PNNL-24472

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

July 2015

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Project period: From October 1st 2012 to September 30th, 2016

Reporting period end date: June 30th, 2015
Quarterly report submitted to:
Aaron Yocum, National Energy Technology Laboratory, Morgantown, WV 26507

U.S. DEPARTMENT OF ENERGY

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1. Objective

The objective of this project is to advance *predictive engineering (PE) tools* 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 distribution models previously developed and implemented in the Autodesk Simulation Moldflow Insight (ASMI) package for injection-molded long-carbon-fiber thermoplastic composites into a cohesive prediction capability. In our previous US Department of Energy (DOE) funded project, entitled *"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 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 fiber analysis data generated at Oak Ridge National Laboratory on two-dimensional (2-D) structures of edge-gated plaques and center-gated disks injection-molded from long-glass-fiber/polypropylene (PP) and long-glass-fiber/polyamide 6,6 (PA66) pellets. The present effort aims at rendering the developed models more robust and efficient to automotive industry part design to enable 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 (3D) 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 are measured for the model validation based on a 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 2015, the following technical progress has been made toward project milestones:

1) Magna oversaw the tool build and prepared the molding plan for the complex part of Phase II.
2) PlastiComp hosted a visit by Magna and Toyota on April 23rd to finalize the molding scope and schedule. The plan for molding trials including selection of molding parameters for both LFT and D-LFT for the U-shape complex part was established.
3) Toyota shipped the U-shape complex part tool to Magna on May 28th, 2015.
4) Plasticomp provided 30wt% LCF/PP and 30wt% LCF/PA66 compounded pellets to Magna for molding the complex part.
5) Magna performed preliminary molding trials on June 2nd, 2015 to validate wall thickness, fill profile, tool temperature and shot size requirements for the complex part. These molding trials were successful, and there were no anticipated issues with running the new mold with the 200T Engel machine and auxiliary equipment at Magna.
6) Magna performed the first complex part run on June 16th and 17th, 2015 at Magna's Composite Centre of Excellence in Concord, ON, Canada. Dale Roland of Plasticomp, and Umesh Gandhi of Toyota also attended the molding.
7) Magna discussed and finalized the plan with PNNL and the team for cutting samples from molded parts at selected locations for fiber orientation and length measurements.

8) Magna provided the computer-aided design (CAD) files of the complex parts with and without ribs to PNNL and Autodesk to build the corresponding ASMI models for injection molding simulations. Magna also provided the actual parameters used.
9) Plasticomp provided knowledge and experience of molding LCF materials essential to the successful molding of the parts including optimization of fill speed, tool temperatures, and plasticizing conditions for the 30wt% LCF/PP and 30wt% LCF/PA66 materials in both rib and non-rib versions.
10) Magna molded additional parts for evaluation of mechanical property testing including torsional stiffness on June 29th and 30th, 2015 at Magna's Composite Center of Excellence.
11) Toyota began preparation for the torsion test of the specimens. Preparation of a computer-aided engineering (CAE) model to predict the performance is in progress.
12) Autodesk fixed an error in the implementation of the proper orthogonal decomposition (POD) calculation of fiber length that had caused the ASMI solution to crash and provided an updated build of ASMI containing the fix.
13) Autodesk reviewed and provided feedback for the complex part molding and measurement locations.
14) Autodesk provided support to set up the workflow for ASMI-ABAQUS® analysis, and provided a fix and workaround for a bug in the ASMI-ABAQUS® output command.
15) Autodesk helped build ASMI analysis models for the complex parts with and without ribs.
16) Autodesk worked on improving the orientation prediction accuracy in the shearing layer for 3D meshes based on comparison to measured data of the plaque moldings.
17) PNNL installed a new ASMI version received from Autodesk and performed comparative analyses to assess mid-plane versus 3D fiber length predictions using the full fiber length model and the reduced-order model (ROM) using POD.
18) PNNL presented the project scope, accomplishments, significant results and future plans to DOE and the USCAR Materials Tech Team on June 3rd, 2015.
19) PNNL discussed the cutting of samples from molded parts and finalized a plan with Magna and the team suggesting the sample size, locations and number of samples per location.
20) PNNL and Autodesk built ASMI models for the complex parts with and without ribs, and preliminary analyses of the part with ribs were conducted using the actual molding parameters received from Magna.
21) PNNL worked on a procedure to extract fiber orientation and length results from a 3D ASMI analysis to a 3D ABAQUS® model. This procedure is essential to import ASMI fiber orientation and length to a 3D ABAQUS® model of the part allowing future part structural analysis for weight reduction study.
22) University of Illinois (Prof. C.L. Tucker) advised the team on the selection of sampling locations on the complex part.

