Property Prediction Tools for Tailored Polymer Composite Structures

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Pacific Northwest National Laboratory

Oak Ridge National Laboratory

- **CRADA between PNNL and Moldflow Corporation**
- **Subcontract: University of Illinois at Urbana-Champaign**
- **NSF-DOE participants: Virginia Tech, University of Missouri, University of South Carolina, Northwestern University, University of Delaware, University of Massachusetts-Lowell**

This presentation does not contain any proprietary or confidential information

Outline

- Purpose of work
- Barriers
- Approach
- Performance measures
- Technical accomplishments
- Technology Transfer
- Future work
- Summary
- Publications

Purpose of Work

Objective

- **Enable the optimum design of lightweight automotive structural components using long-fiber reinforced injection molded thermoplastics (LFTs)**

Goals and Scopes

- **Develop an integrated approach that links process to structural modeling allowing the optimum design of LFT composite structures**
  - ✓ FY05-FY06: Completed technical feasibility assessment
  - ✓ FY06: Developed thermoelastic property prediction models accounting for LFT microstructure (fiber orientation/length distributions, initial debonding)
  - ✓ FY07: Developed a fiber orientation model for LFTs – Developed an elastic-plastic and strength prediction model for LFTs
- **Develop experimental methodologies for material characterization and testing to establish material property and performance databases and to verify modeling predictions**
  - ✓ FY05-FY06: Completed assessment of characterization techniques
  - ✓ FY06: Developed fiber length measurement technique and validated Leeds fiber orientation technique for LFTs
  - ✓ FY07: Developed coupled mechanical testing and micro-tomography apparatus to observe damage processes within LFTs

Barriers

Vehicle Technology Barriers

- Confidence in applicability of existing predictive models for LFTs
- Confidence in ability to predict long-term performance and behavior of LFT parts
- Cost of design and processing of LFT materials for automotive applications
- Cost of tooling and tooling modifications

