2)$

+ confined
- unconfined

Figure VI-A-28  Same as in Figure VI-A-20
The results from this case are intermediate between those shown in Figures (VI-A-3) and (VI-A-4).

Beyond the value of \( \theta_w = 0.1339 \pi \), the zero-shear viscosity decreases as the solid surfaces collapse toward each other. In such cases the initial configuration of the particles are closer to the shearing plane. This behavior is indicative of the plots of Figures (VI-A-5) to (VI-A-10).

The transient predictions from this approach contain a flaw that is exhibited by the shear overshoot in each figure. When \( \theta_w < \pi/4 \), it is reasonable to anticipate an overshoot because a fraction of the fibers is capable of passing through the principal axis of the rate of strain tensor, and therefore the tension along the fiber reaches a maximum. In the case of \( \theta_w > \pi/4 \), however, the results in Figures (VI-A-7) to (VI-A-10) still exhibit an overshoot in the viscosity curve. This behavior occurs because this model does not prevent particles, whose initial orientations lie between \( \theta_w < \theta < (\pi - \theta_w) \) and \( \pi < \phi < 2\pi \), to poke through the walls during their approach toward the plane of shear. Consequently, this fraction of particles will always pass by the principal axis of the rate of strain tensor. Because of this defect, the kinematics of the particles in the neighborhood of the solid boundaries have to be reconsidered. An attempt to model this situation is described in Section (VI-B). At large strains,
the particles are aligned in the plane of shear. Therefore, the bulk viscosity approaches the solvent shear viscosity.

The results of the dimensionless primary and secondary normal stress coefficients are depicted in Figures (VI-A-11) to (VI-A-28). At the start of the shear deformation, these bulk properties are zero because the configuration of the particles is symmetrical about the x-z plane. At large strains both of these rheological properties converge to zero because the tension along each particle is removed. However, the transient behavior in each case is not clear because a portion of the suspended fibers is able to rotate through the walls.

To conclude this segment on the modeling of the wall effects, a direct renormalization of the particles confined between two rigid boundaries is valid at the inception of the shear flow. However, the transient predictions are doubtful because the model does not prohibit the particles from rotating through the walls. Consequently, a more refined description of the particle motion is necessary to extend the analysis to the transient region.
B. PARTICLE TRACKING METHOD

The objective of this section is to formulate a model that would prevent the particles from penetrating through the walls. The approach taken is to modify the kinematics of the test particle when it encounters the wall surfaces. The particle trajectory is then inserted into the bulk stress tensor, and the result is summed over all initial configurations.

1. Description of the particle motion

The coordinate system for the flow field, and for the particle orientation is shown in Figure (VI-5-1). The center of mass of the test particle is assumed to lie halfway between the walls, and is assumed to be convected affinely by the bulk deformation. However, the trajectory of the test fiber in a confined flow field depends on its initial configuration. Since the initial particle orientation defined by $0 \leq \Theta_0 \leq \pi/2$ and $0 \leq \phi_0 \leq 2\pi$ is symmetrical to the region defined by $\pi/2 \leq \Theta_0 \leq (\pi - \Theta_w)$ and $0 \leq \phi_0 \leq 2\pi$, we need to consider only one of these cases. When $0 \leq \Theta_0 \leq \pi/2$, four regions are identified for the initial azimuthal angle $\phi_0$. These regimes are:

- Region I : $0 \leq \phi_0 \leq \pi$
- Region II : $\pi < \phi_0 < 3\pi/2$
- Region III : $\phi_0 = 3\pi/2$
- Region IV : $3\pi/2 < \phi_0 < 2\pi$

The motions of particles with initial configurations in each
Figure VI-B-1 Schematic drawing of the particle tracking method to model the wall effect
of these regions are described below.

a) Region I

In this regime the ends of the fiber never meet the walls. Consequently the components of the equation of motion (equation IV-A-41) can be written as:

\[
\frac{d\theta}{d\gamma} = \cos^2\theta \sin \phi
\]  
(VI-B-1)

\[
\frac{d\phi}{d\gamma} = \cot \theta \cos \phi
\]  
(VI-B-2)

with the initial conditions,

\[
\gamma = 0, \ \theta = \theta_0, \ \phi = \phi_0
\]  
(VI-B-3)

The particle trajectory is then described by:

\[
\tan \theta = \left(\gamma^2 + 2\gamma \tan \theta_0 \sin \phi_0 + \tan^2 \theta_0\right)^{\frac{1}{2}}
\]  
(VI-B-4)

\[
\tan \phi = \frac{\gamma + \tan \theta_0 \sin \phi_0}{\tan \theta_0 \cos \phi_0}
\]  
(VI-B-5)

Equations (VI-B-4) and (VI-B-5) are the trajectory of any test fiber that starts off in region I. The results indicate that the particles align into the plane of shear as the flow develops.

b) Region II

In the second regime the motion of the test particle is more complicated because the ends of the fiber will meet the wall at some intermediate strain. The initial motion of the particle is to head toward the wall since \(\frac{d\theta}{d\gamma} < 0\) in equation (VI-B-1). This motion is represented by segment 1 in Figure (VI-B-1). When the particle encounters the solid surface, \(\frac{d\theta}{d\gamma} = 0\). This condition would prevent the fiber from penetrating through the wall. At this point we postulate that the tip
of the particle will follow segment 2 in which \( \theta \) remains constant while \( \phi \) varies until \( \phi \) exceeds \( \pi \). Here, the end of the fiber has just cleared the vertical plane shown in Figure (VI-B-1). Thereafter the particle is free from the constraints imposed by the walls. Therefore, during the third part of its journey, the fiber will simply rotate toward the plane of shear, as illustrated by segment 3. Consequently, there are three sub-regions to be modeled.

i) Segment 1: \( \theta_0 < \theta < \theta_w \), \( \phi_0 > \phi > \phi_w \)

Segment 1 is the route traversed by a test fiber, in region II, before the particle meets the wall. Consequently, the kinematics described by equations (VI-B-4) and (VI-B-5) are valid until \( \theta \) equals \( \theta_w \). The time required for the particle to rotate from \( \theta_0 \) to \( \theta_w \), denoted by \( \gamma_w \), can be evaluated from equation (VI-B-4):

\[
\gamma_w = -\sin\phi_0 \tan\theta_0 - (\tan^2 \theta_w - \tan^2 \theta_0 \cos^2 \phi_0)^{\frac{1}{2}} \quad \text{(VI-B-6)}
\]

With \( \gamma_w \) known, \( \phi_w \) can be determined from equation (VI-B-5):

\[
\tan \phi_w = -\frac{(\tan^2 \theta_w - \tan^2 \theta_0 \cos^2 \phi_0)^{\frac{1}{2}}}{\tan \theta_0 \cos \phi_0} \quad \text{(VI-B-7)}
\]

The vector \((\theta_w, \phi_w)\) then specifies the orientation of the fiber when it just touches the wall. The duration is prescribed by equation (VI-B-6), and the motion of test particles in this region are described by equations (VI-B-4) and (VI-B-5).

ii) Segment 2: \( \theta = \theta_w \), \( \phi_w > \phi > \pi \)

When the ends of the fiber meet the wall, the particle orientation is identified by \((\theta_w, \phi_w)\). At this point, the
motion of the particle that was previously governed by equations (VI-B-1) and (VI-B-2) needs to be modified in order to prevent the particle from going through the walls. A proposed mechanism is to allow the fiber to rotate through its azimuthal angle $\phi$, but at constant $\theta_w$. Hence, the governing equations for the particle motion are assumed to be:

$$\frac{d\theta}{dy} = 0 \quad \text{(VI-B-8)}$$

$$\frac{d\phi}{dy} = \cot \theta_w \cos \phi$$

with the conditions that

$$\gamma = \gamma_w, \quad \theta = \theta_w, \quad \phi = \phi_w \quad \text{(VI-B-10)}$$

The solutions to equations (VI-B-8) and (VI-B-9) subject to the conditions in equation (VI-B-10) are then:

$$\theta = \theta_w \quad \text{(VI-B-11)}$$

$$\tan \left( \frac{\pi}{4} + \frac{\phi}{2} \right) = \tan \left( \frac{\pi}{4} + \frac{\phi_w}{2} \right) \exp \left( \cot \theta_w (\gamma - \gamma_w) \right) \quad \text{(VI-B-12)}$$

The motion described by equations (VI-B-11) and (VI-B-12) is halted when $\phi < \pi$ because the particle is no longer driven into the wall by the flow. From here, $\frac{d\theta}{dy} > 0$ indicates that the fiber descends toward the plane of shear.

The time required for a particle to rotate from $\phi = \phi_w$ to $\phi = \pi$, denoted by $(\gamma^* - \gamma_w)$, is obtained from equation (VI-B-12):

$$(\gamma^* - \gamma_w) = -\tan \theta_w \ln \left( -\tan \left( \frac{\pi}{4} + \frac{\phi_w}{2} \right) \right) \quad \text{(VI-B-13)}$$

iii) Segment 3: $\theta_w \leq \theta \leq \frac{\pi}{2}, \quad \phi < \pi$

In the last portion of the particle trajectory, the fiber motion is again governed by equations (VI-B-1) and (VI-B-2).
However the initial conditions have been altered. Instead of the conditions imposed in equation (VI-B-3), the new ones are:

\[ \gamma = \gamma^*, \ \theta = \theta^*, \ \phi = \pi \]  

(VI-B-14)

Consequently the particle motion is described by:

\[ \tan \theta = \left( (\gamma - \gamma^*)^2 + \tan^2 \theta^* \right)^{\frac{1}{2}} \]  

(VI-B-15)

\[ \tan \phi = \frac{-(\gamma - \gamma^*)}{\tan \theta^*} \]  

(VI-B-16)

c) Region III

Region III corresponds to the situation of a test fiber that is initially oriented on the left side of the \((y - z)\) plane. In this case the fiber rotates through \(\theta\) at constant \(\phi\) until its tip meets the wall. Then the particle, in this configuration, translates with the bulk flow because it can neither rotate through \(\phi\) nor poke through the rigid walls. Hence, the motion of the test fiber is governed by equations (VI-B-1) and (VI-B-2) with \(\phi = \frac{3\pi}{2}\) when \(\gamma < \gamma^*\). The kinematics of the particle is then described by:

\[ \tan \theta = \left( \gamma^2 - 2\gamma \tan \theta^* + \tan^2 \theta^* \right)^{\frac{1}{2}} \]  

(VI-B-17)

\[ \phi = \frac{3\pi}{2} \]  

(VI-B-18)

The time required for the fiber to reach the wall, \(\gamma^*_w\), is determined from equation (VI-B-17):

\[ \gamma^*_w = \tan \theta^* - \tan \theta^*_w \]  

(VI-B-19)

Consequently if \(\gamma\) exceeds \(\gamma^*_w\) then the particle orientation is:

\[ \theta = \theta^*_w \]  

(VI-B-20)

\[ \phi = \frac{3\pi}{2} \]  

(VI-B-21)
d) Region IV

In the fourth regime the motion of the fiber follows the same three stages that have been described for Region III because the orientations of particles in these two regions are symmetrical.
i) Segment 1: $\theta_0 < \theta < \theta_w$, $\phi_0 < \phi < \phi_w$

In the first stage, the motion of the test particle is described by equations (VI-B-4) and (VI-B-5), and $\gamma_w$ is given in equation (VI-B-6).

ii) Segment 2: $\theta = \theta_w$, $\phi_w < \phi < 2\pi$

In segment 2, the kinematics of the test fiber have been prescribed by equations (VI-B-11) and (VI-B-12). However, the time required for a particle to rotate from $\phi = \phi_w$ to $\phi = 2\pi$ is given by:

$$ (\gamma^* - \gamma_w) = -\tan \theta_w \ln(\tan\left(\frac{\pi}{4} + \frac{\phi_w}{2}\right)) $$

(VI-B-22)

iii) Segment 3: $\theta_w < \theta < \frac{\pi}{2}$, $\phi > 2\pi$

In segment 3, the particle motion is described by:

$$ \tan \theta = \left( (\gamma - \gamma^*)^2 + \tan^2 \theta_w \right)^{\frac{1}{2}} $$

(VI-B-23)

$$ \tan \phi = \frac{\gamma - \gamma^*}{\tan \theta_w} $$

(VI-B-24)

The motion of the particle has been described in the above. The next step is to insert these kinematics into the bulk stress to arrive at predictions of the rheological properties.

2. Rheological properties

The rheological properties are estimated on the assumption
that the bulk stress has the same form as equation (IV-C-2).

\[
\tau = -\eta_s \dot{\gamma} = \eta_s \left( \frac{\pi}{12} \right)^3 \left( \frac{1}{\psi_N} \right) \left( \frac{1}{2\pi} \right)^2 \int_0^{\pi/2} \int_0^{2\pi} \rho \eta_s \sin^2 \theta \sin \phi \sin \theta d\theta d\phi
\]

(VI-B-25)

where the normalization constant \( \psi_N \) is given by:

\[
\psi_N = \frac{1}{4\pi} \int \int \delta (p - \bar{p}(u, t)) d\rho d\chi
\]

(VI-B-26)

Although equation (IV-C-2) implies that the particle motion follows equation (III-C-5), this model is chosen so that comparison can be made between the predicted values in Section (VI-A) and the results obtained by altering the kinematics of the fiber at the wall.

In the case of a simple steady shear flow, the dimensionless rheological properties are as follows:

a) The dimensionless shear viscosity

\[
\frac{12}{(n \ell^3)^3} \psi_N \left( \frac{\eta^+}{\eta_s} - 1 \right) = \frac{1}{2\pi} \int_0^{\pi/2} \cos^2 \theta \sin^2 \phi \sin \theta d\theta d\phi
\]

(VI-B-27)

b) The dimensionless primary normal stress coefficient

\[
\frac{12}{(n \ell^3)^3} \psi_N \gamma_1^+ = \frac{1}{2\pi} \int_0^{\pi/2} \cos \theta \sin \phi \sin \phi \sin^2 \theta d\theta d\phi - \cos^2 \theta \sin \theta d\theta d\phi
\]

(VI-B-28)

c) The dimensionless secondary normal stress coefficient

\[
\frac{12}{(n \ell^3)^3} \psi_N \gamma_2^+ = \frac{1}{2\pi} \int_0^{\pi/2} \cos \theta \sin \phi \sin \phi (\cos^2 \theta - \sin^2 \phi) \sin \theta d\theta d\phi
\]

(VI-B-29)
In the above equations, \((\theta, \phi)\) is the trajectory followed by a test particle. Therefore, \((\theta, \phi)\) depend on the initial configuration \((\theta_0, \phi_0)\) and the shear strain \(\gamma\).

With the orbits described in Section (VI-B-1), the integrals in equations (VI-B-27) to (VI-B-28) are evaluated by Simpson's rule. The computational scheme is as follows:

a) If the initial configuration belongs to Region I, then for a given \(\gamma\), \((\theta, \phi)\) are evaluated from equations (VI-B-4) and (VI-B-5).

b) If the initial configuration belongs to Region II, then \((\theta, \phi)\) are evaluated according to the numerical value of \(\gamma\).

i) \(\gamma < \gamma_w\)

\((\theta, \phi)\) are determined from equations (VI-B-4) and (VI-B-5)

ii) \(\gamma_w < \gamma < \gamma^*\)

\((\theta, \phi)\) are evaluated from equations (VI-B-11) and (VI-B-12)

iii) \(\gamma > \gamma^*\)

\((\theta, \phi)\) are computed from equations (VI-B-15) and (VI-B-16)

c) If the initial configuration belongs to Region III, then \((\theta, \phi)\) are evaluated according to the numerical value of \(\gamma\).

i) \(\gamma < \gamma_w\)

\((\theta, \phi)\) are determined from equations (VI-B-17) and (VI-B-18)

ii) \(\gamma > \gamma_w\)

\((\theta, \phi)\) are evaluated from equations (VI-B-20) and (VI-B-21)

d) If the initial configuration belongs to Region IV, then the approach used to calculate \((\theta, \phi)\) is identical to the
procedure outlined in part (b).

The results of the calculations are shown by the solid lines in Figures (VI-B-2) to (VI-E-19) for the dimensionless primary normal stress coefficient; and in Figures (VI-20) to (VI-B-28) for the dimensionless secondary normal stress coefficient. The corresponding computer programs to calculate these quantities are listed in Appendix 5. These results are then contrasted to the properties obtained in section (VI-A). The latter results are represented by the "plus" sign. Secondly, the normalization constant for the orientation distribution is given by:

$$\psi_N = \frac{1}{2\pi} \int_{0}^{\pi} \int_{\Theta}^{\pi} (\gamma^2 \cos^2\theta - \gamma \sin 2\Theta \sin\phi + 1)^{-3/2} \sin\Theta d\Theta d\phi$$  \hspace{1cm} (VI-B-30)

The numerical integrations of the rheological properties in equations (VI-B-27) to (VI-B-29) are sensitive to the mesh size because of the different kinematics imposed on the test particles. The computed data, based on a grid of 750X750 for each double integral, are simply connected by the solid lines. Consequently, the shape of each curve may not be smooth.