4. Progress and Status

4.1 Molding the Complex Parts with and without Ribs (Magna, Toyota and PlastiComp)

The molding trials began by running a series of short shot fill profiles (Figure 1). Melt temperatures and tool temperatures were gradually increased until parts began to flash to establish the maximum limits. The team proceeded to optimize fill speed and pack profile to get the best surface finish and fill of the ribs. The processing trials ran very well with very consistent part weights but there were some issues getting complete fill of the ribs (Figure 2). This is likely due to gas trapped in the thin rib areas but strategies to improve rib filling including increasing plasticizing back pressure or screw rotation were not pursued in an effort to preserve fiber length as much as possible. Venting in the deep ribs to alleviate trapped gas is considered another option that could facilitate complete filling of the ribes.

The parts without ribs were filled much more easily since screw rotation (rpm) and plasticizing back pressure were able to be reduced so there was a possibility to achieve longer fiber lengths in the non-ribbed part. Nozzle purgings were saved fromeach of the trials for fiber length measurement. Table 1 reports Magna's molding matrix for the complex parts with and without ribs.

Figure 1. Short shot fill profiles obtained during molding trials.

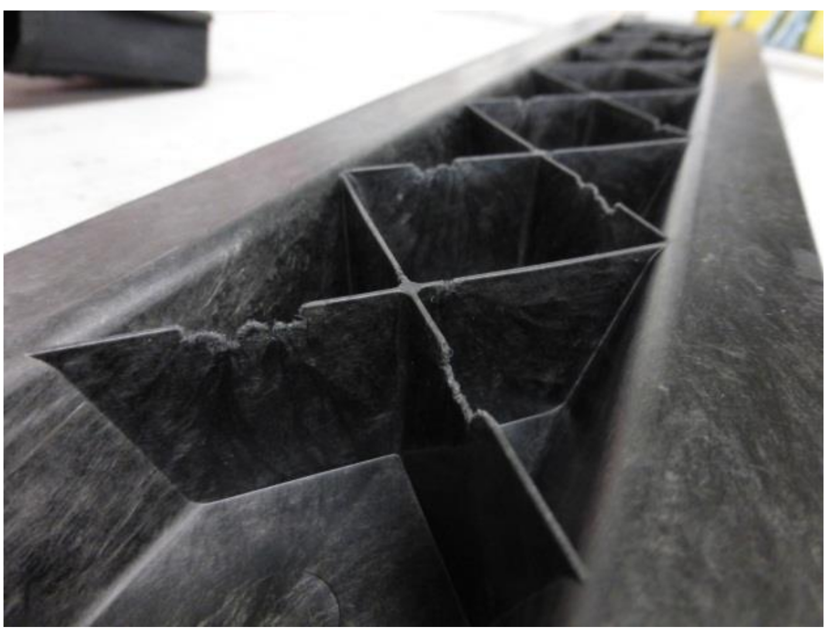

Figure 2. 30CF-PA66 ribs showing incomplete fill due to thin rib and trapped gas.

Table 1. Magna LFT Molding Trial Matrix – U shape Complex Part

Case	Ribs	Resin	CF wt%	LFT/ D-LFT	Trial 1 Date	Parts Molded 1	Trial 2 Date	Parts Molded 2	Total Parts
1	ribs	PP	30%	LFT	06/16/15	13	06/30/15	37	50
2	ribs	PA66	30%	LFT	06/16/15	12	06/30/15	38	50
3	no-ribs	PP	30%	LFT	06/17/15	25	06/29/15	25	50
4	no-ribs	PA66	30%	LFT	06/17/15	22	06/29/15	28	50

Table 2 gathers all the processing parameters that Magna used to mold the parts with and without ribs. Magna also communicated these parameters to PNNL and the team for ASMI process simulations of the complex parts.

Table 2. Magna LFT Molding Trial Processing Conditions – U shape Complex Part

Processing Conditions	
Location:	Magna Exteriors and Interiors - Casmir
Machine	Engel 200 TL
Mold	U-Shape Tool
Molding Date	16/17-June-2015

Material	30CF-PA66	30CF-PA66	30CF-PP	30CF-PP
Rib / No-Rib	Ribs	No Ribs	Ribs	No Ribs
Identification Code	30PALR	30PALN	30PPLR	30PPLN
Mold Temp - Cavity	110 C (230 F)	105 C (220 F)	88 C (190 F)	88 C (190 F)
Mold Temp -Core	115 C (240 F)	105 C (220 F)	82 C (180 F)	82 C (180 F)
Melt Temp	320 C (608 F)	320 C (608 F)	248 C (478 F)	248 C (478 F)
Fill Time	2.64 sec	1.93 sec	2.35 sec	2.24 sec
Fill Speed	70 mm/s (2.75 in/sec)	75 mm/s (2.95 in/sec)	60 mm/s (2.36 in/sec)	60 mm/s (2.36 in/sec)
Packing Pressure (Hydraulic)	33 bar (478 psi)	40 bar (580 psi)	28.3 bar (410 psi)	40 bar (580 psi)
Intensification Ratio	9.0	9.0	9.0	9.0
Packing Pressure (Melt)	297 bar (4,308 psi)	360 bar (5,221 psi)	360 bar (5,221 psi)	360 bar (5,221 psi)
Packing time	3.5 sec	5 sec	3 sec	10 sec
Cooling Time	45 sec	45 sec	46 sec	54 sec
Nomimal wall thickness	2.8 mm	2.8 mm	2.8 mm	2.8 mm
Part Weight (with gate)	274 g	233 g	213 g	193 g
Part Weight (without gate)	269 g	228 g	208 g	188 g

