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

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Project period: From October 1st 2012 to September 30th, 2014 **Reporting** period end date: June 30th, 2014

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 stateof-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 (3-D) long-carbon fiber (LCF) 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

During the third quarter of FY 2014, the following technical progresses have been made toward project milestones:

- 1) Autodesk introduced the options for fiber inlet condition to the 3D solver. These options are already available in the mid-plane/dual domain solver.
- 2) Autodesk improved the accuracy of 3D fiber orientation calculation around the gate.
- 3) Autodesk received consultant services from Prof. C.L. Tucker at the University of Illinois on the implementation of the reduced order model for fiber length, and discussed with Prof. Tucker the methods to reduce memory usage.
- 4) PlastiComp delivered to PNNL center-gated and edge-fan-gated 20-wt% to 30-wt% LCF/PP and LCF/PA66 (7"x7"x1/8") plaques molded by the in-line direct injection molding (D-LFT) process.
- 5) PlastiComp molded ASTM tensile, flexural and impact bars under the same D-LFT processing conditions used for plaques for Certification of Assessment and ascertaining the resultant mechanical properties.
- 6) Purdue developed a new polishing routine, utilizing the automated polishing machine, to reduce fiber damage during surface preparation.
- 7) Purdue used a marker-based watershed segmentation routine, in conjunction with a hysteresis thresholding technique, for fiber segmentation during fiber orientation measurement.

- 8) Purdue validated Purdue's fiber orientation measurement method using the previous fiber orientation data obtained from the Leeds machine and manually measured data by the University of Illinois.
- 9) PNNL conducted ASMI mid-plane analyses for a 30wt% LCF/PP plaque and compared the predicted fiber orientations with the measured data provided by Purdue University at the selected locations on this plaque.
- 10) PNNL put together the DOE 2014 Annual Merit Review (AMR) presentation with the team and presented it at the AMR meetings on June 17, 2014.
- 11) PNNL built ASMI dual domain models for the Toyota complex part and commenced mold filling analyses of the complex part with different wall thicknesses in order to support part molding.
- 12) Toyota and Magna discussed with PNNL on tool modification for molding the complex part. Toyota sent the CAD files of the complex part to PNNL to build ASMI models of the part for mold filling analysis to provide guidance to tooling and part molding.

4. Progress and Status

This section reports the current progress and status vis-à-vis the project milestones and anticipated completion dates set for FY 2014 and the first quarter of FY 2015 (Table 1).

Quarter	Milestone Descriptions	Responsibility	Completed by	Status
FY14 Q1	PlastiCompto deliver 55 lbs of 30 wt% and 50 wt% LCF/PP and LCF/PA66 compound materials to Autodesk for material characterization that is within a 10% batch variation using loss on ignition mass comparison.	PlastiComp	12/31/2013	Completed
FY14 Q2	Deliver 320 edge and centered gated 7x7x0.125 inch plaques to PNNL per statement of work test matrix on 30 wt% and 50 wt% carbon fiber PP and PA resin systems.	PlastiComp	3/1/2014	Completed
FY14 Q3	Autodesk to deliver material characterization report on shear flow, PVT, and mechanical property suite in udb file input for ASMI and PDF on the 30 wt% and 50 wt% PP and PA compound materials from PlastiComp for use in flow simulations in two- and three-dimensional part.	Autodesk	4/1/2014	Completed
	Achieve 10% accuracy of the fiber length distribution measurement relative to referenced standard	Purdue	5/15/2014	In Progress
	Demonstrate a 10% fiber length distribution comparison between the machine purge material between PlastiComp, Magna, and Autodesk that is sufficient in fiber length for plaque and 3D molding to provide a fiber length exceeding 2 mm average.	Team	5/31/2014	In Progress
FY14 Q4	Demonstrate that Purdues fiber orientation process achieves a 10% accuracy of fiber orientation measurement compared to the GM Leeds machine measurements	Purdue	7/15/2014	Completed
	Complete filling analysis on the 3D part for determining the minimum wall thickness for cavity filling and maximizing the average fiber length to exceed 1-2 mm.	PNNL	9/30/2014	On schedule