When $\gamma=0^+$, the two models lead to identical predictions because the particles are still stationary. As the walls begin to close in, the results of the shear viscosity in Figures (VI-B-2) and (VI-B-3) produce an overshoot. This behavior is expected since a fraction of the fibers is passing by the principal axis of the rate of strain. From Figures (VI-B-4) to (VI-B-10), the shear overshoot disappears in the calculations based on the model in section (VI-B). The
Figure VI-B-2 Comparison between the dimensionless bulk shear viscosity versus the shear strain results calculated from the renormalization and the particle tracking methods. Note that the bulk shear viscosity contains the normalization constant $\psi_N$ in these calculations.
Figure VI-B-3  Same as in Figure VI-B-2
Figure VI-B-4  Same as in Figure VI-B-2
Figure VI-B-5  Same as in Figure VI-B-2
$\theta_w = 0.5(\pi/2)$

- renormalization
- particle tracking

Figure VI-B-6 Same as in Figure VI-B-2
$\theta_w = 0.6\left(\pi/2\right)$

+ renormalization

- particle tracking

Figure VI-B-7  Same as in Figure VI-B-2
\[ \theta_w = 0.7(\pi/2) \]

+ renormalization
- particle tracking

Figure VI-B-8  Same as in Figure VI-B-2
Figure VI-B-9  Same as in Figure VI-B-2
$\theta_w = 0.9(\pi/2)$

+ renormalization
- particle tracking

Figure VI-B-10 Same as in Figure VI-B-2
Figure VI-B-11 Comparison between the dimensionless bulk primary normal stress coefficient versus the shear strain results calculated from the renormalization and the particle tracking methods. Note that the bulk primary normal stress coefficient contains the normalization constant $\psi_N$ in these calculations.
$\theta_w = 0.2(\pi/2)$

+ renormalization
- particle tracking

**Figure VI-B-12** Same as in Figure VI-B-11
Figure VI-B-13  Same as in Figure VI-B-11
\[ \theta_w = 0.4(\pi/2) \]

Figure VI-B-14  Same as in Figure VI-B-11

- renormalization
- particle tracking
Figure VI-B-15 Same as in Figure VI-B-11
Figure VI-B-16  Same as in Figure VI-B-11
\[ \theta_w = 0.7(\pi/2) \]

Figure VI-B-17  Same as in Figure VI-B-11
\[ \theta_w = 0.8(\pi/2) \]

Figure VI-B-18  Same as in Figure VI-B-11
\[ \theta_w = 0.9(\pi/2) \]

+ renormalization
- particle tracking

**Figure VI-B-19** Same as in Figure VI-B-11
Figure VI-B-20 Comparison between the dimensionless bulk secondary normal stress coefficient versus the shear strain results calculated from the renormalization and the particle tracking methods. Note that the bulk secondary normal stress coefficient contains the normalization constant $\psi_N$ in these calculations.
$\theta_w = 0.2(\pi/2)$

- renormalization
- particle tracking

Figure VI-B-21  Same as in Figure VI-B-20
\[ \theta_w = 0.3(\pi/2) \]

Figure VI-B-22  Same as in Figure VI-B-20
\[ \theta_w = 0.4(\pi/2) \]

- renormalization
- particle tracking

**Figure VI-B-23** Same as in Figure VI-B-20
$\theta_w = 0.5(\pi/2)$

Figure VI-B-24 Same as in Figure VI-B-20
\[ \theta_w = 0.6(\pi/2) \]

- renormalization
- particle tracking

Figure VI-B-25  Same as in Figure VI-B-20
Figure VI-B-26  Same as in Figure VI-B-20
\[ \theta_w = 0.8(\pi/2) \]

Figure VI-B-27 Same as in Figure VI-B-20
\[ \theta_w = 0.9(\pi/2) \]

- renormalization
- particle tracking

**Figure VI-B-28** Same as in Figure VI-B-20
transition is observed in Figure (VI-B-4) in which the overshoot has been replaced by a kink. From Figures (VI-B-5) to (VI-B-10) the shear viscosity, at a fixed strain, decreases with increasing $\theta_w$ because the average orientation of the fibers is closer to the shearing plane. Secondly, the shear viscosity, in each graph, decreases monotonically toward the solvent viscosity with increasing strain. The results based on the model in section (VI-A), however, still exhibit an overshoot before they too decay to the solvent viscosity at large strains. The difference between these two behaviors is due to the constraint that prevents the tips of the fibers from rotating through the rigid walls.

The computed results of the primary normal stress coefficient are shown in Figures (VI-B-11) to (VI-B-19). Similar to the results of the shear viscosity, the primary normal stress coefficient decreases with increasing $\theta_w$ at a given strain because the average orientation of the particles approaches the plane of shear. However, the estimates based on the model in this section are consistently lower than the predicted values from the model developed in section (VI-A). The differences increase as the walls approach each other. This behavior reflects the constraint on the fiber motion by the walls. Consequently, the normal component of the tension along the fiber is less than the corresponding situation in which the particle can rotate past the wall. Moreover, the differences would be amplified as the walls collapse toward each other.
The secondary normal stress coefficients are plotted in Figures (VI-B-20) to (VI-B-28). The transient behavior of this rheological property is not clearly understood. On a qualitative basis, however, it is interesting to note that the shapes of the results from the model in section (VI-A) follow the behavior of the results in this section. In Figures (VI-B-20) and (VI-B-21) the shapes of the two curves are similar. The oscillation in the solid curve of Figure (VI-B-22) is similar to the shape of the "plus" sign in Figure (VI-B-26). From Figures (VI-B-23) to (VI-B-28) the values on the solid curves are all negative. This behavior later appears on the "plus" sign curve in Figures (VI-B-27) and (VI-B-28).

The model described in this section prohibits the tips of a fiber from rotating into the walls. Whether the kinematics imposed in this model are physically realistic remains to be the subject of future investigations. The next section outlines an improved method for evaluating the motion of a fiber when the later is in contact with rigid boundaries.
C. GENERAL FORMULATION OF THE "WALL-PROBLEM"

The models described in the above two sections are approximate, and have only addressed the case of a simple steady shear flow. In those models, the centers of mass of the particles are all located midway between the two surfaces of the walls. Secondly, the center of mass translates affinely. In section (VI-A) the motion of the test particle is derived from the torque balance that was described in section (III-C). However, this result does not prevent the tips of the fiber from rotating into the solid walls. Consequently, in the next section, the motion of the particle was modified. Although the ends of the fiber can no longer go through the walls, the particle kinematics was imposed instead of being derived from a force balance.

In this section we consider the possibility that the center of mass of the particles are initially randomly distributed. Secondly, we relax the assumption that the centers of mass of a test fiber translates affinely. Thirdly, the motion of the particle is obtained by applying the laws of conservation of linear and angular momentum. The resulting kinematics is then inserted into the bulk stress. The following is an outline to the formulation of such a model in homogeneous flows.

1. The stress tensor

The general form of the bulk stress has been presented in section (III-B) in which:
\[ \dot{I} = -\eta_0 \dot{X} - \frac{1}{V_I} \left[ \frac{1}{l} \int \zeta \left( \frac{1}{l} \int \zeta \right) \psi \dot{r} \, d\psi \, d\sigma \right] \]  \hspace{1cm} (VI-C-1) 

where the distribution function \( \psi \) is governed by:

\[ \frac{\partial}{\partial t} \psi = -\frac{\partial}{\partial r} \left( \dot{r} \psi \right) \]  \hspace{1cm} (VI-C-2) 

The quantity \( \dot{r} \) appearing in equations (VI-C-1) and (VI-C-2), describes the motion of an element of a test fiber. Therefore, \( \dot{r} \) has to be evaluated before equation (VI-C-1) can be used to estimate the bulk rheological properties.

If the fiber never touches the walls, i.e. the distance between the wall and the center of mass of the particle is greater than 1/2, then the dynamics for this fraction of fibers has been determined in Chapters III and IV. The center of mass translates affinely with the bulk deformation. The rotation of the particle is governed by equation (III-C-5), and its solution is given by equation (IV-A-11). The contribution to the bulk stress from such particles is then given by equation (IV-C-6).

If the distance between the center of mass of the particle and the wall is less than 1/2, then this test particle may encounter the solid boundaries. The likelihood of a collision will depend on the type of flow, and on the initial orientation of the test particle. Consequently in cases where the test fiber does not encounter the wall, then the results presented in Chapters III and IV are still valid. In the event that a collision between a test fiber and the wall occurs, then the motion of this particle has to be
re-examined. The formulation to the particle motion in the last case is described below.

2. Dynamics of a fiber in contact with the wall

The situation of a test fiber colliding with a wall is depicted in Figure (VI-C-1). The wall is moving at a velocity $v_w$. When a fiber rotates toward the wall, a reaction force $F_r$ develops at the point of contact. If inertia terms are neglected, the reaction force is balanced by the hydrodynamic drag force. Hence,

$$ F_r = \frac{1}{2} \frac{1}{1/2} \zeta_{\text{eff}} \cdot (\xi \cdot \dot{r} - \ddot{r}) ds $$

$$ = \zeta_{\text{eff}} \{ 2 \dot{\delta} - \ddot{\delta} \} \cdot (\xi \cdot r_c - \dot{r}_c) \tag{VI-C-3} $$

The reaction force is then resolved into a normal component $F_{rn}$, and a shearing component $F_{rs}$,

$$ F_r = F_{rn} \delta_n + F_{rs} \delta_s \tag{VI-C-4} $$

where $\delta_s$ is given by:

$$ \delta_s = \frac{v_w - (\dot{\delta} - \delta_n \delta_n) \cdot (\dot{r}_c + \frac{1}{2} \ddot{r}_c)}{|v_w - (\dot{\delta} - \delta_n \delta_n) \cdot (\dot{r}_c + \frac{1}{2} \ddot{r}_c)|} \tag{VI-C-5} $$

Secondly, if the shearing component is proportional to the normal component in which the constant of proportionality is the kinetic coefficient of friction $\mu_k$, then equation (VI-C-4) can be rewritten as:

$$ F_r = F_{rn} (\delta_n + \mu_k \delta_s) \tag{VI-C-6} $$

and $F_{rn}$ is obtained from equation (VI-C-3):

$$ F_{rn} = \zeta_{\text{eff}} \{ 2 \dot{\delta} - \ddot{\delta} \} \cdot (\xi \cdot r_c - \dot{r}_c) \cdot \delta_n \tag{VI-C-7} $$
Figure VI-C-1  Schematic drawing of a fiber colliding with a wall
The motion of the center of mass is obtained from equation (VI-C-3):

\[ \dot{x}_c = \kappa \cdot x_c - \frac{1}{2 \zeta_{\text{eff}}} \{ \dot{\omega} + \dot{pp} \} \cdot F_r \]  

(VI-C-8)

The solution to this equation is subject to the condition that:

\[ t = t_w, \quad x_c = x_{c,w} \]  

(VI-C-9)

where \( t_w \) is the instant that the particle reaches the wall, and \( x_{c,w} \) is the location of the center of mass of this particle when it hits the wall. Consequently, the center of mass deforms affinely if the reaction force is not present.

The governing equation for the orientation of the test fiber is obtained from a torque balance about the center of mass of the particle. Hence,

\[ \frac{1}{2} \kappa \times \Omega_r = \frac{1}{2} \int_0^{1/2} \kappa \times \left[ \zeta_{\text{eff}} \cdot (v - \dot{r}) \right] ds \]  

(VI-C-10)

Equation (VI-C-10) is then simplified to:

\[ \dot{\omega} = \kappa \cdot \omega - \kappa \cdot \dot{pp} - \frac{6}{4 \zeta_{\text{eff}}} \{ \dot{\omega} - \dot{pp} \} \cdot F_r \]  

(VI-C-11)

The solution to equation (VI-C-11) is subject to the condition that:

\[ t = t_w, \quad \omega = \omega_w \]  

(VI-C-12)

where \( \omega_w \) is the orientation of the fiber at the initial point of contact with the wall.

The complete motion of a test particle is then described by equations (VI-C-6), (VI-C-8) and (VI-C-11) when one end of the fiber is in contact with the wall. Once the tip of the particle leaves the wall then \( F_r \) is zero, and the center of
mass of the fiber will resume moving affinely with the bulk motion.
CHAPTER VII
EXPERIMENTS IN SHEAR FLOW

The purpose of this chapter is to test the strain dependence of the rheological properties in a shear flow. However, experimental difficulties were encountered in the course of obtaining the bulk shear viscosity at intermediary strains. These problems are indicated in Section (VII-D). Nevertheless, the bounds of the suspension shear viscosity have been verified at the high-strain region (Section VII-E), and the zero-strain region (Section VII-F).

Data obtained at large strains would test the asymptotic approach of the bulk viscosity toward the solvent viscosity as the fibers are aligned into the plane of shear. At the other extreme, data recorded at the inception of a shear flow would provide an indication to the validity of the scaling procedure for the effective drag coefficient in a suspension of randomly dispersed fibers, and the renormalization procedure to model the wall effect.

The procedures and the results from these experiments are elaborated in the ensuing sections.

A. MATERIALS

The material tested in this investigation consisted of a suspension of fibers in a Newtonian liquid. Two types of fibers were considered: E-glass and copper fibers. The solvent used in these experiments was pure honey. Each of these ingredients
is briefly described in this section.

1. **Fibers**

Three batches of E-glass fibers were procured from USM Corp., Seabrook, New Hampshire. The average dimensions of the particles in each lot are summarized in Table (VII-A-1) where \( l, w_f, h_f \) are respectively the length, the width and the thickness of the fiber. A schematic diagram of a fiber strand is illustrated in Figure (VII-A-1). Each strand incorporates approximately 200 to 300 glass filaments that are held together by an insoluble size. Consequently the bulk shape of a fiber appears like a parallelepiped.

For the purpose of comparing the experimental data with the model in Chapter IV, we have assigned an equivalent diameter to these fibers. The latter quantity is calculated by assuming that the rectangular cross-sectional area of a cylindrical particle. Hence, the equivalent diameter is given by:

\[
d = \left( \frac{4}{\pi} w_f h_f \right)^{\frac{1}{2}}
\]

(VII-A-1)

The results are listed in the fourth column of Table (VII-A-1).

Copper fibers were used in one set of experiments. This material was acquired in the form of a continuous filament from Magnet Wire Supply, Chatsworth, California. The diameter of the fiber is 0.254 mm, and the length is cut to approximately 1.5 mm. Because the density of this sample is 9,1846 g/cm\(^3\), its usage is limited to experiments of short durations.

2. **Carrying fluid**
Table VII-A-1  Properties of E-glass fibers

<table>
<thead>
<tr>
<th>l (mm)</th>
<th>w_f (mm)</th>
<th>h_f (mm)</th>
<th>d (zm)</th>
<th>l/d</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5</td>
<td>1.118</td>
<td>0.0635</td>
<td>0.301</td>
<td>11.64</td>
</tr>
<tr>
<td>6.4</td>
<td>0.6</td>
<td>0.0725</td>
<td>0.235</td>
<td>27.19</td>
</tr>
<tr>
<td>12</td>
<td>1.75</td>
<td>0.036</td>
<td>0.438</td>
<td>27.41</td>
</tr>
</tbody>
</table>

ρ_f = 2.54 g/cm³
Figure VII-A-1 Schematic diagram of an E-glass fiber
The carrying medium was purchased from a local supermarket (Star's supermarket, Cambridge, Massachusetts) under the brand name of NONAME pure honey. This fluid is Newtonian up to a shear rate of 400 s$^{-1}$, and has a viscosity of approximately 10 Pa.s at room temperature. The density of honey is 1.4291 g/cm$^3$. 
P. APPARATUS

The shear flow experiments have been conducted on the Rheometrics Mechanical Spectrometer (Rheometrics Inc., Union, New Jersey). A schematic diagram of the apparatus is shown in Figure (VII-B-1). The descriptions of the equipment, operational procedures, and limitations of the apparatus have been thoroughly discussed by Nacosko (1975), Yasuda (1979), Yarmoska (1979), Dalal (1980), Oswal (1980), and Weinberg (1981).

The cone and plate, and the parallel plate modes have been utilized to determine the shear viscosity of the suspension. Schematic drawings of the cone and plate, and of the parallel plate fixtures are shown in Figures (VII-B-2) and (VII-B-3) respectively. The diameter, D, of each plate measures 72 mm. In the case of the cone and plate mode, the angle of the cone, \( \theta \), is 0.04 radians. Moreover, the tip of the cone is truncated, hence leaving a clearance of 50 \( \mu m \) between the plates. In the case of the parallel plate mode, the spacing between the plates, \( h \), can be varied.

In both of these fixtures, the sample is placed between the gap of the two concentric plates. The bottom plate is held stationary while the upper plate rotates either in the clockwise or counterclockwise directions at a preset constant angular velocity. The torque required to turn the upper plate, \( T_m \), is then related to the shear viscosity. The normal thrust on the plates, \( F_z \), provides a measure of the elastic properties of the sample. In practice, however, the output of the normal force reading is often plagued by excessive noise.
Figure VII-B-1  Schematic diagram of the Rheometrics Mechanical Spectrometer
Figure VII-B-2  Schematic drawing of a cone and plate viscometer
Figure VII-B-3 Schematic drawing of a parallel plate viscometer
Consequently, only viscosity data are recorded in each test.
C. PROCEDURE

1. Sample preparation

The suspension is prepared by weighing the desired amount of solvent and solids in a small beaker. The two components are then mixed at room temperature. The slurry is stirred slowly to minimize a number of potential experimental complications: a) formation of air bubbles; b) fiber breakage; c) break-up of the fiber bundle into individual filaments. A fresh sample is prepared for each experiment to ensure that the particles are initially randomly oriented.

Since the fractional amount of the ingredients is expressed in terms of weight percentages, a convenient set of formulas is provided to convert this quantity into a volume fraction and a number density of solids:

\[ \phi_v = \left(1 + \frac{\rho_f}{\rho_s} \left(\frac{1}{\phi_w} - 1\right)\right)^{-1} \]  \hspace{1cm} (VII-C-1)

and,

\[ n = \frac{4}{\pi d_i^2} \phi_v \]  \hspace{1cm} (VII-C-2)

2. Experimental technique

In order to determine the shear viscosity of the suspension, the sample is first loaded on the bottom plate of the viscometer. In experiments using the cone and plate mode, fibers are cleared from a small area of approximately 1 mm in diameter at the center of the plate. This fiber-free region would prevent the truncated tip of the cone from rubbing
against the particle surface.

The amount of sample tested in each run depends on the fixture used because the gap thickness of the cone and plate is fixed, whereas the separation between the parallel plates can be adjusted. The latter feature facilitates the tests of the wall effect on the bulk properties. In either case, the amount of sample squeezed out between the plates should be minimized because the orientation of the fibers may be enhanced by the radial flow.

Once the sample is properly put in place, the upper plate is set to rotate at a known angular velocity. At this instant it is assumed that the entire suspension is sheared. Then the history of the bulk shear viscosity is recorded by allowing the experiment to proceed in time at the same apparent shear rate. In the cone and plate fixture, the apparent shear rate is the true shear rate, whereas the apparent shear rate is the rim shear rate in the parallel plate mode. Consequently the torque reading in the later case has to be corrected to accommodate for the variation of the shear rate from the center of the plate to its edge. This correction will be discussed in the next section. The experiment is then repeated for different shear rates, and for different particle geometries and concentrations.

