Optimization of Poly(ethylene terephthalate) Bottles Via Numerical Modeling: A Statistical Design of Experiment Approach

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ABSTRACT: Poly(ethylene terephthalate) bottles, commonly used for carbonated soft drink packaging, occasionally fail because of environmental stress cracking at the petaloid base. At raised temperatures, particularly during hot summer months, increased carbonation pressure of the contents aggravates susceptibility to stress cracking. In this study, numerical modeling with finite element analysis techniques was used to redesign the petaloid base of bottles to improve stress-crack resistance. An experimental design based on an algorithmic partial cubic method was employed. Mathematical modeling of the principal internal stress as a function of key design parameters identified optimal dimensions for the petaloid base. The improvement in stress-crack resistance was verified by experimental studies. © 2009 Wiley Periodicals, Inc. J Appl Polym Sci 114: 1126–1132, 2009

Key words: computer modeling; plastics; polyethylene (PE); simulations; stress

INTRODUCTION

Many different kinds of bottles are used for carbonated soft drink (CSD) packaging, varying in size, material, shape, stability, and cost.[1] Poly(ethylene terephthalate) (PET) has been the most widely used resin, offering excellent clarity, good mechanical and barrier properties, and ease of processing.[2] The most commonly used design is the one-piece bottle with a petaloid base. The petaloid base makes the bottle self-standing, and the one-piece design is easier to manufacture and recycle than the alternative two-piece bottle.

The main problem with the one-piece bottle is that the petaloid base is prone to failure at a stress much lower than the normal failure stress of the material. This failure occurs in the form of either a radial crack or a circumferential crack and is due to the combined effect of stress from the carbonation pressure, the aggressive environment generated by the contents of the bottle, and the line lubricants used in the manufacturing of CSD bottles. This phenomenon, known as environmental stress cracking (ESC), occurs mainly during storage of the bottles; it has been a major inconvenience for manufacturers and distributors.

Although numerous studies have been conducted exploring the cause of the ESC phenomenon in plastics, a clear understanding of the mechanism remains elusive.[3–15] Also, in most of the published research, the focus has been on the characteristics of ESC in PET generally.[3–5] Only a few research articles have addressed the problem of ESC in PET bottles and specifically in the petaloid base.[6,7] In one of the earliest studies, Tekkanat et al.[6] developed a test method to determine the environmental stress crack resistance of blow-molded PET containers. Their method not only gauges the susceptibility of different types of one-piece PET containers to ESC but also provides valuable information on the ESC characteristics of the containers. They identified crazing in the base as a precursor of stress cracking and suggested that the design of the container could be changed to increase the craze initiation pressure by improvements in the dimensional stability of the bottles. In a recent study, Lyu and Pae[7] considered the variation of the physical properties of PET according to the stretch ratio experienced in a blow-molded PET bottle, and they redesigned the petaloid shape of the base. From measurements of the tensile yield stress of stretched PET, they concluded that to improve the mechanical properties of a blow-molded PET bottle, the stretch ratio should be higher than the strain-hardening point of the material. They observed that the structural weakness of the base was related to an abrupt change in material thickness between the center of the base and the bottle walls. In an attempt to eliminate ESC, they shifted the location of the maximum principal stress to a stronger region of the base and reduced the magnitude of the

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principal stress. Their new base design significantly improved the crack resistance of the PET bottles.

Our study also was aimed to improve ESC resistance by modifying the design of the petaloid base. Commercial computer-aided design/finite element analysis software was used to simulate the internal stresses arising from the carbonation pressure of the bottle content. An experimental design and optimization program was then used to mathematically model the simulated internal stress as a function of key design parameters to optimize the dimensions of the petaloid base. Experimental verification was performed through the testing of the new base according to environmental stress crack resistance test methods.