Quarter		Milestone Descriptions	Responsibility	Completed by	Status
FY15 Q1		Complete the improvement of the 3-D ASMI solver and demonstrate a fiber orientation prediction within 15% of measured fiber orientation distributions for the LCF/PP and LCF/PA66 plaque moldings.	Autodesk	10/30/2014	In progress
	Go/no-go	Validate the ASMI predictions for the injection molding of long-carbon-fiber/PP and long-carbon-fiber/PA6,6 center and edge gated plaques using the available ASMI version for mid-plane modeling to achieve a 15% agreement with the experimental fiber orientation and length results.	PNNL	10/31/2014	In Progress
		Complete the implementation of the reduced-order fiber length model in ASMI and demonstrate accuracy equivalent to the full model while decreasing the memory required for fiber length calculation by at least 70%	Autodesk	10/30/2014	In progress

Table 1. Project milestones for FY 2014 and FY 2015 first quarter.

4.1 Plaques Molding (PlastiComp, Inc.)

During the second quarter of FY 2014, PlastiComp had molded 30-wt% and 50-wt% LCF/PP and LCF/PA66 edge-gated and center-gated (7"x7"x1/8") plaques using the conventional injection-molding process. During the third quarter, the edge-gated and center-gated plaque molds used in earlier experimental molding trials were used for further molding trials in PlastiComp, Pushtrusion[®], D-LFT processing to complete the milestone on plaques molding. As opposed to earlier molding trials with pre-compounded pellets, Pushtrusion[®] directly feeds the molten resin and cut fibers into the mixing zone of the injection barrel. The principle is illustrated in Figure 1.



Pushtrusion[®] Operating Principle

The resin drags the fiber strands along with it

The csa of the capillary tube determines the volumetric ratio of fiber to resin



Fiber lengths in the molten resin stream are cut to desired length by a rotary cutter (not shown in Figure 1) at the exit of the capillary tube. The rotary speed of the cutter, the number of cutting edges and the lineal speed of the fiber/resin stream determine cut or chopped fiber-lengths, and are programmable. As with the pre-compounded pellets, fibers were cut to 12-mm lengths. Since fiber-chopping in Pushtrusion[®] occurs in the molten phase, there is tight control on fiber-length distribution, whereas fibers in pre-compounded pellets are subject to severe length attrition during pellet melting in the injection barrel. Pushtrusion[®] routinely compounds, 20 to 50 wt% glass-fiber compounds and is currently used for molding PlastiComp customer parts. Table 2 relates nozzle/capillary size to the fiber weight fraction in

Nozzle Size (in)	Fiber Wt.%	Tows	Fiber	Resin	
0.061	13%	1	Glass	Polyamide	
0.068	23%	2	Glass	Polyamide	
0.068	36%	3	Glass	Polyamide	
0.118	58%	7	Glass	Polyamide	
·					
Nozzle Size (in)	Fiber Wt.%	Tows	Fiber	Resin	
0.124	20%	6	Carbon	Polyamide	
0.136	-	7-8	Carbon	Polyamide	

these composites. This Table shows the dependence of fiber weight fraction on the nozzle-size at the fiber-inlet and the number of tows used.

Table 2. The dependence of fiber weight fraction on the nozzle size and the number of tows.

The type of resin used only affects operating temperatures. Thus, polypropylene requires lower processing temperatures than polyamides, and processing the latter resin at higher temperatures means that resin degradation in the apparatus, especially in the capillaries and nozzles can lead to blockages and process interrupts. A second contrast exists between fiber tows, where carbon fiber tows (12,000 to 24,000) have substantially more fiber filaments than glass fiber tows (4,000 - 6,000). The impact of the filament count on flow in capillaries is not well documented, nor is there a study of the role of nozzle opening on capillary flow. It should be noted that the nozzle opening is not identical to the capillary diameter but controls the number of fiber tows that can be used. The capillary diameter is strictly responsible for the flow cross-section area (csa) and hence, the volume of resin flowing through. A systematic study of these process parameters and equipment modifications based on results were outside the scope of the program. For example, the capillary tubes and nozzles that constitute the fiber-resin entrainment section, shown as the "Entrainment Barrel" in Figure 1, are made from metal carbides for dimensional accuracy at elevated temperatures and for wear resistance. These flow elements cannot be machined at short notice to suit experimental outcomes. Some of the available nozzles also showed degradation from wear, especially with the glass fiber tows and had to be abandoned. Modifications to the equipment, to eliminate dead spaces that could lead to resin entrapment and in-situ resin-degradation were also not carried out. The undertaking of these tasks was not limited by budget, but by time constraints and the estimated probability of successful technical outcomes.