4.2 ASMI Fiber Length Comparative Analyses (PNNL, Autodesk)

Upon receiving an updated ASMI research version from Autodesk, PNNL performed injection molding mid-plane and 3D simulations for the PlastiComp slow-fill 30wt% LCF/PP edge-gated plaque using the full fiber length model and reduced-order model (ROM) using proper orthogonal decomposition (POD) [1-2]. The goal of this study was to assess the prediction accuracy using the ROM-POD model. In all the simulations, the fiber length distribution (FLD) data in the injection molding machine nozzle measured by Purdue was applied as the fiber inlet condition at the injection location (Figure 3). Also, the same set of model parameters were used in all the analyses. The accuracy in fiber length prediction was determined using the 15% accuracy criterion. This criterion was evaluated via the principal tensile and flexural moduli computed using predicted vs. measured FLDs for a prescribed fiber orientation distribution. In this work, predicted fiber orientations at Locations A, B, and C were used in the computation of elastic moduli for these locations (Figure 4).

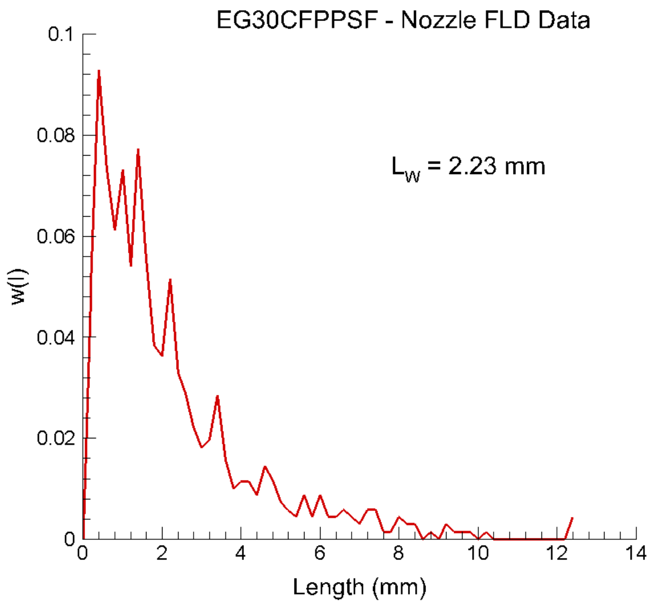

Figure 3. Measured fiber length distribution for the slow-fill 30wt% LCF/PP purge material from the injection molding machine nozzle.

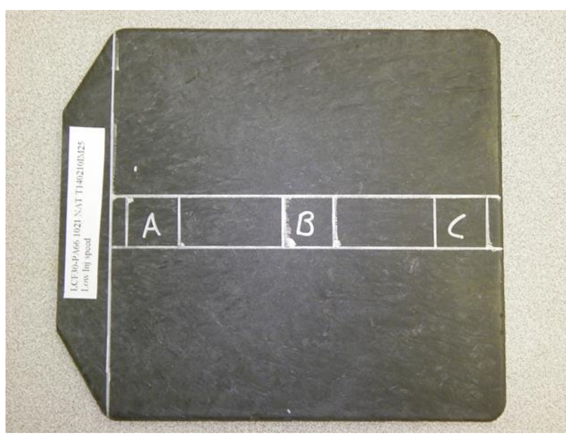

Figure 4. Locations A, B and C defined on an edge-gated plaque where samples were cut out for fiber orientation and length measurements.

Figures 5 to 7, respectively, report the predicted FLDs compared to FLDs measured by Purdue for Locations A, B and C on the slow-fill 30wt% LCF/PP plaque. The weight-average lengths resulting from the predicted and measured distributions are also given in these figures. Both the full fiber length model and the ROM-POD, as well as both mid-plane and 3D ASMI solutions are able to capture the measured length distributions quite well. There is also reasonable agreement between all the predicted FLDs and the corresponding weight-average lengths with the experimental results. Tables 3 to 8 provide the tensile and flexural moduli calculated based on the predicted and measured FLDs for Locations A, B and C on this plaque. Very good agreement of results for the tensile moduli E_{11} and E_{22} as well as for the flexural moduli D_{11} and D_{22} are observed for all three locations. The excellent agreement in predicted stiffness performance is not surprising since the fiber length distributions achieved represent truly long fibers producing high fiber aspect ratio values that bring the elastic moduli near their maximum limits. Modest changes in fiber length in this high aspect ratio range have only very little effect on the composite elastic moduli. A sensitivity study of the fiber length effect on the elastic moduli was completed and reported in our previous quarterly report [3].

