Effects of Preform Deformation Behavior on the Properties of the Poly(ethylene terephthalate) Bottles

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ABSTRACT: Plastics bottles made out of poly(ethylene terephthalate) (PET) are usually produced by injection stretch blow molding. Optimization of the process parameters is necessary to achieve bottles with adequate top load and burst strength. However, doing so experimentally is time-consuming and costly. To overcome this difficulty, simulation packages based on finite element analysis methods have been developed. In this study, process optimization of a 350-mL PET fruit juice bottle was carried out by means of BlowView and ANSYS simulation packages. BlowView was used for the ISBM process simulation and ANSYS for structural analysis of the bottles. The bottles were produced under different process conditions where the timing of the stretch rod movement was varied in relation to the activation of the blow pressure. The simulation results obtained through the both simulation packages were compared with experimental results. It was found that bottles of highest quality were produced if the sequencing of axial stretching and radial inflation results in simultaneous biaxial deformation of the preform. Truly biaxial orientation of PET molecules improved both top-load and burst resistances of the bottles. The structural simulation studies performed by the ANYSYS simulation package validated most of our experimental findings. © 2012 Wiley Periodicals, Inc. J Appl Polym Sci 000: 000–000, 2012

Key words: simulation; stress; polyethylene terephthalate; injection molding; mechanical properties

INTRODUCTION

Poly(ethylene terephthalate) (PET) is the material of choice for fruit juice packaging due to its excellent clarity, good mechanical and barrier properties, and ease of processing. PET bottles used for the fruit juice packaging are generally made by injection stretch blow molding (ISBM). An injection molded preform is deformed radially by the internal (blow) pressure and axially by the stretch rod. The air pressure loading consists of two consecutive stages: preblow and final blow. The preblow forms most parts of the bottle with a low pressure, whereas the final blow exerts a higher pressure to form the intricate details of the bottle.[1] Both process parameters and the preform design are known to affect bottle qualities such as top load and burst strength.[2] The process parameters comprise preform temperature, the timing of the stretching and blowing stages, stretch rod speed, and preblow and final-blow pressures. There are numerous studies related to the effect of process parameters on the bottle properties.[3–7] Haddad et al. investigated the ISBM process for a 600-mL PET bottle utilizing B-SIM simulation software; for a given preform shape and temperature, they obtained wall thickness and von Mises stress distribution along the arc of the bottle. The simulated bottle file was exported to the ANSYS finite element analysis software for structural analysis to verify the mechanical strength of the bottles. The ANSYS results were used to identify key areas of structural weakness in relation to the thickness distribution from B-SIM simulation.[3] Yang et al. studied the processing of a 330-mL PET bottle using a finite element model incorporating heat transfer between the stretch rod, the preform, and the mold with a view to optimizing process conditions. Comparison of the predicted wall thicknesses with the measured showed good agreement along most parts of the bottle.[4] In one of the earlier studies, an integrated simulation of preform reheating, stretching and inflation was conducted in a two-stage ISBM process for the manufacture of 250-mL PET water bottle.[5] Experimentally measured preform temperature profiles were used in the simulations. The predicted bottle wall thickness distribution was found to be within the limits of experimental scatter. McEvoy et al. simulated the ISBM process for 1/3 and 2 L bottles based on production line setting.[6] To evaluate the

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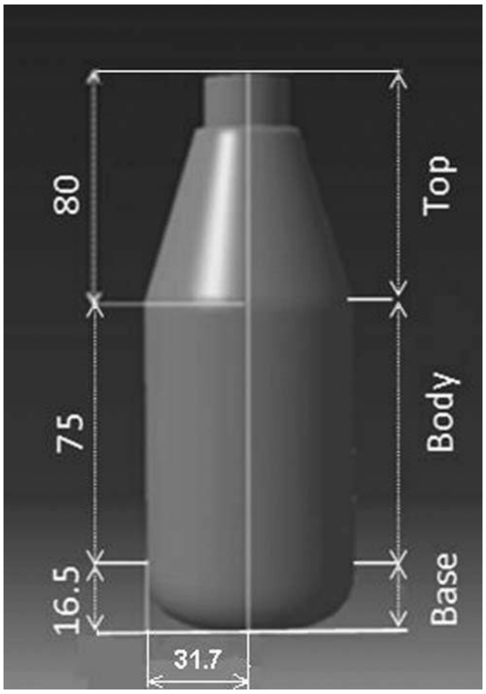

