L. Simulation of Injection Molding of Thermoplastics Reinforced with Short and Long Fibers

Principal Investigator: Donald G. Baird
Virginia Polytechnic Institute and State University
Department of Chemical Engineering
Blacksburg, VA 24061
(540) 231-5998, fax: (540) 231-2732, email: dbaird@vt.edu

Co-Principal Investigator: Peter Wapperom
Virginia Polytechnic Institute and State University
Department of Mathematics
Blacksburg, VA 24061
(540) 231-7252, email: pwappero@vt.edu

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

Participants
Aaron P. R. Eberle, Ph.D. student, email: eberle@vt.edu
Gregorio Velez, PhD. student, email: gvelez@vt.edu

Contractor: Virginia Polytechnic Institute and State University
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Objective

- Improve predictions of fiber orientation in thermoplastics during injection and compression molding by:
  - Using a theory that couples fiber orientation with flow (Doi Theory).
  - Incorporating the effects of viscoelasticity and the frontal flow region (which is dominated by extensional flow) in the calculations.
- Define and evaluate rheological tests to determine the material parameters for the constitutive relation.
- Evaluate predicted orientation distribution by comparing results to glass-fiber orientation found in an injection-molded part (end and center-gated parts).

Approach

- Conduct transient rheological tests (stress growth/relaxation) on glass-fiber-filled polypropylene systems in which fibers of various length (from 11 mm to 0.5 mm) are used.
- Demonstrate the feasibility of extending Doi's Theory for rigid-rod molecules to the glass-fiber-filled polypropylenes by comparing the transient rheology to that predicted by the theory.
- Fit the model to the transient rheological results to obtain empirical constants for the theory.
- Use the finite element method (FEM) to simulate the flow in three basic mold geometries (tubular element, planar element, center-gated disk).
- Injection mold samples of varying fiber length and matrix viscosity, and quantify fiber orientation.
- Compare model predictions for fiber orientation to that of experimental findings.

Accomplishments

- Rheological characterization and stress growth/relaxation tests were performed on glass-filled polypropylenes containing fibers of various lengths in order to establish a methodology for determining model rheological parameters.
- Model predictions for stress growth/relaxation were performed, and parameter effects on model predictions were investigated.
- The development of a finite element code for simulating Hele-Shaw flow was initiated.
- Two presentations were given, one at the Society of Rheology meeting in Vancouver, BC, Oct. 2005, the other at the annual American Institute of Chemical Engineers (AIChE) meeting in Cincinnati, OH, Nov. 2005.

Future Direction

- Validate transient rheology by comparing data found with parallel-plate rheometer to that of sliding-plate rheometer.
- Fit Doi Model to transient stress growth/relaxation data.
- Develop a unique method for determining model parameters.
- Finish phase one of the FEM model.
- Begin injection molding parts using glass-fiber-filled systems.

Introduction

The purpose of this project is to improve the predictions of fiber orientation during processing of thermoplastics and, hence, the ability to predict stiffness and part dimensional stability. The improvements will be accomplished by using constitutive relations which contain the micro-structural aspects of the reinforced melts and viscoelastic effects.

Glass-Fiber-Filled Polypropylene Rheology

Two fiber-filled polypropylene samples have been used in this work. The first sample is a glass-fiber-filled polypropylene pellet that is formed by pultrusion and then cut into 2.75 mm, 5.5 mm and 11 mm fiber-length samples allowing for the evaluation of fiber length on rheology. The other sample is a glass-fiber-filled polypropylene that has been processed (extruded) and pelletized with an average fiber length of 1 mm. The two samples have a different matrix viscosity.

Rheological testing in the low shear-rate region (0.1-100 s^{-1}) is performed with a Rheometrics Mechanical Spectrometer (RMS-800) fitted with parallel-plate geometry, which allows for gap control. A Göttfert Rheograph 2001 capillary rheometer is used for high shear-rate data (10-2000 s^{-1}). As seen in Figure 1, at low shear rates (.1-10 s^{-1}) there is an obvious increase in the magnitude of stress with increasing fiber length; but at high shear rates the magnitude of the stress for varying fiber length converges to that of the matrix values.

An analysis of the storage modulus (G') of different fiber-filled systems compared to that of the matrix material suggests that the fiber has a dramatic effect on the viscoelasticity of the systems, i.e., relaxation time spectrum. Also, the fiber length is a factor in the relaxation time spectrum as seen in Figure 2.