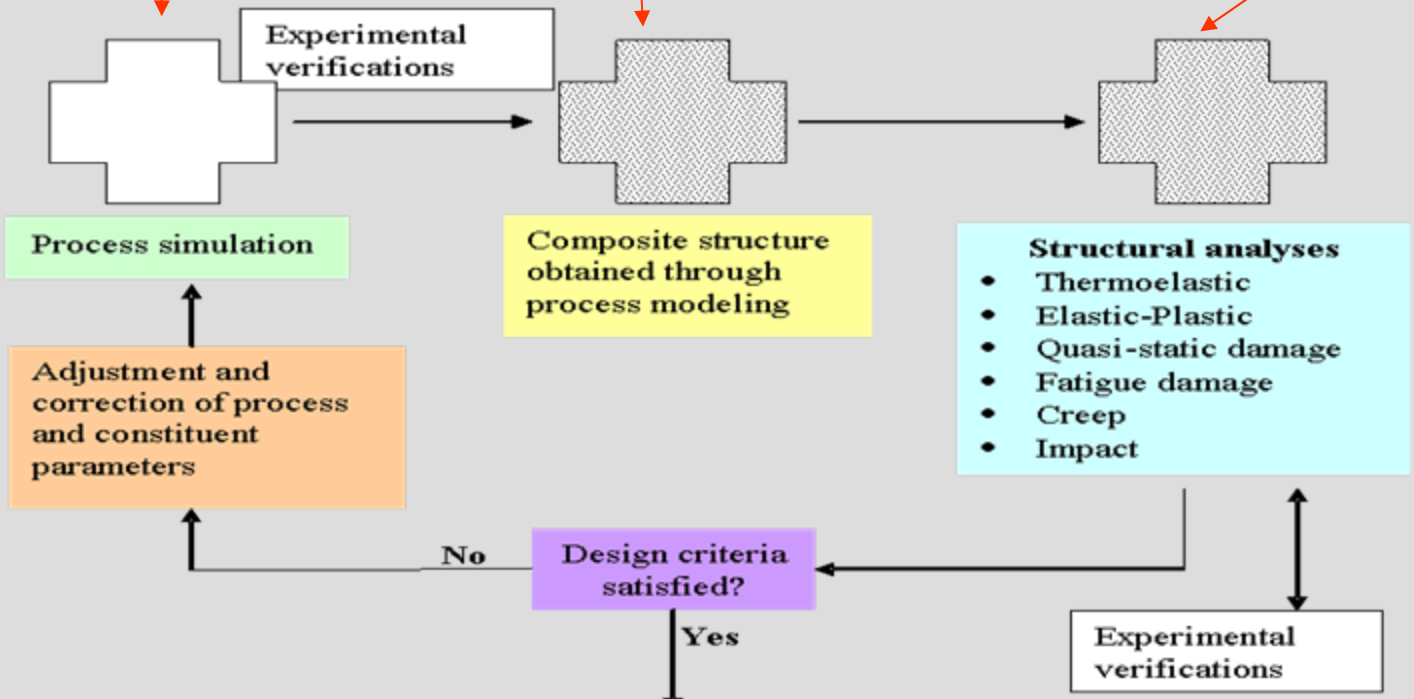
Technical Barriers

- Inadequate process models for LFTs
- Lack of property prediction models for LFTs
- Lack of interface between process models and property prediction models
- Inadequate characterization methods and tools
- Insufficient understanding of differences from short fiber reinforced thermoplastics
- Limited understanding of factors influencing durability of LFTs

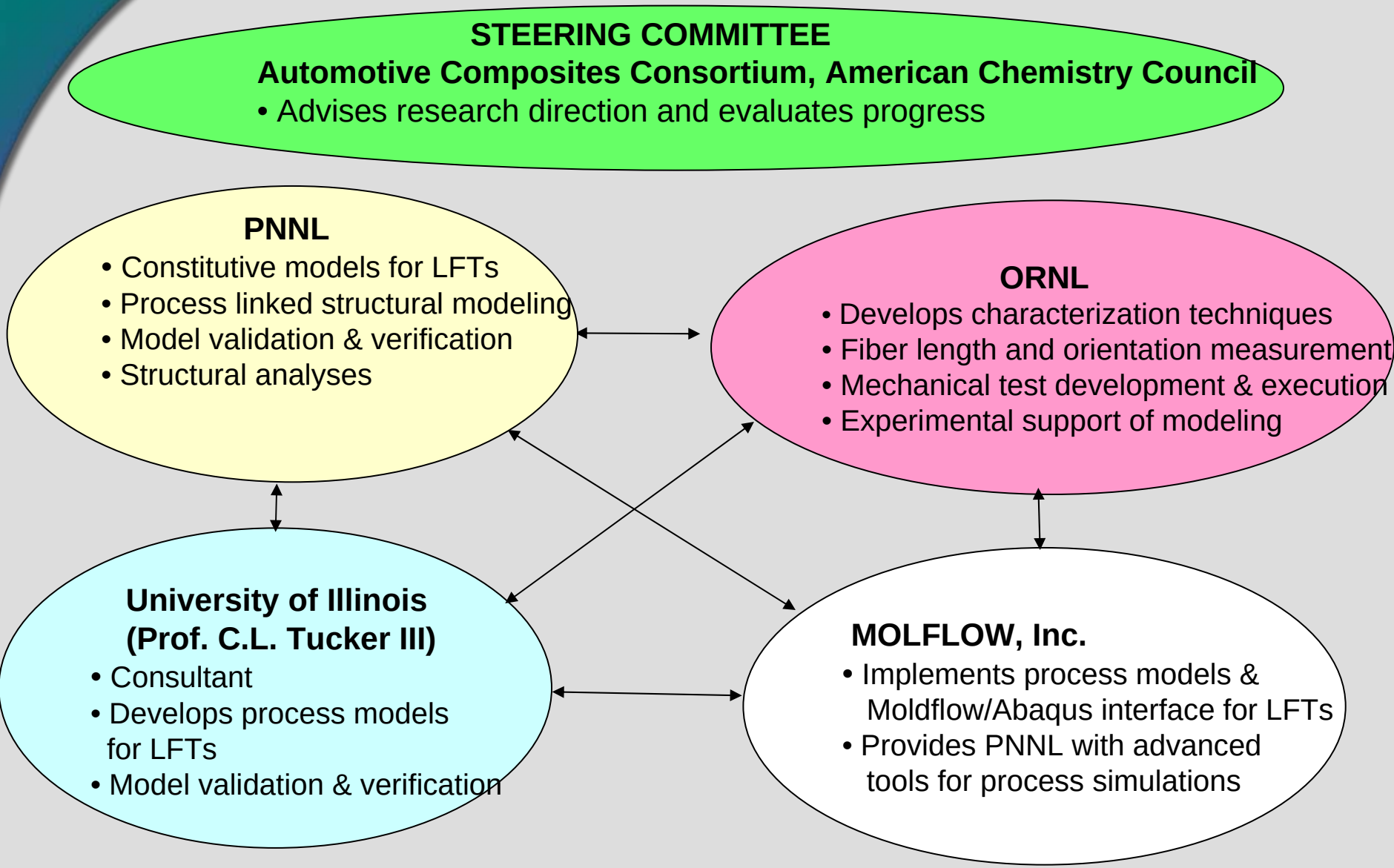
Approach: Integrated Approach Linking Process to Structural Modeling

