O. Incorporating Higher-Order Tensors in the Computation of Polymer Composite Mechanical Properties

Principal Investigator: Douglas E. Smith
University of Missouri at Columbia
E2411 Lafferre Hall / MAE Dept., Columbia, MO 65211
(573) 884-6552; fax: (573) 884-5090; e-mail: smithdoug@missouri.edu

Technology Area Development Manager: Joseph A. Carpenter
(202) 586-1022; fax: (202) 586-1600; e-mail: joseph.carpenter@ee.doe.gov

National Science Foundation (NSF) Monitor: Mary Lynn Realff
(703) 292-7088; fax: (703) 292-9056; email: mlrealff@nsf.gov
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Participants: David A. Jack, University of Missouri at Columbia

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Objective

- Develop a predictive capability that incorporates higher-order orientation tensors to evaluate mechanical properties of short- and long-fiber-reinforced polymer composites.

Approach

- Development of a model for predicting mechanical properties from higher-order orientation tensors derived from flow simulations or measurements that are not limited by the material symmetry requirements imposed by current models.
- Development of an automated three-dimensional voxel-based finite element modeling technique that may be used to predict the effective mechanical properties of short- and long-fiber suspensions.
- Integration of Micro-CT-derived fiber reconstructions to illustrate the applicability of the proposed approach on production hardware to be obtained from industry or DOE.
- Statistical assessment of mechanical property calculations to address sampling issues associated with using the proposed averaging techniques.
- Demonstration of the proposed methodology on an industrially-relevant polymer composite product where flow simulation software is to be provided by Moldflow Corporation.

Accomplishments

- Developed a statistical sampling approach for predicting the variability of short-fiber composite properties from the mechanical properties of the constituent materials and a fiber-orientation distribution function.
- Derived an analytical relationship between mechanical properties and fiber-orientation tensors for statistically independent short fibers.

Future Direction

- Investigate methods for incorporating fiber interaction into the current statistical sampling methodology.
- Develop a voxel-based, three-dimensional, finite element modeling capability for evaluating effective mechanical properties for short- and long-fiber composites.
- Develop an automated procedure for defining three-dimensional finite element models of a representative cell that may be used with analytically-derived, fiber-orientation distribution functions, or fiber-orientation states obtained from Micro-CT measurements.

Introduction

The purpose of this project is to develop a predictive capability that incorporates higher-order orientation tensors to evaluate mechanical properties of short- and long-fiber-reinforced polymer composites. To realize this goal, the project will develop a computational methodology to predict elastic mechanical properties from orientation tensors of second- and fourth-order which are computed during melt-low simulations. The micromechanics of both short- and long-fiber suspension will be simulated with a voxel-based finite element modeling approach, so that the mechanical properties of randomly-oriented fiber samples can be computed. Simulated fiber- orientation states, as well as those obtained from Micro-CT scans, will serve as input. Finally, fiber-orientation states from industrially-relevant products will be evaluated with the new methodology to assess its applicability for complex geometries.

This report provides a brief description of the three-year project and some preliminary results that have been obtained since its start in September, 2005.

Project Deliverables

The primary deliverable of this research will be a relationship between higher-order (i.e., fourth) orientation tensors and the elastic mechanical properties for short- and long-fiber suspensions. An assessment of the variability of mechanical properties among fiber-orientation states will be provided, along with a computational procedure for evaluating the same properties for a specific orientation state. A final report will be generated to communicate the functional form of the mechanical properties and the relevant model parameters for specific examples studied.

Background

Orientation tensors are used extensively to represent the stochastic nature of polymer-composite fiber suspensions in a form that is suitable for large-scale melt-flow simulations. Orientation tensor research over the past two decades has advanced the state-of-the-art related to polymer composites; however, the use of tensors today is still basically the same as it was when these methods were first developed nearly twenty years ago. In addition, the application of orientation tensors to long-fiber composites is nearly non-existent.

The continued advancement of our basic understanding of short- and long-fiber-reinforced polymer composites is critical in numerous industries including consumer products and automotive which rely heavily on the low cost, design flexibility, and superior performance offered by these materials. A major focus of the National Science Foundation/U.S. Department of Energy/American Plastics Council sponsored workshop[1],co-organized by the PI in June 2004, was the need for the U.S. automotive industry to incorporate more fiber-reinforced polymer composites in the design of future vehicles to reduce the weight, emissions, and fuel consumption.

