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BN Nguyen
SE Sanborn
KL Simmons
RN Mathur
MD Sangid
X Jin
F Costa
UN Gandhi
S Mori
CL Tucker III

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# Predictive Engineering Tools for Injection-molded Long-Carbon-Fiber Thermoplastic Composites

Ba Nghiep Nguyen, Scott E. Sanborn, Kevin L. Simmons,
Pacific Northwest National Laboratory, Richland, WA 99352
Raj N. Mathur
PlastiComp, Inc., Winona, MN 55987
Michael D. Sangid
Purdue University, West Lafayette, IN 47907
Xiaoshi Jin, Franco Costa
Autodesk, Inc., Ithaca, NY 14850
Umesh N. Gandhi
Toyota Research Institute North America, Ann Arbor, MI 48105
Steve Mori
MAGNA Exteriors and Interiors Corp., Aurora, Ontario, Canada
Charles L. Tucker III
University of Illinois at Urbana-Champaign, Urbana, IL 61801

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Reporting period end date: December 31st, 2013

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Richland, Washington 99352

## 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 (PP) or long-glass-fiber/polyamide 6,6 (PA66) 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 PP and PA66 are 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 CRADA between PNNL, Autodesk, Toyota and Magna has been effective since October 28th, 2013. The whole team including CRADA and subcontract partners kicked off the project technically on November 1st, 2013. During the first quarter of FY 2014, the following technical progresses have been made toward project milestones:

1) The project kickoff meeting was organized at PlastiComp, Inc. in Winona on November 13th, 2013 involving all the project partners. During this meeting the research plan and Gantt chart were discussed and refined. The coordination of the research activities among the partners was also discussed to ensure that the deliverables and timeline will be met.

2) Autodesk delivered a research version of ASMI to PNNL for process modeling using this tool under the project. PNNL installed this research version on a PNNL computer and tested it. Currently, PNNL is using ASMI to prepare the models for PlastiComp plaques.

3) PlastiComp has compounded long carbon-fiber reinforced (LCF) PP and PA66 compounds for rheological and thermal characterization tests by the Autodesk laboratories in Melbourne, Australia.

4) Initial mold flow analysis was carried out by PlastiComp to confirm that the 3D complex part (Figure 1) selected by Toyota as a representative automotive part is moldable.

5) Toyota, Magna, PlastiComp and PNNL finalized the planning for molding the Toyota 3D complex part.

6) Purdue University worked with PNNL to update and specify the test matrix for characterization of fiber length/orientation.

7) Purdue University developed tools to automate the data collection and analysis of fiber length and orientation measurements.

8) Purdue University designed and specified equipment to replace the need for equipment using the technology established by the University of Leeds (LEEDs equipment) at General Motors (GM).

## 4. Progress and Status

This section reports the progress and status of the activities for each project participants for the first quarter of FY 2014.

### 4.1 PNNL

PNNL has assumed the overall project management for the project and the process modeling tasks. Under these roles PNNL finalized the research plan and revised the GANTT chart with the team. PNNL also coordinated the research activities among the project partners through the project kickoff meeting, teleconferences, and separate discussions. While most of the Phase 1 process modeling work at PNNL cannot begin until other team members complete specific tasks, PNNL nonetheless took technical steps this quarter to be prepared. During this quarter the following technical progress was made:

- **Installation of Moldflow:** Autodesk provided PNNL with a research version of ASMI. While the *current* research version of ASMI does not contain the 3-D solver improvements and reduced order fiber length model that will be implemented during Phase 1, this version is useful to prepare models in preparation for plaques that will be molded by PlastiComp and whose fiber orientations and lengths will be measured by Purdue University. PNNL successfully installed the current research version and tested some models developed as part of the past predictive engineering work in long-glass-fiber composites. During the next quarter, PNNL expects to get dimensions and processing parameters of the plaques molded by PlastiComp and to build ASMI models that match these inputs.