- **PNNL**: Molded materials, process modeling
- **ORNL**: Fiber orientation & length distribution measurements
- **Univ. Illinois**: Process modeling, models for LFTs
- **Modflow**: Rheological & physical data

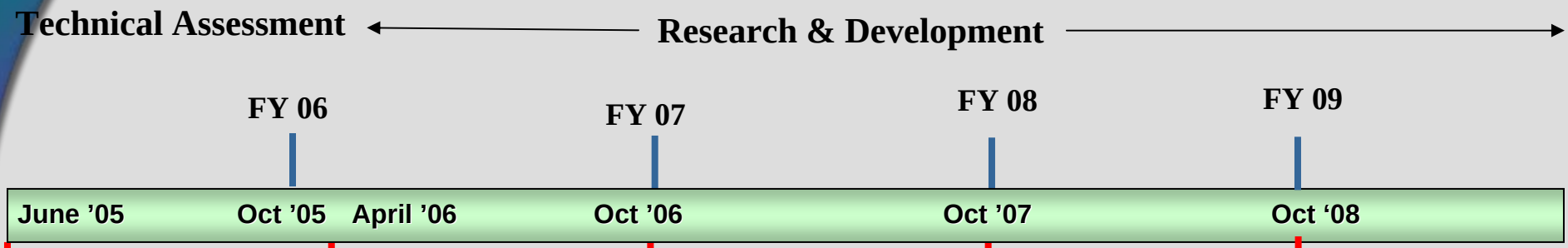
- **PNNL**: Develops and implements constitutive models for LFTs in Abaqus, Moldflow/Abaqus Interface
- **ORNL**: Mechanical testing & microstructural characterization
- **Moldflow**: Implements process models for LFTs in Moldflow, Moldflow/Abaqus interface



Approach: Project Participants' Roles



Performance Measures - Project's Timelines



June '05 – Oct '05

1. Evaluate Characterization techniques for LFTs (fiber morphology, orientation, etc.)
2. Assessment of process models
3. Comparative evaluation of molding behavior of glass and carbon

Oct '05 – April '06

1. Develop material-process matrix
2. Develop process models for LFTs
3. Develop constitutive models for LFTs (thermoelastic property)
4. Develop LFT characterization techniques
5. Experimental LFT characterization

April '06 – Oct '06

1. Develop a fiber orientation for LFTs
2. Develop constitutive models for LFTs (elastic-plastic & strength)
3. Develop LFT characterization techniques
4. Experimental characterization & mechanical testing

Oct '06 – Oct '07

1. Develop a fiber breakage model for LFTs
2. Develop constitutive models for LFTs (creep and damage)
3. Complete LFT characterization techniques
4. Experimental characterization & mechanical testing

Oct '07 – Oct '08

1. Implement LFT process models in Moldflow
2. Complete constitutive models for LFTs (fatigue & impact)
3. Experimental characterization & mechanical testing
4. Demonstrate integrated tools

Performance Measures - Completed Milestones

- **June 2005 to March 2006 Completed Milestones**
  - First injection-molding trials to produce LFT samples
  - Complete technical assessment of existing process models applied to injection-molded LFT materials
  - Complete technical assessment of characterization methods for LFT microstructures
- **FY 2006 Completed Milestones**
  - Complete thermoelastic property prediction for LFTs
  - Determine effect of fiber curvature on elastic properties
  - Validate the Leeds method for fiber orientation measurement for LFTs
  - Develop a method for fiber length measurement
  - Measure fiber length and orientation in LFT samples
- **FY 2007 Completed Milestones**
  - Develop an anisotropic rotary diffusion (ARD) model for fiber orientation in LFTs
  - Develop and implement in ABAQUS an elastic-plastic model for LFTs and predict strength of LFTs
  - Establish a CRADA with Moldflow
  - Develop an X-ray tomography unit to identify microstructural evolution of damage

