Engineering Property Prediction Tools for Tailored Polymer Composite Structures

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Pacific Northwest National Laboratory
Oak Ridge National Laboratory

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Project ID #LM068

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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 Consoritum (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)

Project Status

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.)

Technical Relevance

- 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

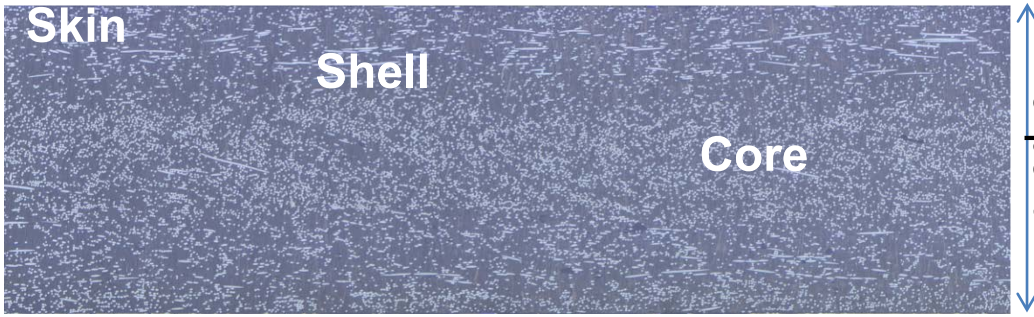
- LFT automotive use by applications:
  - Front End Modules (17%)   Instrument Panel Carriers (16%)
  - Underbody Shields (13%)   Door Modules (8%)

- 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)

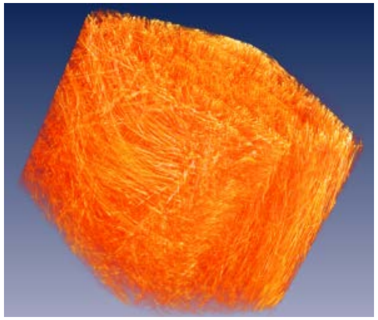
Long Fiber Thermoplastics (LFT) Microstructure

- Injection-molded LFTs possess a complex microstructure characterized by spatial variations of fiber orientation, length and entanglement

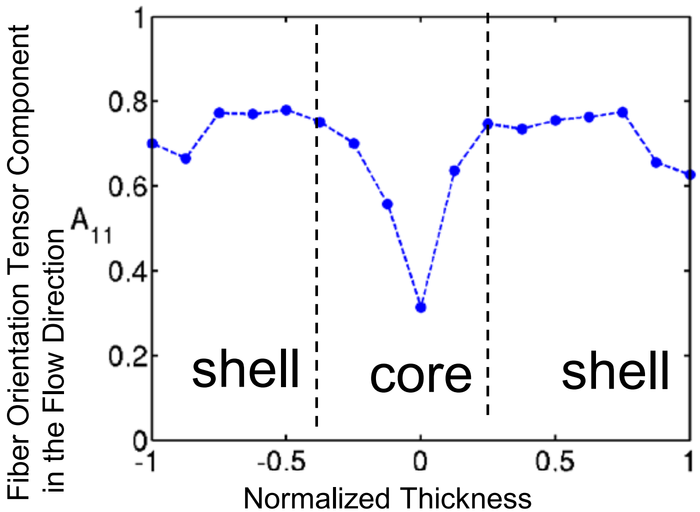


Skin/shell/core orientation layer structure in LFTs

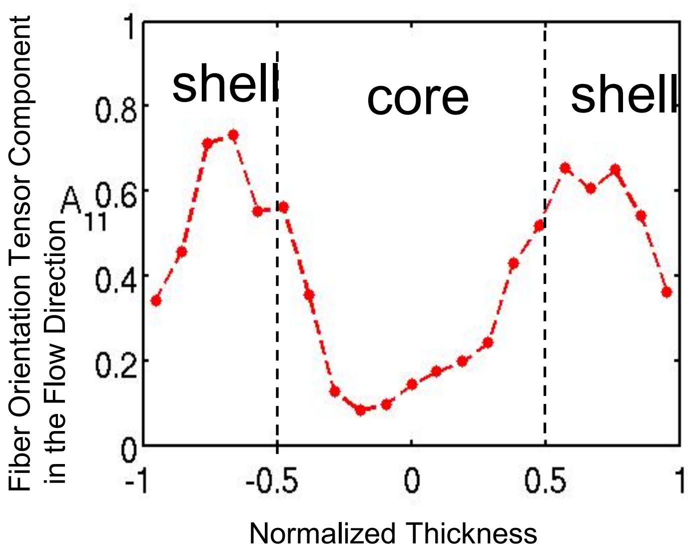
Tangled network of fibers in LFTs



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



Injection-molded LFT (long fiber 3+)



