Basic Concepts of Rigid Fiber Suspensions Rheology

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Abstract

In this work, fiber suspension rheology in any orthogonal system of coordinates is described in terms of the second- and fourth-order orientation tensors. At present, the theoretical basis of the dilute and semi-dilute fiber suspensions are reviewed generally. Due to the symmetry properties of the orientation tensors and normalization condition of the orientation distribution function the independent components of the second-order tensor are reduced from original “9” to “5” while the independent components of the fourth-order tensor are reduced from “81” to “13” components in any orthogonal system of coordinates. Moreover in contracted notation, these components are reduced to “3” and “5” for the second and fourth-order tensors; respectively. The closure approximation method, i.e. to approximate the even higher order tensors in terms of the lower order one; herein the fourth-order tensor in terms of the second-order tensor, is used to solve the equation of state. Various closure approximations are reviewed. Basis of some constitutive models that describe the rheological stresses in fiber suspensions are outlined. The transition from macrostructure state to the microscopic one are briefly investigated through the Folgar-Tucker as well as Advani-Tucker models. Finally, exact solutions of simple shearing flow for dilute and semi-dilute rigid fiber suspensions are performed.

Indexing terms/Keywords

Fiber suspensions, Rigid fibers, Orientation distribution function, Advani-Tucker model, Closure approximation.

Academic Discipline and Sub-Disciplines

Physics, Fluid Mechanics

SUBJECT CLASSIFICATION

Rheology of Polymers

TYPE (METHOD/APPROACH)

Theoretical Study.

INTRODUCTION

A fiber is the fundamental unit of textiles and fabrics and can be defined as a unit of matter having a length at least 100 times its width or diameter. In this range the material is said to be rigid-fibers or short-fibers. Other than these dimensions, fibers are termed as long-or flexible fibers. In industrial applications, fibers are classified into four types, namely glass fibers, carbon fibers, synthetic fibers and natural fibers. Glass and carbon fibers are added into plastic materials to reinforce the mechanical and thermal properties with negligible change in weight. The short fibers composite products are commonly manufactured by injection molding, compression molding and extrusion processes [1]. Most commercial composites contain 10% to 50% fibers by weight, which can be regarded as being concentrated suspensions. Hence, composite materials are become increasingly important due to improved physicomechanical properties. Fiber reinforced composites are of interest in many fields.

The term suspension means any solid particles suspending into a viscous or viscoelastic solvent matrix [2]. Suspensions occur in a variety of natural and man-made materials:

1. Paints – latex paints, for instance, are stable water-based emulsions of solid monomers.
2. Nano-particle suspensions, nano-fluids, are suspensions of nano-metre sized metal suspended in aqueous solvents.
3. Bacterial suspensions – the fluid mechanics of suspensions of micro-organisms is becoming an increasingly interesting topic for study. Hydrodynamic interactions in groups of microbes may play a crucial role in the formation of bio-films, since they serve as a model of non-equilibrium system.
4. Paper-pulp – the process of paper manufacture involves the processing of cellulose fiber suspensions in an aqueous medium. The orientation of fibers under flow conditions decides the property of final paper product.

Vast quantities of some of the aforementioned products are handled by the chemical, bio-chemical and pharmaceutical industries. Thus, there is a clear need for understanding the flow behavior or rheology of these systems. The difficulty in analyzing suspension flow behavior arises because suspensions are quite different of Newtonian fluids. The later, are characterized by a single material property– the shear viscosity. On the other hand, the above examples suggest that suspensions may exhibit a wide range of flow characteristics ranging from solid to gas.
Suspension rheology is more than 100 years old. Einstein's inaugural dissertation [3] can be considered as the starting point of suspension rheology. Jeffery is the pioneering one who carried out the theoretical work which the theoretical study of suspensions continued in earnest from the 1970s with a series of papers by Hinch et al. on various aspects of suspensions [4, 5, 6]. Jeffery studied theoretically the motion of an ellipsoid immersed in a simple shear Newtonian viscous flow neglecting inertia and Brownian rotation. He found that the force acting on ellipsoid reduces to two couples, one tending to make the ellipsoid adapt to the same rotation as the surrounding fluid, and the other tending to set the ellipsoid with its axes parallel to the principal axes of distortion of the surrounding fluid. In Hinch et al. work, it was found that including small Brownian motion in a fiber suspension resulted in a stationary distribution of orbits. Further researches by Hinch et al. included constitutive modeling [7, 8], characterization of fiber suspensions with Brownian motion [9, 10], and time dependent modeling [11]. Batchelor [12] provided a method of determining bulk stress from the microstructure of a fiber suspension. He also specified the conditions for the validity of ensemble and its equivalence to statistical process used often in subsequent theoretical and numerical works.

The properties of a fiber-reinforced composite are highly dependent on the orientation of the fibers. Fiber orientation affects elastic modulus, thermal expansion, and strength when the matrix is solid; viscosity when the matrix is liquid; and thermal and electrical conductivity for both solid and liquid matrices. When the composite is deformed during processing, the fibers reorient and the properties of the material change [1]. The rheological properties and fiber structure are the results of the interaction among fibers in the suspension flow. The volume fraction \( V_f \) (total volume of particles in a unit volume of suspension) and aspect ratio \( a_r \) (ratio of fiber length to diameter) are two parameters influencing the fiber structure and rheological properties of suspensions. Fiber interactions depend not only on its concentration, \( V_f a_r^2 \), but also on the length of fibers. Hence, on the basis of mechanical and hydrodynamic suspension interacting forces, a suspension is said to be [13, 14]:

\[
\begin{align*}
\text{dilute} & : \quad V_f a_r^2 < 1, \\
\text{semi-dilute} & : \quad 1 < V_f a_r^2 < a_r, \\
\text{concentrated} & : \quad V_f a_r^2 > a_r.
\end{align*}
\]

The rheological properties of these fiber suspensions are classified as the following:

i. Dilute, low fiber concentration is one in which the fibers are never close to one another and do not interact [15, 16]. Therefore, each fiber can freely rotate without any hindrance from surrounding fibers with three rotational degrees of freedom.

ii. Semi-dilute or semi-concentrated, intermediate fiber concentration suspension would have no mechanical contact between the fibers, but the hydrodynamic interactions become significant. As a consequence, each fiber has two degrees of rotational freedom.

iii. Concentrated suspensions, in which the fiber orientation behavior becomes very complex [17, 18]. The average distance between two neighboring fibers is less than its diameter. Therefore, a fiber cannot rotate independently, except about its own symmetrical axis. Any motion of the fibers must involve a cooperative effort of all surrounding fibers and fiber-fiber contacts are dominate.

Usually, polymers reinforced by short fibers are molded or extruded as suspensions with the viscoelastic matrix in a liquid state. The resulting product is then cooled to make a solid composite with a given fiber orientation that is a key feature of the finished product since it affects elastic modulus, thermal and electrical conductivity, and strength of the composite material [19, 20]. Therefore, it is important to model the flow as accurately as possible in order to design and control manufacturing processes that would generate favourable fibre orientation state, which will ultimately lead to the best mechanical and thermal properties of the composite.

There are two main aspects in the research of fiber suspension flows. One aspect is to investigate the movement of fibers in flows. This research field belongs to low Reynolds number hydrodynamics. The other aspect is to investigate into the new properties of flows caused by the addition of fibers. This research field belongs to rheology. It is basically the additional stress induced by the fiber suspensions. On the other hand, there are two main ways to depict fiber orientation; namely, experimental studies, statistical and continuum mechanics theory as well as numerical simulation studies. On this basis, Physicists, Engineers and Mathematicians has conducted in the past few decades a huge of scientific and industrial researches including dilute and semi-dilute fiber suspensions. Recently, a few theoretical works concerning concentrated fiber suspensions have been done in the last period [21].

The present article is organized as the following:

- After this introduction, the mathematical basis of the fourth-order stiffness tensor is outlined in section 2.
- Section 3 is concerned with fiber orientation description in the flow domain.
- In section 4 fiber suspension rheology are investigated.
- Some closure approximation models are reviewed in section 5.
- In section 6 constitutive equations for fiber suspensions are examined briefly.
- In section 7 examples of constitutive equations for dilute and semi-dilute fiber suspension are investigated.
• An exact solution of orientation tensor is discussed in the appendix.