At the end of a run, the suspension containing glass fibers is discarded. However, the metal fibers are washed, dried and reused for later experiments.
3. **Data reduction**

The readings gathered from these two rotational viscometers are the variations of the torque with time at a preset rate of rotation. This section outlines the procedure to convert these primary data into relations between the shear viscosity and the shear strain.

a) Cone and plate data

The shear rate in a cone and plate viscometer is assumed to be uniform. This quantity can be obtained from the angular velocity by:

\[ \dot{\gamma} = \frac{\omega}{2} \quad \text{(VII-C-3)} \]

The shear strain is evaluated from the product of the shear rate and the elapsed time \( t \),

\[ \gamma = \dot{\gamma}t \quad \text{(VII-C-4)} \]

and the transient viscosity is related to the torque by:

\[ \eta^* = \frac{12\beta T_M}{\pi \omega D^3} \quad \text{(VII-C-5)} \]

where \( t \) and \( T_M \) are read off from the output of the strip chart recorder.

b) Parallel plate data

The shear rate in a parallel plate viscometer is assumed to vary linearly from the center to the edge of the plate. The shear rate at the center is zero. At the rim, the shear rate is related to the angular velocity by:

\[ \dot{\gamma}_R = \frac{\omega D}{2h} \quad \text{(VII-C-6)} \]

Consequently the rim shear strain is:
\[ \dot{\gamma}_R = \dot{\gamma}_R \]  

(VII-C-7)

The measured torque is an average of the shearing stress on the circular surface of the upper plate. Hence,

\[
T_M = 2\pi \int_0^{D/2} \eta^+(\gamma) \dot{\gamma} r^2 dr = \frac{2\pi R^3}{3} \int_0^{\dot{\gamma}_R} \eta^+(\gamma) \dot{\gamma} \gamma^3 d\gamma = \frac{2R}{t\gamma_R^3} \int_0^{\dot{\gamma}_R} \eta^+(\gamma) \gamma^3 d\gamma \]  

(VII-C-8)

To extract \(\eta(\gamma_R)\) from equation (VII-C-8), the later is differentiated with respect to \(\gamma_R\). After a few manipulations,

\[
\eta^+(\gamma_R) = \frac{4T_M}{\pi \gamma_R^3 D^3} (3 + \frac{\text{dln}(4T_M/\pi D^3)}{\text{dln}\gamma_R}) 
\]  

(VII-C-9)

In a given experiment, \(D\) and \(\dot{\gamma}_R\) are predetermined; \(T_M\) and \(t\) are obtained from the output of the strip chart recorder; and \(\gamma_R\) is evaluated from equation (VII-C-7). A sample calculation is illustrated in Appendix 6.
D. EXPERIMENTAL OBSERVATIONS

In the shear flow experiments using the parallel plate viscometers, the following observations have been made.

1. The degree of fiber breakage is minimal in the course of the experiment. Although the glass fibers are more prone to damage, breakage has not been observed probably because each strand contains a bundle of fibrils. Secondly, the size which holds the fibrils together is insoluble. Hence, the fibrils do not disperse into the suspension, and the integrity of the fiber bundle is maintained throughout the entire experiment. Thirdly, there are no sharp edges within the parallel plate environment to abrade the glass particles.

2. The suspensions of glass fibers are characterized in the parallel plate viscometer because the fiber lengths are too long for these particles to be tested in the cone and plate viscometer. Secondly, the adjustable gap of the parallel plate mode provides a convenient means for testing the effect of the walls on the bulk properties. In the course of these experiments, however, the fibers tend to ooze out of the gap. This undesirable feature is amplified when either the shear rate, the elapsed time, or the fiber length is increased. Hence, the shear rate is typically limited to 0.01 to 0.1 $s^{-1}$, and the experiment is stopped when a substantial quantity of sample is squeezed out of the gap. The elapsed time or the shear strain depends on the test parameters, but the maximum duration lasted one hour.

3. The shear field in a parallel plate viscometer is non-
homogeneous, and therefore presents a problem for comparing the experimental data with the predicted values. However, the suspension viscosity at the inception of the shear flow and at steady-state would be independent of the type of shear deformation. In the zero-strain region, the structural arrangement of the fibers in the suspension has not yet been altered. Consequently, the zero-shear bulk viscosity is a measure of the resistance to deformation from these randomly dispersed fibers. At the other extreme, the particles are all aligned into the plane of shear. Therefore, the bulk viscosity is nearly the same as the solvent viscosity which is a property of the material and not of the measuring apparatus.

4. The suspension of metal fibers was tested in a cone and plate viscometer. However, the particles tend to settle to the bottom plate because of the large difference in densities between the fiber and the solvent. If the particles were neutrally buoyant the cone angle provides a non-uniform wall effect on the suspension. Consequently the results from this apparatus cannot be directly compared with the model in either Chapter IV or VI.

The experimental characterization of fiber suspensions seen to be a difficult task because the dimensions of the particles are often greater than or equal to the dimensions of commercial apparatus. Consequently the bulk properties measured from different equipment may vary substantially because the transient orientation of the particles will depend on the geometry of the apparatus. However, the steady-
state shear viscosity should be independent of the test environment, and the zero-shear viscosity would only depend on the degree of confinement but not on the nature of the shear flow.
E. "HIGH-STRAIN" SHEAR VISCOSITY

The high-strain shear viscosity provides a lower bound estimate of the suspension shear viscosity. According to the calculation presented in Chapter V, the suspension viscosity approaches the solvent viscosity beyond a shear strain of 10.

In this set of experiments, suspensions of 1.5 \( \mu m \) copper fibers were tested in the cone and plate viscometer. The shear rate was set at 100 \( s^{-1} \), and the data were collected at the one second mark. Consequently the shear strain was 100. This value ensured that the suspension had reached steady-rate.

The data are shown in Figure (VII-E-1) and in Appendix 7. As shown in Figure (VII-E-1) the difference between the experimental data and the predicted value is within a factor of 2.5. Secondly, the data suggest that the relative viscosity seems to depend on the number density of solids. The difference between the predicted and experimental results is probably due to the finite thickness of the fiber which has not been accounted for in the model.

In order to assess the contribution from the finite thickness of the particle to the bulk behavior, we assume that all the fibers are stacked up in equally spaced planes of shear. The suspension viscosity is then computed based on the assumption that the bulk energy dissipation in shear flow is equivalent to the energy dissipated by the solvent between the layers of fibers. In this simple analysis,

\[
\frac{n}{n_s} = \frac{d + a_c}{a_c}
\]
Figure VII-E-1 Plot of the "high-strain" bulk viscosity versus the number density for a suspension of 1.5 mm fibers.
\[
\frac{1}{1 - d(nl)^\frac{3}{2}} \quad (\text{VII-E-1})
\]

where \((d + a_o)\) is the distance between the center lines of two fibers located in adjacent fiber layers. With this packing configuration, this spacing is equal \((nl)^{-\frac{3}{2}}\). This result then leads to the relation in equation (VII-E-1). The dash-line in Figure (VII-E-1) represents the result in equation (VII-E-1).

In conclusion, the high-strain data indicate that the suspension shear viscosity is approximately the same as the solvent viscosity at large strains because the particles are all aligned near the plane of shear. Although the experimental data and the model developed in Chapter III agree reasonably well, the previous model can be improved by incorporating the thickness of the fiber.
F. "ZERO-SHEAR" VISCOSITY AND THE WALL EFFECT

The objective of this set of experiments is to verify the scaling of the effective drag coefficient, and the modeling of the wall effect. The tests were conducted on a parallel plate viscometer with a suspension of glass fibers at room temperature. The "zero-shear" viscosities correspond to the measurements at a shear strain of 0.01. Although this value is not obtained instantaneously at the start of the flow, the result in Figure (V-3-2) shows that the initial shear viscosity remains constant up to a strain of approximately 0.1.

The shear viscosity data are summarized in Appendix 8, and in Figures (VII-F-1) to (VII-F-9) for three different lengths of fibers and at three separate gap thicknesses. In each graph the experimental results (+ sign) are compared with the predicted values (solid line). The later is obtained from equation (VI-A-11) in which \( \cos \theta_w = h/l \). In Figure (VII-F-1), for instance, the fiber length, \( l \) is 3.5 mm and the gap thickness is 3 mm. Consequently \( \cos \theta_w = 0.3571 \), and the relative viscosity is:

\[
\frac{n^+}{n_s} = 1 + 6.847 \times 10^{-2} \frac{(n/3)^3}{12}
\]  

(VII-F-1)

Before discussing the results, the limits of the semi-dilute region for each lot of fibers are shown in Table (VII-F-1). These limits are based on an unconfined suspension of randomly dispersed fibers.

The results in Figures (VII-F-1) and (VII-F-2) show that
\[ \frac{n_0}{n_s} - 1 = 6.847 \times 10^{-2} \frac{(n l^3)^3}{12} \]

Figure VII-F-1 Plot of the dimensionless bulk shear viscosity versus the solid concentration for a suspension of 3.5 mm fibers. The gap width of the parallel plate viscometer is 3 mm.
Figure VII-F-2 Same as in Figure VII-F-1 but for a gap width of 2 mm.
$l = 3.5\, \text{mm}; \; \text{gap} = 1\, \text{mm}$

$\log\left(\frac{n^+}{n_s} - 1\right) = 1.294 \times 10^{-2} \frac{(nl^3)^3}{12}$

$\log((nl^3)/12)$

**Figure VII-F-3** Same as in Figure VII-F-1 but for a gap width of 1 mm.
Figure VII-F-4 Plot of the dimensionless bulk shear viscosity versus the solid concentration for a suspension of 6.4 mm fibers. The gap width of the parallel plate viscometer is 3 mm.
Figure VII-F-5  Same as in Figure VII-F-4 but for a gap width of 2 mm.
Figure VII-F-6  Same as in Figure VII-F-4 but for a gap width of 1 mm.
Figure VII-F-7  Plot of the dimensionless bulk shear viscosity versus the solid concentration for a suspension of 12 mm fibers. The gap width of the parallel plate viscometer is 3 mm.
\[ \frac{n^+}{n_s} - 1 = 4.552 \times 10^{-3} \left( \frac{n_1^3}{12} \right)^3 \]

**Figure VII-F-8** Same as in Figure VII-F-7 but for a gap width of 2 mm.
Figure VII-F-9  Same as in Figure VII-F-7 but for a gap width of 1 mm.
<table>
<thead>
<tr>
<th>l (mm)</th>
<th>Volume fraction</th>
<th>log((nl^3)/12)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5</td>
<td>0.007 &lt; (\phi_v) &lt; 0.086</td>
<td>-1.079 to 2.119</td>
</tr>
<tr>
<td>6.4</td>
<td>0.001 &lt; (\phi_v) &lt; 0.037</td>
<td>-1.079 to 3.224</td>
</tr>
<tr>
<td>12</td>
<td>0.001 &lt; (\phi_v) &lt; 0.037</td>
<td>-1.079 to 3.235</td>
</tr>
</tbody>
</table>
the experimental data and the predicted values agree closely up to a value of \( \log((nl^4)^3/12) = 3 \). Although this value has exceeded the upper limit of the solid concentration in the semi-dilute regime (Table VII-F-1), the close agreement is perhaps due to the presence of the wall. The role of the solid boundaries is to enhance the alignment of the particles. Consequently the separation between adjacent fibers would increase. Therefore it is possible to extend the upper concentration limit of the semi-dilute regime so that the distance between nearest neighbors in a confined environment is the same as the corresponding case in an unconfined situation.

In Figure (VII-F-3) the difference between the measured values and the estimated values by approximately an order of magnitude at the lower concentration end is unclear. The close agreement at the high end of the concentration regime is again due to the presence of the wall.

In Figures (VII-F-4) to (VII-F-9), the concentration of solids in each graph has exceeded the corresponding upper limit that is indicated in Table (VII-F-1). Secondly, the model slightly overestimates the experimental data. However the difference between the measured value and the theoretical line decreases as the concentration of solids increases. This behavior is consistent with the above discussion of the wall effect. The model overestimates the measured data because it is based on a renormalization of the distribution function. Therefore, the estimated values do not account for the
variation of the separation between adjacent particles with respect to the distance between the walls. This effect is equivalent to adding more fibers into the suspension. Consequently, the differences between the theoretical and experimental results decrease as the solid concentration increases.

In summary, the experimental results agree reasonably well with the predicted values. The encountered differences, which are within an order of magnitude, are probably due to the method in which the wall effect has been modeled. An improved model should relate the distance between neighboring fibers to the orientation of the particles.
CHAPTER VIII

A GENERAL MODEL OF FIBER SUSPENSIONS IN ARBITRARY FLOWS

The general form of the rheological equation of state for a suspension of particles has been described previously by Batchelor (1970). In Chapter III we have presented a method to convert a multi-body problem into a single particle problem in which the analysis is focused on a test fiber that is immersed in an effective medium. Furthermore, the drag force on the test particle is represented by a Stokes-Burgers model.

In order to elucidate the usage of this model for predicting the macroscopic behavior of this type of material while simultaneously reducing the amount of computations, we have restricted the analysis to the case of a suspension of rigid fibers in homogeneous flows. The analytical solutions for the bulk rheological properties have been presented in Chapter IV, and are illustrated in Chapter V for various homogeneous flows.

The governing equations for the constitutive equation of a suspension of deformable but inelastic fibers in general flows are outlined in this chapter as means of furthering the previous results to more realistic flow conditions. The formulation of the model follows the same procedure as in Chapter III. First, the bulk stress is modified from the volume average result of Batchelor. Secondly, the distribution function is identified. Thirdly, the equation of motion is constructed to describe the evolution of the test particle
configuration.

In closing, special cases from the general model are related to the earlier results, and to the work of Hinch (1976).

A. STRESS TENSOR

The bulk stress derived by Batchelor is given by:

\[ \mathbf{I} = -\eta_s \dot{\mathbf{\gamma}} + \frac{1}{V} \sum \mathbf{n} \cdot \mathbf{n} dA \]  \hspace{1cm} (VIII-A-1)

where the summation is over all the particles in the suspension.

The next stage of the development is to reduce the above multi-body problem to a single particle problem by focusing the analysis on a test particle that is immersed in an effective medium. Hence,

\[ \mathbf{I} = -\eta_s \dot{\mathbf{\gamma}} + \frac{1}{V} \int \mathbf{I}_{\text{eff}} \cdot \mathbf{n} \psi dr dA \]  \hspace{1cm} (VIII-A-2)

where \( \psi (\mathbf{r}, t) \) is the probability of locating a particle point in the neighborhood of \( \mathbf{r} \) to \( \mathbf{r} + dr \) at time \( t \). The position vector \( \mathbf{r} \), as sketched in Figure (VIII-A-1), is used to situate a point on the center line of the fiber. Therefore, \( \mathbf{r} \) depends on the arc length, \( s \), and the history of the flow, \( t \). The volume \( V \) is chosen such that \( V^{1/3} \) is greater than a differential element of the fiber \( ds \), but smaller than the length scale over which the bulk flow is varying.

Similar to Section (III-B), the drag force per unit length \((\pi d) \mathbf{I}_{\text{eff}} \cdot \mathbf{n}\) is approximated by a Stokes-Burgers model. Consequently,

\[ \mathbf{I} = -\eta_s \dot{\mathbf{\gamma}} - \frac{1}{VI} \int_{-1/2}^{1/2} \zeta_{\text{eff}} \{ 2\dot{\mathbf{\gamma}} - \mathbf{r}' \mathbf{r}' \} \cdot (\mathbf{v} - \dot{\mathbf{r}}) r_w dr ds \]  \hspace{1cm} (VIII-A-6)
Figure VIII-A-1  Schematic diagram of an inextensible fiber
To make use of equation (VIII-A-6), the distribution function $\psi(r, t)$ and the rate of change of a particle point $\dot{r}(r, t)$ need to be evaluated. The governing equations for these two quantities are presented in the next two sections.
B. DISTRIBUTION FUNCTION

The distribution function \( \psi (r, t) \) describes the likelihood that a particle point can be found in the range of \( r \) to \( r + dr \) at time \( t \). The governing equation for \( \psi \) is analogous to the one for the orientation distribution function discussed in Section (III-D). In the present case a point on the fiber is conserved in configuration space. Consequently,

\[
\frac{\partial \psi}{\partial t} = -\frac{\partial}{\partial r} \cdot (r \psi) \tag{VIII-B-1}
\]

with the initial condition that \( \psi \) is a constant. This constant can be determined by applying the normalization condition. Hence,

\[
\psi (r, 0) = C = (\int \psi dr)^{-1} \tag{VIII-B-2}
\]

The formal solution for \( \psi \) from the above conservation equation can be obtained by the method of characteristics for a suspension of non-Brownian particles. In such case \( \dot{r} \) does not depend on the gradient of \( \psi \). Therefore, the procedure is to first rewrite equation (VIII-B-1) in terms of a set of ordinary differential equations.

\[
\frac{d}{dt} r = \dot{r} \tag{VIII-B-3}
\]

and,

\[
\frac{d}{dt} \psi = -\frac{\partial}{\partial r} \cdot (r \dot{r} \psi) \tag{VIII-B-4}
\]

with the initial conditions,

\[
r = r_0 \quad \text{at} \quad t = 0 \tag{VIII-B-5}
\]
\[ \Psi = C \quad \text{at } t = 0 \]  

(VIII-B-6)

Equation (VIII-B-4) can be directly integrated to yield:

\[ \Psi(r_0, t) = C \exp\left( - \int_{0}^{t} \left( \frac{\partial}{\partial r} \cdot \mathbf{\hat{r}} \right) dt \right) \]  

(VIII-B-7)

At this point it is necessary to obtain an expression for \( \mathbf{\hat{r}} \) in terms of \( r \) and \( t \) so that \( \frac{\partial}{\partial r} \cdot \mathbf{\hat{r}} \) can be rewritten as functions of \( r \) and \( t \). Secondly, \( \mathbf{\hat{r}} \) can be inserted into equation (VIII-B-3) to arrive at a relation for \( r(r_0, t) \). The result for \( r(r_0, t) \) then enables the integration in equation (VIII-B-7) to be carried out. The last step is perhaps the most difficult part of the entire solution procedure because it requires the conversion of \( r_0 \) back to \( r \). As an example the solution to a simpler situation has been presented in Section (IV-B).
C. EQUATION OF MOTION

The equation of motion provides a relation for \( \dot{\mathbf{r}}(\mathbf{r}, t) \) which is subsequently employed to obtain \( \Psi \) from equation (VIII-E-8) and \( \mathbf{I} \) from equation (VIII-A-6). Furthermore, the shape of the test fiber is described by \( \mathbf{r} \). The evolution of the particle shape portrays the configuration of the fiber, and predicts the possibility of fiber breakage when the local radius of curvature reaches a critical value. The governing equations for the motion of the particle are set up in this section. A summary of the assumptions is listed in Table (VIII-C-1).