EXPERIMENTAL

Material specifications

The PET resin used was a food grade (9921) from Eastman Kodak Company (USA) with an intrinsic viscosity of 0.80 dL/g. The material properties for the virgin PET were a Young's modulus of 2.9 GPa, a yield strength of 55 MPa, a Poisson ratio of 0.4, a thermal expansion coefficient of $7 \times 10^{-5}\,{}^{\circ}\mathrm{C}^{-1}$, and a density of 1200 $\mathrm{kg/m^3}$.

Bottle processing conditions

Bottles with a 1500-mL volume were produced with a two-stage injection stretch blow-molding machine under standard operating conditions. Injection-molded preforms were reheated to temperatures in the range of 90–115°C, that is, between the glass-transition temperature and the cold-crystallization temperature of PET. Reheating of the perform was done with infrared radiation from an array of lamps in conjunction with convection. The neck above the support ring was kept cooler than the body of the preform to prevent distortion of the bottle closure region; similarly, the base of the preform was kept cooler to prevent piercing by the stretch rod. After axial temperature profiling, the preform was stretched axially by the stretch rod and radially by the blow pressure until it took up the shape of the bottle mold.

NUMERICAL SIMULATION

Simulation via CATIA

Maximum von Mises stress values were simulated via finite element analysis with CATIA software (version 5, release 14).

Computer-aided design of the bottle

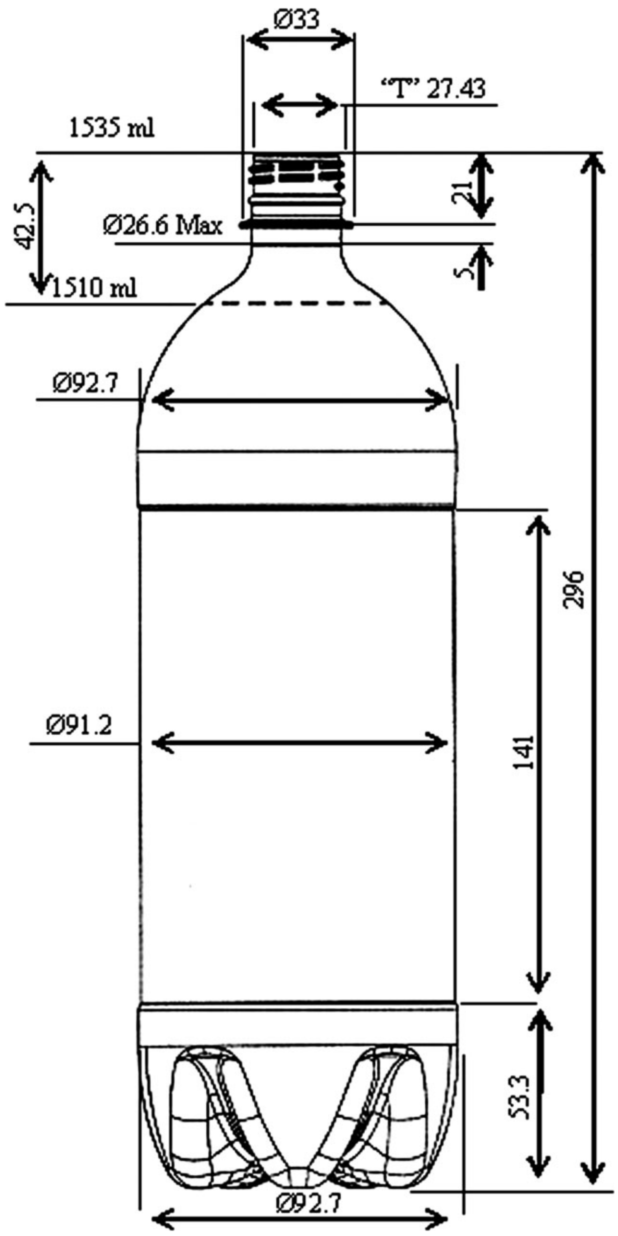

Figure 1 Current 1500-mL bottle design.