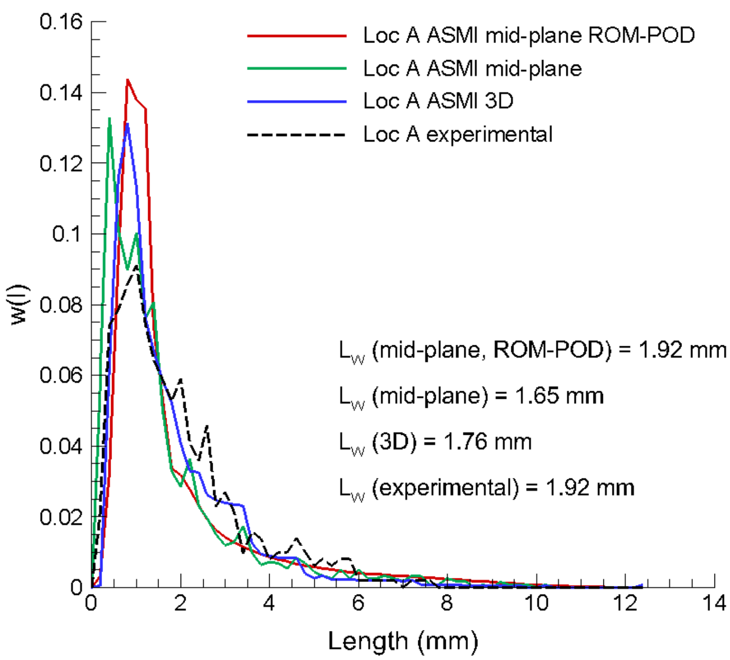

Figure 5. Predicted and measured fiber length distributions for Location A on the slow-fill 30wt% LCF/PP plaque.

Table 3. Computed E_{11} and E_{22} from measured and predicted fiber length distributions at Location A in the slow-fill 30wt% LCF/PP edge-gated plaque.

Tensile Modulus	***E*₁₁** (mid-plane ROM-POD) MPa	***E*₁₁** (mid-plane) MPa	***E*₁₁** (3D) MPa	***E*₁₁** (measured length) MPa
Loc. A	14978 (0.79%)	14387 (3.18%)	14919 (0.4%)	14860

Tensile Modulus	***E*₂₂** (mid-plane ROM-POD) MPa	***E*₂₂** (mid-plane) MPa	***E*₂₂** (3D) MPa	***E*₂₂** (measured length) MPa
Loc. A	17990 (0.82%)	17254 (3.30%)	17917 (0.41%)	17843

Table 4. Computed D_{11} and D_{22} from measured and predicted fiber length distributions at Location A in the slow-fill 30wt% LCF/PP edge-gated plaque.

Flexural Modulus	D_{11} (mid-plane ROM-POD) MPa.mm^3	D_{11} (mid-plane) MPa.mm^3	D_{11} (3D) MPa.mm^3	D_{11} (measured length) MPa.mm^3
Loc. A	59243 (0.75%)	57027 (3.02%)	59024 (0.38%)	58802
Flexural Modulus	D_{22} (mid-plane ROM-POD) MPa.mm^3	D_{22} (mid-plane) MPa.mm^3	D_{22} (3D) MPa.mm^3	D_{22} (measured length) MPa.mm^3
Loc. A	45378 (0.69%)	43817 (2.77%)	45224 (0.35%)	45067

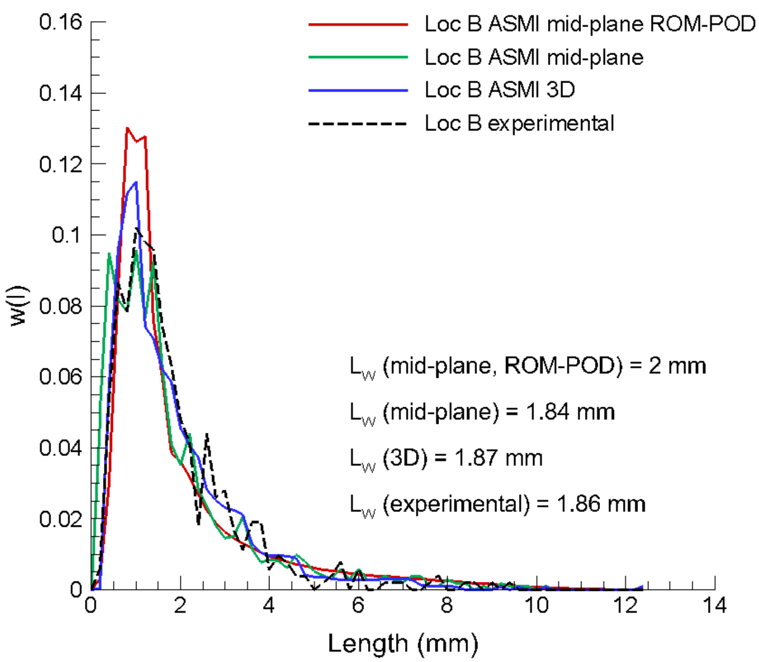

Figure 6. Predicted and measured fiber length distributions for Location B on the slow-fill 30wt% LCF/PP plaque.

