Bottom Design of Carbonated Soft Drink Poly(ethylene terephthalate) Bottle to Prevent Solvent Cracking

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ABSTRACT: The use of a petaloid shape for the bottom design for carbonated PET bottles is widespread. Through this study, the causes of bottom cracking were investigated and a novel petaloid bottom was designed. The variations of the physical properties of PET according to the stretch ratio were examined and the stretch ratios in the blown bottle were analyzed. Cracking phenomena of the bottom were observed by a solvent-cracking test. The effective stress and the maximum principal stress in a carbonated bottle were analyzed by computer simulation. It was concluded that the bottom crack occurs because of not only the insufficient strength of material due to the insufficient stretch of PET but also to the coarse design of the petaloid shape. The highest maximum principal stress occurred at the valley in the petaloid bottom of the bottle and this strongly affected the cracking in the bottom. The petaloid shape was redesigned to minimize the maximum principal stress, and this resulted in increasing the crack resistance. © 2003 Wiley Periodicals, Inc. J Appl Polym Sci 88: 1145–1152, 2003

INTRODUCTION

The use of poly(ethylene terephthalate) (PET) bottles for carbonated soft drinks (CSDs) is widespread.[1–6] CSD bottles had previously consisted of two pieces: a PET blown bottle and a bottom cap for standing. The PET blown bottle had a hemispherical bottom shape, and the cap was made of polyethylene. These were assembled for the CSD bottle. However, the two-piece bottle was changed to a one-piece bottle in the middle of the 1980s. A one-piece bottle consists of only a PET blown bottle without a cap. The bottom shape of a one-piece bottle for CSDs is petaloid in shape to allow it to be self-standing. This one-piece bottle has advantages in reducing the manufacturing processes and material by eliminating the bottom supporter and cap, compared with a two-piece bottle. However, there has been a crack problem in the one-piece bottle at the petaloid bottom.

Published research articles for the study of cracks in PET bottles are very limited. Most of the research articles were about the characteristics of the fracture and cracking phenomena of the PET material itself without considering the geometry of the product.[7–13] Articles concerning the bottom cracks of PET bottles have appeared in patents.[14–17] Those patents were limited to the modifications of the process to give high stretch in stretch blow molding and preform designs. However, increasing the stretch ratio above the natural draw ratio[1] in the petaloid bottom would be difficult since it complicated the geometry of the bottom. Thus, a robust design of the petaloid bottom to resist cracking is important.

This article investigated the variations of the yield stress of PET according to the stretch ratio. The stretch ratio and the thickness distributions of a blown bottle were examined to check the strength of the bottle. A solvent-cracking test was performed to observe the cracking phenomena of CSD PET bottles and the main design factors associated with the cracking of the petaloid bottom were found. Stresses in the CSD PET bottle were simulated to examine the stress concentration in the bottles. The petaloid geometry that can prevent stress concentration and also enhance the resistance of bottom cracking was redesigned through this study. Cracking resistance of the newly designed petaloid bottom of the bottle was verified by the solvent-cracking test.

EXPERIMENTAL AND SIMULATION

Materials

We used PET with different molecular weights, supplied by the Samyang Co. (TRIPET® BI) (Seoul, Korea). The intrinsic viscosities (IVs) of PET were 0.77, 0.80, and 0.83 dL/g.

Tensile yield stresses for the stretched specimens were measured to examine the stretch-related material

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properties of PET. The procedure was as follows: The tensile specimens were prepared by injection molding (BA 750 CD plus, Battenfeld). The temperature of the coolant was maintained at 15°C for cooling the mold. The injection-molded tensile specimens were stretched for various stretch ratios in an Instron 4502 with an isothermal chamber which was maintained at 110°C. The stretched specimens were cooled to room temperature and the tensile yield stresses of variously stretched specimens were measured at room temperature in an Instron 4204.

Preform injection and bottle blowing

The preforms that were used in the blowing process were made by injection molding (XL 500 PET, Husky, 72 cavities). The nozzle and mold temperatures in the injection molding were 305 and 15°C, respectively. The blowing operations for 1.5-L and 350-mL bottles were performed in Sidel (SBO 10/10) and Sipa (ECS 800) blowing machines, respectively. As soon as the perform was heated by lamps to 110°C, the stretching rod stretched the preform axially. Subsequently, the preform was blown by a 4-MPa air pressure. The mold temperature in the blow molding was maintained at 10°C.

