A Fitted Closure of the Sixth-Order Orientation Tensor for Short-Fiber Reinforced Polymer Composite Modeling

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SUMMARY: Orientation tensors are commonly used in short-fiber reinforced injection molding simulations of industrial polymer composite products. Unfortunately, the evolution equation for each even-order orientation tensor is written in terms of the next higher even-order orientation tensor. It has been shown that current fourth-order closures approach the fourth-order truncation limit when representing the fiber orientation distribution function so that an increase in accuracy necessitates the development of a sixth-order closure. A sixth-order fitted closure is presented which assumes that the orthotropic planes of material symmetry of the sixth-order orientation tensor correspond to the principal directions of the second-order orientation tensor. The sixth-order closure is computed using a fitting procedure which minimizes differences between the exact and the fitted sixth-order orientation tensors over a range of orientations encompassing much of the eigenspace of the second-order orientation tensor. The sixth-order closure is demonstrated to approach the sixth-order truncation limit in representing the fiber orientation distribution function over a range of flow fields.

KEYWORDS: Orientation Tensor, Polymer Processing, Fiber Orientation Distribution Function, Closure Approximation

MODELING THE DISTRIBUTION OF FIBERS

Short-fiber polymer composites are used extensively in industrial applications due in large part to their high strength to weight ratio. The orientation state of the short-fibers is critical since it dictates the material properties of the composite structure. Therefore understanding and predicting the fiber orientation is necessary for practical structural design purposes. Most polymer composite fiber orientation simulations begin with the model presented by Folgar and Tucker [1] which superimposes the motion of a single rigid particle in a dilute suspension with that of interacting particles through the use of an interaction coefficient C_I to account for interactions between fibers. The Folgar-Tucker model, which solves the orientation distribution function of fibers $\psi(\theta,\phi)$, is constrained to simple flow simulations due to excessive computation time and memory usage, but is considered to be the benchmark for fiber orientation simulations [2-8]. The solution of the Folgar Tucker model will be referred to as the 'exact' solution throughout the remainder of the paper recognizing that the fiber orientation distribution $\psi(\theta,\phi)$ is solved numerically.

For industrial injection molding applications, Advani and Tucker [2] defined orientation tensors using moments of the fiber orientation distribution function to represent the fiber orientation state. The orientation tensors, a_{ij}, a_{ijkl}, a_{ijklmn}, *etc.* capture the stochastic nature of the fiber orientation distribution in a compact form [2] and are defined through the dyadic products of the unit vector p_i which lies along the fiber axis and the distribution function $\psi(\theta,\phi)$ over the unit sphere

$$a_{ij} = \int_{S^2} p_i p_j \psi(\theta,\phi) dS \qquad a_{ijkl} = \int_{S^2} p_i p_j p_k p_l \psi(\theta,\phi) dS \qquad \cdots \tag{1}$$

By the application of Eqn. (1) the orientation tensors can be shown to be completely symmetric with respect to any pair of indices. Higher order orientation tensors completely describe the lower order orientation tensors using the normalization condition for the distribution function $\psi(\theta,\phi)$ along with Eqn. (1) [2]

$$1 = a_{ii} \qquad a_{ij} = a_{ijpp} \qquad a_{ijkl} = a_{ijklqq} \tag{2}$$

where repeated indices indicate summation, *i.e.* $a_{ii} = a_{11} + a_{22} + a_{33}$. Advani [2] combined Eqn. (1) with the Folgar-Tucker model for the distribution function $\psi(\theta,\phi)$ to obtain the evolution of the even order orientation tensors a_{ij}, a_{ijkl} , etc. The time required to compute the evolution of the second-order orientation tensor is significantly less than the computation time required to evolve the distribution function $\psi(\theta,\phi)$. Unfortunately, the evolution of the second-order orientation tensor a_{ij} is a function of the fourth-order orientation tensor a_{ijkl}, and the evolution equation of the fourth-order tensor a_{ijkl} contains the sixth-order tensor a_{ijklmn} [2]