Table 5. Computed E_{11} and E_{22} from measured and predicted fiber length distributions at Location B in the slow-fill 30wt% LCF/PP edge-gated plaque

Tensile Modulus	E_{11} (mid-plane ROM-POD) MPa	E_{11} (mid-plane) MPa	E_{11} (3D) MPa	E_{11} (measured length) MPa
Loc. B	13053 (0.20%)	12709 (2.44%)	13021 (0.05%)	13027

Tensile Modulus	E_{22} (mid-plane ROM-POD) MPa	E_{22} (mid-plane) MPa	E_{22} (3D) MPa	E_{22} (measured length) MPa
Loc. B	19419 (0.21%)	18864 (1.94%)	19368 (0.68%)	19238

Table 6. Computed D_{11} and D_{22} based on measured and predicted fiber length distributions at Location B in the slow-fill 30wt% LCF/PP edge-gated plaque.

Flexural Modulus	D_{11} (mid-plane ROM-POD) MPa.mm^3	D_{11} (mid-plane) MPa.mm^3	D_{11} (3D) MPa.mm^3	D_{11} (measured length) MPa.mm^3
Loc. B	54131 (0.19%)	52768 (2.33%)	54006 (0.04%)	54030

Flexural Modulus	D_{22} (mid-plane ROM-POD) MPa.mm^3	D_{22} (mid-plane) MPa.mm^3	D_{22} (3D) MPa.mm^3	D_{22} (measured length) MPa.mm^3
Loc. B	46184 (0.18%)	45080 (2.22%)	46083 (0.04%)	46102

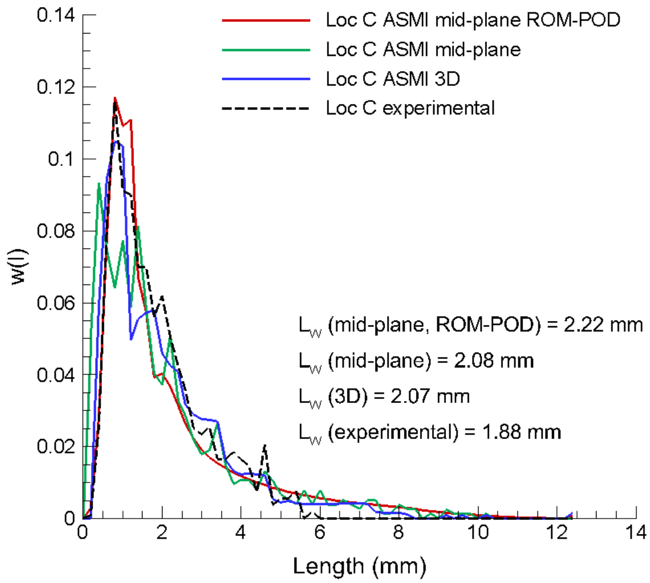

Figure 7. Predicted and measured fiber length distributions for Location C on the slow-fill 30wt% LCF/PP plaque

Table 7. Computed E_{11} and E_{22} based on measured and predicted fiber length distributions at Location C in the slow-fill 30wt% LCF/PP edge-gated plaque.

Tensile Modulus	E_{11} (mid-plane ROM-POD) MPa	E_{11} (mid-plane) MPa	E_{11} (3D) MPa	E_{11} (measured length) MPa
Loc. C	12594 (0.14%)	12271 (2.70%)	12547 (0.52%)	12612

Tensile Modulus	E_{22} (mid-plane ROM-POD) MPa	E_{22} (mid-plane) MPa	E_{22} (3D) MPa	E_{22} (measured length) MPa
Loc. C	18605 (0.15%)	18084 (2.95%)	18528 (0.56%)	18633

Table 8. Computed D_{11} and D_{22} based on measured and predicted fiber length distributions at Location C in the slow-fill 30wt% LCF/PP edge-gated plaque.

Flexural Modulus	D_{11} (mid-plane ROM-POD) MPa.mm^3	D_{11} (mid-plane) MPa.mm^3	D_{11} (3D) MPa.mm^3	D_{11} (measured length) MPa.mm^3
Loc. C	51291 (0.13%)	50040 (2.57%)	51107 (0.49%)	51360
Flexural Modulus	D_{22} (mid-plane ROM-POD) MPa.mm^3	D_{22} (mid-plane) MPa.mm^3	D_{22} (3D) MPa.mm^3	D_{22} (measured length) MPa.mm^3
Loc. C	44323 (0.13%)	43294 (2.44%)	44171 (0.47%)	44379

4.3 ASMI Model for the Complex Parts with and without Ribs (PNNL, Autodesk)

Upon receiving the CAD files of the complex parts (with and without ribs) and the molding parameters from Magna, PNNL worked with Autodesk to build ASMI dual-domain and 3D models for the parts. Preliminary analyses of the complex part with ribs were conducted to exercise the models, to check mold filling, and to prepare for exporting ASMI results to a corresponding ABAQUS® model for future structural analyses of the parts. A 3D ASMI finite element mesh of the complex part with ribs for the injection molding simulation is shown in Figure 8. The mesh is finely discretized for good element aspect ratios for accurate solutions.