ITEM	DESCRIPTION	DESCRIPTION INJECTION SPEED (HIGH)				
1	20-30wt% LCF/PP	20 Plaques	20 Plaques			
2	20-30wt% LCF/PA66	20 Plaques	20 Plaques			

Table 3. Summary of molding conditions and number of plaques D-LFT processed by PlastiComp.

The final realistic solution was to lower carbon fiber contents in both PP and PA66. Therefore, carbon fiber weight fractions in the range from 20 to 30 wt% were adopted, and fast/slow molding conditions for each fiber/resin combination were repeated as in earlier injection molding using the conventional injection molding process. These are summarized in Table 3.

Purge materials or air-shots of the various D-LFT compounded materials were also sent to PNNL. In addition to the molded plaques, ASTM, Tensile, Flexural and Impact bars were also molded under the same processing conditions used for plaques. The fiber content was estimated to be between 20 to 30 weight fractions. The measured properties are listed Table 4.

Material Description	Injection Speed	TS (MPa)	TM (GPa)	Max Strain (%)	FS (MPa)	FM (GPa)	IUN (J/m)
LCF30-20 PP 1004 NAT	Slow	83.81	19.33	0.609	144.61	13.2	366
LCF30-20 PP 1004 NAT	Fast	80.87	20.06	0.575	133.64	13.95	297
LCF30-20 PA66 1021 NAT	Slow	287.08	24.12	1.454	419.34	18.91	744
LCF30-20 PA66 1021 NAT	Fast	292.25	26.5	1.434	401.07	16.7	897

Table 4: Mechanical Properties of D-LFT (Pushtrusion[®]) ASTM Test Specimens.

(TS/FS: Tensile & Flexural Strengths; TM/FM: Tensile & Flexural Moduli; IUN: Un-notched Izod Impact Strength).

4.2 Fiber Orientation Measurement (Purdue University)

Purdue University finalized Purdue's fiber orientation measurement method and validated it using the previous fiber orientation data obtained from the Leeds machine and manually measured data by the University of Illinois. The accomplishments are the following:

- A new polishing routine, utilizing the automated polishing machine, was developed in order to reduce fiber damage during surface preparation.
- A marker-based watershed segmentation routine, in conjunction with a hysteresis thresholding technique, was used for fiber segmentation.
- The orientation measurement method was verified using images and results obtained by Dr. Phelps [1] using the Leeds machine. The orientation results obtained by Purdue's method were compared with the data obtained using the Leeds machine and those obtained using manual segmentation by Dr. Phelps. A good comparison of results was obtained. Purdue's fiber orientation results agree within 10% of a reference analysis on data acquired by the Leeds system, and hence the Purdue method was verified. The milestone related to this task was completed.
- Purdue's method was then used to measure fiber orientations for samples taken at 3 regions (named A, B, and C) on a PlastiComp fast-fill 30wt% LCF/PP edge-gated plaque. The measured data were provided to PNNL.

<u>Validation of Purdue's fiber orientation measurement method</u>: The images obtained by Dr. Phelps [1] using the Leeds machine were used as the reference images. Fiber orientation tensors were calculated at Purdue University using these images, and the results were compared with those obtained using manual segmentation (named Phelps' method) and the Leeds setup. The comparison of the fiber orientation tensor components A_{11} , A_{22} , A_{33} and A_{31} are shown in Figure 2. The 1- and 2-directions denote the flow and cross flow directions, respectively. There was a good agreement between the three methods, thus the validation of Purdue's fiber orientation measurement method was confirmed.



Figure 2: Comparison of fiber orientation tensor components obtained using Purdue's method, Phelps' manual segmentation, and Leeds machine (x_3 denotes the thickness direction).

Following are some representative samples images obtained during the fiber orientation measurement process. This helps illustrate the segmentation and thresholding procedure that was used for fiber orientation measurement. For clarity, only small sections are shown here.



Figure 3: Surface obtained after final polishing. This was used as the input to the fiber orientation measurement software.



Figure 4: A binary image of the section shown in Figure 3 illustrates post fiber segmentation.