**REVIEW OF MATHEMATICAL BASIS**

**Matrix Representation and Contracted Form of the Fourth Order Tensor**  \( C_{ijkl} \)

For most suspensions of fibers in Newtonian and non-Newtonian fluids it is reasonable to assume that the stress tensor \( T_{ij} \) is a linear homogeneity function of the deformation tensor \( \dot{\gamma}_{ij} \) [22, 23]. That is; in component form:

\[
T_{ij} = C_{ijkl} \dot{\gamma}_{kl},
\]

where \( C_{ijkl} \) is the fourth-order stiffness or elasticity tensor and relation (2a) is termed as the law of elasticity. The tensor \( C_{ijkl} \) has 81 components in a matrix form. For a full anisotropic solid (i.e. 3-D random orientation), the following matrix representation can be constructed:

\[
\begin{bmatrix}
T_{11} \\
T_{22} \\
T_{33} \\
T_{21} \\
T_{12} \\
T_{13} \\
T_{23}
\end{bmatrix} = \begin{bmatrix}
C_{1111} & C_{1122} & C_{1133} & C_{1123} & C_{1131} & C_{1112} & C_{1132} & C_{1113} & C_{1121} \\
C_{2211} & C_{2222} & C_{2233} & C_{2223} & C_{2231} & C_{2212} & C_{2223} & C_{2213} & C_{2221} \\
C_{3311} & C_{3322} & C_{3333} & C_{3332} & C_{3331} & C_{3321} & C_{3332} & C_{3323} & C_{3331} \\
C_{2311} & C_{2322} & C_{2333} & C_{2332} & C_{2331} & C_{2321} & C_{2332} & C_{2323} & C_{2331} \\
C_{3111} & C_{3122} & C_{3133} & C_{3132} & C_{3131} & C_{3121} & C_{3132} & C_{3132} & C_{3131} \\
C_{1211} & C_{1222} & C_{1233} & C_{1232} & C_{1231} & C_{1221} & C_{1232} & C_{1232} & C_{1231} \\
C_{1311} & C_{1322} & C_{1333} & C_{1332} & C_{1331} & C_{1321} & C_{1332} & C_{1332} & C_{1331}
\end{bmatrix} \begin{bmatrix}
\dot{\gamma}_{11} \\
\dot{\gamma}_{22} \\
\dot{\gamma}_{33} \\
\dot{\gamma}_{21} \\
\dot{\gamma}_{12} \\
\dot{\gamma}_{13} \\
\dot{\gamma}_{23}
\end{bmatrix},
\]

If the fourth-order tensor \( C_{ijkl} \) demand the symmetry

\[
C_{ijkl} = C_{ijlk} = C_{ijki},
\]

as well as the symmetry property

\[
C_{ijkl} = C_{klji},
\]

then \( C_{ijkl} \) is called a completely symmetric or supper-symmetric tensor. Moreover, the symmetry of \( T_{ij} \) and \( \dot{\gamma}_{ij} \) show that \( C_{ijkl} \) is symmetric not only with respect to i and j but also with respect to k and l. Thus each pair of indices in \( T_{ij} \), \( C_{ijkl} \) and \( \dot{\gamma}_{ij} \); the indices \((ij)\) and \((kl)\), is replaced with a single index that ranges from “1” to “6” [23, 24, 25, 26]; Table 1. Therefore, the number of components of \( C_{ijkl} \) tensor is reduced from a total of 81 to 36 independent one.

**Table 1. Relationship between indices in contracted and tensor notations**

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

As a consequence of \( C_{ijkl} \) symmetry and by using the contracted notation, it is possible to represent equation 2b in the matrix form:

\[
[c_1] = [C_{ij}] [\dot{\gamma}_{ij}],
\]

or equivalently:

\[
\begin{bmatrix}
[\sigma_1] \\
[\sigma_2] \\
[\sigma_3] \\
[\sigma_4] \\
[\sigma_5] \\
[\sigma_6]
\end{bmatrix} = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\
C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\
C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\
C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66}
\end{bmatrix} \begin{bmatrix}
\dot{\gamma}_{11} \\
\dot{\gamma}_{22} \\
\dot{\gamma}_{33} \\
\dot{\gamma}_{21} \\
\dot{\gamma}_{12} \\
\dot{\gamma}_{13}
\end{bmatrix},
\]
in which the contracted notation is used to relate material property matrices \( \sigma, C_{ij}, \) and \( \varepsilon \) to material tensors \( T_{ij}, C_{ijkl} \) and \( \gamma_{ij} \) respectively. In this notation the elements of \( \sigma, C_{ij}, \) and \( \varepsilon \) are given by the substitution of index pairs given in Table 1. The matrix \( [C] \) is known as the elastic stiffness matrix. Its elements, \( C_{ij} \), are called the elastic constants, or the Voigt constants.

**Symmetry Restrictions on Tensor Properties**

If all elements of a second- and fourth-order tensor properties were independent, a very large number of separate properties would have to be measured or computed to predict the behavior of relatively simple systems. Fortunately, the tensor properties obey symmetry relations that reduce the number of independent tensorial elements. If the fourth-order tensor \( C_{ijkl} \) is symmetric, it must be satisfy the relation (3a) as well as the symmetry property given in equation 3b then \( C_{ijkl} \) is called a completely symmetric or supper-symmetric tensor. Moreover, the tensor \( C_{ijkl} \) has a maximum of 36 independent elements and can be represented by the \( (6 \times 6) \) matrix shown in equation 4b. In addition for the symmetry property, it is usually assumed that the \( (6 \times 6) \) contracted matrix representation of \( C_{ij} \) is symmetric with respect to its diagonal

\[ C_{ij} = C_{ji}; \; i, j = 1, 2, ..., 6, \]  

then the total number of independent components is reduced from 36 to 21 (so-called Green elasticity). Thus in the most general case of well-defined anisotropic (triclinic monocrystals) the \( (6 \times 6) \) stiffness matrix has 36 elastic constants, 21 of which can be assumed independent. Furthermore, these elements are reduced due to the symmetry to 16 elements. Moreover, due to the relation \( tr C_{ij} = 1 \), “tr” means the trace of a matrix or a tensor; the independent component reduced to 15 only. Hence, the final form of the stiffness matrix can be written as:

\[
[C_{\text{triclinic}}] = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\
C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\
C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\
C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66}
\end{bmatrix},
\]  

where the matrix elements that are represented by dots are symmetric with the off-diagonal elements.

**Symmetry Groups**

The set of all the point symmetry operations that leave a material unchanged is called its point groups. For crystalline materials, there are 32 point groups. Most of them contain a number of different symmetry elements. Some of the results are given in Table 2, which shows the number of independent elements of second- and fourth-orders for 32 crystallographic point groups and an isotropic group. This is the number of properties that one would have to measure in order to determine the full property tensor. In section 2.2, we assume that, the Green elasticity symmetry condition, \( C_{ij} = C_{ji} \), is valid for the off-diagonal elements in the stiffness matrix \([C]\). By taking Table 2 into account, the number of independent elastic constants for materials of higher symmetry (monocrystals or polycrystalline bodies) is reduced as follows:

**Table 2. Basic symmetry classes and number of independent elements of tensor properties of second- and fourth-orders for 32 crystallographic point groups**

<table>
<thead>
<tr>
<th>Symmetry class (Bravais lattice)</th>
<th>Number of tensor independent coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Second-order tensor</td>
</tr>
<tr>
<td>Triclinic</td>
<td>6</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>4</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>3</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>2</td>
</tr>
<tr>
<td>Trigonal</td>
<td>2</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>2</td>
</tr>
<tr>
<td>Cubic</td>
<td>1</td>
</tr>
<tr>
<td>Isotropic</td>
<td>1</td>
</tr>
</tbody>
</table>
Monoclinic monocrystals (13 independent elastic constants):

\[
[C_{\text{monoclinic}}] = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\
C_{12} & C_{22} & C_{23} & 0 & 0 & C_{26} \\
C_{13} & C_{23} & C_{33} & 0 & 0 & C_{36} \\
0 & 0 & 0 & C_{44} & C_{45} & 0 \\
0 & 0 & 0 & C_{45} & C_{55} & 0 \\
C_{61} & C_{26} & C_{36} & 0 & 0 & C_{66} \\
\end{bmatrix}.
\] \hspace{1cm} (6a)

Orthorhombic monocrystals (9 independent elastic constants):

\[
[C_{\text{orthorhombic}}] = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\
C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66} \\
\end{bmatrix}.
\] \hspace{1cm} (6b)

Tetragonal monocrystals (6 independent elastic constants):

\[
[C_{\text{tetragonal}}] = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\
C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66} \\
\end{bmatrix}.
\] \hspace{1cm} (6c)

Trigonal monocrystals (6 independent elastic constants):

\[
[C_{\text{trigonal}}] = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & 0 & 0 \\
C_{12} & C_{11} & C_{13} & -C_{14} & 0 & 0 \\
C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\
C_{14} & -C_{14} & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & C_{14} \\
0 & 0 & 0 & 0 & C_{14} & \frac{1}{2}(C_{11} - C_{12}) \\
\end{bmatrix}.
\] \hspace{1cm} (6d)

Hexagonal monocrystals (5 independent elastic constants):

\[
[C_{\text{hexagonal}}] = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\
C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & C_{14} \\
0 & 0 & 0 & 0 & 0 & \frac{1}{2}(C_{11} - C_{12}) \\
\end{bmatrix}.
\] \hspace{1cm} (6e)