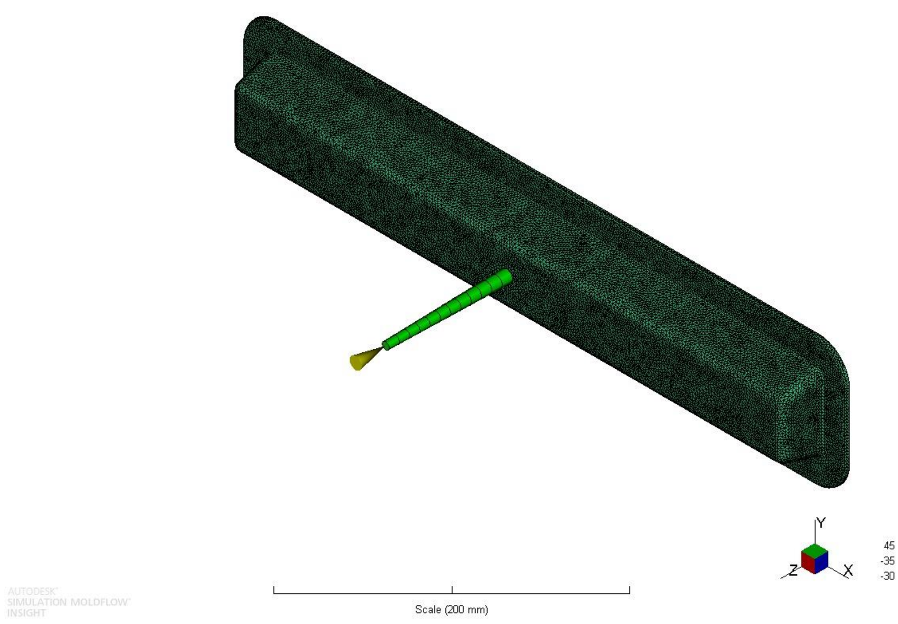

Figure 8. A 3D ASMI finite element model for the complex part with ribs for the analysis.

Figures 9 and 10 show the contours of fill progress based on 3D and dual-domain models of the part molded from the 30wt% LCF/PP material. Similar 3D and dual-domain results are observed.

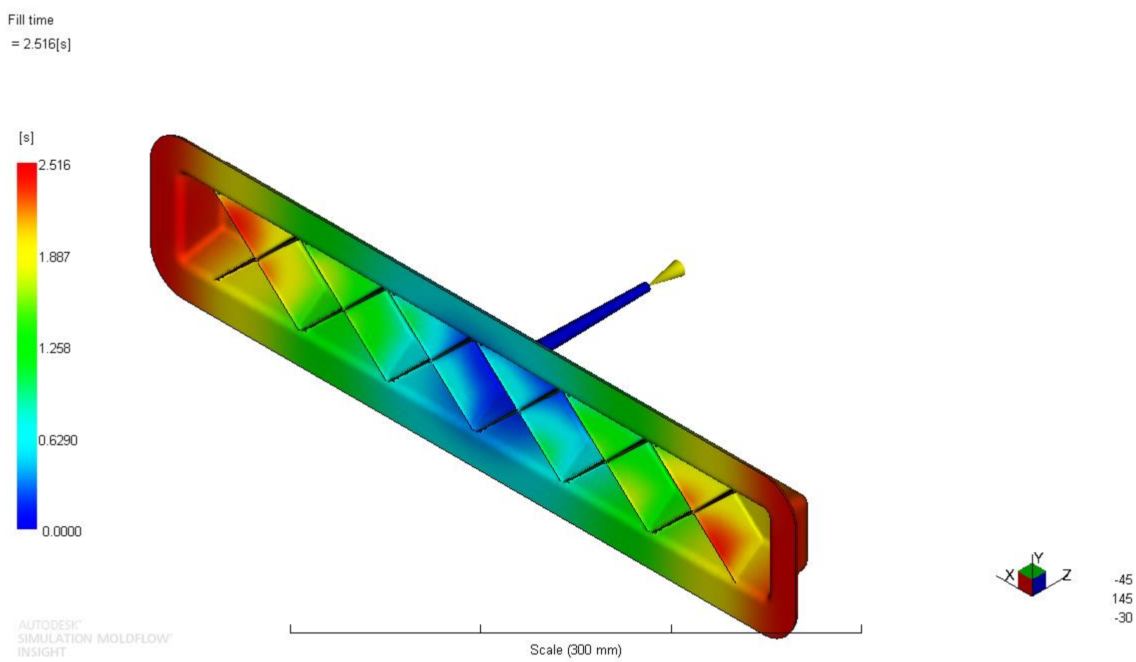

Figure 9. Contour of fill time obtained from the dual-domain model of the complex part with ribs molded from 30wt% LCF/PP.