Solvent-cracking test

Citric acid and sodium bicarbonate were put into a water-containing PET bottle to make carbon dioxide gas. The contents of the carbon dioxide gas were 8.45, 9.23, and 9.82 g/L, respectively. The bottom part of the carbonated PET bottle was merged into a water solution which contains 0.2 wt % of NaOH to stimulate a crack. We then checked the bubble occurrence time and crack location when the bubble appeared through the crack in the bottom of the bottle.

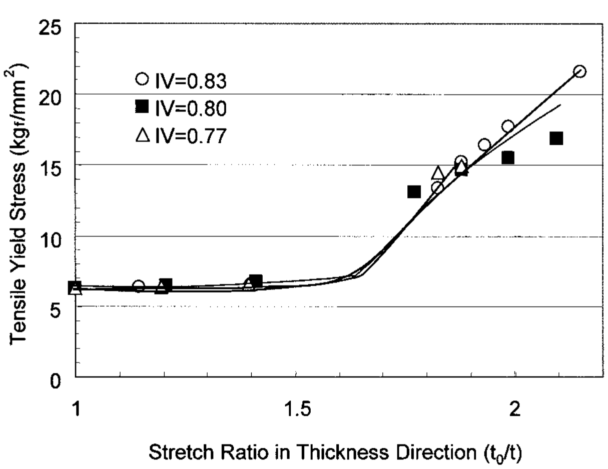


Figure 1 Variation of the tensile yield stresses of stretched PET.

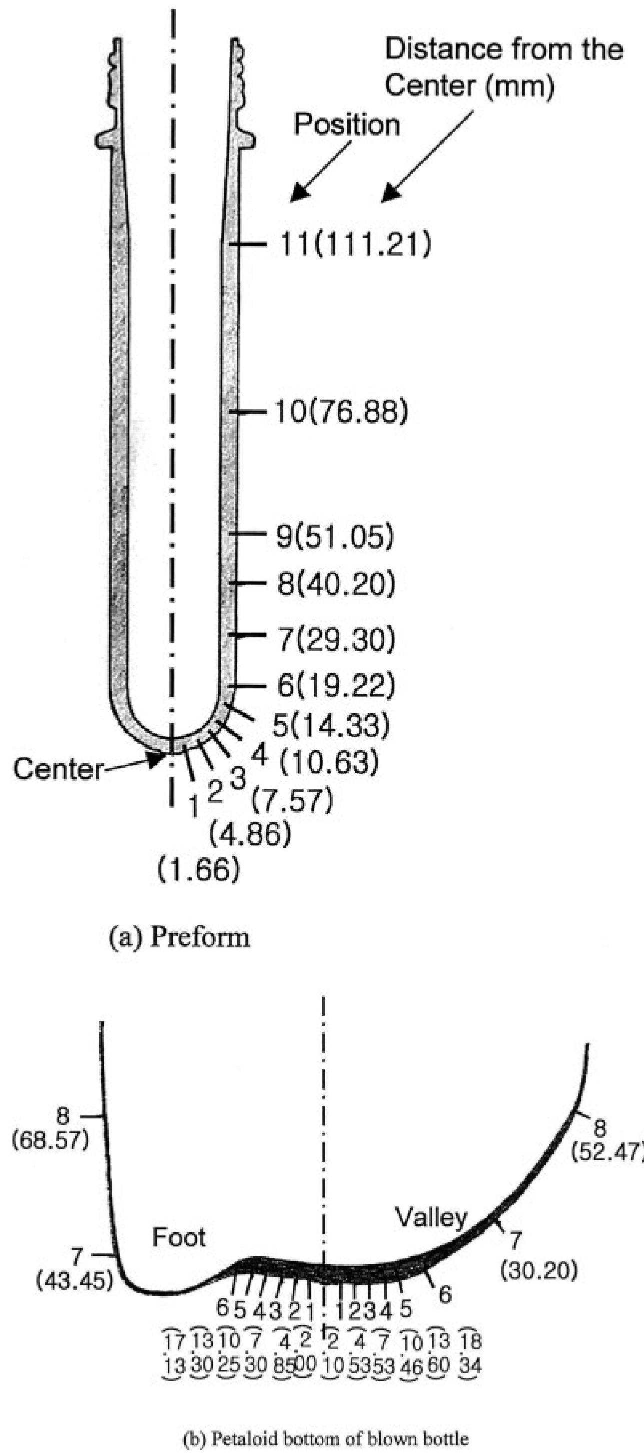


Figure 2 Cross sections of the preform and bottom part of the blown bottle: (a) preform; (b) petaloid bottom of blown bottle.