Cubic monocrystals (3 independent elastic constants):

\[
[C_{\text{cubic}}] = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{13} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44} \\
\end{bmatrix}.
\] \hspace{1cm} (6f)
Isotropic materials (2 independent elastic constants):

\[
\begin{bmatrix}
C_{12} + 2C_{44} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} + 2C_{44} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{12} + 2C_{44} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44}
\end{bmatrix}
\]

(6g)

FIBER ORIENTATION DESCRIPTION

Moments of the Second- and Fourth-Order Tensors

The properties of fiber-reinforced composite are highly dependent on the orientation of the fibers in its flow domain [27]. The orientation of a single fiber within a continuous medium matrix can be described in spherical coordinate system by the unit vector \( \mathbf{p}(\theta, \varphi) \) aligned along the axis of the fiber as shown in Figure 1, where \( \theta \) and \( \varphi \) are the azimuthal and meridian angles; with \( 0 \leq \theta \leq \pi \) and \( 0 \leq \varphi < 2\pi \), \( \mathbf{p} \) is parallel to the major axis of an ellipsoidal particle of a single fiber with components:

\[
p_1 = \sin \theta \cos \varphi; \quad p_2 = \sin \theta \sin \varphi; \quad p_3 = \cos \theta.
\]

(7)

with \( p_1^2 + p_2^2 + p_3^2 = 1 \).

It is unrealistic attempt to develop a theory based on the orientation and motion of individual fibers, and a more useful approach is that of introducing a probability density function \( \Psi(\theta, \varphi) \) whose value for a given orientation gives the probability that a fiber has particular direction. The function \( \Psi(\theta, \varphi) \) defined such that the probability of a fiber oriented between the angles \( \theta_i \) and \( \theta_i + d\theta \) and \( \varphi_i \) and \( \varphi_i + d\varphi \) as:

\[
p(\theta_i \leq \theta \leq \theta_i + d\theta, \quad \varphi_i \leq \varphi \leq \varphi_i + d\varphi) = \Psi(\theta, \varphi) \sin \theta \, d\theta \, d\varphi,
\]

(8a)

with the normalization condition on the unit sphere,

\[
\int_0^{2\pi} \int_0^\pi \Psi(\theta, \varphi) \sin \theta \, d\theta \, d\varphi = 1.
\]

(8b)

The fiber distribution function is a complete description if the orientation of a single fiber is unrelated with that of any of its neighboring fibers. However, the calculations with the distribution function are too computationally cost when applied to industrially relevant flows. Therefore, the introducing of orientation tensors is a suitable way for describing the orientation state of fibers. The orientation tensors are defined as [28].
\[ S_{ij} = \left< p_i p_j \right> = \int_{\mathbb{S}^2} p_i p_j \psi(\mathbf{p}) \, d\mathbf{p}, \]  
\[ S_{ijkl} = \left< p_i p_j p_k p_l \right> = \int_{\mathbb{S}^2} p_i p_j p_k p_l \psi(\mathbf{p}) \, d\mathbf{p}. \]  

In general,
\[ S_{ij ...} = \left< p_i p_j ... \right> = \int_{\mathbb{S}^2} p_i p_j ... \psi(\mathbf{p}) \, d\mathbf{p}, \]  

where \( \mathbb{S}^2 \) is the unit sphere and the bracket " \( \left< \right> \) " means the ensemble average over a volume domain. The second-order tensor \( S_{ij} \) consists of nine components, however, due to symmetry ( \( S_{ij} = S_{ji} \) ) the components is reduced to six. These tensor components can be written as:
\[
S_{ij} = \left< p_i p_j \right> = \begin{bmatrix}
\sin^2 \theta \cos^2 \phi & \sin^2 \theta \sin \phi \cos \phi & \sin \theta \cos \theta \cos \phi \\
\cdot & \sin^2 \theta \sin^2 \phi & \sin \theta \cos \theta \sin \phi \\
\cdot & \cdot & \cos^2 \theta
\end{bmatrix},
\]  

the components of the tensor \( S_{ijkl} \) have all the information needed to describe the fiber orientation. We are left with even-ordered tensors only and all the odd are being zero due to the normalization of \( \psi(\theta, \phi) \). For most efficient numerical simulation of the orientation state of fibers, Advani and Tucker [29] have made use of the orientation tensor which was originally introduced by Hand; [30]. The microstructure is often characterized by these second and fourth-order moments of the fiber distribution function. The normalization conditions in Equations 8b show the two fundamental symmetry properties of \( S_{ij} \):
\[ S_{ij} = S_{ji} \quad \text{and} \quad S_{ii} = 1. \]  

Similarly, any perturbation of the four subscripts keeps \( S_{ijkl} \) constant,
\[ S_{ijij} = 1 \quad \text{and} \quad S_{ijij} = 1. \]  

Moreover, owing to Equations 3 for the symmetry properties of \( S_{ijkl} \), the following relations are obtained easily between the components of the two tensors \( S_{ij} \) and \( S_{ijkl} \); namely:
\[ S_{ij} = S_{ijkl}, \quad S_{ijkl} = S_{ijij} + S_{ij22} + S_{ij33} = S_{ij}, \quad S_{ijkl} = S_{ijkl}. \]  

Therefore, on the basis of Equation 8b the components of \( S_{ij} \) are reduced from original 9 to 5. Similarly, there are \( "13" \) independent components of \( S_{ijkl} \) [20, 31].

Although the tensors may seem an unusual means to describe fiber orientation, they have a simple physical interpretation. The main diagonal components indicate the magnitude of the fiber alignment in the direction of the reference frame, and the off-diagonal components show the rotation of principal orientation axes with respect to the coordinate system. If the fibers are randomly distributed, \( \psi = \frac{1}{4\pi} \), the second- and fourth-order tensors are said to be:
\[ S_{ij} = \frac{1}{3} \delta_{ij}, \]  

or
\[ S_{ij} = \begin{bmatrix}
\frac{1}{3} & 0 & 0 \\
0 & \frac{1}{3} & 0 \\
0 & 0 & \frac{1}{3}
\end{bmatrix}, \]  

where \( \delta_{ij} \) is the components of the second-order identity tensor \( \mathbb{I} \) ( \( \delta_{ij} = 1, 0 \) for \( i = j, \ i \neq j \)) and for
\[ S_{ijkl} = \frac{1}{15} \left( \delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right). \]
Figure 2a shows isotropic orientation state, with equal orientation distribution in all directions. If all the fibers lie in the $x_1x_2$-plane, Figure 2b, which corresponds to planer random orientation state $S_{ij}$ is simply:

$$S_{ij} = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{11d}$$

For perfectly aligned orientation in $x_1$-direction, Figure 2c, $S_{ij}$ is written as:

$$S_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{11e}$$

We can then observe that, the orientation tensor $S_{ij}$ is symmetric and has a unit trace ($\text{tr}S_{ij} = 1$) due to the unit length of $\rho$ and the normalization condition. For a completely random orientation state $S_{ij} = \frac{1}{3} \delta_{ij}$ and the limit that all the fibers are perfectly aligned in the $x_1$-direction the only nonzero component of $S_{ij}$ is $S_{11} = 1$. We limit our discussion to the second-order and the fourth-order tensors because they are rheologically sufficient.

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The Matrix Representation in Six Dimensional Space

As will be indicated in the following subsections, the fiber orientation distribution can be visualized by using eigenvalues I, II and III and eigenvectors $\hat{e}_i$ ($i = 1, 2, 3$) of the second-order orientation tensor $S_{ij}$; Figure 3. The eigenvectors indicate the principal directions of fiber aligned and the eigenvalues give the statistical proportions (0 to 1) of fibers aligned with respect to those directions $\hat{e}_i$ ($i = I, II, III$).

If the stress and the rate of strain deformation second-order tensors $t_{ij}$ and $\gamma_{ij}$ has $t_i$ and $e_i$ components where $t_i$ and $e_i$ are the principal stresses and strains, then in the six-dimensional space the following representation can be observed [32].
\[
\begin{pmatrix}
I_l \\
I_{ll} \\
I_{lll}
\end{pmatrix} = 
\begin{pmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\
0 & C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\
0 & C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\
0 & C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66}
\end{pmatrix}
\begin{pmatrix}
\phi_l \\
\phi_{ll} \\
\phi_{lll}
\end{pmatrix}.
\]

The last equation, in shorthand form, can be rewritten as:

\[
\begin{pmatrix}
I_{\text{princ}} \\
0
\end{pmatrix} = 
\begin{pmatrix}
C_{AA} & C_{AB} \\
C_{BA} & C_{BB}
\end{pmatrix}
\begin{pmatrix}
\phi_{\text{princ}} \\
0
\end{pmatrix},
\]

(12b)

with \( A = 1, 2, 3 \) and \( B = 4, 5, 6 \).
FIBER SUSPENSION RHEOLOGY

A comprehensive treatment of fiber suspension flow in complex geometries involves flow-orientation coupling is investigated [33]. It is well understood that fibers orient in response to flow kinematics, while the suspension rheology is defined in the concentration and orientation of the suspended fiber. Flow simulations that incorporate flow-orientation coupling further emphasize the need for including these fully coupled evaluations to make accurate predictions in certain geometries.