Details of the 1500-mL bottle design, obtained from the production drafting of the CSD packaging industry, are shown in Figure 1. The bottle drawing was generated in CATIA. In the CATIA model, the top, center, and base sections of the bottle design were generated separately and then joined together to form the whole bottle. The bottle base (the focus of this study) was further divided into five 72° segments. The total bottle base was generated by duplication of this slice with CATIA's mirror component feature.

In practice, material thickness is known to vary throughout the bottle, but in this study, for the sake of modeling simplicity and because the objective of the study was to investigate only the effect of the petaloid shape on stress distribution, the bottle thickness was assumed to be uniform. The analysis was repeated for three different wall thicknesses: 2

mm (the wall thickness for current bottles) and then 1 and 0.5 mm. The wall thickness needs to be optimized because it directly affects the material cost.

Method selection

For static case solutions, the problem is defined in two ways: linear and nonlinear. The condition is linear when there is no contact feature or pressure-fitting property; displacement is a linear function of the load. The condition is nonlinear when there is at least one contact feature or pressure-fitting property; in this case, displacement is a nonlinear function of the load.

A new analysis set is an object set corresponding to a new set of specifications of simultaneous environmental actions on a given system. To create object sets for the new specifications, a new static case needs to be inserted. The system response is thus computed on the basis of applied static loads under given restraints. The static solution parameters can be set in the CATIA software. The method is selected according to the type of model: small, medium, or complex. For small models, autoselection is recommended; the stresses can be computed automatically. The Gauss method was chosen for this study; it is recommended for computing stresses in small or medium models.

Application of restraints

In CATIA, the static analysis (e.g., stress and deformation) requires that certain restraints be applied to the body. These restraints may be in one, two, or three dimensions. There are different types of restraints in the generative structural analysis workbench, and the isostatic restraints were selected from them. The restraints were applied to the bottom of the bottle because deformation during bottle filling occurs with the bottle in the upright position. The restraints were simulated in CATIA as clamps applied at eight locations on the bottom of the bottle where it touched the ground, so that the bottle was in an upright position. Once the surfaces were selected, the simulation program automatically chose restraints. The body was prevented from rigid-body translations and rotations by means of the resulting boundary condition.

Application of pressure

The cracks arising at the bottom of the bottle are due to stresses being applied to the inner walls by the carbonation pressure of the bottle contents. The generative structural analysis workbench in CATIA has a feature for applying pressure to selected surfaces, and the magnitude and direction of this pressure can be given as the input. According to the information obtained from the manufacturers and from published studies, the pressure applied by the carbonated contents ranges between 0.4 and 0.6 MPa.[6] These two pressures were used for stress analysis in the CATIA model.

Meshing type and size

Calculation of the locations and magnitudes of the stresses generated on the bottle surface requires the