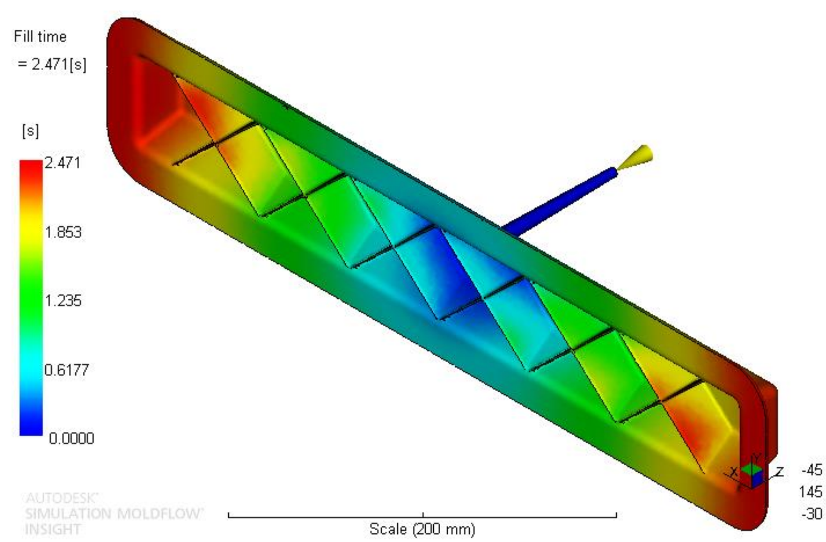

Figure 10. Contour of fill time obtained from the 3D model of the complex part with ribs molded from 30wt% LCF/PP.

4.4 Locations on the Complex Part for Fiber Orientation and Length Measurements (PNNL and Team)

PNNL discussed with the team to define the locations where the (8 mm x 12 mm) samples will be cut out of the molded parts for fiber orientation and length measurements. The locations named A, B, C, and D are illustrated in Figures 11 and 12. Location D is on a rib for the part with ribs (Figure 12). These locations were carefully defined to validate ASMI model predictions. Location A provides the orientation and length data in the immediate gate region. Location B will provide information at a region remote from the gate but on the same surface as Location A. Location C on the wall will allow us to examine fiber orientation and length on another surface, and Location D on a rib will allow investigation of fiber orientation and length in a typical 3D feature.

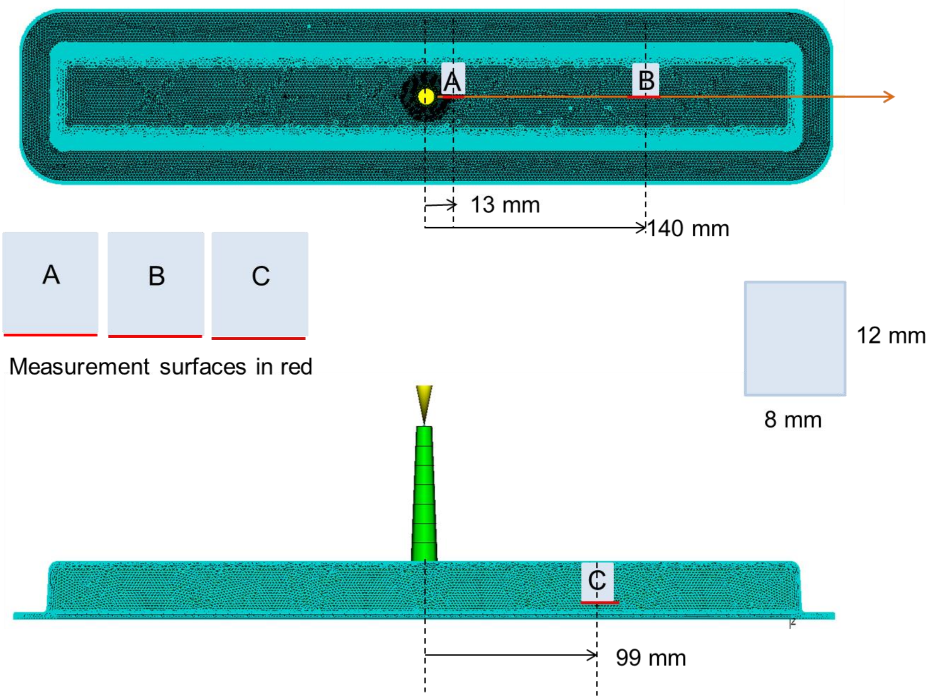

Figure 11. Part locations A, B and C where samples will be cut out for fiber orientation and length measurements. The sample size and the measurement surfaces for fiber orientation measurement are also defined in this figure.