Figure 1 The CAD of the bottle mold.

flexibility of the complete finite element simulations, variations of stretching times and speed were considered for a given preform and bottle. Thickness profiles of the bottles were compared favorably with the experimental results. In another study, the mechanism of preform deformation for a 680-mL bottle was observed by means of a transparent mold; the preform growth was analyzed during stretching and blowing stage.[7] The wall-thickness distributions of the bottles obtained under different preblow delay time were compared. It was found that the delay time of preblow is a key factor in the preform growth; the types of preform growths were found to depend on the geometry and size of preform, the hoop and longitudinal stresses within it, and the temperature distribution along it. In our previous publications, we have shown that the manufacturing of good quality PET bottles depends on both bottle design and processing parameters.[8,9] In this study, we aimed to use an integrative simulation method to investigate the effect of stretch rod timing relative to blow pressure activation. To validate the prediction of the simulation, bottle performance was compared with experimental results. In the first stage of the work, BlowView 8.4 software was used to simulate the PET fruit juice bottle production at four different processing conditions; one being the standard conditions set by the manufacturers of the ISBM machine. Then the ANSYS software was used for structural analysis of the simulated bottles. In the second stage of the work, bottles were produced in the laboratory ISBM machine and the performance of the bottles was assessed in terms of top-load and burst resistances. Finally, the simulation results obtained through the BlowView and the ANSYS simulation packages were compared with the results for the physical bottles.

SIMULATION STUDY

Material

The PET resin used was a food grade (9921W) from Eastman Chemical Company (Tennessee) with an intrinsic viscosity of 0.80 dL/g and viscohyperelastic material model was used in simulation studies. The model has been developed by Pham et al. to represent the behavior of PET during the stretch-blow molding process.[10]

Bottle mold and preform design

The bottle mold used in this study is a 350-mL PET fruit juice bottle (Fig. 1). The preform design, which is generated by BlowView version 8.4; and a typical

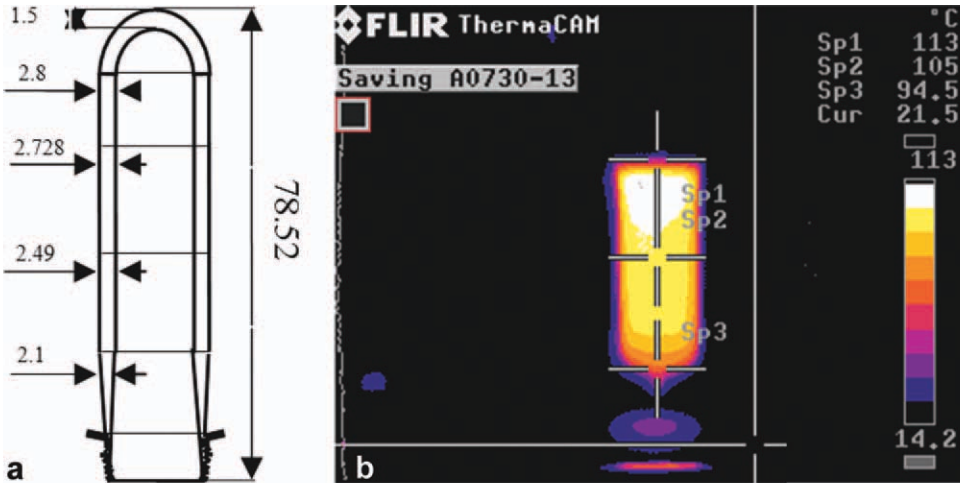

Figure 2 Preform profile (a) thickness and (b) temperature. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