$$\begin{aligned}\frac{Da_{ijkl}}{Dt} = &-(\omega_{im} a_{mjkl} - a_{ijkm}\omega_{ml}) + \lambda(\dot{\gamma}_{im} a_{mjkl} + a_{ijkm}\dot{\gamma}_{ml} - 2\dot{\gamma}_{mn} a_{ijklmn}) + \\ &C_I \dot{\gamma}[-20 a_{ijkl} + 2(a_{ij}\delta_{kl} + a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{jk}\delta_{il} + a_{jl}\delta_{ik} + a_{kl}\delta_{ij})]\end{aligned} \tag{3}$$

where ω_{ij} is the vorticity tensor, λ is the fiber aspect ratio, and $\dot{\gamma}$ is the scalar magnitude of the rate of deformation tensor $\dot{\gamma}_{ij}$. Indeed, the evolution equation of any even-ordered orientation tensor requires information from the next higher even-ordered orientation tensor which necessitates the use of a closure which approximates an orientation tensor in terms of the components of the lower ordered orientation tensors. There exist many closures of the fourth-order orientation tensor as a function of the second-order tensor [2,4-7], along with several closures of the sixth-order orientation tensor [2,8].

A FITTED SIXTH-ORDER CLOSURE

In the literature there exists only a brief investigation into sixth-order closures. Altan *et al.* [8] presented a sixth-order quadratic closure for dilute suspensions of fibers. Their closure is only accurate for highly aligned distributions and has been stated to provide little improvement over fourth-order closure results for the additional computational expenses [5]. Advani and Tucker [2] present a sixth-order hybrid closure, but for most industrial applications the sixth-order hybrid closure overestimates the actual alignment of the fibers [9,10].

This paper presents a sixth-order fitted closure similar in construction to the fourth-order fitted closures of Cintra and Tucker [5], VerWeyst *et al.* [7] and Chung and Kwon [6]. Our sixth-order fitted closure is computed from the components of a_{ijkl} and assumes that the planes of orthogonal symmetry of the sixth-order orientation tensor correspond to the principal directions of the second-order orientation tensor. In this formulation each principal component of the sixth-order orientation tensor is represented as a function of the independent principal components of the second-order orientation tensor.

A general sixth-order orientation tensor has 729 components of which 28 are independent by symmetry arguments for orientation tensors. If we assume that the principal frame of the second-order tensor a_{ij} forms the orthotropic planes of material symmetry for the sixth-order tensor a_{ijklmn}, only 10 independent nonzero components of a_{ijklmn} remain

$$\overline{a}_{111111},\ \overline{a}_{111122},\ \overline{a}_{111133},\ \overline{a}_{112222},\ \overline{a}_{112233},\ \overline{a}_{113333},\ \overline{a}_{222222},\ \overline{a}_{222233},\ \overline{a}_{223333},\ \overline{a}_{333333} \qquad (4)$$

where the overbar indicates that components of the sixth-order orientation tensor are given with respect to the principal frame of the second-order orientation tensor. Using Eqn. (2) for the relation between the fourth- and sixth-order orientation tensors, it can easily be shown that only four unknown components of $\overline{a}_{ijklmn}$ remain from those shown in Eqn. (4) (see *e.g.* [9]). The newly created Eigenvalue Based Fitted sixth-order closure (EBF_6) is formed by arbitrarily selecting the four components $\overline{a}_{111111}$, $\overline{a}_{111122}$, $\overline{a}_{222222}$, and $\overline{a}_{333333}$ to be unknown.

A second-order orientation tensor a_{ij} has three eigenvalues $a_{(i)}$, two of which are independent from Eqn. (2). The two independent principal values of the second-order tensor are selected to be $a_{(1)}$ and $a_{(2)}$ when setting $a_{(1)}\geq a_{(2)}\geq a_{(3)}$. The four unknowns of the EBF_6 are formed by fitting the four remaining independent components of the sixth-order tensor to a second-order polynomial of the eigenvalues of the second-order orientation tensor as

$$\begin{Bmatrix} \overline{a}_{111111} \\ \overline{a}_{111122} \\ \overline{a}_{222222} \\ \overline{a}_{333333} \end{Bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \end{bmatrix} \begin{Bmatrix} 1 & a_{(1)} & a_{(2)} & a_{(1)}a_{(2)} & a_{(1)}^2 & a_{(2)}^2 \end{Bmatrix}^T \qquad (5)$$