Figure 5: Image displaying the ellipses which were fit around the fibers.

<u>Fiber orientation measurement for a PlastiComp plaque:</u> Purdue's method was then applied to measure fiber orientations for samples taken at 3 regions (named A, B, and C) on a PlastiComp fast-fill 30wt% LCF/PP edged gated plaque (Figure 6). Each sample was divided into three parts to allow better segmentation and to improve execution times. Each section is approximately 0.3 in x 0.3 in. The tensors obtained over the three sections and the averaged tensor components for the entire specimen were

compared. The standard deviations were also calculated. However, for clarity of representation, these have not been plotted. The measured and predicted fiber orientations will be discussed in the next section.



Figure 6. Samples were taken at Regions A, B and C on a PlastiComp edge-gated plaque.

4.3 ASMI Analysis of PlastiComp Plaques (PNNL, Autodesk)

PNNL received the first set of fiber orientation data from Purdue University for the PlastiComp fastfill 30wt% LCF/PP edge-gated plaque. On discussion with Autodesk, PNNL used these data to start the validation of ASMI fiber orientation prediction. These data were measured at each location A, B, and C on the plaque (Figure 6). From the measured data a target fiber orientation tensor, A_{ij} , was selected, and from this target, a set of acceptable b_i parameters for the anisotropic rotary diffusion reduced strain closure (ARD-RSC) model [2] were identified. Using this initial set of b_i parameters, ASMI filling simulations of this plaque were run (Figure 7). The ASMI simulations used the actual process parameters that PlastiComp used when molding the plaques. While the b_i parameters were fixed for these initial filling simulations, the reduce-strain closure (RSC) parameter value was varied to control the orientation of the thru-thickness core region. The b_i and RSC parameters identified for this molding are: $b_1 = -0.002074$, $b_2 = 0.1512$, $b_3 = 0$, $b_4 = 0.01209$, $b_5 = 0$, RSC=0.015. Additionally, different pre-set ASMI options for the inlet orientation conditions were explored. It was found that some mesh refinement was required in the region right around the sprue to ensure proper propagation of the inlet conditions downstream. In this analysis, the option "*Fibers aligned at skin/transverse at core*" was used.



Figure 7. An ASMI mid-plane mesh used for the analysis of the PlastiComp edge-gated plaque.

The results of the ASMI analysis of this fast-fill 30wt% LCF/PP edge-gated plaque are promising. Figures 8, 9, and 10 show the experimental and predicted fiber orientations at Regions A, B, and C on the plaque, respectively. The ASMI fiber orientation predictions for all the components agree quite well the experimental orientation data.



Figure 8. Predicted and measured fiber orientation tensor components: (a) A_{11} , (b) A_{22} , (c) A33, and (d) A31 for the edge-gated fast-fill 30wt% LCF/PP plaques at Region A.



Figure 9. Predicted and measured fiber orientation tensor components: (a) A_{11} , (b) A_{22} , (c) A33, and (d) A31 for the edge-gated fast-fill 30wt% LCF/PP plaques at Region B.



Figure 10. Predicted and measured fiber orientation tensor components: (a) A_{11} , (b) A_{22} , (c) A33, and (d) A31 for the edge-gated fast-fill 30wt% LCF/PP plaques at Region C.

4.4 Pre-Analysis and Tooling Preparation for the Complex Part (PNNL, Toyota, Magna, Autodesk, PlastiComp)

PNNL began a mold filling pre-analysis for the Toyota automotive complex part adopted in this project. Toyota sent to PNNL two complex part geometries: one with and one without ribs. The sensitivity study was planned to vary several input parameters (e.g. material, wall thickness, filling control (specified time or automatic), and velocity/pressure switchover) and observe the range of outputs (e.g. maximum inlet pressure, maximum clamp force, and total fill time) that are critical to design a molding process. As this work has just begun, only some preliminary results are available. Figure 11 shows the mold filling results for the 2-mm 50wt% LCF/PP complex part simulation. Figure 11 shows (a) the pressure in the complex part at the end of the fill, and (b) the clamp force vs. time. Additional results will be available for variations on the input and will be discussed in the next report.