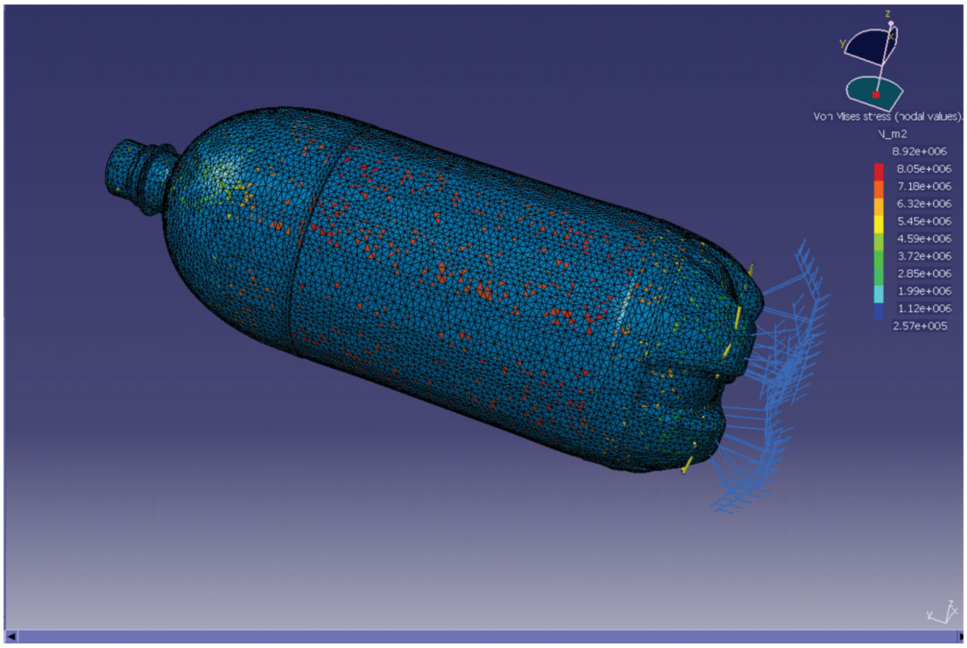

Figure 2 Deformed mesh with the restraints and loads as a result of the deformation. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

analyst to specify the elements and nodes via a finite element mesh. A suitable mesh geometry and dimensions are important to achieve accurate results. CATIA offers a choice between linear tetrahedron and parabolic tetrahedron mesh types. The petaloid base of the bottle, being geometrically a very complicated shape, made the selection of the proper mesh geometry difficult. There is a trade-off between the complexity of mesh generation and the precision of the stress predictions. The linear tetrahedron mesh geometry is the simpler of the two; it covers more surface than the parabolic tetrahedron mesh, and it does this in a much simpler way. The linear tetrahedron mesh geometry was selected, but the mesh size was kept as small as possible. When the mesh size was decreased, the optimized bottle continued to result in lower internal stress values in comparison with the standard bottle. Because the computation time increased as the mesh size was decreased, as a practical compromise, in this study, 2.57 mm was considered the smallest mesh size.

Von Mises stress distribution

When the inner wall of the bottle is subjected to pressure by the carbonated contents, three-dimensional stresses and strains arise; these are usually explained with an equivalent stress, which is represented as the von Mises stress distribution. The CATIA finite element analysis computes the von Mises stress values and displacements; it displays the deformed mesh, showing the stress distribution on the surface in both numerical and color-coded formats (Fig. 2). The von Mises stress distribution obtained from the analysis is given in Figure 3.

Experimental design and mathematical modeling

An experimental design and optimization program (ECHIP-7) from ECHIP, Inc. (USA) was employed to optimize the petaloid base dimensions of the bottle. The design variables were identified as the petaloid base parameters: the foot length, valley width, and clearance [Fig. 4(a,b)]. The optimization range of each parameter was established in accordance with the product identification requirements and processability of the bottles (Table I).

The maximum principal stress values were calculated from the numerical modeling studies in accordance with an experimental design based on an algorithmic partial cubic method. Algorithmic design provides flexibility and allows the introduction of constraints on the design variables. The standard deviation of the test results and the least importance difference (the smallest change in the response that one desires to detect) enable the determination of the minimum number of trials sufficient to provide a statistically significant experimental setup. The number of trials was found by ECHIP-7 to be 21 on the basis of the standard deviation of 0.5×10^6 Pa and the least important difference of 1.5×10^6 Pa. The high G-efficiency of the design confirmed the statistical significance of the analysis based on 21 trials. The G-efficiency of a design gives a measure of how well the design can extract the effects from the data in comparison with an optimum design. For