Jeffery’s Model

Jeffery’s model of fiber suspension requires uninteracting fibers, and hence it is thus valid in the dilute and partially-dilute regimes only. Most typical industrial applications are in the concentrated regime, and as such the Jeffery’s model is clearly not sufficient for industrial use. The motion of a single fiber in a Newtonian flow can be described by Jeffery’s model under the following assumptions [31]: (1) the fiber may be represented by an ellipsoid of revolution; (2) no-slip conditions prevail at the surface of the fiber; (3) the velocity field is only locally perturbed by the motion of the fiber; (4) there is no interaction between fibers; (5) the flow far from the fiber is steady and homogeneous on a length scale that is large compared to the fiber dimensions; (6) the motion is sufficiently slow that inertia forces are negligible; (7) the fiber translates with the fluid velocity as a function of location through the part thickness. Jeffery’s model in its vector form and index notation is written as:

\[
\frac{D\mathbf{p}}{Dt} = \mathbf{p} - \omega \cdot \mathbf{v} + \alpha \left( \gamma \cdot \mathbf{p} - \dot{\gamma} \cdot \mathbf{ppp} \right),
\]

(13a)

\[
\frac{D\mathbf{p}_i}{Dt} = \mathbf{p}_i - \epsilon_{ij} \mathbf{p}_j + \alpha \left( \gamma_{ij} \mathbf{p}_j - \dot{\gamma}_{ij} \mathbf{pp}_j \mathbf{p}_j \right),
\]

(13b)

where \( \alpha \) is a constant defining the ellipticity of the particle and termed as the shape factor of the fiber, it depends on the fiber aspect ratio \( a_r \) as:

\[
\alpha = \frac{a_r^2 - 1}{a_r^2 + 1},
\]

(13c)

for slender fibers \( \alpha \to 1 \). In equations 13a, \( D/Dt = d/dt + (\mathbf{v} \cdot \nabla) \) is the material time derivative, \( \dot{\gamma} = \frac{1}{2} \left[ \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right] \) is the deformation (stretching) tensor and \( \omega = \frac{1}{2} \left( \nabla \mathbf{v} - (\nabla \mathbf{v})^T \right) \) is the vorticity (spin) tensor.

Equation of Continuity (Fokker-Planck Equation)

For dilute suspensions, the kinetics of orientation distribution function \( \Psi \) is governed by the equation of continuity for \( \Psi \) or the so called Fokker-Planck equation [29]; namely,

\[
\frac{D\Psi}{Dt} = -\nabla_p \cdot \left( \mathbf{p} \Psi \right),
\]

(14)

where \( \nabla_p \) is the surface gradient operator in orientation space and \( \left( \mathbf{p} \Psi \right) \) is the flux probability. To solve Equation 14 for \( \Psi \), a constitutive relation for the time rate of change of the fiber orientation vector \( \mathbf{p} \) is needed.

Equations of Motion for \( S_{ij} \) and \( S_{ijkl} \)

Instead of performing the integration and tedious calculation of the distribution function, an equivalent system of differential equations can be written that characterizes the orientation evaluation in terms of the tensors \( S_{ij} \) and \( S_{ijkl} \). Consider the second-order tensor \( B_{ij}(\mathbf{p}) = \mathbf{p}_i \mathbf{p}_j \) for \( i, j \in \{1, 2, 3\} \) is related to the second-order orientation tensor, \( S_{ij} \), through integration as:

\[
\int_{\Omega^2} \Psi B_{ij} \, d\Omega = \int_{\Omega^2} \Psi \mathbf{p}_i \mathbf{p}_j \, d\Omega = S_{ij},
\]

(15a)

multiply the equation of continuity in Equation 14 with \( B_{ij} \)

\[
\frac{D\Psi}{Dt} B_{ij} = -\nabla_p \cdot \left( \mathbf{p} \Psi \right) B_{ij},
\]

(15b)

and performing integration over the unit sphere \( \Omega^2 \).
\[
\dot{D}_{ij} = -\nabla_p \cdot (\mathbf{p} \mathbf{v} - \mathbf{q}_{ij}),
\]

(18)

with the increase of suspension concentration, fiber-fiber contacts also increase, causing deviations from the orientation state observed in dilute suspensions. The diffusive flux vector \( \mathbf{q} \) represents a phenomenological way to account for these deviations. In order to model the diffusive flux vector in Equation 18, Folgar and Tucker suggested the relationship:

\[
\mathbf{q} = -\nabla (D_r \mathbf{v}),
\]

(19)

where \( D_r \) is the rotary diffusivity. At present, it is sufficient to assume that \( D_r \) may be a function of \((\theta, \varphi)\) and as such cannot be brought out of the gradient operator. When the assumption of Folgar-Tucker is taken into consideration, the flow of fiber is given by the equation of continuity:

\[
\frac{D^2 \mathbf{v}}{D t^2} = \nabla \cdot \mathbf{q}.
\]
\[
\frac{D\psi}{Dt} = -\nabla \cdot \left[ \rho \nabla \psi - \nabla \psi (D, \psi) \right] = -\nabla \cdot \left[ \rho \nabla \psi + \nabla \rho [D, \psi] \right],
\]
(20)

where \( \nabla^2 \) represents the Laplacian operator on the orientation space. In case of Jeffery's model, no fiber interaction occurs and hence the rotary diffusion expression \( D_r = 0 \).

By the same method given in section (4.3), the equation of motion for \( S_{ij} \) with introducing the diffusion term, is given by:

\[
\frac{DS_{ij}}{Dt} = -\left( \alpha \gamma_{ij} S_{ij} - \gamma_S \gamma_{ij} \right) + \left( \alpha \gamma_{ij} S_{ij} + \gamma_{ij} - 2\gamma_S S_{ij} \right) + 2\gamma S \delta_{ij} - 3S_{ij},
\]
(21a)

or equivalently

\[
\frac{DS_{ij}}{Dt} = \left( \frac{\omega S - S \cdot \omega}{2} + \gamma \frac{S \cdot \gamma S}{2} + \frac{\gamma - 2\gamma : S}{4} \right) + 2\gamma S \delta_{ij} - 3S_{ij},
\]
(21b)

In the same manner, the equation of motion of the fourth-order tensor \( S_{ijkl} \) is:

\[
\frac{DS_{ijkl}}{Dt} = -\left( \alpha \gamma_{ijkl} S_{ijkl} - \gamma_S \gamma_{ijkl} \right) + \left( \alpha \gamma_{ijkl} S_{ijkl} + \gamma_{ijkl} - 2\gamma_S S_{ijkl} \right) + 2\gamma S \delta_{ijkl} - 3S_{ijkl},
\]
(21c)

The evaluation of the second-order orientation tensor requires knowledge of the fourth-order orientation tensor \( S_{ijkl} \), which induces the classic closure problem. The time required to compute the evaluation of the second-order orientation tensor \( S_{ij} \) is significantly less than the computational time required to evolve \( \psi(p) \) once an approximate method is selected to approximate the fourth-order orientation tensor \( S_{ijkl} \).

More about the Constant \( D_r \)

For three decades, approaches to model fiber orientation while incorporating fiber interaction effects, are based on Folgar-Tucker model [34]. Their model introduces interaction between fibers through forces similar to Brownian motion. For non-dilute suspensions, Folgar and Tucker hypothesized that fiber interaction acted similarly to isotropic diffusion and a result added diffusion like term to Jeffery's equation. They proposed a diffusivity function based on the rate of deformation tensor \( \gamma \) and an empirically derived parameter \( C_\gamma \) termed as the interaction coefficient; defined as:

\[
D_r = C_\gamma \| \gamma \|,
\]
(22a)

where \( C_\gamma \) is assumed to be a function of volume fraction \( V_f \) (a large \( C_\gamma \) implies more fiber-fiber interactions) and \( \| \gamma \| \) is the scalar magnitude of the rate of deformation tensor; \( \| \gamma \| = \frac{1}{2} (\gamma : \gamma) \) with \( \gamma : \gamma = \gamma_{ij} \gamma_{ji} \).