LFTs possess <u>larger cores</u> and <u>thinner shell</u> layers

An Integrated Approach Linking Process to Structural Modeling with Experimental Verifications

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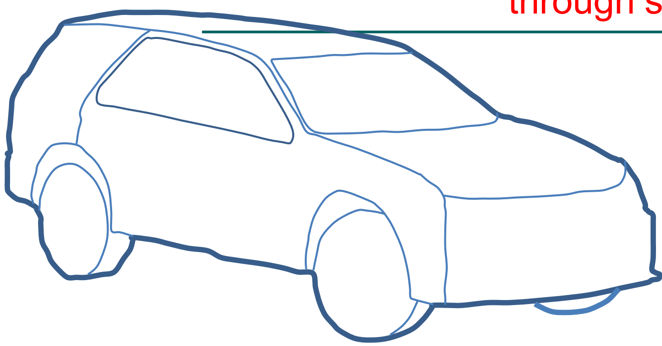
Creation of a composite part through simulations



LFTs for structural and semi-structural applications

Univ. Illinois/PNNL/Autodesk

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

Prediction of the composite microstructure

Map fiber length and orientation results into Modeling

Provide data to validate models

EXPERIMENTS (ORNL)

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*

Modeling (PNNL)

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*

Accomplishments: Process to Property Prediction

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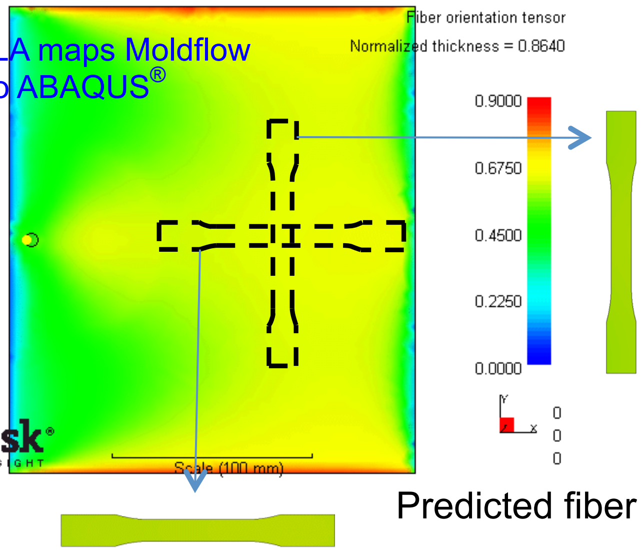
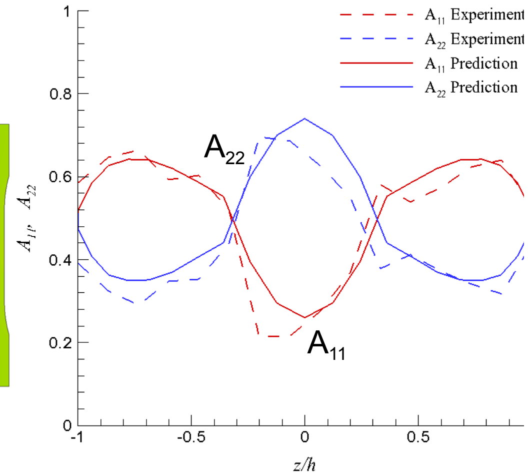
Moldflow® process modeling to predict fiber orientation and length distribution