For example, a specific goal of FreedomCAR is to reduce the weight of an automotive structure by 50% for the same cost and durability as seen in today's products. The key to meeting these objectives is a comprehensive predictive engineering approach that is capable of accurately simulating critical attributes associated with the design of both the product and its manufacturing process. To this end, Figure 1 captures the long-standing vision of an integrated

[1] See http://www.missouri.edu/~desy9b/nsf/index.htm for workshop information.

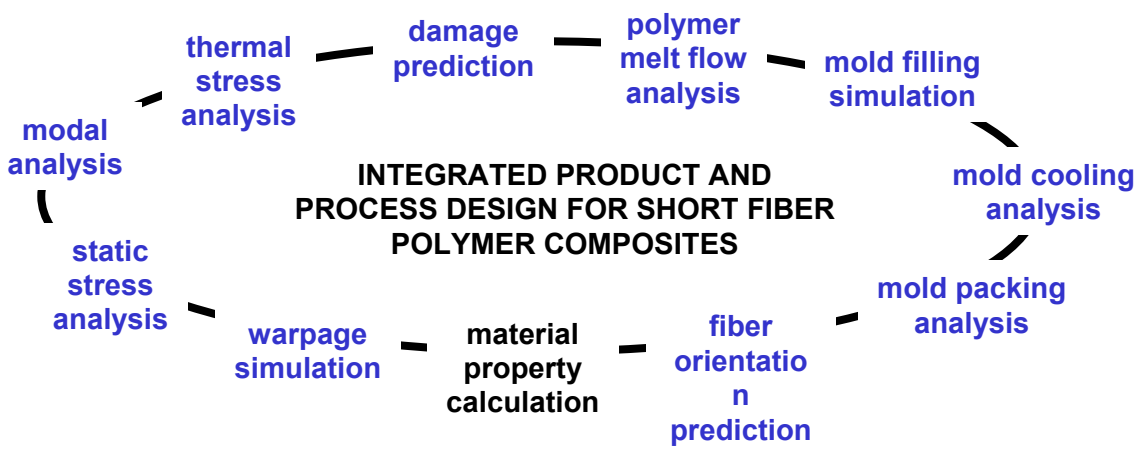

Figure 1. Relationship of product and process attributes in the analysis of short- and long-fiber polymer composites.

product and process design environment for short-fiber reinforced polymer composites. Here, the critical link that connects the computation of materials processing attributes with the prediction of a composite product's performance is the evaluation of structural mechanical properties from melt-flow predictions.

Given the dramatic increases in affordable computing over the past decade, and the anticipated demands on our predictive capabilities for composite materials over the next decade, it is now time to reconsider assumptions that compose today's fiber-orientation models. For example, limiting fiber-orientation predictions to solving for only the second-order orientation tensor components in an effort to reduce computational effort may not be necessary. This project will provide a higher-order approximation to more accurately describe suspension mechanics for complex flow fields such as those where both shear and elongational velocity gradients exist in all three different planes.

Statistical Approach for Computing Mechanical Properties

One task of this research is to develop a statistical approach that may be used to evaluate the variability of mechanical properties of short- and long-fiber composites. Current methods for computing the mechanical properties are limited to short fibers, and provide the deterministic (i.e., averaged) values of properties such as elastic moduli and Poissons ratios. Unfortunately, a finite region within an injection-molded part would be better represented by a statistical sample of the orientation distribution, rather than its mean values. This is particularly important since elastic properties computed by integrating through the thickness of a polymer composite rely on data evaluated over finite sub-regions that may have dimensions on the order of 100 μm.