Computer simulation of stress in CSD bottle

Stresses at the bottom of the bottle were quantitatively examined by computer simulation using commercial software, Abaqus (Version 5.8-16). The CSD bottle was simulated for six different input data and three thicknesses for two pressures. The uniform thickness was

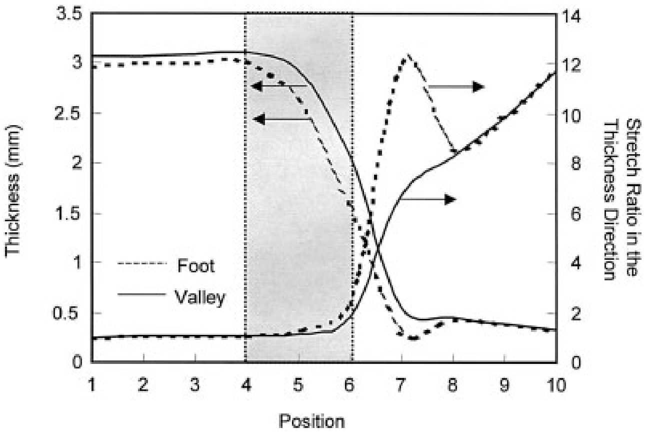


Figure 3 Variations of thicknesses and stretch ratios at foot and valley in the bottom of the bottle.

used in each simulation. The actual thickness in the bottle was distributed unevenly. However, a uniform thickness was used in the simulation for simple modeling since the objective of this simulation was the investigation of the stress distribution that comes from the geometrical shape of the petaloid bottom. The thicknesses were 0.35, 2.0, and 3.36 mm and the corresponding moduli were 77.6, 173.1, and 173.1 kg_f/mm^2. Those thicknesses were the average values of the sidewall, bottom part, and preform, respectively. Two pressures, 0.04 and 0.06 kg_f/mm^2, were applied. Those were the pressures in the bottle for 8.45 and 9.82 g/L of carbon dioxide gases, respectively. The 8.45 g/L of the carbon dioxide gas is common in carbonated beverages.

RESULTS AND DISCUSSION

Physical property of material

The tensile yield stresses of the stretched PET are shown in Figure 1. The yield stresses remained at almost the same value for low stretch ratios, less than 1.6. However, these increase as the stretch ratio increases for high stretch ratios, higher than 1.6. In the stretching of PET at elevated temperature, the increments of the stress was very small for low stretch ratios.[18–20] As the stretch ratio increases, the polymer chains are arranged in the stretching direction. Subsequently, the stress increases drastically as the stretch ratio increases after a certain point of the stretch ratio. That is the hardening of material through molecular orientation. Figure 1 shows the yield stresses for variously stretched PET specimens and this shows the physical behavior of hardening. Through this examination, we could see that the stretch ratio in bottle blowing should be higher than the hardening point to ensure a high mechanical property. The effect of IV for the tested range, between 0.77 and 0.83 dL/g, on the yield stress for stretched PET would be negligible.

Stretch ratio and strength of the bottom in the bottle

The cross sections of the preform and the blown bottle of 1.5 L are shown in Figure 2. We marked points on the preform surface and then blew it. The stretch ratio in the thickness direction (thickness ratio of preform to bottle) of the blown bottle was calculated by measuring the thicknesses at marked points on the preform and the corresponding marked points in the blown bottle. Figure 3 shows the profiles of the thicknesses and stretch ratio at the foot and valley in the petaloid bottom of the bottle. The thickness near the center of the bottom was much thicker than was the sidewall of the bottle, and the stretch ratio in the thickness direction at this center region was near one.

The stretch ratios at the foot and valley in the thickness direction increased slowly after point 4 and those increased drastically from point 6. However, the material strength would not be improved by the molecular orientation until point 6 because the stretch ratios were lower than was the hardening point. The material strength increased after point 6, although the stretch ratio began to increase after point 4. Thus, the material strength at the bottom from point 1 to point 6 would be the same. However, the thickness of the bottom decreased from point 4. Through this examination, we can see the structural weakness of the bottom because of an abrupt change of thickness between points 4 and 6 without increment of the material strength. Figure 4 shows profiles of the yield stresses along the foot and valley which were estimated using the results of Figures 1 and 3. Similar results were found in the 350-mL bottle in our study.