By assuming the diffusivity term is of the form given by Folgar and Tucker, Equation 21a, and using Equation 22a the resulting equation of motion of the second-order orientation tensor is written as:

\[
\frac{DS_{ij}}{Dt} = -\left( \alpha \gamma_{ij} S_{ij} - \gamma_S \gamma_{ij} \right) + \left( \alpha \gamma_{ij} S_{ij} + \gamma_{ij} - 2\gamma_S S_{ij} \right) + 2C_\gamma \| \gamma \| (\delta_{ij} - 3S_{ij}),
\]
(22b)

the particle shape factor is very close to unity due to the large length-to-radius ratio of fibers; i.e. slender model. This model yields exceptional results compared to previous theories, and has been considered the standard throughout both the industrial and academic communities. The Folgar and Tucker model is considered to be the benchmark for fiber orientation analysis during processing and has found wide acceptance in the literature. The empirically determined interaction coefficient \( C_\gamma \) ensures that the final orientation state is accurately captured.

The Folgar-Tucker model allows for the control of the steady state fiber orientation through the magnitude of \( C_\gamma \) but the rate of fiber reorientation is still dominated by the flow field for typical values of \( C_\gamma \). Small values (16 x 10^{-4} to 1 x 10^{-4}) [29] typically provide a good fit to experimental fiber orientation data. Bay [35] developed an empirical expression for concentrated suspensions (\( V_f > a_r^{-1} \)),

\[
\Delta V_{p}^{\psi} = V_{p}^{\psi} - V_{p}^{\psi}(D, \psi) = -V_{p}^{\psi} \cdot \left[ \rho \nabla \psi + \nabla \rho [D, \psi] \right],
\]
Equation 23a predicts that $C_i$ decreases for increasing $V_f a_r$, a result explained by a proposed caging effect.

Phan-Thien et al. (2002) [36] proposed a model in which $C_i$ increases with increasing $V_f a_r$ as:

$$C_i = M [1 - \exp(-NV_f a_r)] ,$$

(23b)

where $M$ and $N$ are constants. Phan-Thien et al. [36] determined $M=0.03$ and $N=0.224$ by fitting Equation 23b to experimental data in comparison with Folgar and Tucker model for various suspensions of nylon fibers subject to simple shear flow. Recently, the parameter proposed by Sepehr et al. (2004a); [37], can be incorporated into the Folgar-Tucker model as follows:

$$\frac{DS_{ij}}{Dt} = \alpha \left[ \varepsilon_{ikji} S_{ij} - S_{ik} \delta_{ij} \right] + \left[ \gamma_{ik} S_{ij} + S_{ik} \gamma_{ij} - 2 \gamma_{ik} S_{ij} \right] + 2 \gamma_i \left[ \delta_{ij} - 3 S_{ij} \right].$$

(23c)

To solve Equations 22b and 23c closure approximation approach is needed to express the fourth-order tensor $S_{ijkl}$ in terms of the second-order tensor $S_{ij}$.

**CLOSURE APPROXIMATION**

The evolution equation of any orientation tensor contains next higher even-order tensor; say $S_{ij}$ in Equation 20a contains $S_{ijkl}$ and $S_{ijkl}$ in Equation 20c contains $S_{ijklmn}$ and so on. Thus, one needs a closure approximation to close the set of the evolution equations of the orientation tensors. A fourth-order closure may be expressed as:

$$S_{ijkl} \approx F_{ijkl}(S_{mn}),$$

(24)

where $F_{ijkl}$ is a function of the second-order tensor $S_{mn}$. There have been many methods proposed to address the closure problem.

Most types of closure approximations are Linear (L), quadratic (Q) and a Hybrid (H) which is being a combination of (L) and (Q) closure approximations. One of the popular models used in the numerical simulation of real manufacturing processes, such as injection molding, compression molding, is the (H) closure approximation [29, 38, 39] since it shows stable behavior of fiber orientation state with reasonable computational efficiency.

A Hybrid closure approximation has readily been used for its stable behaviors in spite of its over prediction of orientation components compared with distribution function approximation. Cintra and Tucker [26] developed orthotropic fitted closure approximation by assuming that the principal directions of the fourth-order orientation tensor $S_{ijkl}$ are functions of the eigenvalues of the second-order orientation tensor $S_{ij}$. Known parameters where determined by fitting selected flow data obtained from probability distribution function.

Orthotropic closure approximation shows better behaviors than previous closure approximation but unfortunately suffers from non-physical oscillations at low value of fiber-fiber interaction coefficient $C_i$. Chung and Kwon [40] have proposed Orthotropic closure approximation [41] which overcome such problems of non-physical oscillations. However, such orthotropic type closure approximation require additional computation time for the transformation between the global coordinate system and the principal coordinate system. In this respect, Chung and Kwon [42] have proposed invariant based optimal fitting closure approximation, which significantly reduces the computation time. Finally; equation of the hybrid closure approximation which is a combination of linear and quadratic closure approximations as well as other closure approximations are, summarized by the following equations:

**Linear Closure Approximation (L)**

An even simpler closure approximation is the linear one which originally introduced by Hand [43]:

$$S_{ijkl}^L = -\frac{1}{35} \left( \delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) + \frac{1}{7} \left( S_{ij} \delta_{kl} + S_{ik} \delta_{jl} + S_{il} \delta_{jk} + S_{jk} \delta_{il} + S_{jl} \delta_{ik} + S_{kl} \delta_{ij} \right).$$

(25a)

In general form:

$$S_{ijkl}^L = \frac{-1}{\left(4 + N_L\right)\left(2 + N_L\right)} \left( \delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) + \frac{1}{\left(4 + N_L\right)} \left( S_{ij} \delta_{kl} + S_{ik} \delta_{jl} + S_{il} \delta_{jk} + S_{jk} \delta_{il} + S_{jl} \delta_{ik} + S_{kl} \delta_{ij} \right),$$

(25b)

where $N_L$ refers to a space dimensions; i.e.,

$$N_L = \begin{cases} 2 & \text{in 2D}, \\ 3 & \text{in 3D}. \end{cases}$$

(25c)
This closure approximation is exact for a random distribution of fiber orientations (an isotropic suspension). Also, it is exact for a completely isotropic distribution of fiber orientations,
\[
S_{ijkl}^N = S_{ij}S_{kl},
\]
(25d)
which is exact for aligned fibers.

**Quadratic Closure Approximation (Q)**

This closure is exact (and not approximation) for perfectly aligned fibers;
\[
S_{ijkl}^Q = S_{ijkl}. \tag{26a}
\]
Although the quadratic closure is frequently used with an other closures, it does not obey the symmetry requirements for a fourth-order orientation tensor, i.e.
\[
S_{ijkl}^Q = S_{klij} \quad \forall \quad i, j, k, l. \tag{26b}
\]

**Hybrid Closure Approximation (H)**

The hybrid closure proposed by Advani and Tucker [29] is the most widely used method in industry because of its algebraic simplicity and numerical robustness. As we have seen in the last two subsections, the linear closure approximation is exact for random distribution of orientation while the quadratic one is exact for highly aligned fibers. The hybrid closure approximations have proposed to improve the accuracy for the intermediate cases of fiber orientations and still remain exact at two limits. It is a linear combination between the quadratic closure and the linear closure as:
\[
S_{ijkl}^H = (1 - f) S_{ijkl}^Q + f S_{ijkl}^L, \tag{27a}
\]
where "f" represents the scalar measure of orientation (weighting function) with,
\[
f = 1 - N_H \det(S_{ij}), \tag{27b}
\]
and
\[
N_H = \begin{cases} 
4 & \text{in 2D}, \\
27 & \text{in 3D}. 
\end{cases} \tag{27c}
\]

Two expressions for the weighting function "f" in terms of the tensor $S_{ij}$ have been suggested by Advani and Tucker [29], such that "f = 1" for perfectly aligned fibers (as one expects in steady uniaxial extension) and "f = 0" for completely random distribution of fiber orientations (an isotropic suspension):

**Natural Closure Approximation (N)**

The natural closure approximation [44] is formed through the fitting process of the general expression of a fully symmetric $S_{ijkl}$ in terms of $S_{ij}$. This type of closure in two dimensional case takes the form:
\[
S_{ijkl}^N = \frac{1}{6} \left[ \det(S_{ij}) (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \frac{1}{3} (S_{ij} \delta_{ik} + S_{ij} \delta_{jl} + S_{ij} \delta_{jk}) \right], \tag{28}
\]