In our preliminary work, material properties are obtained from the aggregate of unidirectional fibers by computing expected values of the material properties from a known fiber-distribution function. The orientation average, or expectation value, of the material properties of the composite sample is defined for discrete non-correlated fiber distributions as

$$\left\langle C_{ijkl} \right\rangle = \frac{1}{N}\sum_{n=1}^{N}(Q_{pi}(\theta_n,\phi_n)Q_{qj}(\theta_n,\phi_n) \\ Q_{rk}(\theta_n,\phi_n)Q_{sl}(\theta_n,\phi_n)\overline{C}_{pqrs})$$

where N is the number of fibers considered in the sample which is defined by the fiber volume fraction, fiber size, and the volume of a sample of the composite of interest. In this calculation, $\left\langle C_{ijkl} \right\rangle$ is the expectation value of the compliance tensor, $\overline{C}_{pqrs}$ is the underlying unidirectional compliance tensor for a single fiber (computed using the Mori-Tanaka, Halpin-Tsai, or similar inclusion model) and $Q_{ij}(\theta_n,\phi_n)$ is a rotation tensor that transforms

the *n*th fiber into a selected coordinate system. The angles θ and ϕ define the fiber direction as shown in Figure 2. It is important to note that this computation does not account for spatial interactions between individual fibers, and assumes a homogeneous volume fraction, as do other techniques that appear in the literature[2].

The material property expectations are evaluated in this research through Monte Carlo simulations by generating *N* randomly-oriented fibers for a polymer-composite sample. Then, a similar analysis is used to randomly generate multiple samples which are used to compute the mean and variance of the mechanical properties of interest.

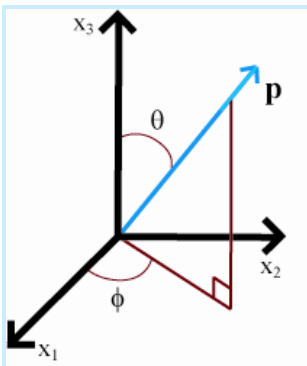

Figure 2. Coordinate system defining fiber direction with the unit vector p(θ,ϕ).

Example Calculations

To illustrate the statistical nature of the mechanical properties of short-fiber composites, we consider the fiber-orientation distribution function

$$\psi(\theta,\phi) = k \sin^n \theta \quad \cos^m \phi$$

where *n* and *m* define the amount of fiber alignment, and *k* is a constant chosen to satisfy the normalization condition. As n and m increase, fibers become more aligned in the x_2-direction in Figure 2. In the first example, we consider a short-fiber sample having a fiber aspect ratio $a_r = 100$ and a volume fraction $V_f = 0.2$. A highly-aligned flow is assumed here with $n = m = 60$ which defines the normalization parameter $k = 61/4\pi$. In this example, the fiber and matrix moduli are 10.5 Mpsi and 0.5 Mpsi, respectively, and the fiber and matrix Poissons ratios are 0.2 and 0.35, respectively. The orthotropic material properties computed for this composite appear in Table 1 where mean property values for the Young's moduli (E_1, E_2, and E_3), Poissons ratio (ν_{12}) and shear moduli (G_{12} and G_{23}) are evaluated. Also shown are results computed by the statistical approach presented here for N = 100,000. Table 1 shows that the mean orthotropic material properties obtained from our statistical approach are nearly identical to results published by Advani and Tucker.

Table 1. Elastic properties evaluated from Advani and Tucker, and by the Monte Carlo sampling approach presented here.

material property	Advani and Tucker properties	expected value from 10^5 fiber simulations
E_1 (Mpsi)	2.220	2.224
E_2 (Mpsi)	0.813	0.814
E_3 (Mpsi)	0.813	0.813
ν_{12}	0.333	0.330
G_{12} (Mpsi)	0.293	0.292
G_{23} (Mpsi)	0.254	0.254

In a second example, our statistical approach is used to evaluate the variability in mechanical properties of a short-fiber composite. Figure 3 illustrates a cube of uniformly-random and aligned fibers sampled from the orientation distribution function given above. A Monte Carlo simulation was performed using 100,000 samples from each distribution and histograms of the resulting elastic moduli and Possions ratio appear in Figure 4.

The effect of volume fraction on material property variability is also evaluated using the Monte Carlo simulation method and statistical evaluation described above. Figure 5 illustrates the coefficient

[2] See e.g., Advani, S. and Tucker, C., 'The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites', *Jn. of Rheology*, Vol. 31, No. 8, pp. 751-784, 1987.