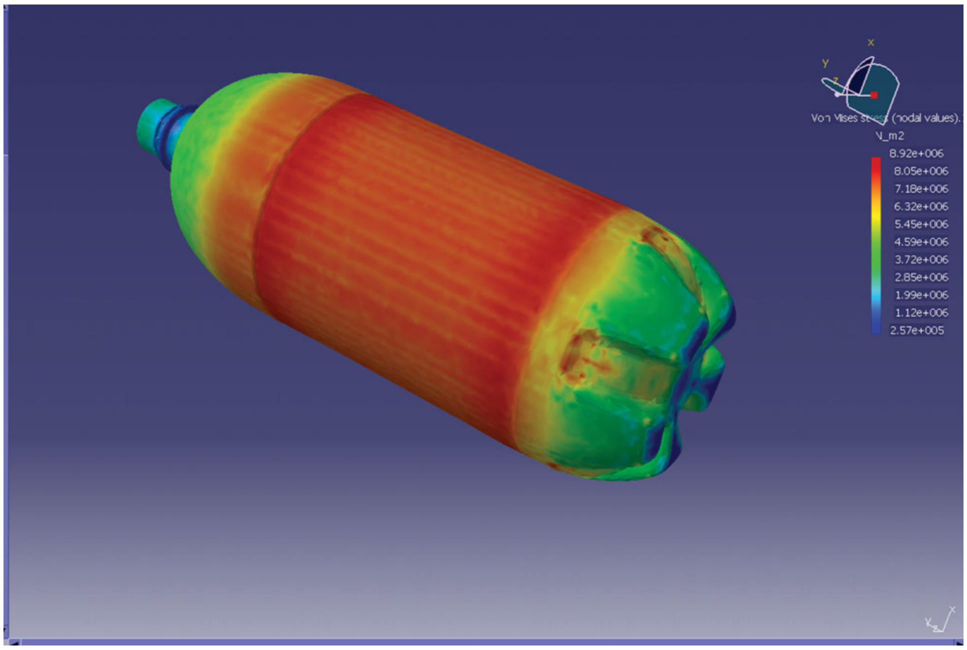

Figure 3 von Mises stress distribution at an amplification magnitude of 63.7. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

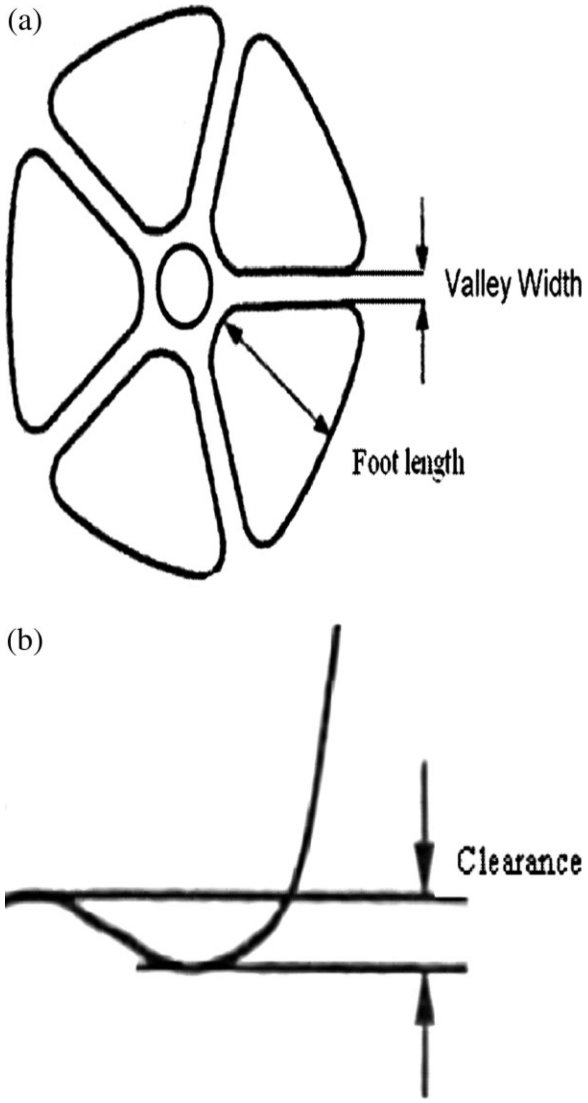

Figure 4 Design parameters of the petaloid base of the PET bottle: (a) foot length and valley width and (b) clearance.

two designs with an identical number of trials, the lower efficiency design will provide less ability to resolve the differences in the output.[16] The simulated stress values were imported back into the optimization program as the response variables. The simulated von Mises stress was modeled by a partial cubic polynomial function. Hence, the simulated stress data were fitted as a function of base parameters to generate a response surface. The response surface readily contained the optimum base dimensions, that is, the foot length, valley width, and clearance, which minimized the von Mises internal stresses.