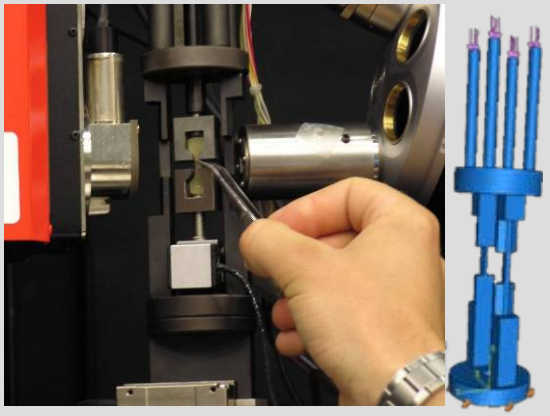
Technical Accomplishments

- **PNNL**
  - Material preparation and molding trials
  - Complete technical assessment of process models for short- & long-fiber systems
  - Micromechanical models to predict elastic properties and CTEs for LFTs (**code EMTA**). These models account for fiber length and orientation distributions
  - Constitutive model to predict the strength and elastic-plastic response of LFTs
  - Implement constitutive models into ABAQUS and validate them
  - CRADA with Moldflow
  - Apply Moldflow code to simulate injection-molding of LFT samples
- **University of Illinois**
  - Assess and apply the current fiber orientation model to predict fiber orientation in LFT samples
  - Validate the Leeds' fiber orientation method for LFTs
  - Develop a new fiber orientation model (anisotropic rotary diffusion model) for LFTs
- **Moldflow**
  - CRADA with PNNL
  - Rheological and physical data measurements
  - Deliver to PNNL a research version of Moldflow
  - Technical support

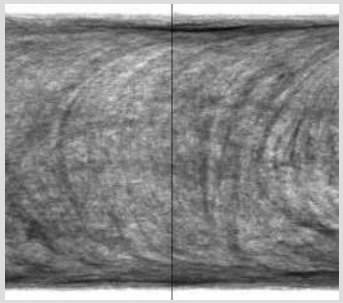
Technical Accomplishments (cont.)

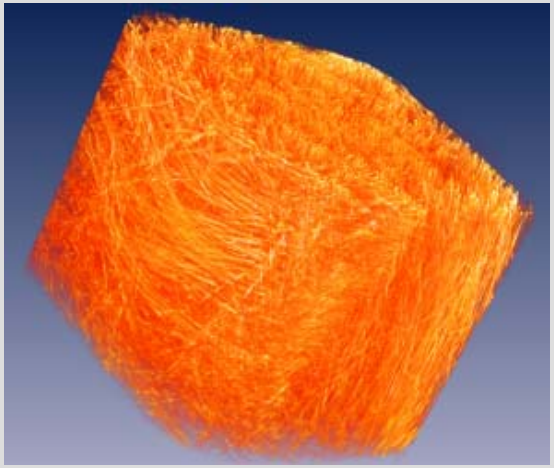
ORNL

- Complete technical assessment of characterization methods for LFTs
- Develop and validate methods for fiber length and orientation measurement
- Develop method for long carbon filament separation
- LFT specimen preparation
- Microstructural characterization & mechanical testing to support modeling
- Develop an X-ray tomography unit to identify microstructural evolution during loading of LFT specimens



durability evaluation

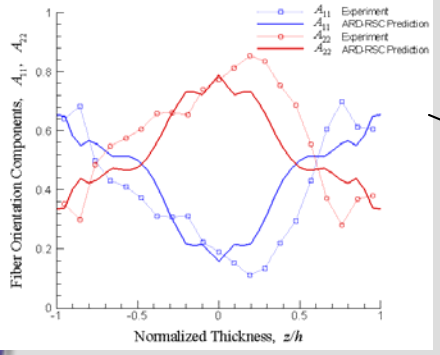




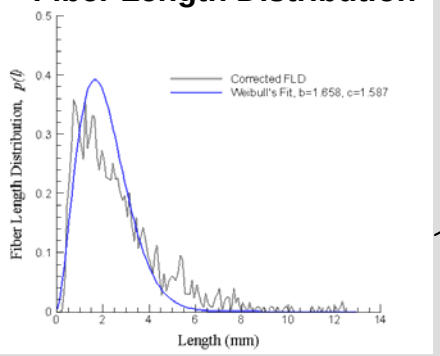
microstructure characterization

Technical Accomplishments (cont.)

