Engineering Property Prediction Tools for Tailored Polymer Composite Structures

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2012 DOE Annual Merit Review
May 17, 2012

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PROJECT OVERVIEW

Timeline

Phase 1 - Feasibility
  Start  August 2005
  End    March 2006

Phase 2 – 2D Structures
  Start  April 2006
  End    September 2011

Barriers

- Barriers addressed
  - Existing modeling tools cannot predict LFT processing and molding behavior accurately, resulting in non-optimal design, processing, mold design and component over design.
  - Significant cost barrier due to mold retooling.
  - Weight savings limited due to part over design.

Partners

- The University of Illinois-Urbana Champaign (by PNNL subcontract)
- Autodesk®, Inc. (by PNNL CRADA)
- American Chemistry Council – Plastics Division & Member Companies (Cost Share)
- OEMs Through Automotive Composites Consortium (Cost Share)

FY11 Budget & Expenses

FY 2011 (PNNL): $40,000
  PNNL Expense: $136,144

FY 2011 (ORNL): $0
  ORNL Expense: $101,812
Outline

- Project Objective and Goals
  - Objective, gap and project status
  - Technical relevance
- LFT Microstructural Aspects
  - Difference between long and short fiber thermoplastics
- Results and Discussion
  - Process-property prediction
  - Validation – 15% match with experimental results
  - Collaborations
  - Proposed future work
- Summary
  - Accomplishments and gaps
- Key Publications
Objectives

Develop Predictive Tools to enable the optimum design of lightweight automotive structures using injection-molded long-fiber thermoplastics

Technology Gap: Existing modeling tools cannot predict LFT processing and molding behavior accurately, resulting in non-optimal design, processing, mold design and component over design

Approach: Knowing the initial fiber length, concentration and other input parameters going into the mold

1. Be able to first predict the final fiber orientation and length distributions in the injection-molded part by process modeling
2. Then use predicted fiber orientation and lengths to predict the mechanical properties in any given location and in any direction.
3. Then use that in a feedback loop to allow for mold design and control of input parameters to obtain properties where desired.

Phase 1 – Feasibility
Phase 2 – Two dimension part (plaques)
Phase 1 – Feasibility assessment  
(09/01/2005 to 03/31/2006)

Phase 2a – Development of new models and experimental methods  
(04/01/2006 to 09/30/2009)

Phase 2b – Validation on large plaques  
(10/01/2009 to 9/30/2011)

Project brings together:
PNNL, ORNL, University of Illinois, Autodesk, Inc., American Chemistry Council – Plastics Division, OEM participants, and material suppliers (SABIC-IP, Ticona, DuPont™, DOW, etc.)
Current automobiles contain 330 lb. of polymer and polymer composites per vehicle and injection molded thermoplastics comprise significant percentage of the per-vehicle total of polymers and polymer composites.

Injection molding is cost-effective – parts with complex geometry can be made:

Inject ---> Demold ---> Part

LFT automotive use by applications:
- Front End Modules (17%)  
- Instrument Panel Carriers (16%)
- Underbody Shields (13%)  
- Door Modules (8%)

Existing modeling tools cannot predict LFT processing, molding behavior and properties accurately, resulting in over design.

New process and property prediction models have been developed using data from six molding trials (Delphi, RTP, DuPont, SABIC-IP, GM, and Injection Technologies).
Injection-molded LFTs possess a complex microstructure characterized by spatial variations of fiber orientation, length and entanglement. Skin/shell/core orientation layer structure in LFTs:

Skin

Shell

Core

Tangled network of fibers in LFTs

Injection-molded SFT (short fiber 0-3mm)

Injection-molded LFT (long fiber 3+)

LFTs possess larger cores and thinner shell layers.

Fiber Orientation Tensor Component in the Flow Direction

Normalized Thickness

shell core shell

Normalized Thickness

Normalized Thickness
An Integrated Approach Linking Process to Structural Modeling with Experimental Verifications

LFTs for structural and semi-structural applications

Creation of a composite part through simulations

Process simulations using
- A new fiber orientation model
- A fiber length attrition model

Prediction of the composite microstructure

Model performs homogenization (EMTA):
- Elastic properties
- Coefficients of thermal expansion

Model is implemented in ABAQUS (EMTA-NLA):
- Elastic-plastic analysis and strength prediction
- Creep analysis
- Damage and fatigue damage analyses
- Impact analysis

Microstructural characterizations
- Fiber length distribution
- Fiber orientation distribution
- Fiber dispersion
- Fiber/matrix debonding and other microdefects

Mechanical testing
- Quasi-static and fatigue tests
- Creep and impact tests

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EXPERIMENTS (ORNL)

Provide data to validate models

Map fiber length and orientation results into Modeling

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- Impact analysis
Accomplishments: Process to Property Prediction

Moldflow® process modeling to predict fiber orientation and length distribution.