**Invariant Based Optimal Fitting Closure Approximation (IBOF)**

This closure starts with the most general expression of the fourth-order tensor $S_{ijkl}$ in terms of the two second-order tensors $S_{ij}$ and $\delta_{ij}$ as follows [42]:
\[
S_{ijkl} = \beta_1 F(\delta_{ij} S_{kl}) + \beta_2 F(S_{ij} S_{kl}) + \beta_3 F(S_{ij} S_{km} S_{ml}) + \beta_4 F(S_{ij} S_{km} S_{ml} S_{pq}) + \beta_5 F(S_{mn} S_{mj} S_{mr} S_{ni}), \tag{29a}
\]
where the operator "F" indicates the symmetric part of the argument for instance; i.e.,
\[
F(T_{ijkl}) = \frac{1}{24} \left[ T_{ijkl} + T_{ijlk} + T_{lijk} + T_{ljik} + T_{iljk} + T_{jkil} + T_{klji} + T_{laji} + T_{ilkj} + T_{jkli} + T_{klji} + T_{laji} + T_{ilkj} + T_{jkli} + T_{klji} + T_{laji} + T_{ilkj} + T_{jkli} + T_{klji} + T_{laji} \right]. \tag{29b}
\]
Invantin based closure assumes that the coefficients $\beta_1 \rightarrow \beta_6$ are polynomial expansions of the second and third invariants of $S_{ij}$; i.e., II and III. It can be easily shown that, among the six $\beta_i$’s in equation 29a, there are only three independent values with the rest being determined in terms of the three independent ones with the help of the normalization conditions and full symmetry between indices together with Cayley-Hamilton theorem.
The Neural-Network-Based Optimal Fitting Closure Approximation (NNBOF)

This closure approximation was developed recently by Jack et al. [44]. It assumes two-layer neural-network between the second and fourth-order orientation tensors \( \mathbf{S}_2 \) and \( \mathbf{S}_4 \) as follows:

\[
\mathbf{S}_4 = \tau_2 \left[ \Omega_2 \cdot f_1 \left( \mathbf{S}_2 + \mathbf{b}_1 \right) + \mathbf{b}_2 \right],
\]

where \( \mathbf{S}_4 \) and \( \mathbf{S}_2 \) are, respectively the independent values of \( \mathbf{S}_4 \) and \( \mathbf{S}_2 \), \( \Omega_i \) (i = 1, 2) are the net-work weights, \( \mathbf{b}_i \) are the net-work bases and \( f_1 \) are respectively the hyperbolic tangent transfer function and the pure linear transformation function. The neural-network closure approximation is accurate for a wide range of the flow fluids, and also its computational time is much lower than the orthotropic closures.

CONSTITUTIVE EQUATION FOR FIBER SUSPENSIONS

There are two ways to construct the constitutive equations for fiber suspensions: the continuum mechanics approach and microstructure modeling. Several constitutive models have been proposed to describe the stress tensor for a suspension of particles in a Newtonian fluid. The constitutive equations for such systems, either obtained by invoking continuum mechanics or by using microstructure information, have the same form despite different starting points. In general, the total viscous stress tensor for the suspension, \( \tau_{ij} \), is taken to be the sum of the stress contributions from the Newtonian suspending fluid, \( \tau_{ij}^n \), and from the fiber, \( \tau_{ij}^f \). Hence, the resulting constitutive equations for the suspension can be expressed as:

\[
\tau_{ij} = \tau_{ij}^n + \tau_{ij}^f,
\]

where \( \mu_0 \) is the solvent (dynamical) viscosity and \( P \) is the hydrostatic pressure. To model the fiber stress tensor, Advani and Tucker [29] assume that:

\[
\tau_{ij}^f = \mu_0 V_l \left[ \mu_1 \gamma_{kl} S_{ijkl} + \mu_2 \gamma_{ik} S_{ij} + \mu_3 \gamma_{ij} + 2\mu_4 D_{ij} S_{ij} \right],
\]

or, in component form,

\[
\tau_{ij}^f = \mu_0 V_l \left[ \mu_1 \gamma_{kl} S_{ijkl} + \mu_2 \gamma_{ik} S_{ij} + \mu_3 \gamma_{ij} + 2\mu_4 D_{ij} S_{ij} \right].
\]

\( \mu_i \) (i = 1, 2, 3, 4) are positive material parameters specified by the particle aspect ratio, \( a_r \). The term involving \( D_{ij} \) accounts for Brownian motion. Most constitutive models for dilute and semi-dilute suspensions differ from each other based on how the material parameters \( \mu_i \) are defined. The explicit expressions for \( \mu_i \) suggested by different constitutive models have been discussed and reviewed [9, 31, 45]. Examples of these parameters are shown in Table 3.

### Table 3. Explicit expressions for \( \mu_i \) suggested by different constitutive models.

<table>
<thead>
<tr>
<th>Models</th>
<th>Material Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hinch et al. (1972)</td>
<td>( \mu_1 = 2 ), ( \mu_2 = \frac{a_r^2}{2[\ln(2a_r) - 1.5]} ), ( \mu_3 = \frac{6\ln(2a_r) - 11}{a_r^2} ), ( \mu_4 = 0 )</td>
</tr>
<tr>
<td>Lipscomb et al. (1988)</td>
<td>( \mu_1 = 2 ), ( \mu_2 = \frac{a_r^2}{2\ln a_r} ), ( \mu_3 = \mu_4 = 0 )</td>
</tr>
<tr>
<td>Shaqfeh et al. (1990)</td>
<td>( \mu_2 = -\frac{16a_r^3}{3\ln V_l} \left[ 1 + \frac{\ln(-\ln V_l)}{\ln V_l} - 0.6634 \right] ), ( \mu_1 = \mu_3 = \mu_4 = 0 )</td>
</tr>
</tbody>
</table>

For a slender particle, particle thickness can be ignored producing \( \mu_2 \) and \( \mu_3 \) equal to zero. If the particle is large enough so that Brownian motion can be ignored, last term containing \( D_{ij} \) can be omitted. Therefore, typical fiber stress tensor for dilute suspensions can be expressed as follows:

\[
\tau_{ij}^f = \mu_0 \mu_1 V_l \gamma_{kl} S_{ijkl},
\]

(33a)
and
\[ \mu_1 = \frac{a_r^2}{\ln (2a_r - \frac{3}{2})} \approx \frac{a_r^2}{\ln a_r}, \] (33b)

In semi-dilute suspensions a hydrodynamic interaction between the particles exists. For such material systems, an expression similar to equation 33a was proposed by Dinh and Armstrong [46] as:
\[ \tau_{ij} = \mu_0 \left( \frac{\pi \ell^3}{6 \ln(2h/d)} \right) \delta_{ij} S_{ijkl} \text{ijklkl} \frac{3}{o} f_{ij} S_d h^2 \ln(6 n \gamma \pi \mu \eta \bar{\lambda} \bar{\lambda} = \tau_{ij}, \] (34a)

where "n" is the fiber number density, "\ell" and "d" are the length and diameter of the fiber and "h" is defined to be the average fiber spacing as:
\[ h = \begin{cases} (n \ell)^{-1/2} & \text{for aligned orientations,} \\ (n \ell^2)^{-1} & \text{for random orientations.} \end{cases} \] (34b)

Finally, the constitutive equations are supplemented by:

The equation of conservation of linear momentum; Cauchy's dynamical equation of motion,
\[ \rho \frac{D\mathbf{u}}{Dt} = \mathbf{\nabla} \cdot \mathbf{\tau} + \rho \mathbf{b}, \] (35a)
in which "\rho" is the mass density and "\mathbf{b}" the body force per unit mass and \( \mathbf{u} \) is the velocity.

Continuity equation (for incompressible fluid);
\[ \mathbf{\nabla} \cdot \mathbf{u} = 0, \] (35b)

Fiber equation of state;
\[ \frac{DS}{Dt} = -\left( \mathbf{\omega} \cdot S_4 - S_4 \cdot \mathbf{\omega} \right) + \beta \left( \mathbf{\gamma} \cdot S_4 + S_4 \cdot \mathbf{\gamma} - 2S_4 \right) + 2D_1 \left( I - 3S_4 \right), \] (36)

In addition, we have to specify boundary conditions. Therefore, we assume for convenience the non-slip condition:
\[ \mathbf{u} = 0 \quad \text{on the boundary} \quad \Gamma, \] (37a)
(no boundary condition is specified in respect of the orientation tensor) and the initial conditions:
\[ \mathbf{u}(x, 0) = \mathbf{u}_0, \quad S_4(x, 0) = S_4^0 \quad \text{on} \quad \Gamma. \] (37b)

**Examples of Constitutive Equations for Dilute Fiber Suspensions**

**Ericksen Equation**

In the dilute range, the fluid behavior around each fiber is unaffected by the other. The medium is known to be governed by the Ericksen equation of state [47],
\[ \tau = -P_{\delta} + 2\mu_0 \gamma + \mu_2 \gamma P_{\delta} \] (38a)

where the rheological parameter \( \mu_2 \), for a given aspect ratio \( a_r \), is given by:
\[ \mu_2 = \frac{a_r^2 \mu_0}{\ln a_r}. \] (38b)

**Lipscomb et al. Equation**

Following Batchelor [48] and Evans [49], Lipscomb et al. [31] have proposed a model for dilute particle suspension, which can be written for ellipsoids with high aspect ratio as:
\[ \tau = -P_{\delta} + 2\mu_0 \gamma + \mu_2 \gamma V(\mu_1 \gamma + \mu_2 \gamma S_4), \] (39)
Examples of Constitutive Equations for Semi-Dilute Fiber Suspensions

In the semi-dilute range, the medium is submitted to two additional types of interactions namely, the “fiber-boundaries” and the “fiber-fiber” which affect the dynamics of the flow. These interactions appear either between the fiber and the boundaries or between neighboring fibers. The “fiber-boundaries” interactions are negligible with respect to the “fiber-fiber” interactions.