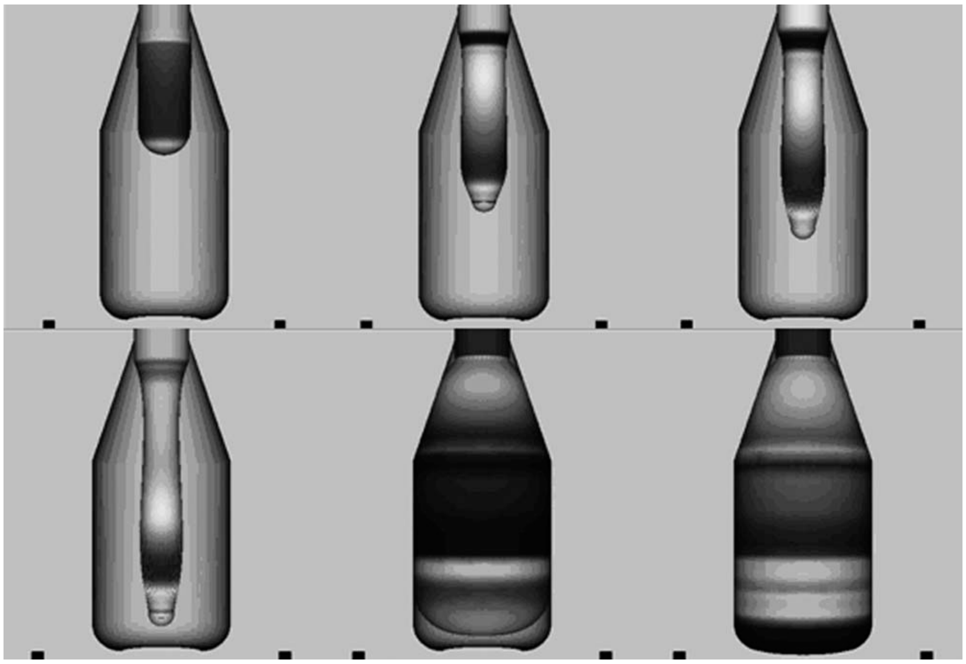

Figure 3 Preform deformation steps—Model 1.

temperature profile of preform, which is obtained by a thermal imaging camera (*FLIR ThermaCAM PM 595*), are shown in Figure 2(a,b), respectively.

Process simulation

In this study, a total of three different processing models were generated; each model has a different set of stretch rod movement and pressure profile as a function of time. Processing conditions suggested by the manufacturers of the machine (AOKI, Japan) were also included under "standard model."

1. Model 1: The stretch rod is engaged at the same time with the preblow pressure (Fig. 3).
2. Model 2: The stretch rod moves only half way down the bottle mold prior to the application of the preblow (Fig. 4).
3. Model 3: Preblow pressure is applied without any stretch rod movement generating free-blow conditions (Fig. 5).
4. Standard Model: Preblow is applied shortly after the stretch rod touches the bottle base (Fig. 6).

The process parameters used in the simulation and the experimental study are given in Table I. Preform weight and preform temperature profile were kept the same for all the models used. The preblow pressure and the final-blow pressure were set at 0.4 and 2 MPa, respectively, throughout the study. The BlowView (version 8.4) simulation software was used to obtain thickness and stress distributions on the bottles; whereas the ANSYS software was used for the analysis of bottle top-load and burst pressure resistance.

The BlowView and ANSYS simulation packages

The BlowView Plastic Blow molding software, which has been developed at the Industrial Materials Institute-Canadian National Research Centre (IMI-CNRC), simulates and optimizes blow molding processes.[11]

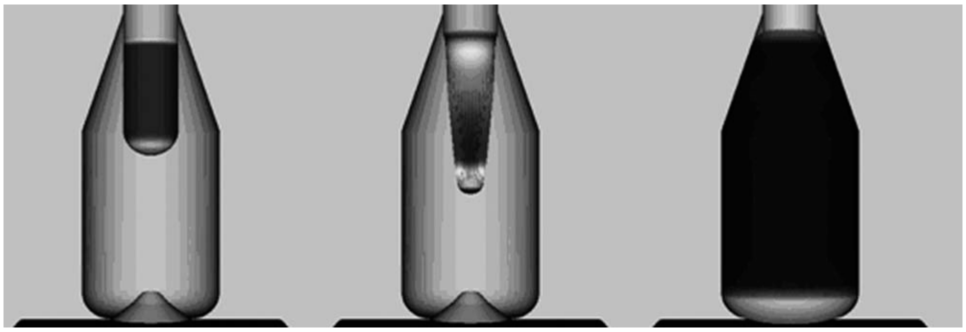

Figure 4 Preform deformation steps—Model 2.

Figure 5 Preform deformation steps—Model 3.