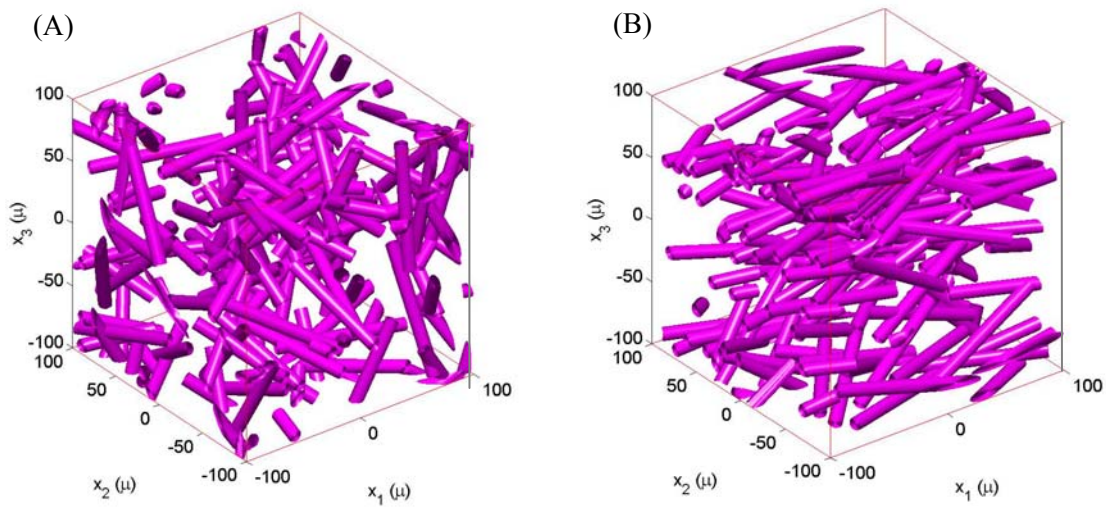

Figure 3. Short-fiber composite samples with $V_f = 0.1$ and $a_r = 10$ for A) a uniformly-random distribution having $k = 1/4\pi$ and $n = m = 0$ and B) a distribution aligned in the x_2 direction with $k = 7/4\pi$ and $n = m = 6$.