EMTA-NLA maps Moldflow results to ABAQUS®.

Predicted fiber orientation and length distributions compared with measurements.

Predicted stress-strain responses up to failure compared well with experiments.

Flow-direction results and Cross-flow direction results.
**Accomplishments: Model Validation for ACC Plaques**

**Metrics:** Predictions of fiber orientation and length distributions are within 15% of experimental measurements

- Performed with one set of material parameters (no modification for gating, fill speed etc.)
- Validated for all eight molding conditions of ACC molding trial
- Three locations at each plaque (near gate, mid-flow, and end-of-flow)

![Global flow, orientation & fiber length prediction in the part](Image)

![Local comparison of predictions (solid line) with experiments (dashed line)](Image)

- Average mismatch of 7.7% for fiber orientation
- Fiber orientation match within 15% target for 21/24 cases
- Fiber length match within 15% target for 15/24 cases
EMTA-NLA maps Moldflow results to ABAQUS

Predicted crack

Specimens cut from slow-fill glass/PP center-gated plaque

Specimens cut from slow-fill glass/PP center-gated plaques

Accomplishments: Model Validation for ACC Plaques

<table>
<thead>
<tr>
<th>Properties</th>
<th>ABAQUS/EMTA-NLA Predictions (MPa)</th>
<th>Experiments (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow-direction Modulus</td>
<td>8431 (2%)</td>
<td>8598</td>
</tr>
<tr>
<td>Cross-flow direction Modulus</td>
<td>6156 (4%)</td>
<td>5921</td>
</tr>
<tr>
<td>Flow-direction Strength</td>
<td>87.9 (9.7%)</td>
<td>80.2</td>
</tr>
<tr>
<td>Cross-flow direction Strength</td>
<td>53.3 (10.8%)</td>
<td>59.7</td>
</tr>
</tbody>
</table>

Materials

LM0

68
Partners:

- University of Illinois at Urbana-Champaign subcontracted by PNNL (Prof. CL Tucker III) developed fiber orientation and length models for LFTs – provided consultant services to PNNL

- Autodesk, Inc. had CRADAs with PNNL to implement new process models for LFTs in Autodesk® Moldflow® Insight research versions and delivered these versions to PNNL for testing and validation – performed rheological measurements for LFTs for the project

- American Chemistry Council – Plastics Division and their members provided pellet materials for molding trials - consultant services and project reviews

- OEMs through the Automotive Composite Consortium provided molding trials, consultant services, and project reviews

Technology transfer:

- Results were transferred through model implementations in finite element packages (Autodesk® Moldflow® Insight and ABAQUS®) and through journal and conferences articles publications, and reports
Consider a three-dimensional (3-D) complex LFT part possessing 3-D features representative of real-world automotive structures using LFTs.

- Validate new process models for fiber orientation and length distributions for the complex part.

- Validate the basic property prediction models (stiffness, local stress-strain responses, damage accumulations) for the complex part.
Summary of Accomplishments and Gaps

Key accomplishments to date:

- Developed a fiber orientation model
- Developed a fiber attrition model for fiber length distribution in mold
- Fiber orientation and length models implemented in Moldflow research versions
- Developed models for predicting thermoelastic properties, elastic-plastic, damage, and creep behavior
- Integrated Moldflow’s process modeling to ABAQUS
- Developed characterization tools for determining microstructural features (fiber orientation & length distributions, etc.)
- Developed of LFT property database, including linear and non-linear properties
- Developed novel testing methods to determine fiber location, size and orientation
- Validated against 6 molding trials

Gaps:

- Tools are yet to be validated on complex 3-dimensional parts
- Molders are continually challenged to produce parts with long fibers
- 3-D Moldflow model requires additional work for refinement