The simulation package helps to predict how the blow molded parts will preform before committing to expensive tool manufacture. The software solves the nonisothermal solid mechanics constitutive equations specifically for the individual phases of the blow molding process. It incorporates thermomechanical material models: viscoelastic models for polyolefins and viscohyperelastic material models for PET. The viscohyperelastic material model is based on the assumption of an additive decomposition of the stress into hyperelastic and viscous contributions. The model takes into account strain-rate and temperature effects, effectively represents strain hardening properties of PET. Coefficients used to characterize the hyperviscoelastic material properties are obtained by biaxial stretching tests performed on the Brucker machine, available at the IMI-CNRC.

The ANSYS simulation softwares have been developed by ANSYS, a leading simulation software company. The "ANSYS Structural" module addresses the unique concerns of pure structural simulations. It offers both linear and nonlinear structural capabilities. The software is capable of reading the output files generated by BlowView simulation software for structural analysis purposes.[12]

Simulation of top-load and burst pressure resistances with ANSYS software

ISBM bottles are required to demonstrate high top-load and burst pressure resistances. To compare the effect of changes in the timing of the stretch rod movement in relation to the blow pressure activation on the bottle properties, the processing of the bottles were simulated under different processing regimes by means of the BlowView software. The resultant simulation files were then transferred into the ANSYS software to analyze the burst pressure and top-load resistance of the bottles. For the structural analysis of the bottles, instead of using a constant

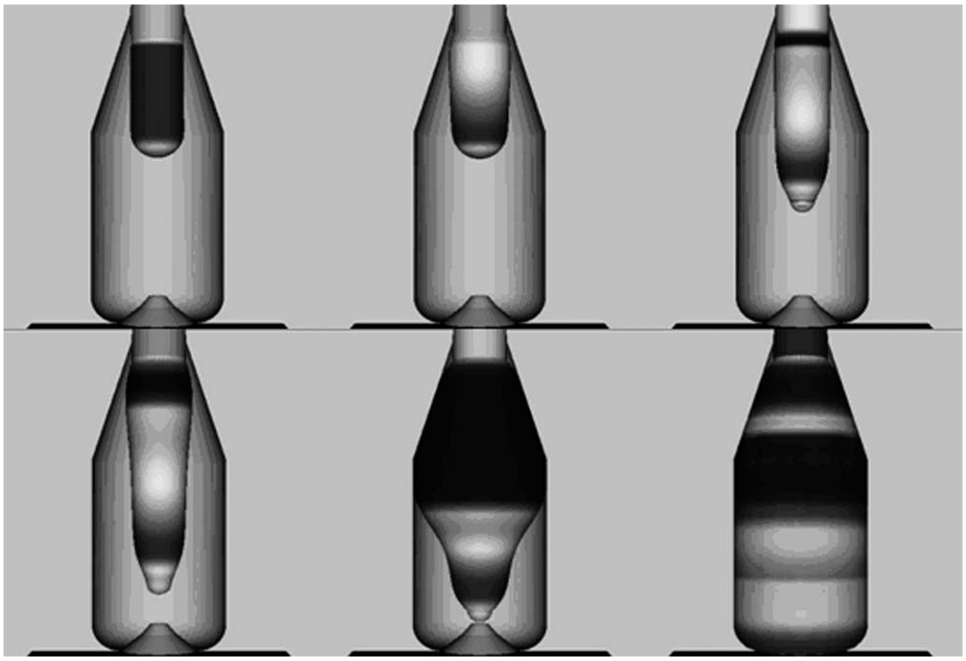

Figure 6 Preform deformation steps—standard model.

TABLE I
Process Parameters used in the Simulation and Experimental Study

	Model 1	Model 2	Model 3	Standard model
Preblow pressure start (s)	0.10	0.12	0.12	0.12
Final blow pressure start (s)	0.18	0.14	0.12	0.12
Blow pressure finish (s)	3.18	3.14	3.12	3.12
Stretch rod start (s)	0.10	0.10	3.00	0.30
Stretch rod finish (s)	0.17	0.14	3.07	0.37

value to define the material properties, microstructure-dependant mechanical performance models were used to calculate typical mechanical properties including Young's Modulus, yield stress as shown in our recent publication.[13]

In the top-load analysis, the constraints were applied at the base section of the bottle. Loads varying from 200 to 400 N were then applied to the top section of the bottle. The maximum equivalent stresses and the maximum deformation on the bottle surface were recorded. In the burst resistance analysis, the top section of the bottle was clamped, pressures varying from 1.0 to 1.5 MPa were applied inside the bottle. Maximum stress and deformation values were then recorded.