Observations of cracks in the bottom

Cracks were observed through the cracking test for commercialized PET bottles which have different petaloid shapes. The typical crack patterns in the bot-

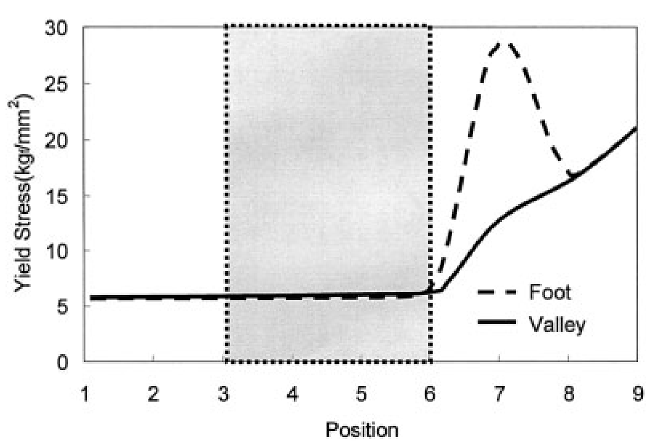


Figure 4 Profiles of yield stresses in the bottom of the bottle.

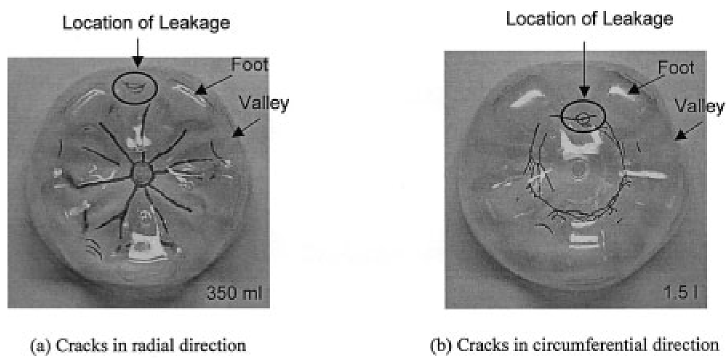


Figure 5 Cracks in the petaloid bottom of the bottle: (a) cracks in radial direction; (b) cracks in circumferential direction.

tom of the bottle are shown in Figure 5. There are two directions of the cracks: One is the radial direction [Fig. 5(a)]. In this case, cracks began bottom center and propagated to the outside, radial direction. The other is the circumferential direction [Fig. 5(b)]. The cracks were located at some distance from the bottom center and the direction was circumferential.

The cracks that finally caused leakage at the valley of the petaloid bottom and the direction of the cracks was circumferential as indicated by the arrows in Figure 5. The locations of these cracks were distributed between points 4 and 6 as indicated in Figures 3 and 4. In that area, the material strength was weak because of insufficient stretch of the material and the abrupt decrease of thickness as discussed in the previous section.

Through the cracking experiments, we could find design factors which affected the circumferential cracks at the valley. The design factors are indicated in Figure 6. These are clearance, foot length, and valley width. The petaloid shape with a large clearance, large foot length, and narrow valley width had the tendency of reducing the circumferential cracks at the valley regardless of the bottle size. These design factors should be considered important in the design of the petaloid bottom.

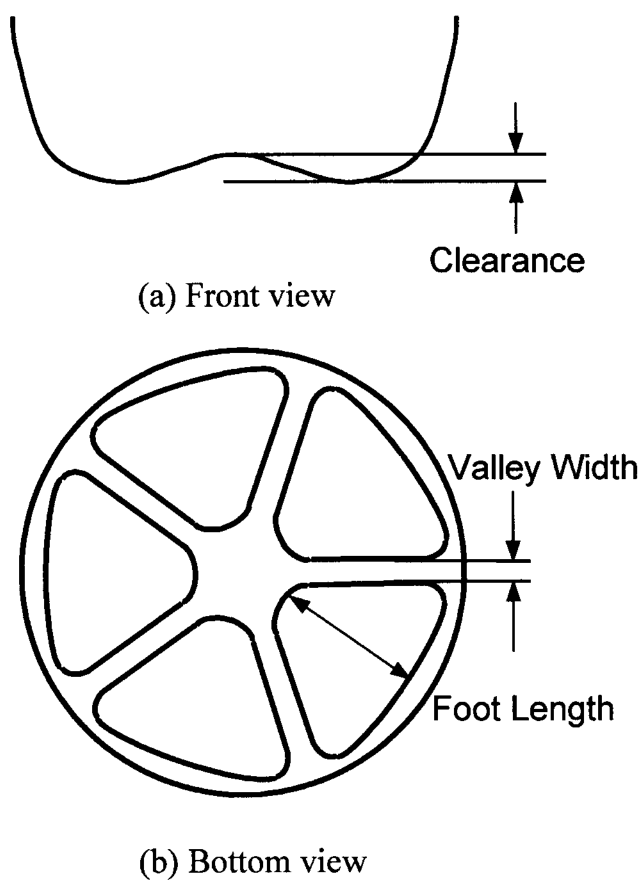


Figure 6 Design factors in the petaloid bottom: (a) front view; (b) bottom view.