EMTA-NLA maps Moldflow results to ABAQUS®

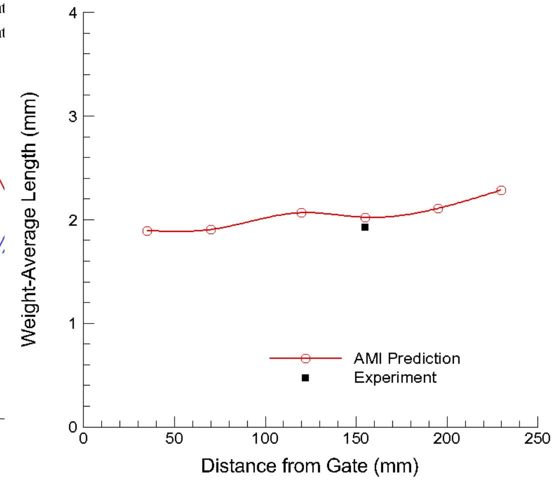


Autodesk® MOLDFLOW® INSIGHT

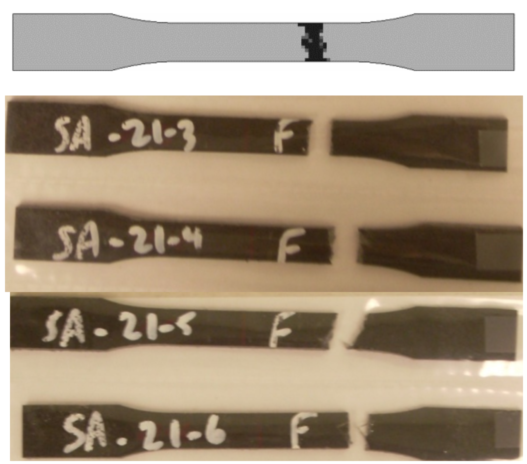
Fiber orientation distribution



Fiber length distribution

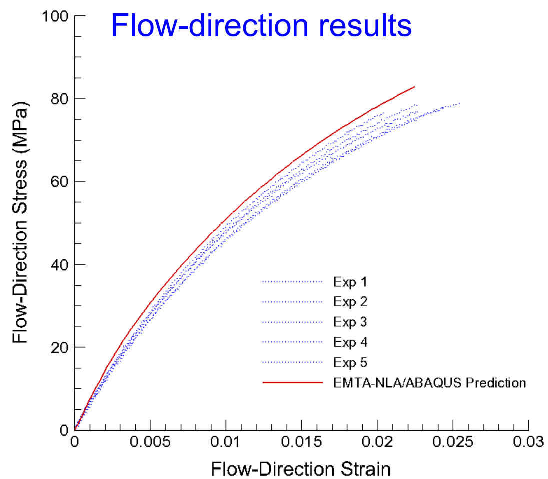


Predicted fiber orientation and length distributions compared with measurements

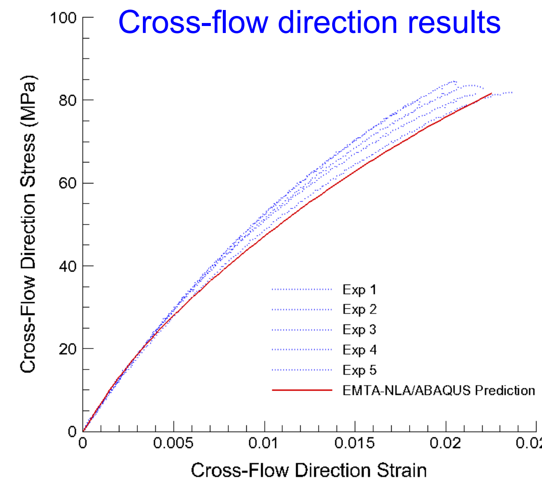


Predicted failure locations agree with experimental observations

Flow-direction results



Cross-flow direction results



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

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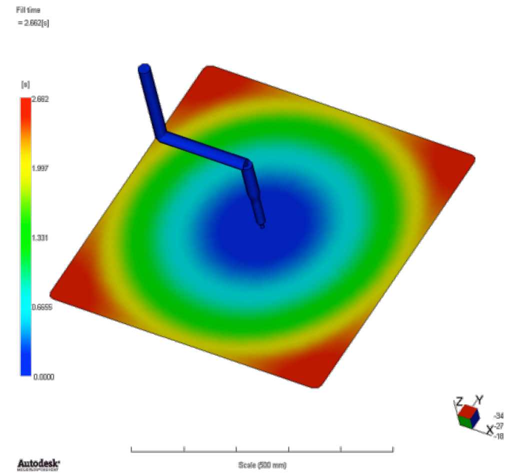
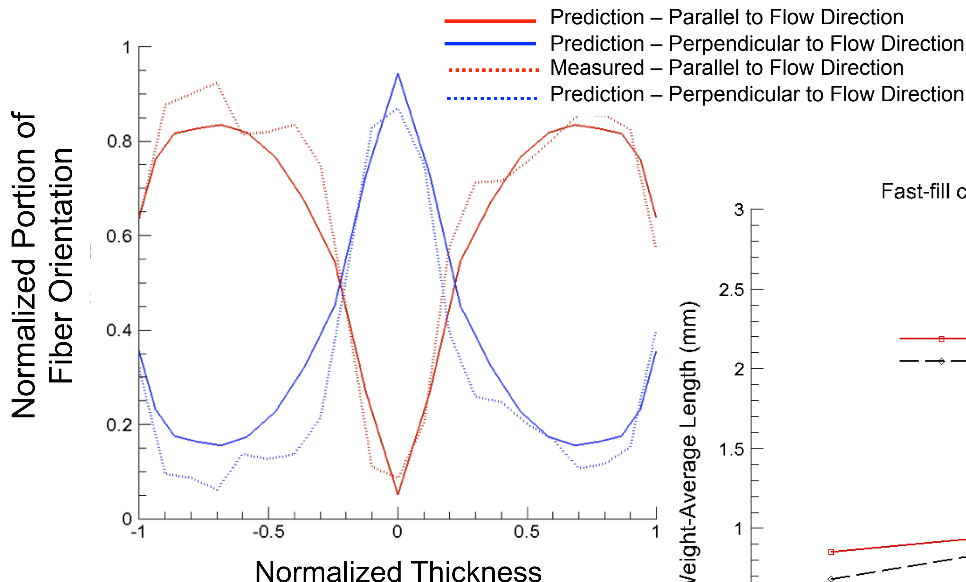
Accomplishments: Model Validation for ACC Plaques