The coordinate system used to locate a point on the test fiber is illustrated in Figure (VIII-A-1). A free-body diagram on a segment of length \( ds \) on this deformable but inelastic test fiber is shown in Figure (VIII-C-1). The unit vectors denoting the internal coordinates of the test fiber are labelled by \( (\hat{\delta}_X, \hat{\delta}_Y, \hat{\delta}_Z) \). Their relations with the fixed reference frame are listed in Table (VIII-C-2), and the differential properties of these unit vectors are summarized in Table (VIII-C-3). In Figure (VIII-A-1), the vectors \( \hat{T} \) and \( \hat{M} \) are respectively the tension and the moment at the ends of the segment \( ds \). The quantities \( d\hat{T} \) and \( d\hat{M} \) represent the infinitesimal change in the tension and the moment over a segment \( ds \) of the fiber. The external force acting on the element \( ds \) is \( F_h \). This hydrodynamic force is approximated by a Stokes-Burgers model:

\[
F_h = \zeta_{eff} (2\hat{\delta} - \mathbf{r}' \mathbf{r}') \cdot (\mathbf{v} - \dot{\mathbf{r}}) \frac{ds}{t} \tag{VIII-C-1}
\]
Table VIII-C-1  Summary of assumptions used to describe the shape of a test fiber in arbitrary flows.

1. Inertia terms are neglected in the conservations of linear and angular momentum.

2. The fiber is deformable but inextensible.

3. The fiber is thin.

4. Terms containing the product of the differential arc length \((ds)^2\) are neglected.

5. The fiber only undergoes pure bending.

6. Torsional terms are neglected.

7. The stress in the fiber is linearly proportional to the strain.
\[ F_n = \zeta_{\text{eff}} \cdot (\mathbf{y} - \mathbf{r}) \frac{ds}{l} \]

**Figure VIII-C-1**  A free-body diagram on a segment ds of an inextensible fiber
Table (VIII-C-2) Relations between the unit vectors of the internal coordinates and the fixed reference frame.

\[
\delta_X = \mathbf{r}'
\]
\[
= \left(\frac{\partial r_X}{\partial s}\right) \delta_x + \left(\frac{\partial r_Y}{\partial s}\right) \delta_y + \left(\frac{\partial r_Z}{\partial s}\right) \delta_z
\]

\[
\delta_Y = (\mathbf{r}'' \cdot \mathbf{r}'')^{-\frac{1}{2}} \mathbf{r}''
\]
\[
= R \left[ \left(\frac{\partial^2 r_X}{\partial s^2}\right) \delta_x + \left(\frac{\partial^2 r_Y}{\partial s^2}\right) \delta_y + \left(\frac{\partial^2 r_Z}{\partial s^2}\right) \delta_z \right]
\]

\[
\delta_Z = \delta_X \times \delta_Y
\]

where,

\[
R \equiv (\mathbf{r}'' \cdot \mathbf{r}'')^{-\frac{1}{2}} = \text{radius of curvature}
\]
Table VIII-C-3 Derivatives of the unit vectors with respect to arc length in the internal coordinate frame.

\[ \frac{\partial}{\partial s} \delta_X = \frac{1}{R} \delta_Y \]

\[ \frac{\partial}{\partial s} \delta_Y = -\frac{1}{R} \delta_X + \frac{1}{\Omega} \delta_Z \]

\[ \frac{\partial}{\partial s} \delta_Z = -\frac{1}{\Omega} \delta_Y \]

where,

\[ \frac{1}{\Omega} = R^2 ( (r' \times r'') \cdot r''' ) \]

and,

\[ |\Omega| = \text{radius of torsion} \]
where \( \mathbf{v} \) is the bulk velocity field.

In order to arrive at an expression for \( \mathbf{\dot{r}} \), conservation of linear and angular momentum is applied over the element \( ds \).

With the inertia terms neglected, a force balance yields:

\[
-\mathbf{\hat{T}} + \mathbf{\dot{T}} + \frac{d\mathbf{T}}{ds} + \zeta_{\text{eff}}(2\mathbf{\hat{\omega}} - \mathbf{r}' \mathbf{\dot{r}}') \cdot (\mathbf{v} - \mathbf{\dot{r}}) \frac{ds}{l} = 0
\]  
(VIII-C-2)

Equation (VIII-C-2) can be rearranged to give:

\[
\mathbf{\dot{r}} = \mathbf{v} + \frac{1}{2} \mathbf{T}' + \frac{1}{2} \mathbf{r}' \mathbf{r}' \cdot \mathbf{T}'
\]  
(VIII-C-3)

where,

\[
\mathbf{T} = \frac{1}{\zeta_{\text{eff}}} \mathbf{\hat{T}}
\]  
(VIII-C-4)

and the symbol (') represents differentiation with respect to \( s \).

The above result is subject to the constraint that the rod is inextensible. This condition is given by:

\[
\mathbf{\dot{r}}' \cdot \mathbf{r}' = 0
\]  
(VIII-C-5)

By differentiating equation (VIII-C-3) with respect to \( s \) and by performing the scalar product of the result with \( \mathbf{r}' \), we obtain:

\[
0 = (\mathbf{r}' \mathbf{r}': \mathbf{\nabla} \mathbf{v}) + \mathbf{r}' \cdot \mathbf{T}'' + \frac{1}{2} \mathbf{r}' \cdot \mathbf{T}''
\]  
(VIII-C-6)

In arriving at equation (VIII-C-6) the relation \( \mathbf{r}' \cdot \mathbf{r}'' = 0 \) has been utilized.

At this junction equations (VIII-C-3) and (VIII-C-6) are insufficient for calculating \( \mathbf{r} \) because \( \mathbf{\dot{r}} \) and \( \mathbf{T} \) are vectorial quantities while equation (VIII-C-6) is a scalar equation.

However, if \( \mathbf{T} \) is in the \( \mathbf{r}' \) direction then the above equations form a closed set of relations to determine \( \mathbf{r} \). This case
corresponds to a suspension of zero Young's modulus fibers. The shape of these particles in homogeneous flows has been worked out by Hinch (1976). The special cases will be summarized in the next section.

In order to acquire additional equations, the conservation of angular momentum is applied. With the inertia terms neglected, we obtain:

\[ M - \dot{M} - \dot{\delta}_x ds \times (-\mathbf{T}) - \dot{\delta}_x ds \times \mathbf{F}_h = 0 \]  (VIII-C-7)

Furthermore, by neglecting the product of the differential arc length, \((ds)^2\), equation (VIII-C-7) is reduced to (Landau and Lifshitz, 1959):

\[ \frac{\partial}{\partial s} M = \dot{\delta}_x \times \mathbf{T} \]  (VIII-C-8)

By assuming that the thin test fiber only experiences a pure bending deformation in the \((X,Y)\) plane, and by neglecting all torsional terms, equation (VIII-C-8) is simplified to:

\[ \frac{\partial}{\partial s} M_Z = \mathbf{T}_Y \]  (VIII-C-9)

where \(M_Z\) is the component of the moment in the \(Z\) direction, and \(\mathbf{T}_Y\) is the component of the tension in the \(Y\) direction. The moment \(M_Z\) is then evaluated by assuming a linear stress-strain relationship for the fiber. Hence,

\[ M_Z = \int_S \sigma_{XX} Y ds \]

\[ = E \int_S u_{XX} Y ds \]  (VIII-C-10)

where \(\sigma_{XX}\) is the \(XX\) component of the solid stress field; \(Y\) is
the moment arm; $S$ is the cross-sectional surface of the fiber; $E$ is Young's modulus and $u_{XX}$ is the XX component of the strain tensor. When a rod is undergoing a pure bending, the strain $u_{XX}$ is given by (Timoshenko and Gere, 1972):

\[ u_{XX} = \frac{y}{R} \quad (\text{VIII-C-11}) \]

Therefore, the moment $M_Z$ is inversely proportional to the radius of curvature:

\[ M_Z = \frac{EI}{R} \quad (\text{VIII-C-12}) \]

where $I$ is the moment of inertia. For a cylindrical particle, $I$ is related to the diameter of the rod by:

\[ I = \frac{\pi}{64} d^4 \quad (\text{VIII-C-13}) \]

By inserting equation (VIII-C-12) into equation (VIII-C-9), the $Y$ component of the tension is given by:

\[ \hat{T}_Y = EIR(x'' \cdot x'') \quad (\text{VIII-C-14}) \]

In equation (VIII-C-14) the approximate sign is employed because we have neglected the shear deformation within the solid particle. The error introduced by this assumption is not very serious, particularly for a thin fiber.

Since the torsional modes of deformation are assumed to be negligible, then the $Z$-component of the tension is approximately zero.

\[ \hat{T}_Z = 0 \quad (\text{VIII-C-15}) \]

Therefore, the tension $\hat{T}$ is reduced to:
\[ \hat{T} = T_x \hat{\delta}_x + T_y \hat{\delta}_y \]  

(VIII-C-16)

The vectors \( \hat{T}' \) and \( \hat{T}'' \) are then obtained by applying the relations in Table (VIII-C-3):

\[ \hat{T}' = (T_x' - \frac{1}{R} T_y') \hat{\delta}_x + (T_y' + \frac{1}{R} T_x') \hat{\delta}_y \]  

(VIII-C-17)

and,

\[ \hat{T}'' = ((T_x' - \frac{1}{R} T_y')') - \frac{1}{R} (T_y' + \frac{1}{R} T_x') \hat{\delta}_x \\
+ ((T_y' + \frac{1}{R} T_x')') + \frac{1}{R} (T_x' - \frac{1}{R} T_y') \hat{\delta}_y \]  

(VIII-C-18)

In the last two equations, the radius of torsion has been assumed to be infinite. By inserting the above relations into equations (VIII-C-3) and (VIII-C-6), the governing equations that describe the shape of the test fiber are given by:

\[ \ddot{r} = y + (T_x' + EIR^{-3}R') \hat{r} + \frac{1}{2} (2EIR^{-2}(R')^2 \\
- EIR^{-1}R'' + T_x) \hat{r}'' \]  

(VIII-C-19)

and,

\[ T_x'' - \frac{R^{-2}}{2} T_x = -EI(\frac{3}{2}R^{-3}R'' - 4R^{-4}(R')^2) - (\hat{r}' \hat{r}' : \nabla y) \]  

(VIII-C-20)

with the following initial conditions:

\[ r = r_0(s) \quad \text{at } t = 0 \]  

(VIII-C-21)

\[ T_x = 0 \quad \text{at } s = \frac{1}{2} \]  

(VIII-C-22)

The solutions to equations (VIII-C-19) and (VIII-C-20) describe the configuration of a test fiber in an arbitrary flow field \( y \). In addition the local radius of curvature, the center of mass and the drift of the center of mass are respectively given by:
\[ R(s,t) = (\mathbf{r}'' \cdot \mathbf{r}''')^{-\frac{1}{2}} \]  \hspace{1cm} \text{(VIII-C-23)}

\[ \mathbf{I}_c = \frac{1}{I} \int_{1/2}^{1/2} \mathbf{r} \, ds \]  \hspace{1cm} \text{(VIII-C-24)}

\[ \dot{\mathbf{I}}_c = \frac{1}{I} \frac{3}{2} \int_{1/2}^{1/2} \mathbf{r} \, ds \]  \hspace{1cm} \text{(VIII-C-25)}

The radius of curvature indicates the location where fiber breakage may occur. Equation (VIII-C-24) describes the instantaneous location of the center of mass whereas the last equation determines the possibility of particle migration.
D. SPECIAL CASES

The general solutions to the set of equations that describe the particle shape, equations (VIII-C-19) to (VIII-C-22), probably cannot be expressed in simple analytical forms. The purpose of this section is to demonstrate that the model presented in earlier chapters can be retrieved from these general equations. Secondly, we wish to show that the results obtained by Hinch (1976) on the shape of an inextensible thread is a special case of the governing equations in Section (VIII-C).

1. Comparison with the results of Section (IV-A).

In Section (IV-A) the general solution for the motion of a rigid fiber in homogeneous flows has been presented. The same result can be derived from the governing equations of Section (VIII-C). If the test particle is rigid then:

\[ r'(s,t) = r'(t) \]  \hspace{1cm} (VIII-D-1)

Consequently, \( r'' = 0 \) and the radius of curvature is infinite. When these conditions are substituted into equations (VIII-C-19) and (VIII-C-20), then:

\[ \dot{\mathbf{r}} = \mathbf{v} + T_x' \mathbf{r}' \]  \hspace{1cm} (VIII-D-2)

and,

\[ T_x'' = - (\mathbf{r}' \mathbf{r}'') \cdot \mathbf{v} \]  \hspace{1cm} (VIII-D-3)

By taking the derivative of equation (VIII-D-2) with respect to \( s \), and by using equation (VIII-D-3) to replace \( T_x'' \), we obtain:
\[ \dot{r}' = r' \cdot \nabla r' - (r' \cdot \nabla) r' \]
\[ = \kappa \cdot r' - \kappa : r' r' r' \]  \hspace{1cm} (VIII-D-4)

The vector \( r' \) plays the same role as the unit vector \( p \) in Chapter IV. Therefore, if the flow field is homogeneous then \( \kappa = \kappa(t) \), and equation (VIII-D-4) is identical to equation (IV-A-1).

2. Comparison with the work of Hinch

Hinch (1976) considered the shape of a thread in homogeneous flows. The Young's modulus of a thread is zero. Consequently, the governing equations to model this problem can be obtained directly from equations (VIII-C-19) and (VIII-C-20) by setting \( E = 0 \):

\[ \dot{r} = \nabla + T_X' \dot{r}' + \frac{1}{2} T_X \dot{r}'' \]  \hspace{1cm} (VIII-D-5)

and,

\[ T_X'' - \frac{R^2}{2} T_X = -(r r' : \nabla r) \]  \hspace{1cm} (VIII-D-6)

By comparing the above equations with equations (VIII-C-3) and (VIII-C-6), it can be readily seen that the tension is directed tangentially along the center-line of the particle.

For this case Hinch presented an approximate analytical solution for the particle shape near the beginning of the flow, and a finite difference solution to describe the configuration of the fiber in a simple steady shear flow.
CHAPTER IX
CONCLUSIONS AND SUGGESTIONS FOR FUTURE WORK

The rheology of concentrated fiber suspensions has been suspected by previous investigators to be linked to the internal orientation of the particles. This coupling effect may have been the source of the vast disagreement between the experimental data reported in the literature. Our preliminary tests have indicated that the shear viscosity can be lowered by aligning the fibers toward the shearing plane while keeping all other factors constant. Therefore, a logical solution is to model the suspension from a structural approach. However, such attempts have led to an insurmountable degree of difficulty in handling the multi-body problem.

Our approach is to reduce the complexity of the problem by focusing the analysis on an arbitrary test particle, and replace the surrounding particles and solvent by an effective medium. The following is a concise summary of our findings and suggestions for further research.

A. MODELING IN HOMOGENEOUS FLOWS

A model has been constructed to describe the rheological properties a semi-concentrated suspension of rigid fibers in homogeneous flows. This concentration regime is defined to be one in which the distance between nearest neighbors varies from a fiber diameter to a fiber length apart. The model is then derived from either the volume-averaged bulk stress obtained

The analysis is focused on a single test fiber that is immersed in an effective medium. Consequently, a need arises to describe the probability of locating this particle in a given position and configuration along with an adequate representation of the effective drag force on the test particle. In addition a model of the particle motion is required.

The orientation distribution function is obtained by considering conservation of configurations. The effective drag force on a fiber is approximated by a Stokes-Burgers model in which this force is equal to the product between an effective drag coefficient and the relative velocity between the particle and the effective medium. The effective drag coefficient is estimated on the basis that the work required to displace a test fiber to a position that would have been occupied by its nearest neighbor is equivalent to the work done in displacing the nearest neighbor by a distance $l$ along its axis. This argument, however, breaks down when the hydrodynamic length scale is less than the separation between nearest particles. In our model we have neglected the transient behavior of these two length scales. Instead, we have assumed that the separation between adjacent particles for a suspension of randomly oriented particles remains constant. This assumption predicts accurately the bulk properties at the inception of the flow. Furthermore, the error based on this assertion is small in situations where the drag force on
the test fiber decreases with the flow history. Shear flows would fall in this category. More work is required to handle the opposite case typified by elongational flows. The analysis of this problem would require formulating the time dependent behavior of the hydrodynamic length scale since the transient property of the distance between nearest neighbors has already been obtained by Doi and Edwards (1978). The result would redefine the concentration regime based on these two transient length scales so that the correct form of the constitutive equation would be used.

The motion of the particle is determined from the conservations of linear and angular momentum. For a rigid fiber in a homogeneous flow, the conservation of linear momentum requires that the particle center of mass moves affinely with the bulk medium. The conservation of angular momentum shows that the fiber would deform affinely with the exception that it cannot stretch along its axis. Consequently the fiber would simply rotate to a steady-state configuration.
B. GENERAL SOLUTIONS AND ILLUSTRATIVE CALCULATIONS IN HOMOGENEOUS FLOWS

Analytical solutions have been obtained for the particle motion, the orientation distribution function, and the bulk stress tensor of a semi-concentrated suspension of rigid fibers in homogeneous flows. The solutions are given by:

1. **Particle motion**

\[
\mathbf{p} = \frac{\mathbf{E}\cdot\mathbf{p}_0}{(\mathbf{E}^+\cdot\mathbf{E}\cdot\mathbf{p}_0)^{\frac{3}{2}}}
\]  

(IX-B-1)

2. **Distribution function**

\[
\psi(p, t) = \frac{1}{4\pi}(\mathbf{A}^+\cdot\mathbf{A}\cdot\mathbf{p})^{-\frac{3}{2}}
\]  

(IX-B-2)

3. **Stress tensor**

\[
\mathbf{I} = -\mathbf{I}_s - \mathbf{I}_s \mathbf{I}_s (n_1^2)^{\frac{3}{2}} \int \frac{\mathbf{PPPPdp}}{4\pi(\mathbf{A}^+\cdot\mathbf{A}\cdot\mathbf{PP})^{3/2}}
\]  

(IX-B-3)

The above results are then employed to describe the motion of the fibers and the bulk properties in simple steady shear, uniaxial extension and biaxial extension flows.