Fiber Orientation Distribution



Fiber Length Distribution



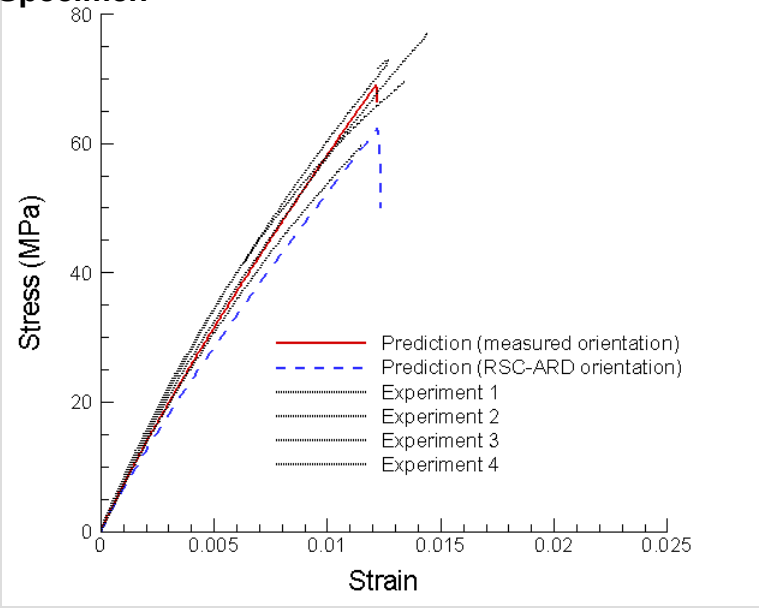
Input to property prediction

Property prediction & Structural Analysis

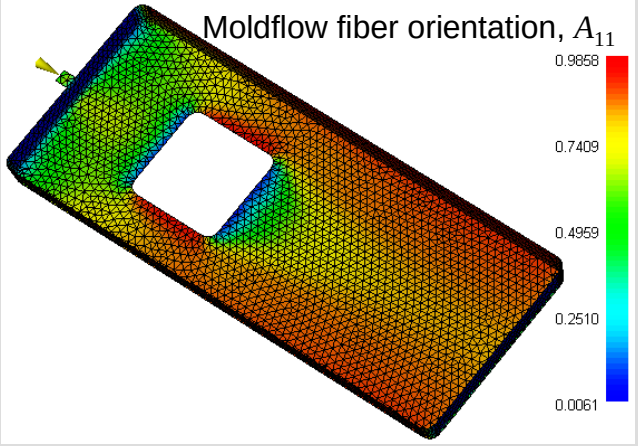
- Code **EMTA**
- **ABAQUS**

Input to property prediction

Stress-Strain Response of A Long-Glass-Fiber/PP Specimen

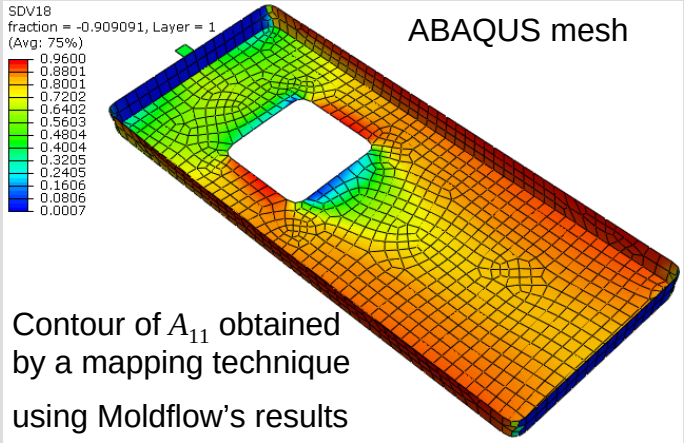


Moldflow fiber orientation, A_{11}



Map Moldflow's fiber orientation results onto an ABAQUS mesh for structural analysis

ABAQUS mesh



Contour of A_{11} obtained by a mapping technique using Moldflow's results

Technology Transfer

- Computational tools for LFTs implemented in leading commercial finite element packages will be available to automotive industry
  - Process models (fiber orientation and fiber length attrition models) are being implemented in Moldflow under CRADA
  - Constitutive models for LFT structural analyses are being implemented in ABAQUS
- Developed microstructural characterization and testing methodologies ready to be applied to actual LFT materials for automotive applications
- Technology is being transferred through publications, presentations and updates of the steering committee
- An integrated tool that links process to structural modeling with experimental verifications will be demonstrated at the end of the project.