The new sixth-order closure is computed from the fourth-order orientation tensor a_{ijkl}. First the second-order orientation tensor a_{ij} is formed from a_{ijkl} using Eqn. (2). Then the eigenvalues $a_{(1)}$ and $a_{(2)}$ are computed and the rotation tensor is formed from the eigenvectors of a_{ij}. Next, the principal components of the sixth-order orientation tensor $\overline{a}_{ijklmn}$ are computed using the EBF_6 closure from Eqn. (5). Finally, the sixth-order orientation tensor in the principal frame is rotated into the material frame yielding a_{ijklmn} for the given a_{ijkl}.

DISTRIBUTION FUNCTION RECONSTRUCTION

Reconstruction of the fiber orientation distribution function provides a quantitative means of assessing the effect of introducing closure approximations on representing $\psi(\theta,\phi)$ [9,10]. Onat and Leckie [11] demonstrated that an approximate distribution function $\hat{\psi}_N$ of N^{th} order can be reconstructed based upon the deviatroic form of the orientation tensors as

$$\hat{\psi}_N(\theta,\phi) = f_o V_o + f_{ij} V_{ij} + f_{ijkl} V_{ijkl} + f_{ijklmn} V_{ijklmn} + \cdots \qquad (6)$$

where f_o, f_{ij}, f_{ijkl}, f_{ijklmn} are the basis functions and V_o, V_{ij}, V_{ijkl}, V_{ijklmn} are the corresponding Fourier coefficients which can be written entirely in terms of the orientation tensors (see *e.g.* [2,9] for a full discussion). This method is identical to expanding the orientation distribution function $\psi(\theta,\phi)$ in terms of orthogonal functions of p_i [11].

To asses the error between the exact distribution function $\psi(\theta,\phi)$ and the Nth order reconstruction of the distribution function, $\hat{\psi}_N(\theta,\phi)$ we use the following error metric [9,10]

$$ERR_N = \sqrt{\int_{S^2} (\psi(\theta,\phi,t_o) - \hat{\psi}_N(\theta,\phi,t_o))^2 \, dS} \qquad (7)$$

where the integration is performed over the unit sphere at the time t_o. Equation (7) may be used to form an Nth order truncation limit from the exact Nth order orientation tensors in Eqn. (1) which is used to assess the accuracy of a given closure. To form the truncation limit for a particular flow field it is necessary to first evolve the exact distribution function $\psi(\theta,\phi)$. The orientation tensors are computed from $\psi(\theta,\phi)$ by Eqn. (1) and the distribution function is reconstructed to the desired order with Eqn. (6). This reconstructed distribution function is then used with the exact distribution function $\psi(\theta,\phi)$ in Eqn. (7) to quantify the error when representing $\psi(\theta,\phi)$. When the exact orientation tensors a_{ij}, a_{ijkl}, a_{ijklmn}, etc. are used in Eqn. (7), the truncation limit of the reconstruction is obtained. Alternatively, when a closure is employed to compute any of the orientation tensors, Eqn. (7) indicates the additional error introduced by the closure. Note that any Nth order closure of an orientation tensor can only be as accurate in representing the distribution function as the exact Nth order reconstruction. As discussed in Jack and Smith [10] the existing fourth-order closures approach the fourth-order reconstruction limit, therefore any substantial increase in accuracy in the representation of the distribution function will need to come from a higher-order closure.

COMPUTING THE EIGENVALUE BASED SIXTH-ORDER CLOSURE

In this study, the finite difference technique of Bay [3] is used to evaluate the distribution function $\psi(\theta,\phi)$ for the five representative flows used in the fitted closure of Cintra and Tucker [5]. All flows have a large interaction coefficient, $C_I = 10^{-2}$, representing the upper range of fiber interactions for industrial applications of injection molding processes. The unknown coefficients C_{ij} in Eqn. (5) are determined by minimizing the difference between the components of the actual a_{ijklmn} in Eqn. (1) and those computed with the closure approximation in Eqn. (5) using the optimization package VisualDOC 4.0 [12]. The cost function is minimized in less than 40 iterations using the BFGS method for unconstrained optimization with the resulting fitted components given as

$$\left[C_{ij}\right] = \begin{bmatrix} 0.07492 & 0.10439 & -0.42312 & 0.27277 & 0.79524 & 0.49666 \\ 0.05126 & -0.13977 & -0.10376 & 0.48791 & 0.09708 & -0.05669 \\ 0.14046 & -0.37744 & -0.26722 & 0.64968 & 0.23585 & 1.07191 \\ 0.97708 & -1.72435 & -1.86763 & 1.60122 & 0.74654 & 0.91396 \end{bmatrix} \qquad (8)$$

