U.S. DEPARTMENT OF ENERGY

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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

PNNL finalized all the documents for a Cooperative Research and Development Agreement (CRADA) with the industrial parties including Autodesk, Inc. (Autodesk), Toyota Motor Engineering and Manufacturing North America (Toyota), and Magna Exterior and Interiors Corporation (Magna). This CRADA (No. 336) entitled: "*Integration of Advanced Process Models in Autodesk Simulation Moldflow Insight and Their Validations for Toyota's Injection-Molded Long-Carbon-Fiber Thermoplastic Structure for Automotive Applications*" has been signed off by all the partners, Department of Energy (DOE) Headquarters, DOE Legal Office, and DOE Pacific Northwest Site Office (PNSO). As a result, the CRADA is effective from October 28th, 2013 to October 28th, 2015.

During the last quarter of FY 2013, no technical progress has been made toward project milestones due to the extended approvals required for the CRADA.

4. Progress and Status

CRADA No. 336 in place has allowed the project to start technically. PNNL Contracts Office has initiated the subcontracts needed for the project. The project kickoff meeting with the team including subcontract and CRADA partners has been scheduled on 11/13/2013 in a facility of PlastiComp, Inc. in

Winona, MN. The project work scope, GANTT chart, individual tasks, and presentations have been prepared and will be discussed with all the project partners at the kickoff meeting.

5. Publications/Presentations

None

6. Patents

None

7. Future Plans

Autodesk starts performing process models improvements and implementations. Under a subcontract by PNNL, PlastiComp will injection mold long-carbon-fiber/polypropylene (PP) and long-carbon-fiber/polyamide 6,6 (PA 6,6) plaques for the project. PlastiComp will also ship long-carbon-fiber/PP and long-carbon-fiber/PA 6,6 pellets compounded for the project to Autodesk for rheological and thermal properties measurements. Autodesk will deliver a research version of ASMI to PNNL for injection molding analyses of PlastiComp plaques. PNNL will start building ASMI models of PlastiComp plaques once the ASMI license is received. Specimens from molded plaques will be prepared and shipped to Purdue University for fiber orientation and length measurements.

8. Participants & Other Collaborating Organizations

Work for each project partner has been planned and will be discussed with the team at the kickoff meeting.

- 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 of 10/27/2013 the project did not start technically awaiting the CRADA 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	$743	$10,087	$418	$10,505								
Non-Federal Share	$0	$0	$0	$0	$0	$0	$0	$0								
Total Incurred Costs	$6,808	$6,808	$2,536	$9,344	$743	$10,087	$418	$10,505								
Variance																
Federal Share	$0	$0	$5,464	$5,464	$237,546	$243,009	$237,870	$480,879								
Non-Federal Share	$0	$0	$0	$0	$285,177	$285,177	$285,177	$570,354								
Total Variance	$0	$0	$5,464	$5,464	$522,723	$528,186	$523,047	$1,051,233								