TABLE II
ISBM (AOKI SB III-100H-15) Process Parameters

Process parameters	
Screw	
Diameter (mm)	38
Screw speed (rpm)	100
Nozzle diameter (mm)	3
Hot runner block (°C)	
Sprue	275
Block	275
Nozzle	295
Barrel temperature (°C)	
Front	275
Middle	275
Rear	270
Nozzle	275
Injection pressure	
Primary (MPa)	13.73
Secondary (MPa)	5.88
Injection speed (m/s)	200
Stretch blow molding	
Mold temperature (°C)	15
Preblow pressure (MPa)	0.4
Final blow pressure (MPa)	2
Machine oil temperature (°C)	50
Stretch rod speed (m/s)	1.0
Stretch rod diameter (mm)	6

TABLE III
Weight Distribution of the Bottle Sections

	Weight distribution (g)		
	Top	Body	Base
Model 1	9.7 ± 0.05	5.0 ± 0.0	4.9 ± 0.05
Model 2	9.5 ± 0.05	5.0 ± 0.0	5.1 ± 0.05
Model 3	9.4 ± 0.05	5.0 ± 0.0	5.2 ± 0.05
Standard model	9.2 ± 0.22	5.1 ± 0.05	5.25 ± 0.16

EXPERIMENTAL STUDY

Injection stretch blow molding process parameters

AOKI SB III-100H-15 single-stage ISBM machine was used for the bottle production in this experimental study. The process parameters are provided in Table II.

Top-load strength

Top-load strength assesses the overall durability of the bottles necessary for filling and stacking the bottles during manufacturing, storage and distribution. The top-load strength tests were conducted using the INSTRON 4466 instrument equipped with a top-load test platform. At least five bottles are tested to achieve an average value.

Burst strength

Burst strength, the pressure at which the bottle bursts, provides an assessment of the overall stability of the bottle under carbonation pressure of the content. It is particularly important in bottles intended for carbonated beverages; to ensure bottles do not blow up at the filling stage and filled bottles do not expand excessively during storage and/or during bottle warming for pasteurization purposes. A Topwave Burst Tester (BR3000), with "Ramp Fill" capability, was used. At least five bottles were tested to achieve an average value.

Material distribution

To measure the material distribution in the bottle, the bottles were cut into three sections: "base," "body," and "top" by a specially designed hot-wire cutter (Fig. 1). The bottle sections were separately weighted on a precision scale and recorded for assessment.

Temperature profile on the preform

The thermal imaging camera (FLIR Systems ThermaCAM PM595)

The thermal imaging camera was used to record the temperature profile of the preforms just before the

TABLE IV
Experimental Burst Pressure Resistance and Volume Expansion Values

	Burst pressure (bars)	Volume expansion (%)
Model 1	12.5 ± 0.2	91.1 ± 13
Model 2	5.2 ± 2	4 ± 0.9
Model 3	12.6 ± 0.68	82.5 ± 25.9
Standard model	13.2 ± 0.27	99.8 ± 8.0

preform is stretched and blown into the bottle mold. The preform temperature profile was then input to the BlowView simulation studies.

RESULTS AND DISCUSSION

Following the bottle production according to the three different models and the standard model, the bottles were weighed to assess the material distribution under different processing conditions. Table III shows the weight of top, body, and base of the bottles for all models.

In Model 1, stretch rod is activated at the same time with the preblow pressure and the stretch rod reaches all the way to the bottle base. During stretching, the preform end-cap moves away from the neck and stretches further, hence the preform end-cap thins out, resulting in lower base weight. In Model 2, stretch rod moves only half-way down the bottle mold, much less axial stretching occurs before the activation of the blow. Hence, the base is heavier compared to the Model 1. In Model 3, the stretch rod is not used; free blow condition becomes prevalent; this improves material distribution across the bottle sections due to truly biaxial deformation of the preform. In the standard model, simultaneous axial and radial deformation of the preform is observed as shown in Figure 6. The biaxial orientation of the preform results in a more even material distribution across all sections. When the PET material is subjected to sequential orientation, stress levels are higher compared to biaxial orientation mode.[14] Hence, under biaxial deformation mode, the preform deformation speed would be higher, improving the overall strength of the bottles.