In a shear flow, the particles are aligned into the plane of shear as the flow progresses. The bulk shear viscosity starts off at a finite value, then exhibits a small shear overshoot before it decays algebraically with increasing shear strain to the solvent viscosity. This phenomenon indicates that the tension along the fibers decrease with the flow.
history. The primary and secondary normal stress coefficients are initially zero because of the random orientation of the fibers. These two properties then become non-zero over a finite range of shear strain because the particles acquire a preferential orientation. However, these two properties vanish at large strain because the tension along these fibers have been removed once the particles lie in the plane of shear.

In extensional flows, the fibers are aligned toward the direction of extension. At the same time the bulk extensional viscosity increases with increasing extensional strain because the particles are rigid. However, the material points within the fiber cannot be stretched along with the materials points in the fluid. Consequently, the increasing tension leads to a rise in the bulk extensional viscosity. However, the separation between the particles increases simultaneously. This effect leads to a lowering of the bulk properties because the interactions between the fibers have been reduced. In order to correctly describe the physics of the problem, there is a need to assess the transient behavior of the hydrodynamic and interparticle length scales mentioned in Section (IX-A).

The above calculations demonstrate that the rheological properties depend strongly on the strain or the history of the flow, and not just on the rate of deformation. Therefore, the strain is a macroscopic representation of the internal fiber orientation.
C. WALL EFFECTS

Two models have been presented to account for the presence of rigid boundaries in a simple steady shear flow.

In the first method, the initial fraction of fibers that would poke through the walls is subtracted out of the contribution to the bulk stress from the particles. Although the model describes accurately the bulk behavior at the inception of the shear deformation, it does not prevent the fibers to penetrate into the wall as the flow develops. Consequently, a stress overshoot is observed for the viscosity irrespective of the separation between the walls. Because of this defect, the kinematics of the particles in the vicinity of the solid boundaries have been reconsidered.

Therefore, the second method consists of following the trajectory of each particle. The kinematics of the test particle are then prescribed so that the ends of the fiber are forbidden to go through the boundaries. However, these modifications do not alter the predictions of the bulk properties from the first model at the start of the flow and at the steady-state regime. Instead the predictions at the intermediate shear strain differ. In particular, the stress overshoot disappears when the suspension is severely constrained by the walls.

In order to extend the analysis to other homogeneous flows, a model has been formulated to describe the interaction between a fiber and a wall. The reaction force at the wall influences the motion of the particle center of mass and the
particle orientation. The governing equations are obtained by applying the conservation of linear and angular momentum. An addition to the model may be included to relate the friction between the fiber and the wall. The solution to this set of equations is a potential area for future investigation.
D. SHEAR VISCOSITY DATA

The results from the model have been compared to the shear viscosity measurements in the high strain and zero-strain regions at room temperature.

In the high-strain regime, suspensions of 1.5 mm copper fibers in pure honey have been tested in a cone and plate viscometer. The results indicate that the suspension shear viscosity is approximately the same as the solvent viscosity at large strains because the particles are all aligned near the plane of shear. Although the data agree reasonably well with the predicted values, the model can be improved by including the thickness of the fiber.

The zero-shear strain data provide a means to verify the scaling of the effective drag coefficient, and the modeling of the wall effect. Suspensions containing glass fibers in honey have been tested in a parallel plate viscometer at various concentrations and different ratios of fiber length to gap width. In each experiment, the results agree reasonably well with the predicted values. The encountered differences, which are less than an order of magnitude apart, are probably due to the method in which the wall effect has been modeled. An improved model would relate the distance between the neighboring fibers to the orientation of the particles.
E. GENERAL MODEL

A general model has been formulated to describe the rheological behavior of a suspension of inextensible non-Brownian particles in arbitrary flows. Similar to the development that has been summarized in Section (IX-A), the bulk stress is derived from Batchelor's work. The modified expression for the bulk stress requires the evaluation of a probability function and an equation for the evolution of the particle.

The probability function is obtained by conserving points in configuration space.

To determine the governing equation for the shape of the particle, the conservation laws for linear and angular momentum are applied over a differential arc length of the fiber. The resulting expressions relate the dimensions and the Young's modulus of the fiber to the properties of the effective medium. The solution to this set of equations, which are subject to future investigations, provides a means to characterize the bulk properties of the suspension. In addition the local radius of curvature will indicate whether fiber breakage will occur.
F. PROCESSING OF FIBER COMPOSITES

The results from this study have a number of implications toward the processing of fiber composites. The shear flow study has shown that the bulk viscosity can be dramatically lowered when the particles are aligned in the plane of shear. Consequently, it would be advantageous to have the fibers stacked up in layers when they are to be conveyed to different sections of the mold cavity. Therefore, the orientation of the fibers can be altered either by another type of flow field or by external means to satisfy the desired mechanical properties.

To have the fibers arranged in laminates, the particles can be manually placed in this configuration such as is done in the processing of sheet molding compounds. However, if the thickness of the part is thin then the study of the wall effect in Chapter VI has shown that the solid surfaces enhance the alignment of the fibers into the shearing planes, thereby eliminating the need for manual labor.

The analysis of the shear flow has also demonstrated the occurrence of normal stresses over a range of shear strains. Since the strain is related to the ratio of the flow length to the gap thickness, the location of the internal gating system, in an injection molding process, can be designed to enhance the flow of the composite into rib sections, by taking advantage of the normal stresses which tend to expand the material normal to the directions of the streamlines.
The results of the extensional flow calculations indicate that the particles are aligned much faster in these flows than in a shear flow. However, the energy dissipated is much higher because the fiber is in tension when it is aligned into the direction of the extension. Therefore, extensional flows are highly efficient to align particles, but not for transporting the fibers to different parts of the mold. Consequently, it may be possible to combine these two types of flows to optimize the transport of fiber composites.

The examples presented above can be extended to more general situations by means of the general solutions of the particle kinematics and the bulk stress developed in Chapter IV. These results coupled with simple experiments permit one to assess the feasibility of a proposed process.
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NOMENCLATURE

$a_c = \text{separation between two adjacent particles, m.}$

$a_i = \text{constants in equation (II-B-1)}$

$a_h = \text{characteristic length scale for the hydrodynamic disturbance, m.}$

$A = \text{surface area of the particle, m}^2$

$b = \text{unit vector describing the orientation of a test particle}$

$b_i = \text{constants in equation (II-B-2)}$

$d = \text{fiber diameter, mm.}$

$D = \text{plate diameter, mm.}$

$\frac{D}{Dt} = \text{substantial time derivative, s}^{-1}$

$E = \text{Young's modulus, Pa.}$

$\mathbf{E} = \text{strain tensor}$

$F = \text{tension along the fiber axis, N.}$

$F_{hn} = \text{hydrodynamic force, N.}$

$F_r = \text{reaction force at the wall, N.}$

$F_z = \text{normal force reading, N.}$

$F_v = \text{average force from the solvent molecules to bead v, N.}$

$h = \text{separation between two rigid boundaries, mm.}$

$h_f = \text{thickness of glass fiber, mm.}$

$H = \text{null vector}$

$I = \text{moment of inertia, m}^2$

$J = \text{Jacobian}$

$k = \text{Boltzmann's constant, m}^3\cdot\text{Pa/}^0\text{K}$
l = fiber length, m.
M = moment vector, N.m
\( \bar{M}_w \) = weight averaged molecular weight, Daltons
M_Z = Z component of the moment vector, N.m
n = number density of solids, mm^{-3}
n = unit vector directed normal to the particle surface
N = total number of beads
P = unit vector denoting the orientation of the particle
\( \dot{P} \) = rate of change of the unit vector \( \vec{P} \), s^{-1}
\( P_0 \) = initial configuration of a test fiber
\( P_W \) = orientation of a fiber at the initial point of contact with the wall
Q = internal coordinates
\( \vec{r} \) = position vector to the surface of the particle from an arbitrary coordinate system, m.
\( \dot{r} \) = rate of change of the vector \( \vec{r} \), m/s
\( \vec{r}' \) = \( \frac{\partial}{\partial s} \vec{r}(s,t) \)
\( \vec{r}'' \) = \( \frac{\partial^2}{\partial s^2} \vec{r}(s,t) \)
\( \vec{r}_c \) = position of the particle center of mass, m.
\( r_e \) = fiber aspect ratio
R = radius of curvature, m.
\( R_v \) = vector from bead \( v \) to the center of mass of the particle, m.
s = arc length, m.
S = cross-sectional surface of a fiber, m^2
t = elapsed time, s^{-1}
\text{tr}(U) = \text{trace of } \{U\}

T = \text{temperature}, \, ^\circ\text{K}

\mathbf{T} = \text{vector defined in equation (VIII-C-4), m}^2/\text{s}

\mathbf{T} = \text{tension, N.}

T_M = \text{torque, N.m}

T_X = \text{X component of } \mathbf{T}, \, \text{m}^2/\text{s}

T_Y = \text{Y component of } \mathbf{T}, \, \text{m}^2/\text{s}

T_Z = \text{Z component of } \mathbf{T}, \, \text{m}^2/\text{s}

u_{XX} = \text{XX component of the strain tensor } \mathbf{\varepsilon}

\mathbf{v} = \text{bulk velocity field, m/s}

\mathbf{v}_s = \text{local velocity field of the solvent, m/s}

\mathbf{v}_w = \text{velocity of a moving wall, m/s}

V = \text{suspension volume, m}^3

w_r = \text{width of a glass fiber, mm.}

W = \text{work, N.m}

\mathbf{x} = \text{displacement function}

\mathbf{x}' = \text{displacement function}

X = \text{internal coordinate}

Y = \text{internal coordinate}

Z = \text{internal coordinate}

\textbf{Greek Letters}

\beta = \text{cone angle, radians}

\beta_i = \text{constants in equation (IV-C-29)}

\gamma = \text{shear strain}

\gamma_w = \text{strain required for a particle to rotate from } \theta_0 \text{ to } \theta_w

\gamma^* = \text{strain at } (\theta, \phi) = (\theta_w, \pi)
\( \gamma(0) \) = strain tensor defined in equation (IV-C-28)
\( \dot{\gamma} \) = magnitude of the shear rate, s\(^{-1}\)
\( \dot{\lambda} \) = bulk rate of strain tensor, s\(^{-1}\)
\( \dot{\lambda}_S \) = local rate of deformation tensor in the solvent phase, s\(^{-1}\)
\( \delta(x-a) \) = Dirac delta function
\( \delta_n \) = unit vector in the normal direction of \( \mathbf{F}_r \)
\( \delta_s \) = unit vector in the shearing direction of \( \mathbf{F}_r \)
\( \mathbf{\dot{\lambda}} \) = unit tensor
\( \dot{\lambda} \) = strain tensor
\( \varepsilon \) = Hencky strain
\( \dot{\varepsilon} \) = rate of strain, s\(^{-1}\)
\( \zeta \) = drag coefficient Pa.s.l
\( \zeta_{\text{eff}} \) = effective drag coefficient, Pa.s.l
\( \eta \) = bulk shear viscosity, Pa.s
\( \eta^+ \) = transient shear viscosity, Pa.s
\( \tilde{\eta}^+ \) = transient extensional viscosity, Pa.s
\( \eta_0^+ \) = zero-shear viscosity, Pa.s
\( \eta_s \) = solvent viscosity, Pa.s
\( \theta \) = internal coordinate denoting the orientation of the particle
\( \theta_w \) = degree of confinement defined in equation (VI-A-1)
\( \theta_0 \) = initial orientation of a particle
\( \mathbf{\kappa} \) = velocity gradient tensor, s\(^{-1}\)
\( \lambda_1 \) = constant in equation (IV-C-24)
\( \lambda_2 \) = constant in equation (IV-C-24)
\( \mu_k \) = kinetic coefficient of friction
\( \mu_s \) = constant in equation (IV-C-24)
\( \nu \) = label for a bead

\( \Pi \) = total bulk stress tensor, Pa.

\( \Pi_{\text{eff}} \) = stress tensor describing the effective medium, Pa.

\( \Pi_s \) = constitutive equation for the solvent, Pa.

\( \rho_f \) = density of the particles, g/cm\(^3\)

\( \rho_s \) = density of the carrying medium, g/cm\(^3\)

\( \sigma_{XX} \) = XX component of the solid stress field, Pa.

\( \Pi_d \) = deviatoric part of the bulk stress tensor, Pa.

\( \Pi^b \) = contribution to the bulk stress from a particle, Pa.

\( \phi \) = internal coordinate denoting the orientation of the particle

\( \phi_v \) = volume fraction of solids

\( \phi_w \) = azimuthal angle of a fiber when it is in contact with the wall

\( \phi_0 \) = initial orientation of a particle

\( \phi_w \) = weight fraction of solids

\( \psi \) = orientation distribution function

\( \psi_N \) = normalization constant for the orientation distribution function

\( \psi \) = distribution function

\( \psi_1^+ \) = transient primary normal stress coefficient, Pa.s\(^2\)

\( \psi_2^+ \) = transient secondary normal stress coefficient, Pa.s\(^2\)

\( \omega \) = angular velocity, rad/s

\( \omega \) = bulk vorticity tensor, s\(^{-1}\)

\( |\Omega| \) = radius of torsion

\( \frac{\partial}{\partial \rho} \) = gradient operator

\( \nabla \) = gradient operator


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Appendix pages are very light in text.
QUALITATIVE SHEAR EXPERIMENTS

SANDERSON, FORGLATER

15% BY WT. OF 1.27CM GLASS FIBERS

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The Orientation Distribution Function

The objective of this section is to verify the solution of the orientation distribution function that has been derived in Chapter IV in which

\[ \psi (p, t) = \frac{1}{4\pi} (\Delta^\dagger \cdot \Delta : pp)^{-1/2} \quad (A-2-1) \]

The governing equation has been provided in equation (IV-B-3),

\[ \frac{3}{\partial t} \psi + (\kappa \cdot p - \kappa : pp) \cdot \frac{\partial \psi}{\partial p} = 3(\kappa : pp) \psi \quad (A-2-2) \]

(term I) (term II) (term III)

and the initial condition is:

\[ t=0 \quad \psi = \frac{1}{4\pi} \quad (A-2-3) \]

To show that the solution to \( \psi \) satisfies the governing equation, we shall insert equation (A-2-1) into each term of equation (A-2-2), and demonstrate that (term I) added to (term II) is identical to (term III).

\[ \text{term I} = \frac{3}{2} \frac{1}{4\pi} (\Delta^\dagger \cdot \Delta : pp)^{-5/2} (\kappa^\dagger \cdot \Delta^\dagger \cdot \Delta : pp + \Delta^\dagger \cdot \Delta \cdot \kappa : pp) \quad (A-2-4) \]

\[ \text{term II} = -\frac{3}{2} \frac{1}{4\pi} (\Delta^\dagger \cdot \Delta : pp)^{-5/2} (\kappa^\dagger \cdot \Delta^\dagger \cdot \Delta : pp + \Delta^\dagger \cdot \Delta \cdot \kappa : pp - 2(\kappa : pp)(\Delta^\dagger \cdot \Delta : pp)) \quad (A-2-5) \]

when (term I) is added to (term II), we obtain:
\[(\text{term I}) + (\text{term II}) = 3\left(\frac{1}{4\pi}\right)(\hat{A}^\dagger \hat{A} : \mathbb{P}\mathbb{P})^{-3/2}(\mathbb{g} : \mathbb{P}\mathbb{P})\]

\[= 3(\mathbb{g} : \mathbb{P}\mathbb{P})\psi\]

\[= (\text{term III})\] \hfill (A-2-6)

Consequently, the solution to \(\psi\) in equation (A-2-1) satisfies its governing equation.

To show that the initial condition is also met, we note that \(\hat{A} = \hat{a}\) at \(t = 0\) (section IV-A). By inserting this relation into equation (A-2-1),

\[\psi(p,0) = \frac{1}{4\pi} (\hat{a}^\dagger \hat{a} : \mathbb{P}\mathbb{P})^{-3/2}\]

\[= \frac{1}{4\pi}\] \hfill (A-2-7)

The last line is obtained by noting that the trace of the dyadic \(\mathbb{P}\mathbb{P}\) is unity.

The solution for the orientation distribution function in equation (A-2-1) has thus been verified.
APPENDIX A

1. THIS PROGRAM COMPUTES THE ORIENTATION DISTRIBUTION FUNCTION, THE DIMENSIONLESS SHEAR VISCOSITY, AND THE DIMENSIONLESS NORMAL STRESS COEFFICIENTS IN A SIMPLE STEADY SHEAR FLOW. THE WALL EFFECT, MODELED BY THE RENORMALIZATION METHOD IS INCLUDED IN THIS COMPUTATION; THE INTEGRATION ON THETA IS EVEN, SIMPSON'S METHOD IS USED.