TABLE I
Design Parameters and Numerical Values

	Numerical value		
Design parameter	Minimum	Maximum	Step
Foot length (mm)	16	41	1
Clearance (mm)	1	12	1
Valley width (°)	3	17	1

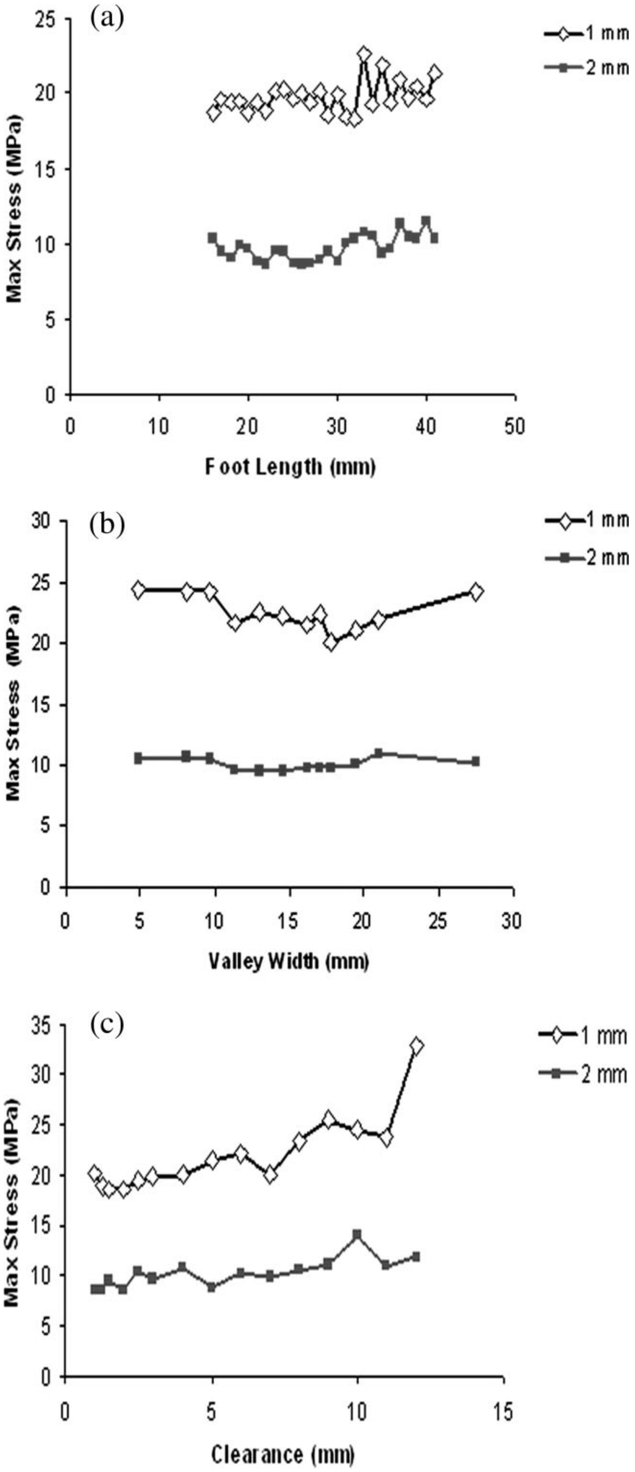

Figure 5 Maximum stress distributions at two different wall thicknesses for (a) the foot length, (b) the valley width parameter, and (c) the clearance parameter.