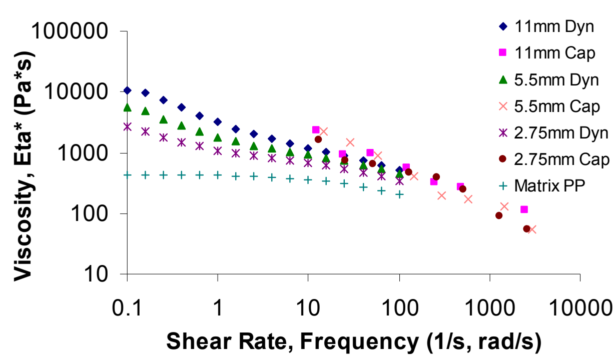

Figure 1. Dynamic and shear viscosity vs. shear rate, frequency for varying fiber length systems, and matrix.

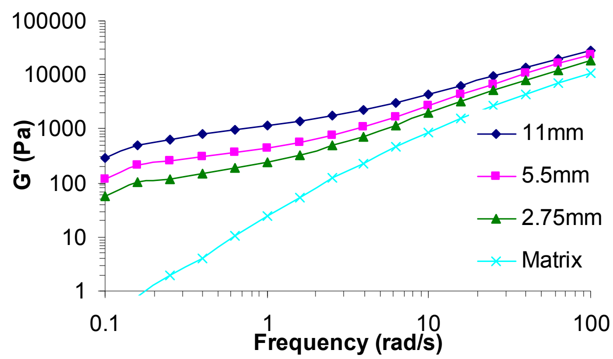

Figure 2. Effect of fiber length on G', compared to matrix viscosity.

Stress growth/relaxation experiments have been performed on all samples. It is found that initial fiber orientation has a large effect on the magnitude of stress overshoot. It is believed that fitting this transient response along with the time for the stresses to relax out of the sample will allow for consistent determination of unique model parameters.

Model: Doi Theory

For this project a constitutive equation is used that couples orientation and flow rather than decouple these events. Doi's Theory was developed for rigid-rod molecules in a solution, and we propose to extend this theory to glass-fiber-filled polypropylene. The model contains two material parameters, ν_1 (constant on the order of unity) and D_r (rotational diffusivity), for which theory gives some methods for calculation. However, when the constants are calculated using this theory, results are unreasonable. This is attributed to the many assumptions made in the development of the theory and the translation from a molecule-solvent system to a fiber-polymer system. For this reason, the material parameters and certain constants have been lumped into three empirical constants for use in fitting the model to transient stress growth/relaxation data. By adjusting these parameters we have found that the Doi theory can predict many of the same transient stress growth/relaxation trends that are found in the fiber-filled systems, i.e., stress growth overshoot, and residual stress in stress relaxation. Though the model can predict stress overshoot, it is still unclear whether the model can predict the magnitude of the overshoot or breadth of time that has been observed for the overshoot to relax to a steady-state stress.

Model: Parameters

A key aspect of this project is determining the material parameters associated with the model. Unique acquisition of these parameters is essential for the accuracy of final results. This is to be accomplished by transient stress growth/relaxation tests on the fiber-filled composites while controlling the initial fiber orientations (initial conditions) in the sample. Evaluation of the model's ability to predict the transient behavior can then be done, and by comparing different initial condition results to model predictions while adjusting the parameters, unique results can be accomplished.

Model: Predicting Fiber Orientation using Finite Element Method (FEM)

Development of a FEM model is a key step to the final goal of increasing the accuracy of predicting fiber orientation in an injection-molded part. The FEM model will be developed and implemented in two phases. In the first phase, the model will be developed for simple pressure-driven flow using the Hele-Shaw approximation, which treats the flow as being dominated by shear flow for the three different die geometries. In the second phase, the code will be adapted to incorporate the kinematics of the flow at the frontal region which has been shown to be dominated by extensional flow (which will play a major role in controlling fiber orientation on the part surface). It is also noted that the quadratic decoupling approximation in Doi's theory will be modified to a Bingham approximation for the frontal flow region.

Conclusions

Although we are in the initial stages of this research project, we have covered a lot of preliminary ground. Rheological classification and transient stress growth/relaxation data for two different glass-fiber-filled systems have been completed. Preliminary model predictions of stress growth/relaxation have shown that Doi's theory simulates many of the interesting phenomena of fiber-filled systems such as stress growth overshoot and stress relaxation which is associated with residual stresses.

Presentations

1. A. P.R. Eberle, D.G. Baird, and P. Wapperom, "Transient Rheology of a Polypropylene Melt Reinforced with Long and Short Glass Fibers," 77th Annual Meeting of The Society of Rheology, October 16-20, 2005, Vancouver, BC, Canada (2005).
2. A. P.R. Eberle, D.G. Baird, and P. Wapperom, "Transient Rheology of a Polypropylene Melt Reinforced with Long and Short Glass Fibers," AIChE Annual Meeting, October 30-November 4, 2005, Cincinnati, OH (2005).