COMPILER DOUBLE PRECISION

DIMENSION PSIT(751),PSIPI(751),UNSHST(751),F(751),
1(51),PSILP(751),PSIIT(751),PSI2P(751),PSI2T(751),
CALL FOPEN(4,'WVISCITT')
CALL FOPEN(5,'WVISCITT')
CALL FOPEN(6,'WPLOTSUIT')
CALL FOPEN(7,'WPLOTN1ITT')
CALL FOPEN(8,'WPLOTN2ITT')
CALL FOPEN(9,'WPLOTSUIT')
CALL FOPEN(10,'WPLOTN11ITT')
CALL FOPEN(11,'WPLOTN21ITT')
PI=3.141592653589793
DO 50 INC=1,11
THETAI=0.05*(INC-1)*PI

C WHEN INC=1 THE WALLS DO NOT RESTRICT THE MOTION C OF A FIBER
C WHEN INC=11 EACH FIBER IS IN THE PLANE OF SHEAR
THETAF=PI/2.
WRITE(4,4)THETAI,THETAF
WRITE(5,4)THETAI,THETAF
4 FORMAT(1X,'THETA RANGES FROM',2X,F20.17,2X,
1*0.05,F20.17)
DO 5 IM=1,751
WRITE (4,5)J,IM
WRITE(5,5)J,IM
5 FORMAT(1X,'JIM=',5X,'GAMMA',12X,'DIST.
1FUNCTION',10X,'SHEAR VISCOSITY',9X,'PAIM,
2NORM, STR',9X,'SEC. NORM, STR')
G(1)=0.0
G(2)=0.005
G(3)=0.01
G(4)=0.05
G(5)=0.1
G(6)=0.5
DO 28 J=1,9
G(J)=1.0+0.1*(J-1)
28 CONTINUE
GO TO 7
C(I) = 10.02, 2, 3, 4
5 CONTINUE
GO TO 8
I = 103, 118
C(I) = 0, 0.03, 0.03, 103
6 CONTINUE
II = 118
I01 = IDIM + 1
C STEP1 IS THE INCREMENT IN THETA
STEP1 = (THETA1 - THETA0) / 10;
C STEP2 IS THE INCREMENT IN PHI
STEP2 = 2 * PI / I01
GO TO 30
K = 1, 11
GO TO 20
J = 1, IDIM
PHI = STEP2 * (I - 1);
A1 = SIN(PHI)
A2 = COS(PHI)
A3 = COS(PHI)
A4 = A3 * A3
GO TO 30
J = 1, IDIM
THETA = THETA0 + STEP1 * (J - 1)
B1 = SIN(THETA)
B2 = COS(THETA)
A3 = 2 * B1 * B2
A4 = B1 * B2
A5 = B2 * B2
PSIT(J) = B1 / (4 * PI * (1 - (GK*B3*A1) / 
  1 - (GK*B3*B5) / (1, 5)))
UNSHST(J) = R4 * B5 * A2 * PSIT(J)
10 CONTINUE
CALL SIMP(STEP1, UNSHST, JDIM, S)
F(I) = S
CALL SIMP(STEP1, PSIT, JDIM, S2)
PSIP(I) = S2
CALL SIMP(STEP1, PSI1T, JDIM, S3)
PSIP(I) = S3
CALL SIMP(STEP1, PSI2T, JDIM, S4)
PSIP(I) = S4
20 CONTINUE
CALL SIMP(STEP2, F, JDIM, WSSUM)
CALL SIMP(STEP2, PSIF, JDIM, WSSUM2)
CALL SIMP(STEP2, PSIP, JDIM, WSSUM3)
CALL SIMP(STEP2, PSI2F, JDIM, WSSUM4)
SSUM = 2 * WSSUM
SSUM2 = 2 * WSSUM2
SSUM3 = 2 * WSSUM3
SSUM4 = 2 * WSSUM4
wSUM = SSUM / SSUM2
wSUM3 = SSUM3 / SSUM2
wSUM4 = SSUM4 / SSUM2
write (4, 40) GK, SSUM2, wSUM, wSUM3, wSUM4
write (5, 40) GK, SSUM2, SSUM, SSUM3, SSUM4
write (6, 45) GK, wSUM
write (7, 45) GK, wSUM3
write (8, 45) GK, wSUM4
write (9, 45) GK, SSUM
write (10, 45) GK, SSUM3
write (11, 45) GK, SSUM4
30 continue
40 format (1x, F10.5, 10x, F14.11, 10x, F14.11,
110x, F14.11, 10x, F14.11)
45 format (1x, F10.5, 10x, F14.11)
50 continue
stop
end
APPENDIX 3

THIS PROGRAM COMPUTES THE ORIENTATION DISTRIBUTION
FUNCTION: THE DIMENSIONLESS TROUTON VISCOSITY
IN UNIAXIAL AND BIAXIAL EXTENSIONAL FLOWS.

SIMPSON'S METHOD IS USED.

COMPILER DOUBLE PRECISION
COMPILER NO STACK

DIMENSION G(51), CPSIT(750), OPSIT(750), CSTRT(750),
       10STR(750), CPSIP(750), OPSIP(750), CSTRP(750), SSTRP(750)

CALL FOPEN(4, 'COMDIV')
JOIN = 748

WRITE(4, S) JOIN

5 FORMAT(1X,'JOIN=',15x, '20X ', 'CONVERGING FLOW', ' 18X ', '1X ', ' DIVERGING FLOW', ' 4X ', ' GAMMA', ' 4X ', ' DIST. FUNCTION', '
3X ', 'ELONG. VISC.' , ' 3X ', 'DIST. FUNCTION ', ' 3X ', 'ELONG. VISC.
0(1) = 0.6
G(2) = 0.005
G(3) = 0.1
G(4) = 0.1
G(5) = 0.1
G(6) = 0.1

DO 6 I = 1, 97
G(1) = 1.0 + 0.1 * (I - 1)
6 CONTINUE

DO 7 J = 98, 102
G(1) = 10.0 + 2.0 * (J - 97)
7 CONTINUE

DO 8 I = 103, 118
G(1) = 25.0 + 5.0 * (I - 103)
8 CONTINUE

PI = 3.141592653589793
PI1 = 0.25 / PI
II = 51
JOIN = JOIN - 1

STEP1 = PI1 / 101
STEP2 = 2 * STEP1

DO 30 K = 1, II

E1 = G(K)
C1 = EXP(E1)
C2 = C1 * C1

II = II - 1

DO 20 I = JOIN

PHI1 = STEP2 * (1 - I)

30 CONTINUE
A1 = SIN(PHI) * SIN(PHI)  
A2 = COS(2, * PHI)  
A3 = TAN(PHI) * TAN(PHI)  
A4 = COS(PHI) * COS(PHI)  
DO 10 J = 1, JDIM  
THETA = STEPIX(J-1)  
B4 = SIN(THETA)  
B1 = B4*B4  
B2 = A1*B4  
B3 = COS(THETA) * COS(THETA)  
CPSIT(J) = FP1*B4 / ((1+0.5*A1*B3) * B1+B4)  
DPSIT(J) = FP1*B4 / ((1+0.5*A4+B3) * B1+B4)  
DUM = (1,-3)*A1*B1*1+B1*A2  
CSTRT(J) = 0.5*DUM*CPSIT(J)  
DSTRT(J) = 0.5*DUM*DPSIT(J)  
10 CONTINUE  
CALL SIMP(STEP1, CPSIT, JDIM, S1)  
CPSIP(1) = S1  
CALL SIMP(STEP1, DPSIT, JDIM, S2)  
DPSIP(1) = S2  
CALL SIMP(STEP1, CSTRT, JDIM, S3)  
CSTRP(1) = S3  
CALL SIMP(STEP1, DSTRT, JDIM, S4)  
DSTRP(1) = S4  
20 CONTINUE  
CALL SIMP(STEP2, CPSIP, JDIM, SUM1)  
CALL SIMP(STEP2, DPSIP, JDIM, SUM2)  
CALL SIMP(STEP2, CSTRP, JDIM, SUM3)  
CALL SIMP(STEP2, DSTRP, JDIM, SUM4)  
WRITE(4, 40) E1, SUM1, SUM3, SUM2, SUM4  
30 CONTINUE  
40 FORMAT(IX, F10.5, 2X, F14.11, 2X, F14.11, 2X, F14.11,  
       12X, F14.11)  
STOP  
END
COMPILER DOUBLE PRECISION
COMPILER NOSTACK
SUBROUTINE SIMP(STEP, YX, JOIM, S)
DIMENSION YX(2500)
  I = JOIM - 1
  J = JOIM - 2
  SUMDD = 0.
  10  K=2, I, J
  SUMDD = SUMDD + YX(K)
  10  CONTINUE
  SUM2EN = 0.
  20  L=3, J, J
  SUM2EN = SUM2EN + YX(L)
  20  CONTINUE
  ODDSUM = 4.*SUMDD
  EVENSUM = 2.*SUM2EN
  S = (YX(1)+YX(JOIM)+ODDSUM+EVENSUM)*STEP/3.
RETURN
END
APPENDIX 5

This program computes the dimensionless shear viscosity, and the dimensionless normal stress coefficients in a simple steady shear flow. The wall effect is modeled by the particle tracking method, the normalization constant for the orientation distribution function is absorbed in the rheological properties, the integration on theta is even.

Compiler double precision
Compiler nostack
Dimension g(500)
Call fopen(4,'visc31')
Call fopen(5,'viscn11')
Call fopen(6,'viscn21')
Call fopen(7,'viscnv1')
Pi=3.141592653589793
Pi4=1./4.*pi
P12=2.*pi
Pi5=1.5*pi
Pi10=0.5*pi
Pi1025=0.25*pi
Do 500 inc=1,11
Thetaw=0.05*(inc-1)*pi
Thetaf=pi/2.
E1=tan(thetaw)
E2=E1**fi.
Write(4,1)thetaw,thetaf
1 Format(1x,'Theta ranges from',2x,F20.17,2x,1'to',2x,F20.17)
Jdim=501
Write(4,2)jdim
2 Format(1x,'Jdim=15/4x,Gamma11x,Primary Normal',8x, 'Secondary Normal',14x,'Shear'
20x,'Stress 5x, Stress Coefficient',10x,'Viscosity')
G(1)=0.0
G(2)=0.005
G(3)=0.01
G(4)=0.05
G(5)=0.1
G(6)=0.5
Do 6 i=1,97
G(i)=1.0+0.1*i-1
   Go continue
DO 7 I=33,100
(1)=10.0+2.0*(1-97)
7 CONTINUE
DO 6 I=103,118
(1)=23.0+3.0*I-.103;
6 CONTINUE
I = 31
II = JI+M - 1
STEP1 = -(THETAM-THETA)/II
STEP2 = 2.*PI/II
DO 300 K = 1,II
OK=6(K)
SK=OR*OK
S1F00=0.
S1P00=0.
V1F00=0.
SIPEV=0.
S1VEV=0.
VIPEV=0.
DO 200 I = 1,II
X=I-1.0)*XI
PHIO = STEP2*(I-1)
AI=SIN(PHIO)
A2=COS(PHIO)
A3=A2*A2
S1T00=0.
S1P00=0.
V1T00=0.
SIPEV=0.
S1VEV=0.
VIPEV=0.
DO 100 J=1,II
Y=(I-1.0)*XI
THETAO = THETAO + STEP2*(J-1)
B1=SIN(THETAO)
B2=TAN(THETAO)
B3=B2*B2
Cl=al*B2
C2=A2*B2
C3=C2*C2
IF(PHIO.EQ.PI5) GO TO 11
IF(PHIO,LE,PI) GO TO 10
IF(PHIO,LT,PI5) GO TO 20
IF(PHIO,GE,PI5) GO TO 40
IF(PHIO,LE,PI2) GO TO 30
10  
11  
15  
16  CONST = F1  
GO TO 15  
11  CONST = 0  
15  THETA = ATAN(SQRT(GK*F1/2 + 6K*C1 + 33))  
PHI = ATAN((GK + C1) / C2) +CONST  
GO TO 50  
20  CRIT = E2 - C3  
IF (CRIT) 10, 11, 15  
21  F1 = SQRT(CRIT)  
6W = -C1 * F1  
IF (GK LE 6W) GO TO 10  
PHIM = ATAN(-F1 / C2) +PI  
DUN = TAN(P1025 + 0.5 * PHIM)  
GPI2 = GW - (G1 * ALOG(1.0))  
IF (GK LE GPI2) GO TO 25  
GDIFF = GK - GPI2  
GDIFF2 = GDIFF * DDIFF  
THETA = ATAN(SQRT(GDIFF2 + E2))  
PHI = ATAN(-GDIFF / E1) + PI  
GO TO 50  
25  ARG = (GK - GW) / E1  
THETA = THETAW  
PHI = 2 * (ATAN(DUN * EXP(ARG)) - P1025)  
GO TO 50  
30  CRIT = E2 - C3  
IF (CRIT) 11, 11, 31  
31  F1 = SQRT(CRIT)  
6W = -C1 * F1  
IF (GK LE 6W) GO TO 11  
PHIM = ATAN(-F1 / C2) +PI  
DUN = TAN(P1025 + 0.5 * PHIM)  
GPI2 = GW - (G1 * ALOG(DUN))  
IF (GK LE GPI2) GO TO 35  
GDIFF = GK - GPI2  
GDIFF2 = GDIFF * DDIFF  
THETA = ATAN(SQRT(GDIFF2 + E2))  
PHI = ATAN(GDIFF / E1)  
GO TO 50  
35  ARG = (GK - GW) / E1  
THETA = THETAW  
PHI = 2 * (ATAN(DUN * EXP(ARG)) - P1025)  
GO TO 50  
40  GW = R2 - E1  
IF (GW - 6W) 91, 91, 42  
41  THETA = ATAN(R2 - GK)
PHI=P115
GO TO 50
42 T H E T A=T H E T A
PHI=P115
50 D1=SIN(T H E T A)
D2=CO S(T H E T A)
D3=SIN(PHI)
D4=COS(PHI)
D5=D1*D2*D3
D6=D1*D3*D4*D5
D7=D1*D4*D4*D4
S1T=B3*(D6-(D2*D2))#B1#P14
S1T2=D5*(D2*D2)-D7)#B1#P14
V1S1=05*DS5*B12#P14
IF (J,J0+1) GO TO 50
IF (J,J0,J01h) GO TO 50
IF (Y,Y0+1,0) GO TO 70
IF (Y,-1,0) GO TO 80
60 S11T0=S11T
S12T0=S12T
V1ST0=V1ST
GO TO 100
70 S11T00=S11T0+S11T
S12T00=S12T0+S12T
V1ST00=V1ST0+V1ST
GO TO 100
80 S1ITEV=S1ITEV+V1ST
S12TEV=S12TEV+S12T
V1STEV=V1STEV+V1ST
GO TO 100
90 S11TF=S11T
S12TF=S12T
V1STF=V1ST
100 CONTINUE
S1IF=(S11T0+S11TF+(4.*S11T0D)+(2.*S1ITEV))#STEP1/3,
S12F=(S12T0+S12TF+(4.*S12T0D)+(2.*S12TEV))#STEP1/3,
V1SF=(V1ST0+V1STF+(4.*V1ST0D)+(2.*V1STEV))#STEP1/3,
IF (I,J0,1) GO TO 160
IF (I,J0,J01h) GO TO 190
IF (X,Y0,1,0) GO TO 170
IF (X,Y0,-1,0) GO TO 180
160 S11PO=S11F
S12PO=S12F
V1SPO=V1ST
GO TO 200
:70  S11F0=F11F0+S11P
S12P0=F12P0+S12P
VISP0=VISP0+VISP
60 TO 200
180  S11FEV=S11FEV+S11P
S12PEV=S12PEV+S12P
VISPEV=VISPEV+VISP
60 TO 200
190  S11FF=S11P
S12PF=S12P
VISFF=VISP
200  CONTINUE
511=VISF0+S11FF+(4, *S11P0)+(2, *S11F0)) *STEP2/3,
S12=(S12P0+S12FF+(4, *S12P0)+(2, *S12F0)) *STEP2/3,
VIS=(VISF0+VISFF+(4, *VISP0)+(2, *VISF0)) *STEP2/3,
FS11=2, *S11,
FS12=2, *S12
VISC =2, *VIS
WRITE(4, 400) GK, FS11, FS12, VISC
WRITE(5, 430) GK, FS11
WRITE(6, 450) GK, FS12
WRITE(7, 430) GK, VISC
300  CONTINUE
400  FORMAT(I6, F10.5, 9X, F14.11), 9X, F14.11)
450  FORMAT(I6, F10.5, 9X, F14.11)
500  CONTINUE
STOP
END
APPENDIX 6

A Sample Calculation for Evaluating $\eta^+ (\gamma_R)$

An illustration of the use of equation (VII-C-9) for evaluating $\eta^+ (\gamma_R)$ is presented in this section.

The experimental data were obtained on a suspension containing 30\% by weight of glass fibers in a honey solution. The dimensions of the fibers were: $l = 3.5$ mm and $d = 0.301$ mm. The viscosity of the pure honey at room temperature was $1.084 \times 10^1$ Pa.s.

The shear flow experiment was conducted in a parallel plate viscometer. The diameter of the parallel plate is 72 mm. For this set of data the rim shear rate was $0.012$ s$^{-1}$, and the gap thickness was 0.3 cm.

The primary data for the elapsed time, $t$, and the torque exerted on the upper plate, $T_m$, Table A6.1. The third column lists the rim shear strain, $\gamma_R$, which is the product of the rim shear rate and the elapsed time (c.f. equation VII-C-7).

In order to compute the transient shear viscosity, $\eta^+$, by means of equation (VII-C-9), the derivative of $\ln(4T_m t/\pi D^3)$ with respect to $\ln \gamma_R$ needs to be determined. This slope, shown in column 6, is obtained from a least square analysis of the quantities in columns 4 and 5. With the slope known, $\eta^+$ is calculated from equation (VII-C-9).
<table>
<thead>
<tr>
<th>$t \times 10^{-2}$</th>
<th>$T_H \times 10^{-5}$</th>
<th>$\gamma_R$</th>
<th>$\ln \gamma_R$</th>
<th>$\ln(4T_H t/\pi D^3)$</th>
<th>Slope $\times 10^{-4}$ Pas</th>
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<tr>
<td>0.008</td>
<td>1.67</td>
<td>0.010</td>
<td>-4.61</td>
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<td>0.100</td>
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<tr>
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<td>-0.511</td>
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<tr>
<td>0.583</td>
<td>1.52</td>
<td>0.700</td>
<td>-0.357</td>
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<td>0.693</td>
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## Appendix 7

### High-Strain Shear Viscosity Data in Figure VII-E-1

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## Appendix C

**Zero-Shear Viscosity Data in Figure VII-F**

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ZERO-SHEAR VISCOSITY DATA IN
FIGURE VII-F-2

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Zero-Shear Viscosity Data in Figure VII-F-3

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ZERO-SHEAR VISCOITY DATA IN
FIGURE VII-E-9

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FIGURE VII-F-5

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**ZERO-SHEAR VISCOSITY DATA IN FIGURE VII-F-6**

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ZERO-SHEAR VISCOSITY DATA IN
FIGURE VII-7.

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APPENDIX 9

THESIS DIGEST
ON THE RHEOLOGY OF CONCENTRATED
FIBER SUSPENSIONS

(Thesis Digest)

by

Steven M. Dinh

SUBMITTED IN PARTIAL FULFILLMENT
OF THE REQUIREMENTS FOR THE
DEGREE OF
DOCTOR OF SCIENCE

at
MASSACHUSETTS INSTITUTE OF TECHNOLOGY
May, 1981

Thesis Supervisor: Professor Robert C. Armstrong
ABSTRACT

A constitutive equation has been developed to relate the microstructure to the bulk behavior of a semi-concentrated suspension of fibers. The calculations, based on this model, in a simple steady shear flow and in uniaxial and biaxial deformations demonstrate that the rheological properties depend strongly on the history of the flow. The strain is found to be a macroscopic representation of the changes in fiber orientation.