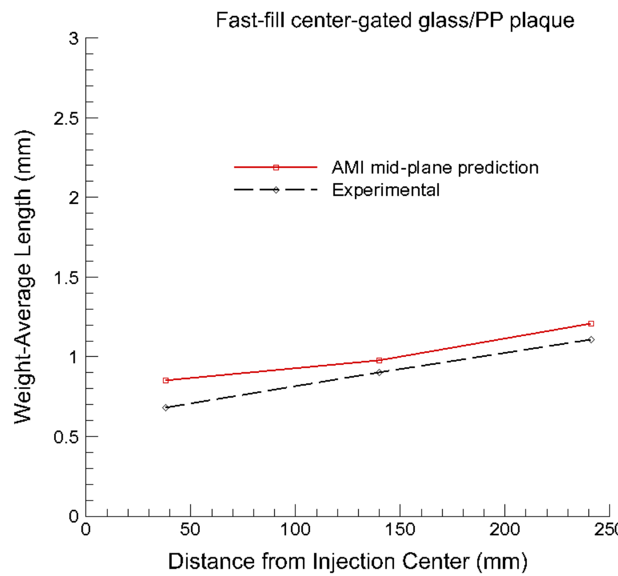
- **Metrics:** Predictions of fiber orientation and length distributions are within <u>15%</u> of experimental measurements
  - Performed with one set of material parameters (no modification for gating, fill speed etc.)
  - Validated for all eight molding conditions of ACC molding trial
  - Three locations at each plaque (near gate, mid-flow, and end-of-flow)



Global flow, orientation & fiber length prediction in the part

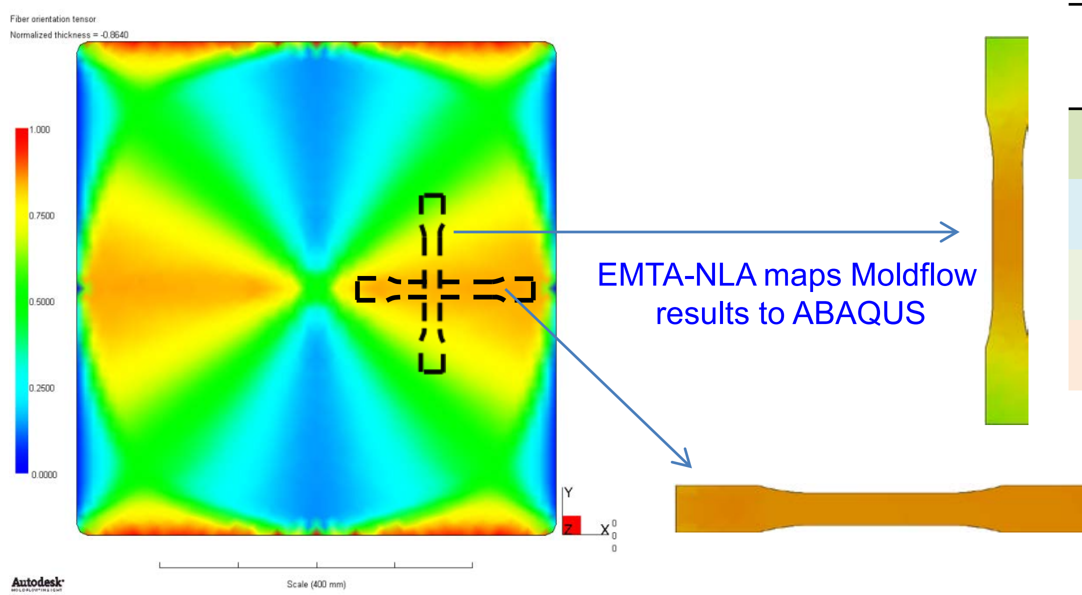
Local comparison of predictions (solid line) with experiments (dashed line)