Future Work

FY 2008 Work

- Characterize damage and non-linear behavior of LFTs
- Enhance the elastic-plastic model with consideration of progressive damage to improve the predictions of strength and stress/strain response
- Develop a creep model for LFTs
- Evaluate the ARD fiber orientation model against new molding trials
- Implement the ARD model in Moldflow
- Develop ways to characterize fiber curvature, contacts, and breakage in LFTs
- Develop a process model for fiber length degradation
- Characterize time dependent behavior of LFTs
- Develop test methods for complex shape samples

FY 2009 Work

- Develop a fatigue model for LFTs
- Characterize fatigue behavior of LFTs
- Develop an impact damage model for LFTs
- Characterize impact behavior of LFTs
- Test samples with complex shape
- Demonstrate an integrated approach for a complex part shape

Summary

- Lightweight automotive structural components made of long-fiber reinforced injection molded thermoplastics can be designed and processed using tools and techniques developed in this project.
- **Key accomplishments to date**:
  - A fiber orientation model for LFTs
  - Models for predicting thermoelastic properties, nonlinear stress-strain responses and strength of LFTs
  - Characterization tools for determining microstructural features (fiber orientation & length distributions, etc.)
  - Novel testing methods for model validation
- Model implementations in commercial leading codes (i.e. Moldflow and ABAQUS) assures that the results will be available in the marketplace.
- Progress of coordinated research to develop predictive and characterization tools is evaluated through periodic review meetings
- Interim results are disseminated via publications and presentations
- Results from this work can be extended to other discontinuous fiber polymer composite processes such as compression molding

Publications & Presentations

Journal Papers

- Bapanapalli SK, BN Nguyen (2007). *"Prediction of Elastic Properties for Curved Fiber Polymer Composites."* Polymer Composites (*in press*).
- Nguyen BN, V Kunc, BJ Frame, JH Phelps, CL Tucker III, SK Bapanapalli, JD Holbery, MT Smith (2007). *"Fiber Length and Orientation in Long-Fiber Injection-Molded Thermoplastics - Part I: Modeling of Microstructure and Elastic Properties."* J. Composite Materials (*in press*)
- Nguyen BN, V Kunc, JH Phelps, CL Tucker III, SK Bapanapalli (2008). *"Prediction of the Elastic-Plastic Stress/Strain Responses for Injection-Molded Long-Fiber Thermoplastics."* Submitted to J. Composite Materials.

Conference Papers and Presentations

- Nguyen BN, JD Holbery, KI Johnson, MT Smith (2005). *"Long-Fiber Thermoplastic Injection-Molded Composites: From Process Modeling to Property Prediction."* In Proceedings of the 5th Annual SPE Automotive Composites Conference & Exposition, Detroit, Sep. 12-14, 2005
- G Velez-Garcia, V Kunc (2006). *"Experimental Methods to Evaluate Fiber Length and Orientation Distribution of Long Glass Fibers in Injection Molded Thermoplastics", Presented by G. Velez-Garcia at Fiber Society Conference, Knoxville, TN, October 10-12, 2006*
- Nguyen BN, V Kunc, BJ Frame, JH Phelps, CL Tucker III, SK Bapanapalli, JD Holbery, MT Smith (2007). *"From Process Modeling to Elastic Property Prediction for Long-Fiber Injection-Molded Thermoplastics."* In Proceedings of the 7th Annual SPE Automotive Composites Conference & Exposition, Detroit, Sep. 11-13, 2007
- Kunc V, BJ Frame, BN Nguyen, CL Tucker III, G. Velez-Garcia (2007). *"Fiber Length Distribution Measurement for Long Glass and Carbon Fiber Reinforced Injection Molded Thermoplastics."* In Proceedings of the 7th Annual SPE Automotive Composites Conference & Exposition, Detroit, 11-13, 2007.
- Nguyen BN, V Kunc, MT Smith (2007). *"Prediction of Elastic Properties for Long-Fiber Thermoplastic Injection-Molded Composites."* Presented by BN Nguyen at the 2007 ASME Applied Mechanics and Materials Conference (McMat 2007), Austin, TX, June 3-7, 2007