Experiments in shear flow confirm that the initial bulk shear viscosity, which corresponds to a suspension of randomly directed fibers, can be orders of magnitude greater than the bulk shear viscosity at steady-state where the particles are aligned in the shearing planes.
I) INTRODUCTION

The use of fiber composites has experienced substantial growth in recent years. In particular glass fiber reinforced plastics are versatile and attractive engineering materials in the polymer and automotive industries because of their high strength to weight ratio, and of their low cost. In order to process the composite optimally, either by injection molding or compression molding or combinations thereof, the material has to be transported to all extremities of the mold cavity with desirable fiber orientation at different locations and with minimum fiber segregation and breakage. Therefore, it would be advantageous to determine a priori the flow behavior of the fiber composite for evaluating the feasibility of a new design.

The basic requirement to simulate the flow field is a stress tensor for the fiber suspension. However little is known about this anisotropic material, especially in the non-dilute regime, because the bulk properties and the microstructure are intertwined. Consequently a fundamental understanding of the behavior of the stress tensor and its interrelation to changes in the fiber orientation is required.

The objective of this research is to develop a rheological model capable of describing the rheological properties of a concentrated suspension of fibers in a Newtonian liquid.

A survey of the literature is presented in the remainder of this section. The construction of the constitutive equation is summarized in Section II. The explicit forms of the stress
tensor and the particle motion are shown in Section III. These results are illustrated for the case of shear and extensional flows in Section IV. Sample comparisons between experimental data and shear flow predictions are given in Section V.

The experimental and structural methods of characterizing the rheology of concentrated fiber suspensions are summarized in Tables 1 and 2.

Blakeney (1966) used a Couette viscometer to measure the shear viscosity of a suspension of nylon fibers, and found that the data collected at steady-state were approximately equal to the solvent viscosity. Rosinger et al. (1974), and Horie and Pinder (1979) also reported transient behavior, but in addition the suspensions exhibited a yield stress. The data gathered by Maschmeyer and Hill (1977), and Tucker (1978) in capillary viscometers showed a power law dependence on the shear rate. However, Mashmeyer and Hill attributed the non-Newtonian character to the small deviation of the silicone oil from a Newtonian fluid at high shear rates.

The results from these experiments indicate that a non-dilute suspension of fibers displays non-Newtonian behavior which can be time-dependent, and can have power law and yield stress regions. Each author suspects that fiber orientation, which results from the type of geometry, strongly influences the shearing properties of the suspension. However, a quantitative description of the effects of particle orientation are unknown. In particular, a stress-strain rate relation may not be sufficient to describe the complete rheological
properties of the suspension.

A structural approach provides a direct link between the microscopic properties and the bulk character of a suspension. However, the analysis is frequently hampered by mathematical complexities that arise from the interactions among the particles.

One of these methods is based on the kinetic theory of dumbbell molecules. The formulation of the stress tensor for a dilute suspension of these particles can be found in Chapter 11 of Bird, Hassager, Armstrong and Curtiss (1977). Doi and Edwards (1978a, b) extended these results to the semi-concentrated regimes by imposing constraints on the motion of a test particle. However, the results presented by Doi and Edwards are not applicable to a suspension of macroscopic fibers because diffusion and Brownian processes will be insignificant. Nevertheless, the idea of restricting the motion of a test particle, as means of extending the dilute theory into the non-dilute regions is physically appealing.

In circumventing the analysis of the different concentration regimes, Batchelor (1970) proposed a general constitutive equation for a suspension of particles in a Newtonian liquid. The macroscopic quantities are formulated from the volume averages of the microscopic variables. In practice, however, Batchelor's formula is extremely difficult to use in the non-dilute concentration regions because the hydrodynamic forces on the particles are coupled with the particle orientations.
II) MODELING

The analysis presented here addresses a semi-concentrated suspension of fibers. In a suspension of randomly oriented particles, the semi-concentrated regime is defined by \((1/l^3) < n < (1/dl^2)\), or \((d/l)^2 < \phi_v < (d/l)\). These concentration limits imply that the spacing between a fiber and its nearest neighbor varies from a fiber length to a fiber diameter apart. Consequently, the motion of a fiber is constrained by the surrounding particles. In particular, the resistances to rotation and to motion perpendicular to the fiber axis are much greater than the resistance to a displacement along the axis of the particle. Therefore, it is unlikely for a fiber to tumble freely from end to end.

When the orientations of the particles are varied, the bulk resistance to deformation will change. At times, the suspension may appear like a solid such as in the shearing of a slurry of randomly packed fibers. In contrast, the bulk resistance is greatly lowered when the particles are aligned in the planes of shear. Consequently the suspension behaves like a visco-elastic material.

The bulk stress can be constructed from either the volume average approach or from the kinetic theory of rod-like polymers. Since the corresponding results can be shown to be identical (cf. Chapter III), only the volume average approach will be discussed here.

The bulk stress for a suspension has been derived by Batchelor:
\[ I = -\eta_s \dot{\gamma} + \frac{1}{V} \iiint \mathbb{H}_c \cdot \mathbf{n} \, dA \]  

(II-1)

where the integral is over the surface of a particle and the sum is over all particles in the volume \( V \). To overcome the difficulty of evaluating the summation of particle surface integrals in a concentrated suspension, the analysis is focused on a test fiber, shown in Figure 1, that is immersed in an effective medium. The effective medium, characterized by a stress tensor \( \mathbb{H}_{\text{eff}} \), is a smeared out picture of the surrounding particles and the solvent. Furthermore, since the position of the test fiber is to be representative of an average particle in the suspension, a distribution function \( \Psi(\mathbf{r}_c, \rho, s, t) \) is introduced to account for the probability that the test fiber has a specific configuration. With these modifications, equation (II-1) becomes:

\[ I = -\eta_s \dot{\gamma} + \frac{(n)}{V} \left[ \frac{1}{2} \right] \iiint \mathbb{H}_{\text{eff}} \cdot \mathbf{n} \Psi d\mathbf{r} d\rho ds \]  

(II-2)

In equation (II-2), the force of the fiber on the surrounding fluid, \( \mathbb{H}_{\text{eff}} \cdot \mathbf{n} \), is approximated by a Stokes-Burgers model in which this force is the product of an effective drag coefficient tensor, \( \zeta_{\text{eff}}(2 \dot{\mathbf{u}} - \mathbf{u}) \), and the relative velocity, \( (\mathbf{v} - \dot{\mathbf{r}}) \), between the effective medium and the test particle. After inserting this relation into equation (II-2), we obtain:

\[ I = -\eta_s \dot{\gamma} + \frac{1}{V} \left[ \frac{1}{2} \right] \iiint \zeta_{\text{eff}}(2 \dot{\mathbf{u}} - \mathbf{u}) \cdot (\mathbf{v} - \dot{\mathbf{r}}) \Psi d\mathbf{r} d\rho ds \]  

(II-3)

Before this relation can be employed, \( \zeta_{\text{eff}}, \dot{\gamma}, \) and \( \Psi \) need to be evaluated. The general formulations for these quantities
are presented in Chapter VIII of the thesis. Here, we review the analysis of a suspension of rigid fibers in homogeneous flows to demonstrate the use of this constitutive equation.

In a homogeneous flow, the velocity gradient tensor is spatially uniform; the bulk velocity can be rewritten as \( \mathbf{V} = \mathbf{K} \cdot \mathbf{P} \); the distribution function \( \Psi \) can be factored into the product of the number density and the orientation distribution function \( \psi \), \( \Psi = n \psi \). For a rigid fiber, a force balance shows that the center of mass translates affinely with the bulk deformation. A torque balance about the center of mass leads to the governing equation for the particle orientation:

\[
\dot{\mathbf{P}} = \mathbf{K} \cdot \mathbf{P} - \mathbf{K} : \mathbf{PPP} \tag{II-4}
\]

with the initial condition that \( \mathbf{P} = \mathbf{P}_0 \) at \( t = 0 \). This equation indicates that the fiber would like to deform affinely, but since it is rigid, it cannot be stretched. Consequently the stretching component, \( \mathbf{K} : \mathbf{PPP} \), is subtracted out of the total deformation \( \mathbf{K} \cdot \mathbf{P} \).

The constitutive equation for a suspension of rigid fibers in homogeneous flows is then reduced to:

\[
\mathbf{I} = -n_s \mathbf{K} - \frac{n \mathbf{l}^2}{12} \int \xi_{\text{eff}} \mathbf{K} : \mathbf{PPP} \psi d\mathbf{P} \tag{II-5}
\]

where \( \xi_{\text{eff}} \) and \( \psi \) have yet to be determined.

The effective drag coefficient is estimated by considering the motion of a test fiber in two equivalent situations that are diagrammed in Figure 2. In the continuum model, the work required to move a test fiber over a distance \( a_o \) in a time
interval $\Delta t$, where $a_c$ is the separation between a particle and its nearest neighbor, is given by $\zeta_{\text{eff}}(a_c/\Delta t)a_c$. To displace the same test fiber over a distance $a_c$ in the structural model, the nearest neighbor has to move out of its original position in order to avoid a head-on collision. To vacate a site that is to be occupied by the test fiber, the adjacent fiber has to displace along its axis by a distance of approximately a fiber length in the same time interval $t$. The work required to execute this motion would be $\zeta(1/\Delta t)l$. By equating the work performed in these two cases, we find:

$$\zeta_{\text{eff}} = \eta_s l(nl^3)^2 \quad \text{(II-6)}$$

In arriving to equation (II-6), the drag coefficient of a cylinder in a Newtonian liquid, $\zeta$, has been approximated by $\eta_s l$, and $a_c = (1/nl^2)$ for a suspension of randomly dispersed fibers (Doi & Edwards, 1978a).

The orientation distribution function $\psi(p,t)$ describes the probability that a fiber would be oriented in the range of $p$ to $p+dp$ at time $t$. Conservation of orientations gives a continuity equation for the rate of change of $\psi$,

$$\frac{\partial}{\partial t}\psi = -\frac{\partial}{\partial p} \cdot (\dot{p}\psi) \quad \text{(II-7)}$$

where $\dot{p}$ is provided in equation (II-4). If the fibers are randomly directed at $t = 0$, then $\psi(t=0) = 1/4\pi$.

At this stage, the microstructure of the suspension is determined by the solution to equation (II-4), and the stress tensor is completely defined with the solution to equation (II-7).
III) RHEOLOGICAL EQUATION OF STATE

The orientation of a particle is described by the solution of equation (II-4). Since the particle is inextensible,

$$\mathbf{P} = \frac{\mathbf{E} \cdot \mathbf{P_0}}{(\mathbf{E}^+ \cdot \mathbf{P_0})^\frac{3}{2}}$$  \hspace{1cm} (III-1)

where the components of \( \mathbf{E} \) in Cartesian coordinates are given by:

$$E_{ij} = \frac{\partial x_i}{\partial x_j}$$  \hspace{1cm} (III-2)

The displacement function \( x_i \) is the position of a material point at the present time, whereas \( x_j \) is the location of the same material particle time \( t_0 \).

The solution to the orientation distribution function is obtained by the method of characteristics. Hence,

$$\psi(P, t) = \frac{1}{4\pi} (\mathbf{\Delta}^+ \cdot \mathbf{P}^0)^{-3/2}$$  \hspace{1cm} (III-3)

Consequently, the rheological equation of state is given by:

$$\mathbf{\Pi} = -\eta_s \dot{\mathbf{\Pi}} - \eta_s \frac{(\mathbf{n1})^3}{12} \mathbf{\Pi} : \left[ \frac{\mathbf{PPPdP}}{4\pi (\mathbf{\Delta}^+ \cdot \mathbf{P}^0)^{3/2}} \right]$$  \hspace{1cm} (III-4)

The first term on the right-hand side of equation (III-4) describes the contribution from the solvent, and the second term arises from the presence of the particles. This stress tensor derived from the structural approach is related to a number of continuum models in Chapter IV.
IV) ILLUSTRATIVE FLOW FIELDS

The above constitutive equation is illustrated in a simple steady-shear flow, and in uniaxial and biaxial extensional flows. The bulk kinematics of these flows are summarized in Tables 3 and 4 along with the corresponding rheological properties of interest.

A. Shear flow

In a simple steady shear flow the motion of a particle is obtained by inserting the strain tensor $E$ in Table 2 into equation (III-1). In terms of the spherical angles shown in Figure 1, the particle motion is described by:

$$\tan \theta = \tan \theta_0 (\gamma^2 \sin^2 \phi_0 + 2 \gamma \sin \phi_0 \cos \phi_0 + 1)^{\frac{1}{2}}$$  \hspace{1cm} (IV-1)

$$\tan \phi = (\cot \phi_0 + \gamma)^{-1}$$  \hspace{1cm} (IV-2)

where the shear strain $\gamma = \dot{\gamma}t$.

At the start of the flow ($\gamma=0$), the orientation of the particle ($\theta, \phi$) is given by ($\theta_0, \phi_0$). As the flow develops or as $\gamma$ increases, the fibers are aligned toward the flow direction ($\theta=\pi/2, \phi=0$), except for the cases in which the particles are initially located in the plane of shear. In the latter situations the fibers would remain there permanently. Hence, it may be concluded that a simple steady shear flow will eventually orient the particles into the shearing planes, and the rate of alignment varies algebraically with the total applied bulk strain.

The rheological properties that characterize the behavior of the suspension in start up of shear flows are the transient
viscosity and the primary and secondary normal stress coefficients, $\eta^+$, $\psi_1^+$, and $\psi_2^+$ respectively. These material functions are evaluated from equation (III-4). The dimensionless forms of these quantities are listed below.

1) Dimensionless bulk transient viscosity

$$\frac{12}{(n_1^3)^3} (\eta^+ - 1) = \int_0^{2\pi} \int_0^{\pi} \frac{\sin^5 \theta \sin^2 \phi \sin^2 \theta \sin^2 \phi}{16\pi (\gamma^2 \sin^2 \theta \sin^2 \phi - \gamma \sin^2 \theta \sin 2\phi + 1)^3/2} d\theta d\phi$$

(IV-3)

2) Dimensionless bulk transient primary normal stress coefficient

$$\frac{12}{(n_1^3)^3} \gamma \psi_1^+ = \int_0^{2\pi} \int_0^{\pi} \frac{\sin^5 \theta \sin^2 \phi \sin \theta \sin 2\phi}{16\pi (\gamma^2 \sin^2 \theta \sin^2 \phi - \gamma \sin^2 \theta \sin 2\phi + 1)^3/2} d\theta d\phi$$

(IV-4)

3) Dimensionless bulk transient secondary normal stress coefficient

$$\frac{12}{(n_1^3)^3} \gamma \psi_2^+ = \int_0^{2\pi} \int_0^{\pi} \frac{\sin^5 \theta \sin 2\phi (\sin^2 \phi - \cot^2 \theta)}{16\pi (\gamma^2 \sin^2 \theta \sin^2 \phi - \gamma \sin^2 \theta \sin 2\phi + 1)^3/2} d\theta d\phi$$

(IV-5)

The results from the integrations for different values of $\gamma$ are depicted in Figures 3 to 5 for the dimensionless $\eta^+$, $\psi_1^+$, and $\psi_2^+$ respectively.

At the inception of the shear flow the suspension behaves as a highly viscous Newtonian fluid because of the isotropic distribution of the fibers. As shown in Figure 3, the zero-shear dimensionless shear viscosity equals 1/15. The zero-shear normal stress coefficients are zero (Figures 4 and 5) because the net effect of the normal components of the drag
force on the fiber summed over all possible configurations is zero.

As the flow develops, the test fiber acquires a preferred orientation which is governed by the hydrodynamic couple. The shear overshoot observed in Figure 3 at a strain of approximately unity is the result of fibers accumulating near the principal axes of the strain rate. Once the fiber passes by this region, the tension along the particle decreases because the particle is heading toward the plane of shear. Subsequently, the bulk shear viscosity decreases algebraically with the shear strain as indicated by the power-law-like dependence of the dimensionless bulk shear viscosity on the shear strain.

The preferential orientation of the fiber, as a result of the bulk flow, produces a net contribution to normal forces in the suspension. Consequently, the normal stress coefficients are finite over a range of shear strain, as indicated in Figures 4 and 5.

At large strain, the tension on the fiber is removed as the particle is aligned in the plane of shear. Therefore, the normal stresses disappear, and the suspension viscosity approaches the solvent viscosity which is orders of magnitude lower than the zero-shear viscosity.

This calculation shows that the rheological properties depend strongly on the history of the flow. The initial resistance is high due to the random orientation of the fibers, but the resistance decreases as the particles are aligned into the planes of shear. Consequently, the macroscopic variable to
characterize the microstructure of the suspension is the shear strain $\gamma$, and not the shear rate.

B. **Extensional flows**

The motion of a fiber in an uniaxial extensional flow is given by:

$$
\tan \theta = e^{-\frac{3}{2} \varepsilon} \tan \theta_0 \tag{IV-6}
$$

$$
\phi = \phi_0 \tag{IV-7}
$$

The results indicate that each particle is rotated toward the direction of the extension ($z$-axis) at a fixed initial azimuthal angle $\phi_0$. The rate of alignment is exponentially in the duration of the flow. Therefore, particles are aligned much faster in an extensional flow than in a shear flow.

In a biaxial extensional flow the motion of a particle is determined by equations (IV-6) and (IV-7) except that the Hencky strain $\varepsilon$ in equation (IV-6) is replaced by $(-\varepsilon)$. The results show that the particles are rotated, at a constant $\phi_0$, into configurations perpendicular to the direction of compression ($z$-axis). Consequently, the particles are eventually aligned in the $x$-$y$ plane of Figure 1. The only exception occurs when $\theta_0 = 0$. In this case the fiber remains in this position for all time because there is no moment arm to rotate this fiber.

The dimensionless transient elongational viscosities for these two types of extensional flows are given by:

1) Uniaxial extensional flow
\[ \frac{12}{(n l^3)^3} \left( \frac{\bar{h}}{\eta_s} - 3 \right) = \int_0^{2\pi} \int_0^{2\pi} \frac{(2-3\sin^2\theta)(\cos^2\theta - \sin^2\theta \cos^2\phi) \sin \theta d\theta d\phi}{8\pi (e^\varepsilon \sin^2 \theta + e^{-2\varepsilon \cos^2 \theta})^{3/2}} \]

(IV-8)

2) Biaxial extensional flow

\[ \frac{12}{(n l^3)^3} \left( \frac{\bar{h}}{\eta_s} - 3 \right) = \int_0^{2\pi} \int_0^{2\pi} \frac{(2-3\sin^2\theta)(\cos^2\theta - \sin^2\theta \cos^2\phi) \sin \theta d\theta d\phi}{8\pi (e^{-\varepsilon \sin^2 \theta} + e^{2\varepsilon \cos^2 \theta})^{3/2}} \]

(IV-9)

These results are plotted in Figures 5 and 6 for the uniaxial and biaxial extensional flows respectively.

