U.S. DEPARTMENT OF ENERGY

PNNL-22473

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

Predictive Engineering Tools for Injection-Molded Long-Carbon-Fiber Thermoplastic Composites

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Quarterly report submitted to Aaron Yocum, National Energy Technology Laboratory, Morgantown, WV 26507

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1. Objective

The objective of this project is to advance the *predictive engineering (PE) tool* to accurately predict *fiber orientation and length distributions* in *injection-molded long-carbon fiber thermoplastic composites* for optimum design of automotive structures using these materials *to meet weight and cost reduction requirements* defined in Table 2 of DE-FOA-0000648 (Area of Interest 1).

2. Background

This project proposes to integrate, optimize and validate the fiber orientation and length distributions models previously developed and implemented in the Autodesk Simulation Moldflow Insight (ASMI) package for injection-molded long-carbon-fiber thermoplastic composites. In our previous US Department of Energy (DOE) funded project titled: *"Engineering Property Prediction Tools for Tailored Polymer Composite Structures"* Pacific Northwest National Laboratory (PNNL), with the University of Illinois and Autodesk, Inc., developed a unique assembly of computational algorithms providing the state-of-the-art process and constitutive models that enhance the capabilities of commercial software packages to predict fiber orientation and length distributions as well as subsequent mechanical properties of injection-molded long-fiber thermoplastic (LFT) composites. These predictive capabilities were validated using the data generated at Oak Ridge National Laboratory on generally two-dimensional (2-D) structures of edge-gated plaques or center-gated disks injection-molded from long-glass-fiber/polypropylene or long-glass-fiber/polyamide 6,6 pellets. The present effort aims at rendering the developed models more robust and efficient to the part design by the automotive industry to achieve weight savings and cost reduction. This ultimate goal will be achieved by optimizing the developed models, improving and integrating their implementations in ASMI, and validating them for a complex three-dimensional long-carbon fiber thermoplastic automotive part. Both polypropylene and polyamide 6,6 will be used for the resin matrices. Local fiber orientation and length distributions at the key regions on the part will be measured for the model validation based on the 15% accuracy criterion. The project outcome will be the ASMI package enhanced with computational capabilities to accurately predict fiber orientation and length distributions in automotive parts designed with long-carbon fiber thermoplastics.

3. Accomplishments

The PNNL team is making progress in the planning phase for the project in order to complete all the legal and contract documents required for establishing the subcontracts needed and a Cooperative Research and Development Agreement (CRADA) with Autodesk, Inc., Toyota Motor Engineering and Manufacturing North America (Toyota), and Magna Exterior and Interiors Corporation (Magna). During the second quarter, our achievements in the planning effort are the following:

- Completion of all the technical and legal documents for the subcontract to PlastiComp, Inc. for long-carbon-fiber/polypropylene and long-carbon-fiber/polyamide 6,6 compounding, and for molding plaques from these pellets,
- Completion of all the technical and legal documents for the subcontract to Purdue University for fiber orientation and length measurements from LFT samples taken from the LFT moldings under this project,
- Completion of all the technical and legal documents for the subcontract to the University of Illinois for providing consultant services to Autodesk for process models improvements and integration,
- The revised CRADA documents were sent to DOE, Autodesk, Toyota, and Magna for final technical and legal reviews and signatures,

- PNNL Legal Services contacted project partners' Legal counterparts for handling all the legal documents for the project. A non-disclosure agreement (NDA) was revised and resent to all the parties for signatures.

4. Progress and Status

The CRADA documents have been processed by PNNL Legal Services. Necessary revisions for the CRADA documents have been performed to address the requested changes and final documents are being sent out for reviews and signatures. DOE has completed the Foreign Entity review.

5. Publications/Presentations

None

6. Patents

None

7. Future Plans

The final CRADA documents will be sent to all the parties for signatures. The subcontracts will be awarded as soon as the CRADA is approved and signed by all the CRADA parties and DOE. The team will have a physical kickoff meeting to start the project technically.