To demonstrate the increased accuracy that may be gained through a sixth-order closure; the error metric presented in Eqn. (7) is shown for two flows, Simple Shear and Shear Stretch B (see *e.g.* [5]). These two flows are used in the fitting procedure for most fitted closures [4-7], and are indicative of flow behavior occurring in injection molding processes. The approximate sixth-order orientation tensor is computed from the exact fourth-order orientation tensor a_{ijkl} from Eqn. (5) and is used to compute the error metric ERR_6EBF_6 from Eqn. (7). The values for the error metric for the transient solution are given in Fig. 1 for both flows. For reference purposes, the error metric for an exact second-order truncation ERR_2, fourth-order truncation ERR_4, and sixth-order truncation ERR_6 are also shown (see *e.g.* [9,10]). Note that any closure of the fourth-order orientation tensor will only approach the fourth-order truncation line ERR_4, whereas throughout the flow history the EBF_6 closure is able to attain a level of error below the fourth-order truncation limit ERR_4 and approaches the sixth-order limit ERR_6.

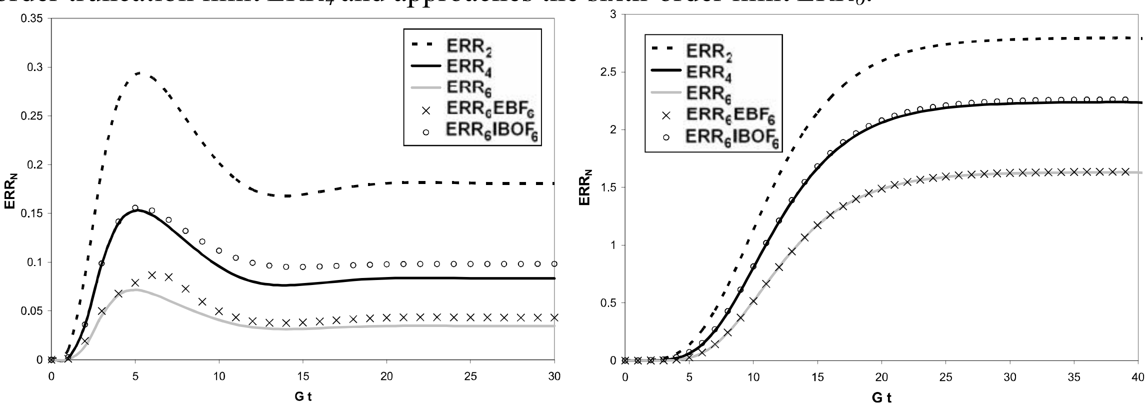

Fig. 1. Transient Error for Simple Shear (left) and Shear-Stretch B (right) for $C_I = 10^{-2}$

CONCLUSIONS

To obtain accuracy greater than the fourth-order truncation limit in representing fiber distributions in short-fiber injection molding simulations, a sixth-order closure becomes necessary. We present a fitted sixth-order closure that is computed from the components of the fourth-order orientation tensor and assumes that the principal directions of the second-order orientation tensor define the orthotropic planes of material symmetry of the sixth-order orientation tensor. The newly formed sixth-order fitted closure is demonstrated to more accurately represent the distribution function under certain flow situations than the fourth- order truncation limit when representing the fiber orientation distribution function. To fully utilize a closure of the sixth-order orientation tensor, it will be necessary to demonstrate the applicability of the higher order closure by evolving the fourth-order orientation tensor for actual injection molding processes.

ACKNOWLEDGEMENTS

The authors are grateful for the financial support of the National Science Foundation (Grant DMI-0327732), the Missouri Research Board, and the Department of Education.

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