PNNL is discussing the pre-analysis results with Toyota, Magna and Autodesk to help design the molding of the complex part. Magna and the team participated in teleconference discussions and project updates pertaining to fiber length and fiber orientation measurements from Purdue University. The

molding and tooling discussions on the complex part are in process, but tooling kick-off will require establishment of wall thickness needed to mold 50wt% LCF/PP and 50wt% LCF/PA66 parts under fast and slow fill conditions. This will be based on predictive modeling of the complex part to be able to maintain an average fiber length of 1 to 2 mm. Magna has received 50wt% LCF/PP and 50wt% LCF/PA66 compounds from PlastiComp. Based on processing recommendations from Plasticomp, Magna will provide the machine purging from these materials to Purdue University that will conduct fiber length distributions studies on the machine purge materials. The objective is to demonstrate fiber length distribution from Plasticomp, Magna, and Autodesk be within 10%. Purge materials should contain sufficiently long fibers for plaques and 3D moldings to provide a fiber length exceeding 2 mm average. The milestone related to this task will now have a target completion for August 31, 2014.



Figure 11. (a) Pressure at end of fill in the complex part, and (b) clamp force vs. time for 2 mm wall thickness 50% LCF PP.

4.6 ASMI 3D Fiber Orientation Prediction Improvement (Autodesk)

The prediction of the ARD-RSC model is strongly influenced by the inlet orientation around the gate of an injection-molded part. As the first crucial step to achieve an accurate fiber orientation prediction, Autodesk focused on improving the fiber orientation prediction around the gate in the ASMI 3D Fiber solver. Two major enhancements were achieved, and the newly introduced options will be available in the upcoming ASMI Technology Preview. First, the options for fiber inlet condition, which are already available in the mid-plane/dual domain solver of the current version, were added in the 3D ASMI fiber solver as shown in Figure 12. The inlet condition is served as the boundary condition for fiber orientation calculation, either at the *gate* or *injection location*. The inlet orientation is assumed axisymmetric at the gate interface, and a user can choose from two typical profiles, *fibers aligned at skin/random at core* and *fibers aligned at skin/transverse at core*, or specify *user-supplied inlet condition*.

Second, the accuracy of fiber orientation calculation around the gate has been improved. In the current 3D fiber solver, fiber orientation is quickly changed after a short flow distance away from the gate and the inlet profile applied at the gate cannot be preserved downstream. If the mesh is not fine enough, it cannot resolve the inlet profile. There was also a solver issue which causes the loss of the inlet orientation after a few layers of elements. Figure 13 shows an exemplary plaque model with the refined mesh around the gate. Figure 14 compares the fiber orientation results for the first principal value contour based on the current (ASMI 2015) solver and the new improved solver. It is clearly demonstrated that the inlet orientation is correctly applied around the injection point axisymmetrically, and the inlet orientation is well preserved downstream.

Calculate fiber orientation using	
Folgar-Tucker model with auto-calculated Ci	•
Apply fiber inlet condition at	
Gate	
Fiber inlet condition	
Fibers aligned at skin / random at core	•
Calculate fiber breakage	
Determined by length	▼ Fiber breakage parameters
	Composite property calculation options

Figure 12. Dialog box for fiber solver parameters, showing the new options for fiber inlet condition.



Figure 13. Exemplary model of a plaque with the refined mesh around the gate.



Figure 14. Comparison of fiber orientation result by ASMI 2015 (left) and the new solver (right). The default inlet profile of *fibers aligned at skin/random at core* is applied.

4.6 Fiber Breakage Model Implementation (Autodesk)

The reduced order model (ROM) for fiber length distribution (FLD) using proper orthogonal decomposition (POD) has been implemented in ASMI and was being prepared for inclusion in a public beta test version of ASMI. However, there were other conflicting changes in the 3D fiber solver which caused some problems while testing the ROM/POD method in a few cases. Further, there was strong opposition inside Autodesk against the inclusion of the ROM/POD method in this public beta because of the reliance on a preliminary snapshot analysis run prior to the actual analysis. The actual analysis uses the POD modes generated from the snapshot-analysis. Basically, it means the full flow analysis must be run twice because the accuracy of the POD method is heavily dependent on the quality of the POD modes generated by the preliminary snapshot analysis. Therefore in this quarter, the focus has been on studying alternative methods to remove the need for the snapshot analysis, or to speed-up the snapshot analysis if we are still to use the proposed POD method.