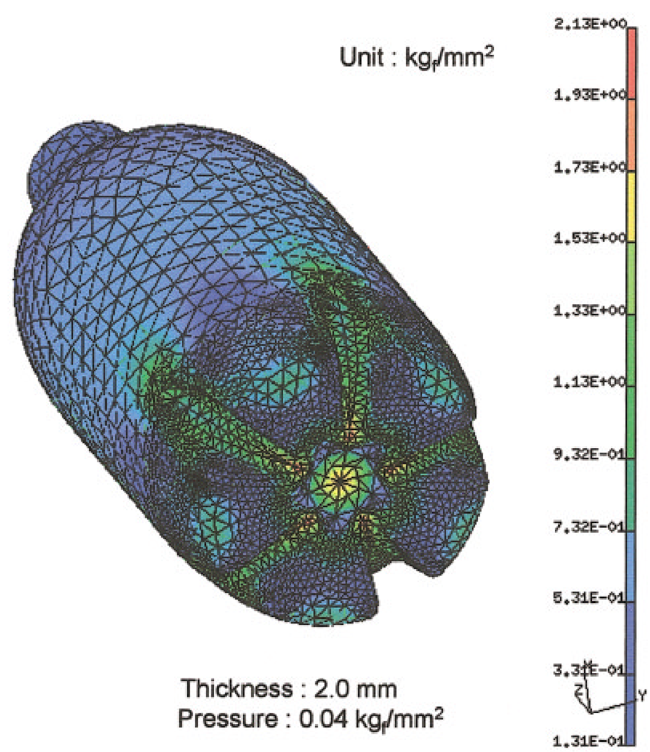


Figure 7 Distribution of effective stress in the CSD PET bottle.

Stresses in carbonated bottle

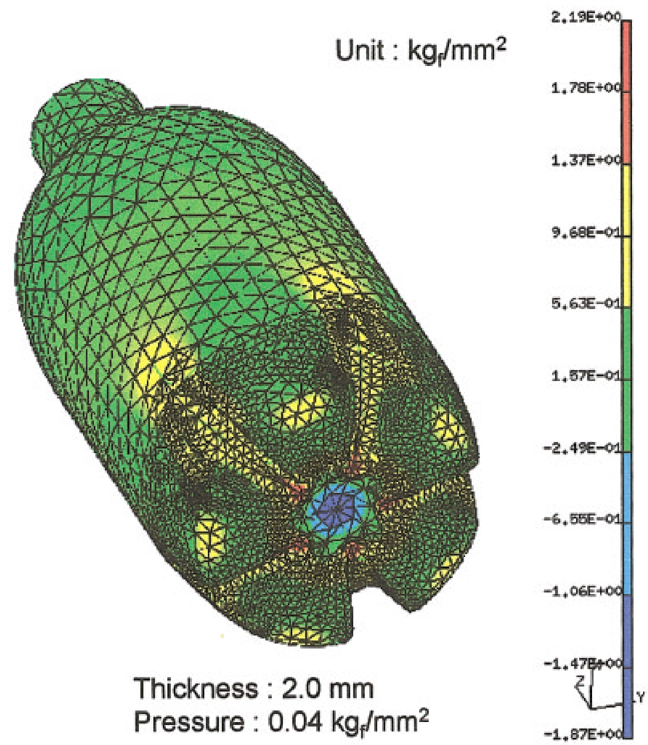
The simulated stresses in the CSD bottle for 350 mL are shown in Figures 7 and 8. The effective stress[21] in Figure 7 at the bottom region is higher than that of the sidewall. The maximum effective stresses are located at the valleys. This implies, geometrically, that the weakest region is the valley. The maximum effective stresses for the thickness of 2.0 mm were 2.13 and 3.2 kg_f/mm^2 for the pressures of 0.04 and 0.06 kg_f/mm^2, respectively. Those are lower than the yield stress of the material, 6.3 kg_f/mm^2 (Fig. 1). Moreover, the actual thickness at the valley where the maximum effective stress occurred was thicker than was the model thickness, 2.0 mm (between points 4 and 6 in Fig. 3). Through this investigation, we concluded that the bottle would be safe in this maximum effective stress.