Batchelor Equation

A general constitutive equation for the bulk stress in a semi-dilute suspension containing cylindrical fibers was originally developed by Batchelor [51]. The equation can be expressed in the form of orientation stress tensors as follows:

$$\tau = \mu_0 \dot{\gamma} + \frac{1}{2} \mu_p \left[ \left( \frac{nL}{2} \right) \cdot \dot{\varepsilon} \right] : \dot{\gamma},$$

(40)

where $\mu_p = \frac{1}{3} nL \mu_o$, is the fiber extra viscosity and $\varepsilon = \left[ \ln \left( 1+p \right) \right]^{-1}$.

Dinh-Armstrong Integral Model

The bulk stress in a suspension of particles in a Newtonian fluid obtained by Batchelor [51] has two separate parts, one due to the viscous dissipation of the fluid and the other due to the presence of particles. This model applies this model to semi-concentrated fiber suspensions and obtained the rheological equation:

$$\tau = -\mu_0 \dot{\gamma} + \frac{1}{2} \mu_p \left[ \left( \frac{nL}{2} \right) \cdot \dot{\varepsilon} \right] : \dot{\gamma},$$

(41a)

with

$$\Psi(p, t) = \frac{1}{4\pi} \left( \dot{\varepsilon}^T \cdot \Delta \cdot \dot{\varepsilon} \right)^{3/2}$$

(41b)

where $\dot{\varepsilon}$ is the deformation gradient; $(\nabla \dot{\varepsilon})^T$. When equation (41a) is combined with equation (41b) the constitutive equation for the fiber suspension is reduced to:

$$\tau = -\mu_0 \dot{\gamma} + \frac{1}{2} \mu_p \left[ \left( \frac{nL}{2} \right) \cdot \dot{\varepsilon} \right] : \dot{\gamma},$$

(42a)

The product $[\dot{\varepsilon}^T \cdot \Delta]$ appearing in equation (42a) is known as the Cauchy strain tensor. It is sometimes convenient to use a finite strain tensor $\dot{\varepsilon}^{[0]} = [\dot{\varepsilon}^T \cdot \Delta - I]$ in terms of which equation (42a) becomes:

$$\tau = -\mu_0 \dot{\gamma} + \frac{1}{2} \mu_p \left[ \left( \frac{nL}{2} \right) \cdot \dot{\varepsilon} \right] : \dot{\gamma},$$

(42b)

Equations (42a) and (42b) are similar in form in the way kinematical tensors appear to results obtained by Doi and Edwards [52] and Curtiss and Bird [53] for concentrated solutions of flexible macromolecules.

In the Dinh-Armstrong model and for cylinder bodies; the stress tensor in the dilute case is given as:

$$\tau = \mu_0 \dot{\gamma} + \mu_o N \dot{\gamma} : \dot{\gamma},$$

(43)

where $N$ is defined as a dimensionless suspension parameter which includes the combined effects of volume fraction $V_1$ and fiber aspect ratio $a_r$.  

The General Constitutive Equation

Finally, a general rheological constitutive equation for suspensions of axisymmetric particles can be represented as follows [22]:

$$\tau = \mu_0 \dot{\gamma} + \mu_o N \dot{\gamma} : \dot{\gamma},$$

(43)
\[
\tau_{ij} = \mu_0 \hat{\gamma}_{ij} + \mu_0 V_l \left[ A \hat{\gamma}_{ik} a_{kj} + B (\hat{\gamma}_{ik} a_{ij} + a_{ik} \hat{\gamma}_{kj}) + C \hat{\gamma}_{ij} + 2 F a_i D_j \right],
\]

where A, B, C and F are material constants which depend on the geometric shape factor. Various theories differ in the way which the constants A, B, C, and F are derived. For a slender particle, where thickness can be ignored, producing B and C equal to zero. If the particle is large enough so that Brownian motion can be ignored, the last term containing \( D_j \) can be omitted. Therefore, typical constitutive equation for fiber suspensions can be expressed as follows:

\[
\tau_{ij} = \mu_0 \hat{\gamma}_{ij} + \mu_0 V_l A \hat{\gamma}_{ik} S_{ikj}.
\]

**APPENDIX**

**Simple shear flow**

Simple shear flow will, as usual, be analyzed in a coordinate system where \( x_1 \) defines the flow direction, \( x_2 \) the direction of the flow gradient and \( x_3 \) the natural direction:

\[
\Psi = \begin{bmatrix}
0 & 0 & 0 \\
\hat{\gamma} & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}, \quad \mathbf{D} = \frac{1}{2} \begin{bmatrix}
0 & \hat{\gamma} & 0 \\
\hat{\gamma} & 0 & 0 \\
0 & 0 & 0
\end{bmatrix},
\]

The rate of shear \( \hat{\gamma} \) may also in general be understood as a function of time, but is a constant, say \( \hat{\gamma} = \hat{\gamma}_0 \), in steady shear flow. For such flows, three rheological properties, namely the transient shear viscosity \( \mu_0 \), first normal stress coefficient \( \psi_1 \), and second normal stress coefficient \( \psi_2 \), are of great importance. These rheological parameters are defined as:

\[
\mu_0 = \tau_{12}, \quad \psi_1 = \frac{\tau_{11} - \tau_{22}}{2}, \quad \psi_2 = -\frac{\tau_{22} - \tau_{33}}{2},
\]

where \( \tau_{11}, \tau_{22}, \) and \( \tau_{33} \) are the normal stresses and \( \tau_{12} \) is the shear stress.

In the following, the solution of Jeffery’s equation of motion for dilute fiber suspension; the exact formula, in simple shear flow is performed.

**Analytical Solution of Orientation Tensors**

Consider the motion of a rigid neutrally buoyant ellipsoidal particle in an arbitrary homogenous flow. The time rate of change of the orientation vector \( p(0, \phi) \) of an ellipsoid of revolution can be expressed as:

\[
\dot{p}_i = \left( \omega_{ij} + \alpha \hat{\gamma}_{ij} \right) p_j - \alpha \dot{p}_i p_k \hat{\gamma}_{kj}.
\]

Following Bretherton’s work \([54]\), the solution of equation A-3 with the initial condition \( p_i = p_i^0 \) at \( t = t_0 \) can shown to be,

\[
p_i = \frac{E_i p_i^0}{\left( E_{mm} p_m^0 \right)^{\frac{1}{2}}},
\]

where \( E_{ij} \) are the components of the particle rotation tensor, defined by:

\[
\frac{dE_{ij}}{dt} = \left( \omega_{ik} + \alpha \hat{\gamma}_{ik} \right) E_{kj}.
\]

Equation (A-4), with the initial condition \( E = I \) (unit tensor), provides the analytical solution of the rotation vector \( p(0, \phi) \) and is valid for both two and three-dimensional flows and orientation fields. For infinite aspect ratio fibers (i.e., slender fibers) \( \alpha = 1 \) the rotation tensor \( E_{ij} \) becomes the actual strain tensor of the flow field and equation A-5 reduces to:

\[
E_{ij} = \frac{\partial x_i}{\partial x_j^0},
\]

where \( x_i \) and \( x_i^0 \) are the fluid particle coordinates at \( t \) and \( t^0 (t^0 < t) \), respectively. Hence, for \( \alpha = 1 \); \( E_{ij} \) is defined as the strain tensor for the undistorted flow.
In order to determine the particle rotation tensor components in terms of velocity gradients for planer orientations, two sets of differential equations, given by equation A-5, need to be solved with the initial condition \( E = I \), [55]. Each set contains two coupled ordinary differential equations and can be solved independently. After obtaining analytical solutions of equation A-5, the orientation vector components can be easily calculated for any initial fiber orientation by using equation A-4.

For any two-dimensional homogenous flow, the velocity gradient tensor can be specified as:

\[
\mathbf{u}_{ij} = \begin{bmatrix}
\frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} \\
\frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2}
\end{bmatrix} = \begin{bmatrix}
c & c_1 \\
c_2 & -c
\end{bmatrix},
\]

(A-7)

where \( c, c_1 \) and \( c_2 \) are arbitrary constants, and the trace of \( \mathbf{u}_{ij} \) should be zero to satisfy the conservation of mass for incompressible flow. A single parameter \( w^2 \) can be utilized to define the solution families of equation A-7 with an arbitrary velocity gradient tensor.

\[
w^2 = \frac{\alpha^2 (B^2 + 4c^2) - A^2}{4},
\]

(A-8)

where \( B = c_1 + c_2 \) and \( A = c_1 - c_2 \). Depending on the value of \( w^2 \), three different solution families are possible as shown by Akbar and Altan [55].