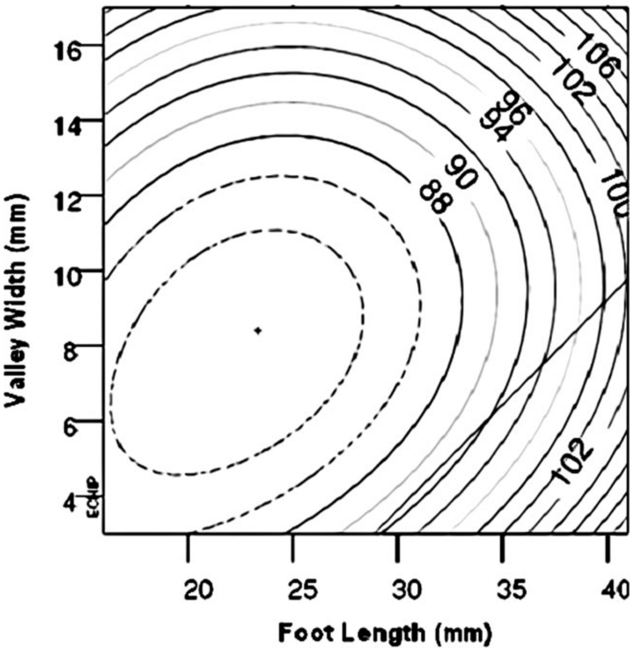

Figure 6 Minimum stress distribution for the bottle with a thickness of 2 mm at 40 Pa on a two-dimensional contour plot.

RESULTS AND DISCUSSION

Simulated stress analysis

Results from the stress analysis of the PET bottle can be concisely summarized as follows.

- The stresses on the surface of the bottle occurred most intensively in the middle sidewall section. Stresses on the base of the bottle were lower than those on the sidewalls, and those on the edges between the base and sidewall increased. In general, the highest stresses were on the sidewall, and the lowest stresses were on the base section.
- Increases in the maximum stress values were nearly the same for the pressures of 0.4 and 0.6 MPa. Some combinations of petaloid base parameters produced a convex shape at the bottom and sidewall of the bottle, which would destroy the self-standing feature of the petaloid base. Constraints were applied in the optimization process, fixing the clearance parameter to preserve the freestanding geometry of the base.
- A short foot length and a small clearance were the best combination for a sound petaloid shape. The valley width had no appreciable influence on the stress distribution in the bottle base.
- At two different wall thicknesses, the maximum stress distributions were given as a function of the foot length, valley width, and clearance, as shown in Figure 5(a–c), respectively. The maximum stress values decreased as the thickness of the bottle wall increased; nevertheless, for a given base parameter (foot length, valley width, and clearance), the maximum stress values were found to be different at different wall thicknesses (1 and 2 mm). The wall thickness of the bottle needs to be optimized for lower production costs and physical properties such as gas permeation, thermal stability, and burst pressure.

Mathematical modeling and optimization

The simulated stress values were obtained as explained previously for internal pressures of 0.40 and 0.60 MPa, which represent the inner gas pressure due to the CSD being in the bottle. These simulated stress values were empirically fitted to a partial cubic polynomial function of petaloid base parameters to define a response surface. Equation (1) mathematically defines the response surface for the stress [σ (N/m^2)] as a function of design variables [the foot length (x), the clearance (y), and the valley width (z)]:

$$\begin{aligned}\sigma = {} & 9589338 + 37339.13x + 242434.5y + 16873.82z \\ & - 1999.54xy + -3902.05xz - 16788.95yz + 2663.71x^2 \\ & + 4895.10y^2 + 18138.44z^2 + 267.25xy^2 - 570.08x^2y \\ & + 402.75xz^2 + 128.70x^2z - 563.74yz^2 - 1999.20y^2z\end{aligned} \tag{1}$$