Figure 8 shows the maximum principal stress among the three principal stresses in the carbonated bottle. The crazing occurs in brittle materials under tensile stress.[22,23] Thus, the crazing is strongly related to the tensile principal stresses. The crazing contour is below the yield contour for the tensile principal stresses.[22,24,25] The highest maximum principal tensile stress occurs at the valleys, and the direction is radial as shown in Figure 8. This radial direction is perpendicular to the crack direction that caused leakage in the bottom as we observed in the cracking test. Through these examinations, we could realize that the maximum principal stress among the stresses has the major role in the cracking of the bottom of the bottle.

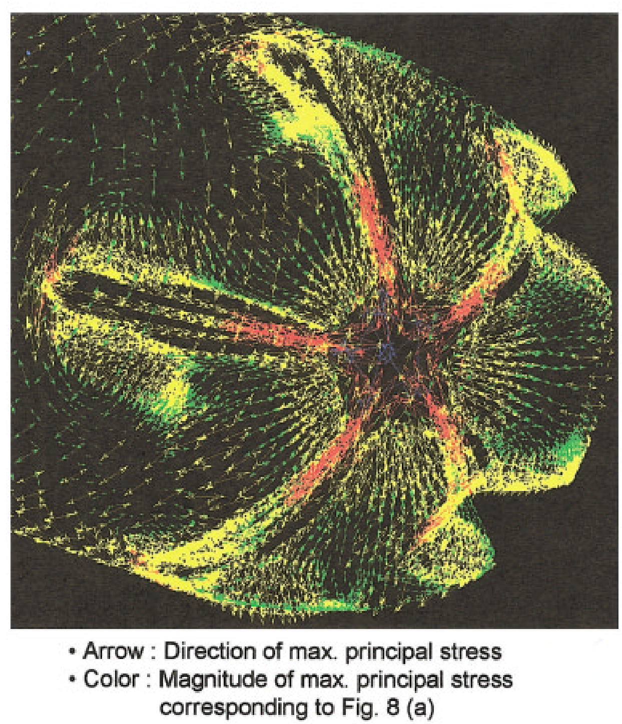
Design the petaloid bottom and evaluation

The petaloid bottom of the 1.5-L bottle was redesigned. To modify the petaloid shape, we considered the three design factors, clearance, foot length, and valley width, that were found in the cracking test. The petaloid shape that could reduce the maximum principal stress was designed through computer simulation. Figure 9 shows the variations of maximum principal stresses for three design factors. Through these examinations of the design factors, the petaloid shape was redesigned as follows: Large clearance, long foot length, and medium valley width were chosen in the studied geometries. This implies that the clearance and the foot length in the petaloid bottom were increased by 50 and 5%, respectively, with the same dimension of the valley width compared with the existing shape of the old design.

The effect of the redesigned petaloid shape on the cracking resistance was examined by computer simulation and the cracking test. Figure 10 shows the maximum principal stresses at the petaloid bottom for the old and the newly designed bottles. The highest value of maximum principal stress was decreased by 21% from 4.59 to 3.62 kg_f/mm^2. The location of the highest maximum principal stress was moved to the sidewall from the valley. This means the high stress concentration occurs at the strong region. The cracking resis-



(a)



(b)

Figure 8 Maximum principal stresses and their directions in the bottom of the bottle: (a) distribution of maximum principal stress; (b) directions of maximum principal stress.