TABLE V
Experimental Top-Load Resistance and Compressive Strength Values

	Max compressive load (*N*)	Extension (mm)	Compressive strength (MPa)
Model 1	321 ± 30	−5.26 ± 0.54	5.43 ± 0.51
Model 2	205 ± 27	−2.54 ± 0.32	3.47 ± 0.45
Model 3	374 ± 11	−6.03 ± 0.31	6.3 ± 0.19
Standard model	394.54 ± 31	−6.2 ± 0.09	6.67 ± 0.52

TABLE VI
Maximum Stress Values under the Burst Resistance Simulations via ANSYS

Internal pressure (MPa)	Maximum stress (N/mm^2)			
	Model 1	Model 2	Model 3	Standard
0.8	134.07	287.36	135.01	124.55
0.9	150.83	323.28	151.89	140.13
1	167.59	359.2	168.77	155.71
1.1	184.35	395.12	185.65	171.29
1.2	201.11	431.04	202.52	186.86
1.3	217.86	466.96	219.4	202.43

The highest burst resistance value was achieved in the standard model and the lowest one in Model 2 (Table IV). However, the burst resistance values for the Model 1, the Model 3, and the standard model are found to be very close to each other.

The top-load resistance of the bottles shows the same trend as in burst resistance (Table V). The maximum top-load resistance value was reached for the bottles produced by standard model, closely followed by the bottles produced according to the Model 3 and the Model 1. The high biaxial orientation of PET molecules would be achieved under simultaneous axial and radial deformation (standard model) and under free blow conditions (Model 3). That is most likely to be the reason for high mechanical performance of the bottles produced according to standard model and Model 3.

The bottles were produced by the BlowView 8.4 simulation software according to the three models proposed and the standard model currently in use. These simulated bottles were then transferred into ANSYS software to carry out top-load and burst resistance tests. The burst resistance and top-load values obtained by ANSYS are given in Tables VI and VII, respectively.

According to the burst resistance results obtained through ANSYS simulation software, bottles produced according to the Model 1 and the standard model were found to be stronger than the Model 2 and Model 3 bottles (Table VI). In this context, the burst pressure values obtained by means of ANSYS simulation are in harmony with the actual burst

TABLE VII
Maximum Stress Values under the Top-Load Simulations via ANSYS

	Maximum stress (MPa)			
Load (*N*)	Model 1	Model 2	Model 3	Standard
200	4.98	15.71	16.7	5.52
250	6.24	19.67	20.89	6.91
300	7.49	23.63	25.08	8.3
350	8.73	27.53	29.27	9.67
400	9.98	31.49	33.46	11.06

pressure values obtained by the experimental study (Table IV).

Top-load resistance simulations carried out via ANSYS are shown in Table VII. While standard model and Model 1 resulted in strong bottles, Model 2 and Model 3 bottles were found to be inferior in terms of their top-load resistance. The simulation results from ANSYS are not in harmony with the experimental results for all models (Table V). In particular, Model 3 bottles showed high top-load resistance experimentally. However, the simulation via ANSYS predicts a very low top-load resistance. We were not able to validate our experimental finding for the top-load strength of the bottles produced under Model 3.

CONCLUSIONS

In this study, we used an integrative simulation method to investigate how the timing of the stretch rod in relation to blow pressure activation affects the bottle properties and also aimed to validate our predictions via experimental work. A total of four different processing models were considered. Preform weight and preform temperature profile were kept constant for all processing models. Each model had a different stretch rod and blow pressure activation timing, resulting in different preform deformation behavior.

We found that the 350-mL PET fruit juice bottle produced by the standard model has achieved the best qualities in terms of top-load and burst resistances. In this model, the sequencing of axial stretching and radial inflation introduced simultaneous biaxial deformation of the preform as demonstrated by the simulation studies. The truly biaxial orientation of PET molecules improved the overall strength of the bottles. The structural simulation studies performed by ANYSYS simulation package validated most of our experimental findings.

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