- **Program to Calculate the ARD-RSC Model Parameters:** The ARD-RSC (Anisotropic Rotary Diffusion-Reduced Strain Closure) model implemented in ASMI requires a number of parameters as inputs. Several of these parameters ($b_1$, $b_2$, $b_3$, $b_4$, $b_5$) must be selected such that they are consistent with the model and result in physically acceptable solutions. To achieve this, one pair of $b_3$-$b_5$ parameters are chosen for a target second order orientation tensor in simple shear flow. Then a closure method, in this case the orthotropic closure approximation, is applied to get the fourth order orientation tensor and a set of equations are used to determine $b_1$, $b_2$, and $b_4$ (see Phelps and Tucker, 2009[1] for details on this procedure). After this, the second order tensor **C** (which depends on the invariants of the second order orientation tensor and rate-of-deformation tensor) is checked for positive eigenvalues indicating a physically acceptable tensor. These parameters are then checked in other simple types of flows. The procedure is repeated over a map of $b_3$-$b_5$ values to determine the set of $b_i$ parameters that are furthest from boundaries determining the acceptable/unacceptable regions; since the exact flows that will be encountered during the simulation are not known, it is best to choose parameters closest to the interior of the acceptable regions in the simple flows. PNNL wrote a simple Matlab program to achieve the selection and checking of the $b_i$ parameters for use in the ASMI models.

The calculated sets of $b_i$ parameters were compared to some sets identified under the past effort and very close agreement was found. However, ASMI uses a different closure approximation, the hybrid closure approximation, than the one tested. During the next quarter, PNNL plans to implement the hybrid closure approximation in this $b_i$ parameter selection program to be consistent with ASMI.

### 4.2 Purdue University

Purdue University developed tools to automate the data collection and analysis. To improve throughput for capturing the fiber length and orientation measurements over a large number of samples, automation of data collection and analysis methods consisted of the following:

- **Fiber length measurement:** Manually burning off the matrix and thus down selecting the number of fibers in the sample (using an actuator controlled syringe and 18 gage hypodermic needle) can be performed in batches. The fiber aggregate will be separated using a combination of a corona generator (made in house during the first quarter of this project) and manually perturbing the system, while ensuring the fibers do not break. High-resolution images of the fibers are captured and an automated image analysis program was written to segment the fibers, isolate fibers especially across potential nodes/junctions, locate their end points, and determine their length. Next quarter, Purdue will work on creating sensitivity analysis of the characterization process.

- **Fiber orientation measurement:** A program was written to digitize images captured, perform an edge detection algorithm to fit an ellipse on each fiber's cross-section, and capture the second-order orientation tensor. As an option to replace the need to use the GM's LEEDs instrument, Purdue University has investigated and specified a system composed of an optical microscope and computer controlled motorized stage. The system will automate the focus and capture of images for the fiber's cross-section and then move the stage to the next position. This will enable a large field of view to be recorded and stitched together for accurate statistics of the fiber orientation distributions. Once the automated system is operational, Purdue will compare the results of the in house equipment to those results obtained by the LEEDs machine

### 4.3 PlastiComp

The kick-off meeting was held at PlastiComp Global Headquarters in Winona, MN. Quarterly milestones were revisited and defined. PlastiComp has compounded long carbon-fiber (LCF) reinforced PP and PA66 compounds as listed in Table 1.

[1] J.H. Phelps, C.L. Tucker III/J. Non-Newtonian Fluid Mech. 156 (2009) 165-176.

**Table 1.** 30 wt% and 50wt% LCF/PP and LCF/PA66 compounds made by PlastiComp for shipment to Autodesk for rheological and thermal tests.

| Serial No | Compound | Amount | Remarks |
|---|---|---|---|
| 1 | PP+LCF30 Natural | 55 lbs. | Shipped to Autodesk, Australia |
| 2 | PP+LCF50 Natural | 55 lbs. | Shipped to Autodesk, Australia |
| 3 | PA66+LCF30 Natural | 55 lbs. | Shipped to Autodesk, Australia |
| 4 | PA66+LCF50 Natural | 55 lbs. | Shipped to Autodesk, Australia |

Representative samples of these 12 mm-long pellets or granules were sent to Purdue University so as to establish a laboratory procedure for fiber-length analyses. Additionally, PlastiComp will perform pellet-microscopy to reveal fiber dispersion in the polymer matrices.