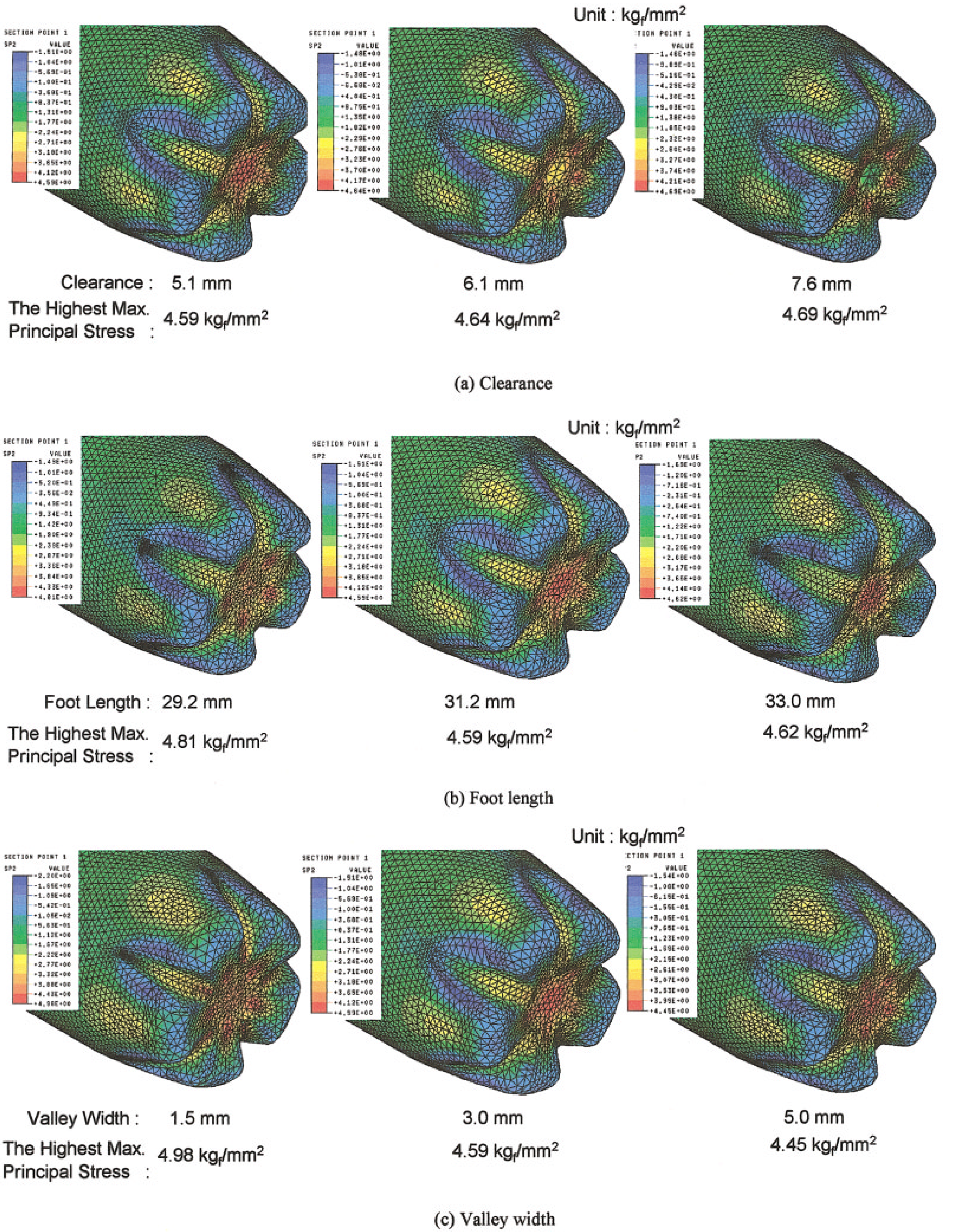
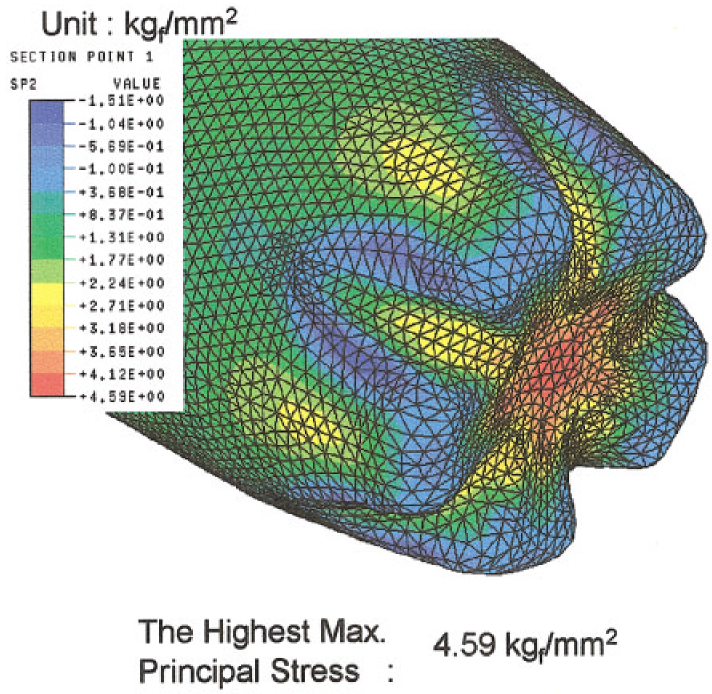
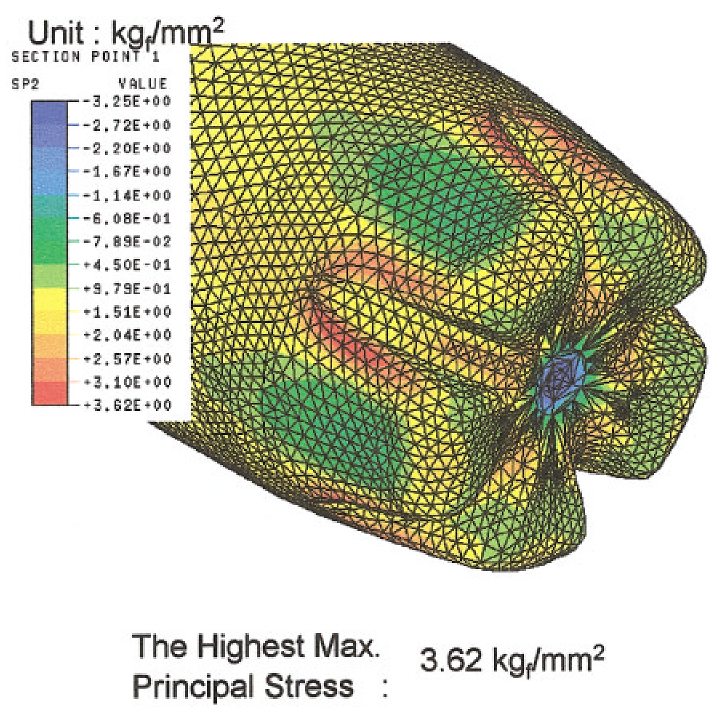