When \( w^2 = 0 \),

\[
\mathbf{E}_{ij} = \begin{bmatrix}
1 + \alpha ct & \frac{(\alpha B + A)t}{2} \\
\frac{(\alpha B - A)t}{2} & 1 - \alpha ct
\end{bmatrix}.
\]

(A-9)

When \( w^2 > 0 \),

\[
\mathbf{E}_{ij} = \begin{bmatrix}
w \cosh(\omega t) + \alpha c \sinh(\omega t) & \frac{(\alpha B + A) \sinh(\omega t)}{w} \\
\frac{w (\alpha B - A) \sinh(\omega t)}{2w} & \frac{2w}{w \cosh(\omega t) - \alpha c \sinh(\omega t)}
\end{bmatrix}.
\]

(A-10)

When \( w^2 < 0 \),

\[
\mathbf{E}_{ij} = \begin{bmatrix}
w \cos(\omega t) + \alpha c \sin(\omega t) & \frac{(\alpha B + A) \sin(\omega t)}{w} \\
\frac{w (\alpha B - A) \sin(\omega t)}{2w} & \frac{2w}{w \cos(\omega t) - \alpha c \sin(\omega t)}
\end{bmatrix}.
\]

(A-11)

In equation A-10 \( w \) is defined as \( w = \sqrt{-w^2} \). Equations (A-9) – (A-11) are the possible solutions for particle rotation tensor and can be used in equation A-4 to specify the rotation of both oblate and prolate spheroids subjected to an arbitrary homogenous flow.

If the initial distribution of particle orientation is known, the time-dependent evolution of orientation distribution function can be obtained analytically. For planer orientations, using normalization condition as given in equation 8b, the initial condition for randomly oriented particles becomes:

\[
\Psi(\Omega, t = 0) = \frac{1}{\pi}.
\]

(A-12)

Therefore, for random initial condition, the solution of the Fokker-Planck equation; equation 14 with equation A-3 can be expressed as:

\[
\Psi(\Omega, t) = \frac{1}{\pi} (\Lambda_m \Lambda_p p_m)^{-1},
\]

(A-13)

where \( \Lambda_{ij} \) is the inverse of particle rotation tensor \( \mathbf{E}_{ij} \). Equation (A-13) can be rearranged by using planer orientation angle \( \phi \) as:

\[
\Psi(\Omega, t) = \frac{1}{\pi} (a_1 \cos^2 \phi + \frac{1}{2} a_2 \sin 2\phi + a_3 \sin^2 \phi)^{-1},
\]

(A-14)
where 
\[ a_1 = \lambda_{11}^2 + \lambda_{21}^2, \]
\[ a_2 = 2(\lambda_{11}\lambda_{12} + \lambda_{21}\lambda_{22}), \]
\[ a_3 = \lambda_{12}^2 + \lambda_{22}^2. \]  
(A-15)

Determining analytical solutions of the second- and fourth-order orientation tensors involves calculation of the integrals given by equations 9a and 9b. For the second-order orientation tensor \( S_{ij} \), the resulting integral becomes:
\[
S_{ij} = \frac{1}{\pi} \int_0^\pi \cos((i-j)\varphi) \sin((i-j)\varphi) \left[ a_1 \cos^2 \varphi + \frac{a_2}{2} a_2 \sin 2\varphi + a_3 \sin^2 \varphi \right] d\varphi,
\]
where \( \zeta = i + j \). Similarly, the fourth-order orientation tensor \( S_{ijkl} \) can be expressed as:
\[
S_{ijkl} = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \cos((i-j-k+l)\varphi) \sin((i-j-k+l)\varphi) \left[ a_1 \cos^2 \varphi + \frac{a_2}{2} a_2 \sin 2\varphi + a_3 \sin^2 \varphi \right] d\varphi.
\]
where \( \zeta = i + j + k + l \). Consequently, the \( S_{ij} \) components are obtained as:
\[ S_{11} = \frac{1}{2\lambda_1} \left[ a_2^2 - 2(a_3 - a_1)(1 - a_3) \right], \]  
(A-18)
\[ S_{12} = \frac{1}{2\lambda_1} \left[ 2a_2 - a_2(a_1 - a_3) \right], \]  
(A-19)
\[ S_{22} = \frac{1}{2\lambda_1} \left[ a_2^2 + 2(a_3 - a_1)(1 - a_1) \right]. \]  
(A-20)

From equation A-17, the \( S_{ijkl} \) components becomes:
\[
S_{1111} = \frac{a_1 - 3a_3}{2\lambda_1} \left[a_2^2 - 2(a_3 - a_1)^2 - a_3^2 + 4a_2(a_1 - a_3) + 2a_3^2 + 2a_2a_2^2 + a_2^2 - 4a_3a_3^2 - 4a_3^2a_3 + 2a_3^2a_3^2 \right], \]  
(A-21)
\[
S_{1112} = \frac{4a_3a_2(a_1 - a_3) + a_2[(a_1 - a_3)(2 - a_3)]}{2\lambda_1} \left[a_2(3a_3^2a_3 - a_3^2 - 2a_3^2) - a_3 - a_3^2 \right], \]  
(A-22)
\[
S_{1122} = \frac{(a_1 + a_3)[(a_1 - a_3)^2 - a_3^2]}{2\lambda_1} \left[a_2^2a_2 - 2a_1a_3 + 4a_2a_3^2 + a_2a_2^2 - 2a_3^2a_3 \right], \]  
(A-23)
\[
S_{1222} = \frac{a_2[(a_1 - a_3)^2 - a_3^2 + 4a_3a_2(a_1 - a_3)]}{2\lambda_1} \left[a_2(3a_3^2a_3 - a_3^2 - 2a_3^2) - a_3 - a_3^2 \right], \]  
(A-24)
\[
S_{2222} = \frac{(a_3 - 3a_3)[(a_1 - a_3)^2 - a_3^2] - 4a_3(a_1 - a_3)}{2\lambda_1} \left[a_2^2 - 4a_1a_3a_3 + 2a_2a_3^2 + 2a_2a_3^2 + a_2^2 - 4a_3^2a_3 \right]. \]  
(A-25)

where \( \lambda_1 = (a_1 - a_3)^2 + a_3^2 \) and \( \lambda_2 = \sqrt{4a_3a_3 - a_3^2} \).

**Second and Fourth Order Tensor Components of Simple Shear Flow**

The velocity gradient tensor for a simple shear flow is expressed as:
\[
u_{ij} = \begin{bmatrix} 0 & c_1 \\ 0 & 0 \end{bmatrix}, \]  
(A-26)

where \( c_1 \) represents the shear rate. It can be easily seen that \( w^2 \), defined in equation A-8, becomes
\[
w^2 = \frac{c_1^2(a^2 - 1)}{4}. \]  
(A-27)

Since \( a^2 < 1 \) for finite aspect ratio particles, \( w^2 < 0 \). Therefore, the second- and fourth-order orientation tensor components for the simple shear flow simplify as:
\[ S_{11} = \Delta_3 (b_1 + b_1 b_3 - b_3 + b_3^2 - 2), \]  
\[ S_{12} = \frac{1}{2} \Delta_3 b_2 (2 - b_1 - b_3), \]  
\[ S_{22} = \frac{1}{2} \Delta_3 (b_1^2 - b_1 + b_3^2 + b_3 - 2), \]  
\[ S_{1111} = \frac{1}{2} \Delta_3^2 (b_1 + b_3 - 2)^2 (4 + b_1 + 5b_3 + 2b_3^2), \]  
\[ S_{1112} = \frac{1}{2} \Delta_3^2 b_2 (b_1 + b_3 - 2)^2 (1 + b_3), \]  
\[ S_{1122} = \frac{1}{2} \Delta_3^2 b_2 (b_1 + b_3 - 2)^2 (b_1 + 2b_3^2 + b_3), \]  
\[ S_{1222} = \frac{1}{2} \Delta_3^2 b_2 (b_1 + b_3 - 2)^2 (1 + b_3), \]  
\[ S_{2222} = \frac{1}{2} \Delta_3^2 (b_1 + b_3 - 2)^2 (4 + 2b_3^2 + 5b_1 + b_3), \]  

where

\[
\Delta_3 = \left[(b_1 + b_3)^2 - 4\right]^{-1}, \\
b_1 = 1 - \frac{2a}{1 + a} \sin^2 wt, \\
b_2 = \frac{2a}{\sqrt{1 + a^2}} \sin 2wt, \\
b_3 = 1 + \frac{2a}{1 - a} \sin^2 wt.
\]

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