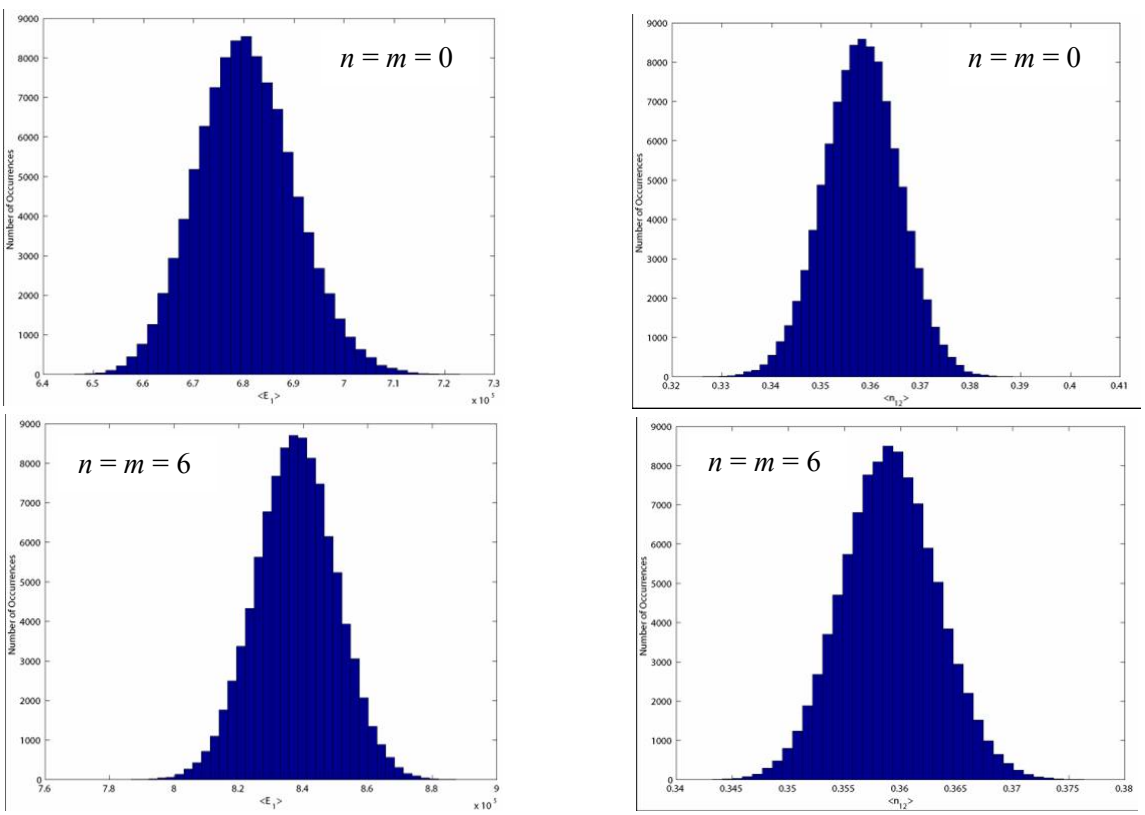

Figure 4. Histograms of selected elastic properties generated from 100,000 samples of fiber-orientation states for uniformly-random and aligned distributions.

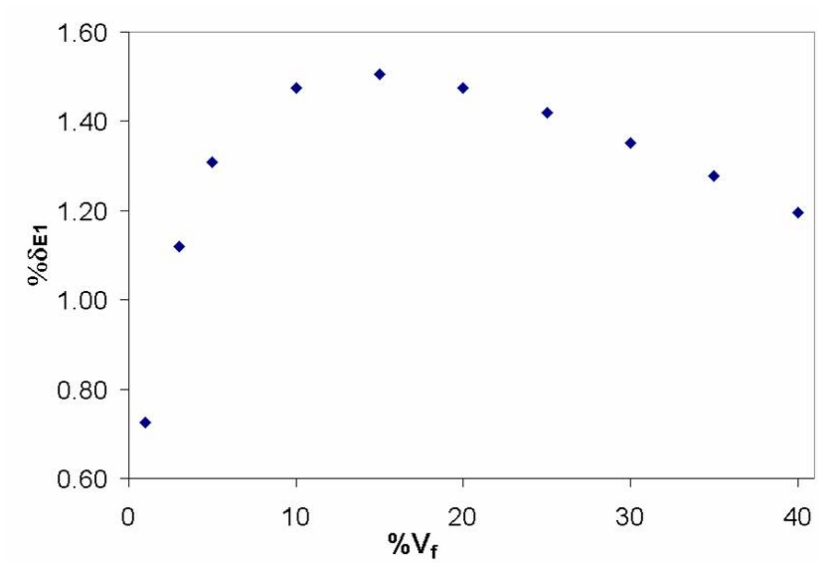

Figure 5. Coefficient of variation as a function of volume fraction for a highly aligned fiber-orientation state ($n = m = 6$).

of variation for the elastic modulus in the x_2 direction defined as

$$\%\delta = \frac{\sigma}{\mu}(100\%)$$

where μ and σ are, respectively, the mean and standard deviation of an elastic property determined through statistical sampling. The results presented here are for the highly-aligned distribution described above. The values illustrated in Figure 5 show that as the volume fraction gets large or small, the decreased influence of orientation reduces δ. It is also seen that δ is a maximum near a volume fraction of approximately 12% for the conditions evaluated here.

Conclusions

This research project focuses on the prediction of elastic mechanical properties from higher-order fiber orientation tensors. As part of this study, computations are being performed to assess the variability in these properties that occurs due to sampling the fiber-orientation distribution function. Preliminary results are presented here for short-fiber composites based on a statistical evaluation of the mechanical property's expected value and Monte Carlo sampling. These results show that both fiber orientation and volume fraction influence property variability

Presentations/Publications/Patents

1. D.A. Jack and D.E. Smith, 'A Statistical Method to Obtain Material Properties from the Orientation Distribution Function for Short-fiber Polymer Composites', IMECE2005-81263, Proceedings of ASME IMECE'05, Orlando, Florida, Nov. 5-11, 2005.