Figure 9 Variations of maximum principal stresses according to the design factors: (a) clearance; (b) foot length; (c) valley width.



(a) Old design



(b) New design

Figure 10 Comparison of maximum principal stresses for old and newly designed bottom of bottle: (a) old design: (b) new design.

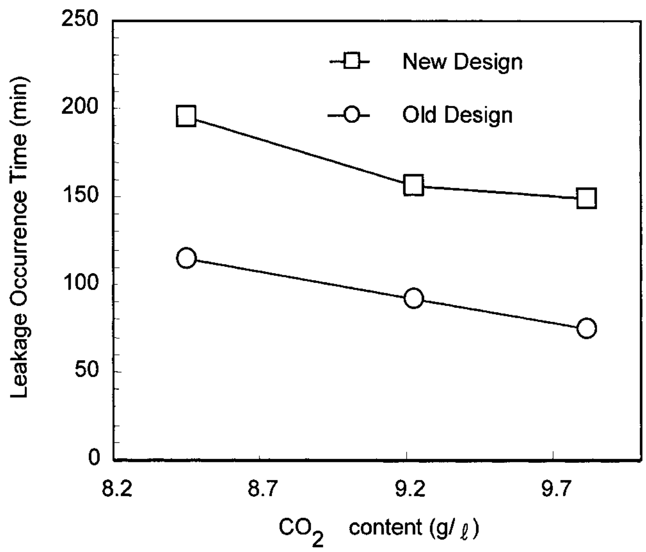


Figure 11 Comparison of leak occurrence time for old and newly designed bottoms of the bottle.

tance of the redesigned petaloid shape was verified through the cracking test. Figure 11 shows the leakage occurrence times at the bottom for the old and the newly designed bottoms. The leakage occurrence time of the redesigned bottle was increased by about 70%. The results of the computer simulation and the cracking test showed that the crack resistance of the bottle increased through the modification of the petaloid shape.

CONCLUSIONS

The bottom-cracking phenomena in the CSD bottle were investigated and the petaloid shape of the bottom was redesigned to prevent cracking. The strength at the bottom part of bottle was weak structurally because of the abrupt decrease of the thickness as the stretch ratio increases without improvement of the mechanical strength. The stretch ratio in the bottom of the bottle was below the hardening point of the material in the stretching process. The stretch ratio at the petaloid bottom should be increased over the hardening point to improve the mechanical property associated with the molecular orientation.

The cracks that caused leakage in the CSD PET bottle were located on the valleys and the direction was circumferential in the petaloid bottom. The highest maximum principal stress occurred at the valleys. The direction of this stress was radial and this caused a crack circumferentially through crazing. The maximum tensile principal stress should be lowered or minimized at the valleys of the petaloid bottom to prevent cracking.

There were three design factors, clearance, foot length, and valley width, that affected the cracking at the petaloid bottom of the bottle. The crack resistance of the petaloid CSD bottle was improved by the modification of the petaloid shape considering the design factors. Through the modification of the petaloid shape, the location of the highest maximum principal stress shifted to the safe region, near the sidewall, as well as the highest maximum principal stress being reduced. The improvement of the crack resistance of the newly designed petaloid bottom in the CSD PET bottle was verified by the cracking test.

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