Figure 11. Location D on a rib where samples will be cut out for fiber orientation and length measurements. The surface for fiber orientation measurement is marked in red.

5 Publications/Presentations

L.S. Fifield and B.N. Nguyen *"Predictive Engineering Tools for Injection-Molded Long-Carbon Fiber Thermoplastic Composites"* presented to the USCAR Materials Tech Team on June 3rd, 2015.

4 Patents

None

5 Future Plans

Magna will prepare cut-out samples from the designated locations of the part for fiber length and fiber orientation measurements. These location areas have been scribed into the tool for exact location reference (Figure 13). Nozzle purgings will also be extracted for fiber length measurement. The U-shape complex mold will be shipped to Plasticomp in early July, and Magna will support D-LFT molding trials at Plasticomp. The Virginia Polytechnic Institute and State University (Virgina Tech) joined the team in July 2015 and will perform fiber orientation and length measurements for the samples cut out from the parts. Autodesk continues 3D fiber orientation improvement. Autodesk will provide technical support to PNNL to validate fiber orientation and length predictions upon receiving measured data from Virginia Tech. Toyota will perform mechanical testing to assess mechanical performance of the parts under torsion and bending.

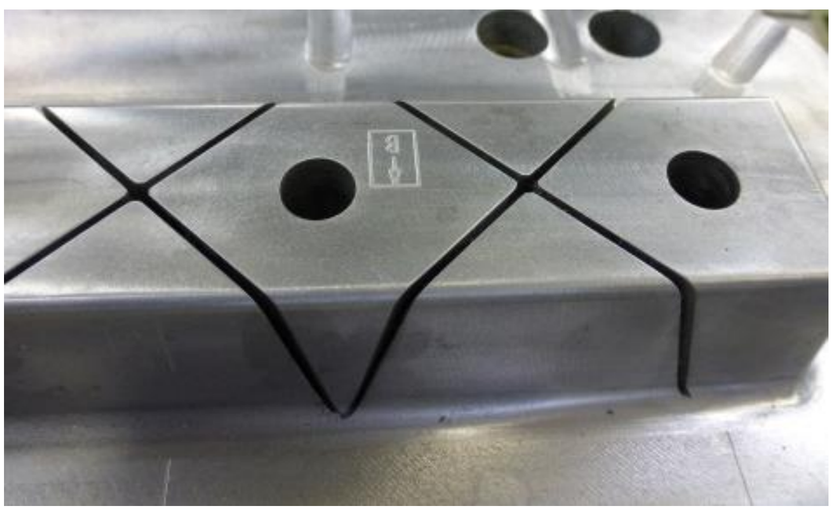

Figure 13. Scribing of a selected location where samples will be cut out from the molded part for fiber orientation and length measurements. This picture shows a view of the core side of tool insert.

6 Budgetary Information

	Budget Period 2									
	FY15-Q2		FY15-Q3		FY15-Q4		FY16-Q1		FY16-Q2	
Baseline Reporting Quarter	1/1/2015 - 3/31/2015		4/1/2015 - 6/30/2015		7/1/2015 - 9/30/2015		10/1/2015 - 12/31/2015		1/1/2016 - 3/31/2016	
	Q2	Cumulative Total	Q3	Cumulative Total	Q4	Cumulative Total	Q1	Cumulative Total	Q1	Cumulative Total
Baseline Cost Plan										
Federal Share	$101,927	$593,312	$56,013	$649,325	$131,920	$781,245	$131,920	$913,166	$87,855	$1,001,021
Non-Federal Share	$102,294	$672,648	$102,294	$774,942	$102,294	$877,235	$102,294	$979,529	$102,294	$1,081,822
Total Planned	$204,221	$1,265,960	$158,307	$1,424,267	$234,214	$1,658,480	$234,214	$1,892,694	$190,149	$2,082,843
Actual Incurred Cost										
Federal Share	$71,374	$588,765	$58,637	$647,402		$647,402		$647,402		$647,402
Non-Federal Share	$127,783	$1,083,395	$135,147	$1,218,542		$1,218,542		$1,218,542		$1,218,542
Total Incurred Costs	$199,157	$1,672,160	$193,784	$1,865,944		$1,865,944		$1,865,944		$1,865,944
Variance										
Federal Share	$30,553	$4,547	-$2,624	$1,923						
Non-Federal Share	-$25,489	-$410,747	-$32,853	-$443,601						
Total Variance	$5,064	-$406,200	-$35,477	-$441,678						

The variance of the budget federal share cost plan to actual incurred cost cumulative for this quarter is small. The large negative variance of budget non-federal share cumulative contributing to the large total variance as of this quarter is due to the generous cost-share contributions of partner Autodesk. As of this quarter, Autodesk has contributed $746,435, or $386,435 above their $360,000 total cost-share contribution planned for the project.

7 References

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