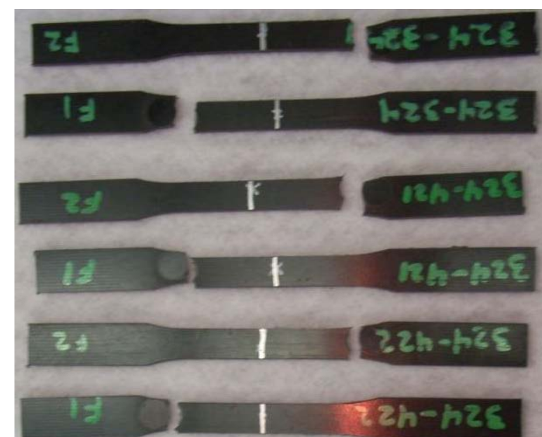


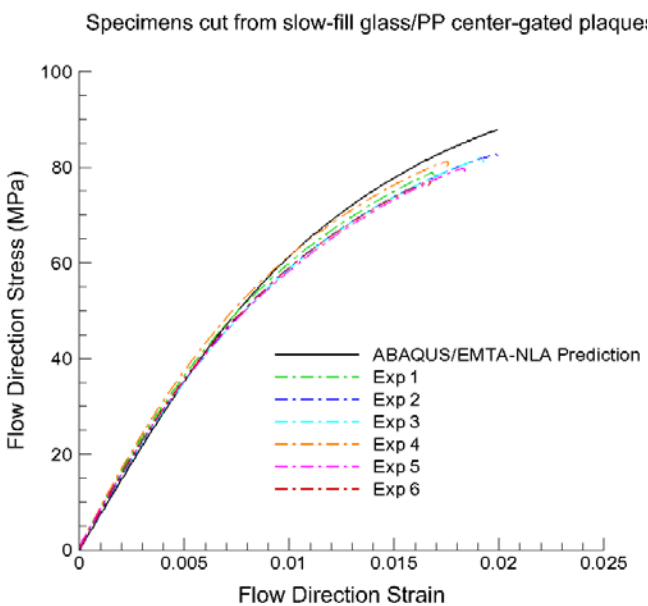
- Average mismatch of <u>7.7%</u> for fiber orientation
- Fiber orientation match within <u>15% target</u> for 21/24 cases
- Fiber length match within <u>15% target</u> for 15/24 cases

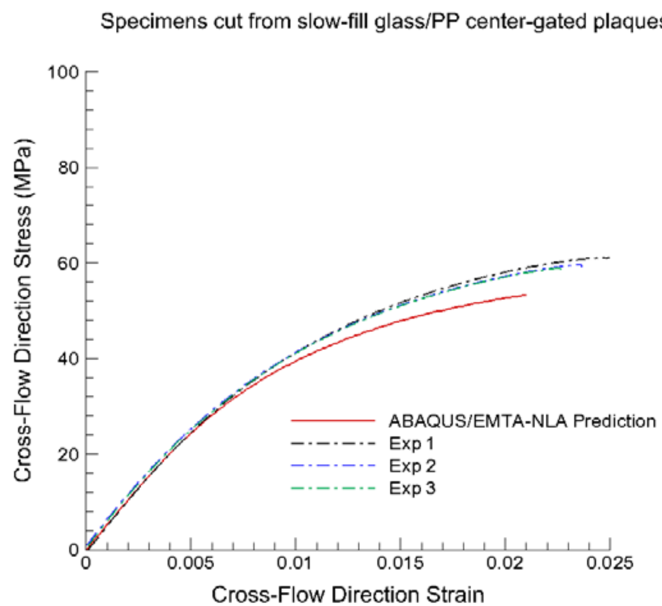
Accomplishments: Model Validation for ACC Plaques



Properties	ABAQUS/EMTA-NLA Predictions (MPa)	Experiments (MPa)
Flow-direction Modulus	8431 (2%)	8598
Cross-flow direction Modulus	6156 (4%)	5921
Flow-direction Strength	87.9 (9.7%)	80.2
Cross-flow direction Strength	53.3 (10.8%)	59.7







Collaborations

- **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

Proposed Future Work

- 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