Initial analyses of flow in the mold were carried out to confirm that the 3D part selected by Toyota as a representative automotive part is moldable (Figure 1). These analyses indicate that the part wall thicknesses in specific sections of the part will have to be increased from the current 2 mm wall thickness to approximately 2.8 mm, to ensure filling at reasonable injection pressures that are not adverse to preserving fiber-lengths.

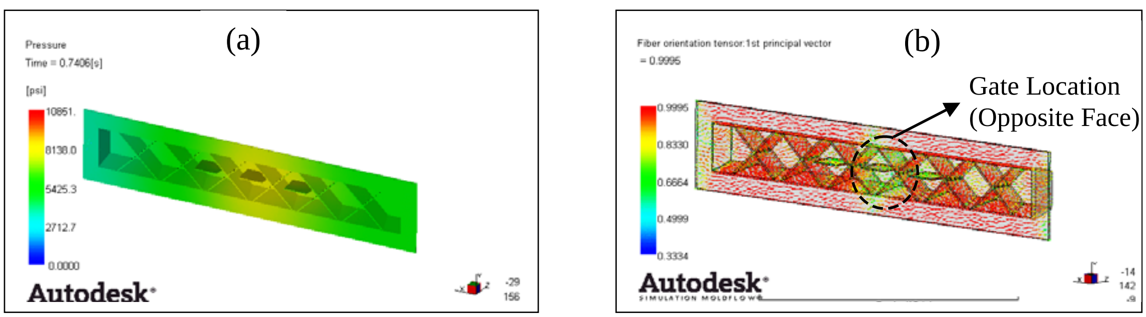


**Figure 1:** (a) High injection pressures (≥ 76 MPa) for 2 mm wall thicknesses, and (b) A center gate location is appropriate for lengthwise fiber orientation and testing of part in bending mode.

### 4.4 Autodesk

Autodesk's staff attended the project kickoff meeting and addressed the technical questions regarding the characterization tests needed for the project. These tests should adequately identify the response of the matrix of the as-formed composite. Autodesk delivered a research version of ASMI to PNNL for process modeling, and provided support to PNNL to install this version on PNNL's computers. In the meantime, Autodesk commenced work on ASMI 3D fiber orientation prediction improvements and used PNNL models and other measured data to check the progress on the improvement.

### 4.5 University of Illinois

Prof. C.L. Tucker at the University of Illinois has worked to put Autodesk in a position to implement the reduced-order model for fiber length attrition. PNNL consulted Prof. Tucker on gating configurations for the plaques and characterization tests needed for acquiring the data for modeling. In particular, Prof. Tucker provided recommendations to PNNL on the locations on PlastiComp plaques where samples will be cut out and prepared for fiber orientation and length measurements.

### 4.6 <u>Toyota</u>

Toyota's staff attended the project kickoff meeting and participated in refining the research plan for the project at this meeting and the follow-up teleconferences and discussions. In particular, Toyota has engaged the discussions with Magna, PlastiComp and PNNL on the preparation for molding the 3D complex part (provided by Toyota).

### 4.7 <u>Magna</u>

Magna's staff attended the project kickoff meeting and participated in refining the research plan for the project at this meeting and the follow-up teleconferences and discussions. In particular, Magna has engaged the discussions with Toyota, PlastiComp and PNNL on the preparation for molding the 3D complex part (provided by Toyota).

## 5. Publications/Presentations

None

## 6. Patents

None

## 7. Future Plans

Autodesk continues performing process models improvements and implementations. PlastiComp will injection mold LCF/PP and LCF/PA66 plaques for the project. PlastiComp has already shipped LCF/PP and LCF/PA66 pellets compounded for the project to Autodesk for rheological and thermal properties measurements. Autodesk will perform these characterization tests for the compounds defined in Table 1. PNNL will start building ASMI models of PlastiComp plaques. 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 was refined and discussed with the team at the kickoff meeting and follow-up teleconferences.