Prof. C.L. Tucker communicated with Dr. Xiaoshi Jin (Autodesk) in May on other ideas that could reduce the memory usage. One of them is to use "Average-Length Models for Fiber Length Attrition" and the other is to explore "A Galerkin Approach to Reduced-Order Fiber Length Modeling", Prof. C.L. Tucker also proposed an approach to speed up the calculations for the ROM model for FLD. The discussion between Prof. Tucker and Dr. Xiaoshi Jin has continued, and a face-to-face meeting on this subject and on fiber orientation model improvement has been planned in the first week of August 2014. In this quarter, a lot of efforts have been exerted attempting to remedy the first snapshot analysis to determine if the accuracy can still be achieved, and to implement the average-length model to assess the effectiveness of this model. So far, the average-length model appears good in terms of average length calculations, but it lacks a length probability profile calculation model that can show the length probability distribution. Autodesk is currently working on including the probability calculation and will then compare these overall results with the full-length model solution.

The Autodesk Moldflow development team has now set up a separate prototype version of ASMI independent from other public beta tests. This new version will include the proposed models specific to this project and will be well tested before sending to PNNL and other project partners for model validation.

5. Publications/Presentations

The Annual Merit Review presentation was given by Dr. B.N. Nguyen at the DOE 2014 Annual Merit Review and Peer Evaluation Meetings, Washington D.C.

6. Patents

None

7. Future Plans

The team will meet at Purdue University on August 6 and 7, 2014 to evaluate the progress, discuss the project milestone status and plans for the coming months and next year. Autodesk continues performing process models improvements and implementations as discussed above. Purdue University continues performing fiber orientation and length measurements for samples cut out from PlastiComp plaques. PNNL continues the ASMI model validation for fiber orientation and length predictions against the experimental data when available for the remaining PlastiComp plaques molded under this project. Molding analysis of the complex part will be refined with the introduction of fiber length distribution in the nozzle (when available) to estimate the remaining average length in the part and make sure that the remaining average length is within 1 to 2 mm. Magna, PlastiComp, and Toyota continues planning for molding the complex part.

8. Budgetary Information

COST PLAN/STATUS

	Budget Period 1								Budget Period 2							
		Q1		Q2	(23	C	14		Q1	(22		Q3	(Q4
Baseline Reporting Quarter	9/11/2012	- 12/31/2012	1/1/2013	3 - 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
		Cumulative		Cumulative		Cumulative		Cumulative		Cumulative		Cumulative		Cumulative		Cumulative
	Q1	Total	Q2	Total	Q3	Total	Q4	Total	Q1	Total	Q2	Total	Q3	Total	Q4	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	\$117,143	\$190,508	\$90,514	\$281,022		
Non-Federal Share	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$178,823	\$178,823	\$219,222	\$398,045	\$160,040	\$558,085		
Total Incurred Costs	\$6,808	\$6,808	\$2,536	\$9,344	\$743	\$10,087	\$418	\$10,505	\$241,683	\$252,188	\$336,365	\$588,553	\$250,554	\$839,107		
Variance																
Federal Share	\$0	\$0	\$5,464	\$5,464	\$237,546	\$243,009	\$237,870	\$480,879	\$64,550	\$545,429	\$10,266	\$555,695	\$36,895	\$592,590		
Non-Federal Share	\$0	\$0	\$0	\$0	\$285,177	\$285,177	\$285,177	\$570,354	-\$50,956	\$519,398	-\$91,355	\$428,043	-\$32,173	\$395,870		
Total Variance	\$0	\$0	\$5,464	\$5,464	\$522,723	\$528,186	\$523,047	\$1,051,233	\$13,593	\$1,064,827	-\$81,089	\$983,738	\$4,722	\$988,460		

9. References

- 1. Phelps JH. 2009. "Processing-Microstructural Models for Short- and Long-Fiber Thermoplastic Composites," PhD Thesis, University of Illinois at Urbana-Champaign, Urbana, IL 61801.
- 2. Phelps JH and CL Tucker III. 2009. "An Anisotropic Rotary Diffusion Model for Fiber Orientation in Short- and Long-Fiber Thermoplastics," *Journal of the Non-Newtonian Fluid Mechanics*, 156(3):165-176.