At the start of the flow (\( \varepsilon = 0 \)), the dimensionless Trouton viscosity in each case can be integrated analytically from equations (IV-8) and (IV-9) to yield 0.2. As the flow continues, the particle progressively aligns with the streamline. Consequently, the tension along the particle increases because the fiber is rigid. Therefore, the steady-state Trouton viscosity is greater than the initial value in both situations. The difference in the shape of the curve in Figures 6 and 7 is due to the different bulk kinematics.

In a more refined calculation, the estimate of the effective drag coefficient in this kind of flow will need to be reconsidered because an initially concentrated suspension may become hydrodynamically dilute as the separation between adjacent particles becomes sufficiently large relative to the hydrodynamically length scale. However, this difficulty is not serious in a shear flow because the tension on the fiber vanishes at steady-state.
V) SHEAR FLOW EXPERIMENTS

The shear flow experiments are intended to test the strain dependence of the rheological properties. However, experimental difficulties were encountered in the course of obtaining the bulk shear viscosity at intermediate strains because the suspension tended to ooze out of the gap of the viscometer. In spite of this difficulty, the bounds of the suspension shear viscosity have been verified at the high-strain and the zero-strain regions.

A. High-strain shear viscosity

The high-strain shear viscosity provides a lower bound estimate of the suspension shear viscosity. According to the shear flow calculations, the suspension viscosity approaches the solvent viscosity beyond a shear strain of 10. In a set of experiments conducted at room temperature, copper fibers (l = 1.5 mm, d = 0.254 mm) suspended in honey were tested in a cone and plate viscometer at high shear rates of short durations to minimize the amount of material squeezed out of the gap.

The data were collected at a shear strain of 100 and at room temperature. As shown in Figure 8, the data and the model are in close agreement. The difference, by a factor of 2.5 between the experimental and predicted results, is probably due to the finite thickness of the fiber which has been neglected in the model.

In order to assess the contribution from the finite thickness of the particle to the bulk behavior, we assume that
all the fibers are stacked up in equally spaced planes of shear. The suspension viscosity is then computed based on the assumption that the bulk energy dissipation in shear flow is equivalent to the energy dissipated by the solvent between the layers of fibers. In this simple analysis,

\[
\frac{n}{n_s} = \frac{1}{1 - d(nl)^2}
\]  

(V-1)

Equation (V-1) is represented by the dash-line in Figure 8.

These results in the high-strain region are also confirmed by the experiments performed by Blakeney (1966) who used a set of concentric cylinders.

B. **Zero-shear viscosity**

The objective of this set of experiments is to verify the scaling of the effective drag coefficient. The tests were carried out at room temperature on a parallel plate viscometer with three batches of glass fibers suspended in honey. The dimensions are: 1) \( l = 3.5 \) mm, \( d = 0.301 \) mm; 2) \( l = 6.4 \) mm, \( d = 0.235 \) mm; 3) \( l = 12 \) mm, \( d = 0.438 \) mm.

In these experiments, the "zero-shear" viscosities correspond to measurements at a shear strain of 0.01. Although this value is not obtained instantaneously at the start of the flow, the result in Figure 3 shows that the initial shear viscosity remains constant up to a strain of 0.1. The shear viscosity data for the three different lots of fibers, measured at a separation of \( h = 2 \) mm between the parallel plates, are shown in Figures 9 to 11, is given by:
\[
\frac{12}{(n_1^3)^3} \left( \frac{n_s^4}{n_s^4} - 1 \right) = \frac{1}{10} \left( \sin^2 \theta_w \cos^2 \theta_w + \frac{2}{3} \cos^3 \theta_w \right) \quad (V=2)
\]

where the degree of confinement is described by \( \theta_w \) \( (= \cos^{-1} n/1) \).

In Figures 9 to 11 the experimental results agree reasonably well with the predicted values. The encountered differences, which are less than an order of magnitude, are due to the method in which the wall effect has been modeled. The estimated values which are based on the renormalization of the distribution function do not take into account the influence of the walls on the particle spacing. The presence of the walls enhance the alignment of the fibers closer to the shearing planes. Consequently, the spacing between nearest fibers increases and leads to a lowering of the bulk shear viscosity. Therefore, the model, which is based on a random suspension, would slightly overestimate the experimental data.
VI) CONCLUSIONS

A rheological model interrelating the microstructure to the bulk properties has been developed for a semi-concentrated suspension of rigid fibers in homogeneous flows. The semi-concentrated regime is defined by $1/dl^2 < n < 1/d^2l$ when the particles are randomly dispersed.

The results show that the bulk stress depends on the dynamics of the suspended particles. A force balance about a test fiber indicates that the center of mass of the particle translates affinely with the bulk deformation. The remaining part of the fiber rotates affinely but without stretching.

Sample calculations in shear flow demonstrate that the initial shear viscosity is much larger than the viscosity at steady-state. This huge zero-shear viscosity is attributed to the structure formed by the randomly oriented fibers. However, as the particles become aligned toward the shearing plane, the resistance to deformation reduces to the solvent viscosity. The transient normal stress, which appear only over a finite range of the shear strain, are due to the preferred orientation acquired by the fibers during the flow.

Calculations in uniaxial and biaxial extensional flows show that the fibers are aligned much faster into the respective directions of the extension. The bulk elongational viscosities also increase as the flow proceeds. These results along with the shear flow calculations suggest that the rheological properties depend on the strain, and not on the rate of strain. The strain is then a macroscopic representation of the internal
structure of the suspension.

The zero-shear viscosity and the steady-state viscosity have been experimentally verified. The difference between the predicted and the test data is less than an order of magnitude apart. At steady-state the model can be improved by including the thickness of the fiber.

This study suggests that extensional flows are efficient to orient the fibers. Once the particles are aligned, the composite can be transported without much effort by a shear flow.
a_c = separation between two adjacent particles, mm.
A = surface area of a particle, m^2
d = fiber diameter, mm.
E = strain tensor
h = separation between two rigid boundaries, mm.
l = fiber length, mm.
k = Boltzmann's constant
n = number density of solids, mm^-3
n = unit vector directed normal to the particle surface
p = unit vector denoting the orientation of the particle
\dot{p} = rate of change of the unit vector p, s^-1
p_0 = initial configuration of a test fiber
r = position vector to the surface of a particle from an arbitrary coordinate system, m.
\dot{r} = rate of change of the vector r, m/s
r_c = position of the particle center of mass, m.
s = arc length, m.
t = time, s^-1
T = temperature, °K
\gamma = bulk velocity field, m/s
V = suspension volume, m^3
\dot{X} = displacement function
\dot{X'} = displacement function
X, Y, Z = internal coordinates
\gamma = shear strain
\dot{\gamma} = bulk rate of strain tensor, s^-1
\dot{\gamma} = unit tensor
\dot{A} = strain tensor
\varepsilon = Hencky strain
\dot{\varepsilon} = rate of strain, s^-1
\zeta_{df} = effective drag coefficient, Pa.s.m.
\eta_s = solvent viscosity, Pa.s
\eta_t = transient shear viscosity, Pa.s
\eta^+ = transient extensional viscosity, Pa.s
\[ \eta^+ \] = zero-shear viscosity, Pa.s
\[ \theta^0 \] = internal coordinate denoting the orientation of the fiber
\[ \theta^0 \] = initial orientation of a particle
\[ \dot{\varepsilon} \] = velocity gradient tensor, s\(^{-1}\)
\[ \Pi_{\text{eff}} \] = stress tensor describing the effective medium, Pa.s
\[ \Pi_s \] = constitutive equation for the solvent, Pa.
\[ I \] = deviatoric part of the bulk stress tensor, Pa.
\[ \phi \] = internal coordinate denoting the orientation of the fiber
\[ \phi_v \] = volume fraction of solids
\[ \phi^0 \] = initial orientation of a particle
\[ \psi \] = orientation distribution function
\[ \psi \] = distribution function
\[ \psi^+ \] = transient primary normal stress coefficient, Pa.s\(^2\)
\[ \psi^+ \] = transient secondary normal stress coefficient, Pa.s\(^2\)
\[ \frac{\partial}{\partial x} \] = gradient operator
REFERENCES


<table>
<thead>
<tr>
<th>Author</th>
<th>Flow</th>
<th>Apparatus</th>
<th>Solvent</th>
<th>Fiber</th>
<th>l</th>
<th>l/d</th>
<th>$\phi_v$</th>
<th>Yield Stress</th>
<th>Power Law</th>
<th>Transient Behavior</th>
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</thead>
<tbody>
<tr>
<td>Blakeney (1966)</td>
<td>Shear</td>
<td>Concentric cylinders</td>
<td>Tetrachloroethylene</td>
<td>Nylon</td>
<td>16.9-19.2</td>
<td>0-43.1</td>
<td>20.3</td>
<td>0.009 µm</td>
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<td>Rosinger et al. (1974)</td>
<td>Shear</td>
<td>Cone and plate</td>
<td>Water</td>
<td>Asbestos</td>
<td>0.6-9.5 mm</td>
<td>$\sim 10^4$</td>
<td>0.01</td>
<td>Yes (by weight)</td>
<td>Yes</td>
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<td>Mashmeyer and Hill (1977)</td>
<td>Shear</td>
<td>Capillary</td>
<td>Silicone</td>
<td>Glass</td>
<td>0.025 cm</td>
<td>20</td>
<td>0.15,</td>
<td>No</td>
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<td>0.025-0.12</td>
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<td>Horige and Pinder (1979)</td>
<td>Shear</td>
<td>Concentric cylinders</td>
<td>Polyethylene-glycol-water-sodium chloride-dextran</td>
<td>Nylon</td>
<td>0.987 mm</td>
<td>22.9-6.72</td>
<td>0.04-0.17</td>
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Survey of rheological tests on concentrated fiber suspensions in a Newtonian liquid.
## Table 2  Summary of structural models

<table>
<thead>
<tr>
<th>Author</th>
<th>Concentration</th>
<th>Particle Geometry</th>
<th>Stress Tensor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kramers*</td>
<td>Dilute</td>
<td>Dumbbell</td>
<td>( \mathbf{I} = -\eta_{S} \dot{\gamma} - \frac{n\xi_1^2}{2} \mathbf{K}: \langle \mathbf{ppp} \rangle )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(- 3n\kappa T \langle \mathbf{pp} \rangle + n\kappa T \mathbf{\dot{\phi}} )</td>
</tr>
<tr>
<td>Giesekus*</td>
<td>Dilute</td>
<td>Dumbbell</td>
<td>( \mathbf{I} = -\eta_{S} \dot{\gamma} + \frac{n\xi_1^2}{4} (\frac{d}{dt} \langle \mathbf{pp} \rangle )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(- \kappa \cdot \langle \mathbf{pp} \rangle - \langle \mathbf{pp} \rangle \cdot \kappa^T )</td>
</tr>
<tr>
<td>Doi and Edwards</td>
<td>Semi-concentrated</td>
<td>Rod</td>
<td>( \mathbf{I} = -3n\kappa T \langle \mathbf{pp} \rangle + n\kappa T \mathbf{\dot{\phi}} )</td>
</tr>
<tr>
<td>(1978)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Doi and Kuzuu</td>
<td>Concentrated</td>
<td>Rod</td>
<td></td>
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<td>(1980)</td>
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<tr>
<td>Batchelor</td>
<td>Arbitrary</td>
<td>Arbitrary</td>
<td>( \tau = -\eta_{S} \dot{\gamma} + \frac{1}{V} \int_{\Omega_{S}} n\mathbf{r} \cdot \mathbf{A} )</td>
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<tr>
<td>(1970)</td>
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</tbody>
</table>

* Bird, Hassager, Armstrong, Curtiss (1977), Chapter 11
Table 3  A summary of the type of flows investigated

<table>
<thead>
<tr>
<th>Flow fields</th>
<th>Velocity components, $v_i$</th>
<th>Velocity gradient tensor $\mathbf{\dot{\kappa}} = (\nabla \mathbf{v})^T$</th>
<th>Rheological properties</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Shear flow</strong></td>
<td>$v_x = \gamma y$</td>
<td>$\mathbf{\dot{\kappa}} = \begin{bmatrix} 0 &amp; \gamma &amp; 0 \ 0 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 \end{bmatrix}$</td>
<td>$\eta^+, \psi_1^+, \psi_2^+$</td>
</tr>
<tr>
<td></td>
<td>$v_y = 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$v_z = 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\gamma = 0, t &lt; 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\gamma = \dot{\gamma}, t &gt; 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Uniaxial extensional flow</strong></td>
<td>$v_x = -\frac{1}{2} \dot{\varepsilon} x$</td>
<td>$\mathbf{\dot{\kappa}} = \begin{bmatrix} -\frac{1}{2} \dot{\varepsilon} &amp; 0 &amp; 0 \ 0 &amp; -\frac{1}{2} \dot{\varepsilon} &amp; 0 \ 0 &amp; 0 &amp; \dot{\varepsilon} \end{bmatrix}$</td>
<td>$\eta^+$</td>
</tr>
<tr>
<td></td>
<td>$v_y = -\frac{1}{2} \dot{\varepsilon} y$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$v_z = \dot{\varepsilon} z$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\dot{\varepsilon} = 0$ for $t &lt; 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Biaxial extensional flow</strong></td>
<td>$v_x = \frac{1}{2} \dot{\varepsilon} x$</td>
<td>$\mathbf{\dot{\kappa}} = \begin{bmatrix} \frac{1}{2} \dot{\varepsilon} &amp; 0 &amp; 0 \ 0 &amp; \frac{1}{2} \dot{\varepsilon} &amp; 0 \ 0 &amp; 0 &amp; -\dot{\varepsilon} \end{bmatrix}$</td>
<td>$\eta^+$</td>
</tr>
<tr>
<td></td>
<td>$v_y = \frac{1}{2} \dot{\varepsilon} y$</td>
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<tr>
<td></td>
<td>$v_z = -\dot{\varepsilon} z$</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>$\dot{\varepsilon} = 0$ for $t &lt; 0$</td>
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<tr>
<td>Flow fields</td>
<td>Displacement function</td>
<td>Strain tensor $\mathbf{E}$</td>
<td>Strain tensor $\mathbf{A}$</td>
</tr>
<tr>
<td>---------------------</td>
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<td>-----------------------------</td>
</tr>
<tr>
<td>Shear flow</td>
<td>$x = x' + \gamma y$</td>
<td>$\begin{bmatrix} 1 &amp; \gamma &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 1 - \gamma &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{bmatrix}$</td>
</tr>
<tr>
<td></td>
<td>$y = y'$</td>
<td></td>
<td></td>
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<tr>
<td></td>
<td>$z = z'$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniaxial extensional</td>
<td>$x = x' \exp(-\frac{1}{2} \varepsilon)$</td>
<td>$\begin{bmatrix} e^{-\varepsilon/2} &amp; 0 &amp; 0 \ 0 &amp; e^{-\varepsilon/2} &amp; 0 \ 0 &amp; 0 &amp; e^{\varepsilon} \end{bmatrix}$</td>
<td>$\begin{bmatrix} e^{\varepsilon/2} &amp; 0 &amp; 0 \ 0 &amp; e^{\varepsilon/2} &amp; 0 \ 0 &amp; 0 &amp; e^{-\varepsilon} \end{bmatrix}$</td>
</tr>
<tr>
<td>flow</td>
<td>$y = y' \exp(-\frac{1}{2} \varepsilon)$</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>$z = z' \exp(\varepsilon)$</td>
<td></td>
<td></td>
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<tr>
<td>Biaxial extensional</td>
<td>$x = x' \exp(\frac{1}{2} \varepsilon)$</td>
<td>$\begin{bmatrix} e^{\varepsilon/2} &amp; 0 &amp; 0 \ 0 &amp; e^{\varepsilon/2} &amp; 0 \ 0 &amp; 0 &amp; e^{-\varepsilon} \end{bmatrix}$</td>
<td>$\begin{bmatrix} e^{-\varepsilon/2} &amp; 0 &amp; 0 \ 0 &amp; e^{-\varepsilon/2} &amp; 0 \ 0 &amp; 0 &amp; e^{\varepsilon} \end{bmatrix}$</td>
</tr>
<tr>
<td>flow</td>
<td>$y = y' \exp(\frac{1}{2} \varepsilon)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$z = z' \exp(-\varepsilon)$</td>
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</tbody>
</table>
Figure 1  Schematic diagram of a test fiber immersed in an effective medium
Figure 2. Estimate of the effective drag coefficient

\[ W = \zeta_{\text{eff}} \left( \frac{a_c}{\Delta t} \right) a_c \]

\[ W = \zeta \left( \frac{l}{\Delta t} \right) l \]
Figure 3: Log-log plot of the dimensionless bulk shear viscosity versus the shear strain.
Figure 4: Plot of the dimensionless bulk primary normal stress coefficient versus the shear strain.
Figure 5: Plot of the dimensionless bulk secondary normal stress coefficient versus the shear strain.
Figure 6: Plot of the dimensionless Trouton viscosity versus the Hencky strain in an uniaxial extensional flow.
Figure 7: Plot of the dimensionless Trouton viscosity versus the Hencky strain in a biaxial extensional flow.
Figure 8  Plot of the "high-strain" bulk viscosity versus the number density for a suspension of 1.5 mm fibers.
Figure 9  Plot of the dimensionless bulk shear viscosity versus the solid concentration for a suspension of 3.5 mm fibers. The gap width of the parallel plate viscometer is 2 mm.
Figure 10  Plot of the dimensionless bulk shear viscosity versus the solid concentration for a suspension of 6.4 mm fibers. The gap width of the parallel plate viscometer is 2 mm.
Figure 11 Plot of the dimensionless bulk shear viscosity versus the solid concentration for a suspension of 12 mm fibers. The gap width of the parallel plate viscometer is 2 mm.
Steve Dinh is an overseas Chinese born on July 29, 1955 in Saigon, Vietnam. His family immigrated to New York City in 1968. After graduating from Forest-Hills High School in 1972, he earned a Bachelor of Engineering in Chemical Engineering from Cooper Union in June, 1976, and moved on to Cornell University to complete a M.S. in January, 1978 under the direction of Dr. James F. Stevenson. He came to MIT in February, 1978 to further his study in Chemical Engineering. After completing this work, he will join the faculty of the Chemical, Nuclear and Thermal Engineering department at the University of California, Los Angeles as an Assistant Professor.