- PNNL is leading the overall project management task. In addition, it assumes
    - 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. a CRADA partner performs 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 intermediate updates and a license to PNNL for process modeling.

- Toyota at Ann Arbor, Michigan, a CRADA partner performs 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 LCF/PP and LCF/PA66 compounds,
   - Building a fixture to evaluate part stiffness and compare weight reduction to other material options (Year 2).

- Magna in Ontario, Canada, a CRADA partner performs the following tasks:

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

- PlastiComp, Inc. subcontracted by PNNL performs the following tasks:

   - Compounding LCF/PP and LCF/PA6,6 pellets,
   - Molding 7 in. × 7 in. × 0.125 in. plaques from these materials under slow-fill and fast-fill conditions using conventional LFT and direct LFT (D-LFT) technologies,
   - Molding the 3D complex part adopted using D-LFT (Year 2).

- Purdue University subcontracted by PNNL performs 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 provides consultant services to Autodesk for improvement of process models and model integration in ASMI.

**Milestones status:**

As of 12/31/2013 the project team is on tract to complete two important sub-milestones on:

1) Completion of moldings for 30wt% and 50wt% LCF/PP and LCF/PA66 center-gated and edge-gated plaques (Table 2).
2) Completion of rheological and thermal tests by Autodesk Labs for the PlastiComp compounds given in Table 1.

These sub-milestones are part of the milestone on completing ASMI models validation for the injection molding of LCF/PP and LCF/PA66 plaques.

**Table 2.** Molding matrix for PlastiComp LCF/PP and LCF/PA66 7 in. × 7 in. × 0.125 in. plaques molded under slow fill and fast fill conditions

| Weight Fraction | Materials | Processing | Condition | Number of edge-gated plaques | Number of center-gated plaques |
|---|---|---|---|---|---|
| 30% | CF/PP | LFT | Slow | 10 | 10 |
| | | | Fast | 10 | 10 |
| | | D-LFT | Slow | 10 | 10 |
| | | | Fast | 10 | 10 |
| | CF/PA6,6 | LFT | Slow | 10 | 10 |
| | | | Fast | 10 | 10 |
| | | D-LFT | Slow | 10 | 10 |
| | | | Fast | 10 | 10 |
| 50% | CF/PP | LFT | Slow | 10 | 10 |
| | | | Fast | 10 | 10 |
| | | D-LFT | Slow | 10 | 10 |
| | | | Fast | 10 | 10 |
| | CF/PA6,6 | LFT | Slow | 10 | 10 |
| | | | Fast | 10 | 10 |
| | | D-LFT | Slow | 10 | 10 |
| | | | Fast | 10 | 10 |

## 9. Budgetary Information

COST PLAN/STATUS

| Baseline Reporting Quarter | Budget Period 1 | | | | | | | | Budget Period 2 | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Q1 | | Q2 | | Q3 | | Q4 | | Q1 | | Q2 | | Q3 | | Q4 | |
| | 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 | $62,859 | $73,365 | | | | | | |
| Non-Federal Share | $0 | $0 | $0 | $0 | $0 | $0 | $0 | $0 | $18,485 | $18,485 | | | | | | |
| Total Incurred Costs | $6,808 | $6,808 | $2,536 | $9,344 | $743 | $10,087 | $418 | $10,505 | $81,345 | $91,850 | | | | | | |
| **Variance** | | | | | | | | | | | | | | | | |
| Federal Share | $0 | $0 | $5,464 | $5,464 | $237,546 | $243,009 | $237,870 | $480,879 | $64,550 | $545,429 | | | | | | |
| Non-Federal Share | $0 | $0 | $0 | $0 | $285,177 | $285,177 | $285,177 | $570,354 | $109,382 | $679,736 | | | | | | |
| Total Variance | $0 | $0 | $5,464 | $5,464 | $522,723 | $528,186 | $523,047 | $1,051,233 | $173,931 | $1,225,165 | | | | | | |