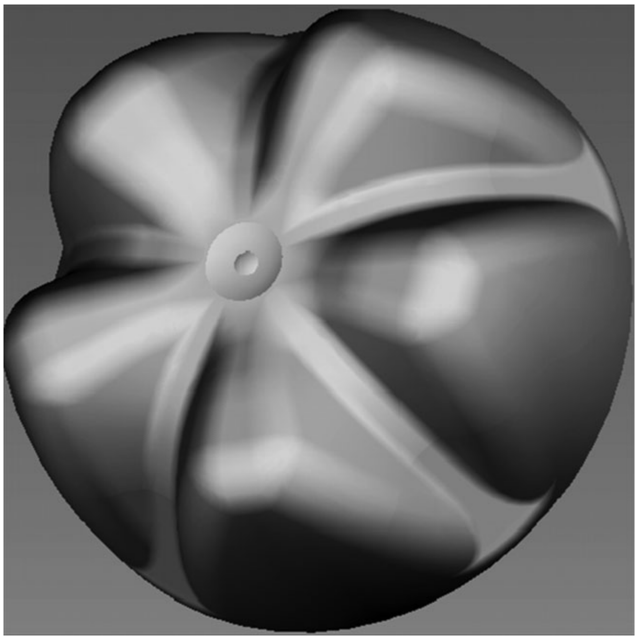

Figure 7 Computer-aided design drawing of the existing PET bottle base.

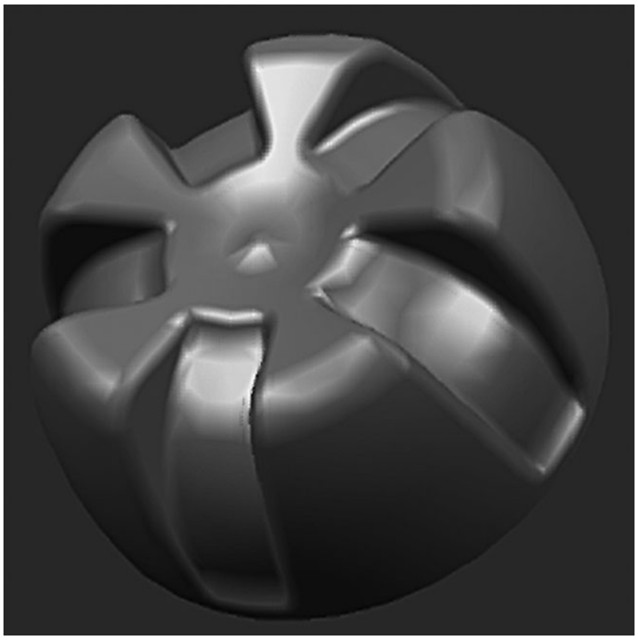

Figure 8 Computer-aided design drawing of the optimized PET bottle base.

The optimum parameters of the bottle base resulting in minimum stress distribution were 22.45, 8.03, and 1 mm for the foot, valley, and clearance, respectively (Fig. 6). However, the minimum clearance value was set to 5.8 mm to preclude the convex base, as mentioned earlier. In this case, the optimum foot length and valley width of 29 and 8.40 mm, respectively, were obtained with this clearance set value of 5.8 mm. In addition, the parameters of the bottle base currently used are as follows: 20, 4.25, and 5 mm for the foot length, valley width, and clearance, respectively. The current and optimized bottle base shapes are given in Figures 7 and 8, respectively. In this case, the maximum stress value of 10 MPa of the current bottle was reduced by approximately 1 MPa down to 8.92 MPa

A number of optimized bottles were produced under the same processing conditions used for the current bottles and were subjected to accelerated stress crack resistance testing according to a proprietary test method in which a high temperature is used to accelerate the failure of the bottles. Stress crack resistance was 88% higher with the optimized base design.

CONCLUSIONS

In this study, numerical modeling employing a statistical design of experiment approach was used to identify the geometry for the petaloid base that minimizes the stresses associated with ESC; the current petaloid base of the bottle was optimized.

The design of the experimental study produced a number of base geometry combinations for minimum stress. The next step was to simulate the stress distribution generated by each geometry combination by the incorporation of the geometry into the CATIA model of the bottle. However, some of the geometry combinations represented unacceptable deformation of the base and/or the sidewall–base intersection, and it was necessary to make compensating modifications. Occasionally, there were slight deviations of the combinations generated by ECHIP-7 and of the stress values accordingly. However, the standard deviation calculation took these into consideration. The new base design imparts enhanced environmental stress crack resistance, which will be the subject of a follow-up article.

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