8. Participants & Other Collaborating Organizations

We expect that the project could technically start at the end of the third quarter or at the beginning of the fourth quarter. Work for each project partner has been planned and is summarized below:

- PNNL will be leading the overall project management task. In addition, it will be:
    - Coordinating the research activities among project partners,
    - Performing process modeling using ASMI to validate the integrated predictive tool,
    - Performing weight and cost saving study on selected Toyota's complex automotive structures (in Year 2 of the project).

- Autodesk, Inc. at Ithaca, New York, a CRADA partner will be performing the following tasks:
    - Performing rheological and thermal tests on adopted materials to obtain data for process modeling,
    - Improving three-dimensional fiber orientation modeling and implementing the reduced order length model in ASMI,
    - Delivering an ASMI research version and license to PNNL for process modeling.

- Toyota at Ann Arbor, Michigan, a CRADA partner will be performing the following tasks:
    - Providing a candidate automotive structure that can be molded and analyzed for weight saving,

  - Modifying its preexisting mold that can be used to produce the complex automotive structure using injection molding with long carbon-fiber/polypropylene and long-carbon-fiber/PA6,6 compounds,
  - Building a fixture to evaluate part stiffness and compare weight reduction to other material options.

- Magna in Ontario, Canada, a CRADA partner will be performing the following tasks:

  - Participating in mold building,
  - Injection-molding Toyota's complex 3D structures adopted for the project.

- PlastiComp, Inc. subcontracted by PNNL will be performing the following tasks:

  - Compounding long-carbon-fiber/PP and long-carbon-fiber/PA6,6 pellets,
  - Molding 7 in. x 7 in. x 0.125 in plaques from these materials using conventional LFT and direct LFT (D-LFT) technologies,
  - Providing assistance in the molding of Toyota's complex 3D structures (Year 2).

- Purdue University subcontracted by PNNL will be performing the following tasks:

  - Fiber orientation and length measurements on samples taken from molded plaques (Year 1) and from the complex 3D parts (Year 2).

- University of Illinois subcontracted by PNNL will be providing consultant services to Autodesk, Inc. for improvement of process models and model integration in ASMI.

Milestones status:

As the project has not yet started technically awaiting the CARDA in place with the industrial partners, there are no updates on the milestones status at this time.

9. Budgetary Information

COST PLAN/STATUS																
	Budget Period 1								Budget Period 2							
	Q1		Q2		Q3		Q4		Q1		Q2		Q3		Q4	
Baseline Reporting Quarter	9/11/2012 - 12/31/2012		1/1/2013 - 3/31/2013		4/1/2013 - 6/30/2013		7/1/2013 - 9/30/2013		10/1/2013 - 12/31/2013		1/1/2014 - 3/31/2014		4/1/2014 - 6/30/2014		7/1/2014 - 9/30/2014	
	Q1	Cumulative Total	Q2	Cumulative Total	Q3	Cumulative Total	Q4	Cumulative Total	Q1	Cumulative Total	Q2	Cumulative Total	Q3	Cumulative Total	Q4	Cumulative Total
Baseline Cost Plan																
Federal Share	$6,808	$6,808	$8,000	$14,808	$238,289	$253,097	$238,288	$491,385	$127,409	$618,794	$127,409	$746,203	$127,409	$873,612	$127,409	$1,001,021
Non-Federal Share	$0	$0	$0	$0	$285,177	$285,177	$285,177	$570,354	$127,867	$698,221	$127,867	$826,088	$127,867	$953,955	$127,867	$1,081,822
Total Planned	$6,808	$6,808	$8,000	$14,808	$523,466	$538,274	$523,465	$1,061,739	$255,276	$1,317,015	$255,276	$1,572,291	$255,276	$1,827,567	$255,276	$2,082,843
Actual Incurred Cost																
Federal Share	$6,808	$6,808	$2,536	$9,344												
Non-Federal Share	$0	$0	$0	$0												
Total Incurred Costs	$6,808	$6,808	$2,536	$9,344												
Variance																
Federal Share	$0	$0	$5,464	$5,464												
Non-Federal Share	$0	$0	$0	$0												
Total Variance	$0	$0	$5,464	$5,464												