OPTIMUM DESIGN OF PET BOTTLE BASES AGAINST STRESS CRACKING

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Abstract

The polyethylene terephthalate (PET) bottles with petaloid shaped base are widely used for the carbonated soft drinks. There are currently various bottle designs with different petaloid shaped base in the market. While the PET bottles provide safe transportation and storage of soft drinks, occasional cracking of the petaloid base presents problems to the manufacturers of the PET bottles.

In this study, dimensions of the petaloid shaped base are optimized against stress cracking by means of finite element analysis (FEA) and process simulation software. Based on the results, a new design for the petaloid shaped base is proposed.

Introduction

While there are many different kinds of bottles for carbonated soft-drink varying in size, material, shape, stability and $cost^1$, PET has been the most widely used material since it offers excellent clarity, good mechanical and barrier properties, and ease of processing².

The bottles with petaloid shaped base are the ones most commonly used in industry. This petaloid shaped base not only gives a self standing feature to the bottles but its production cost is also less than that of the two-pieces bottle. One-piece bottles are advantageous over the two-pieces bottles in terms of lower production times, ease of processing and convenience of use.

There is a number of parametric modeling in the literature for the ISBM process. Computer aided design and computer aided manufacturing software programs are needed to produce bottle-mould initial design with minimal modeling and production time as processing and mould design are time consuming and expensive³. Compared to injection moulding, it is more convenient to use blow moulding systems in the manufacture of plastic items due to favorable cost factors, possibility of variable wall thicknesses, low stresses ⁴.

Main problem with the one-piece bottle is the cracking of the petaloid shaped base during the storage of the soft-drinks, hence causing major inconvenience for carbonated soft-drinks distributors and producers. For this reason, bottle and petaloid shaped base need to be redesigned by using FEA computer programs to prevent cracking at the base of the bottles before being produced with the injection stretch blow molding (ISBM) process. So far, a few computer simulation programs have been used for this purpose⁴. Both the bottle design and the ISBM processes parameters are optimized by means of these programs, reducing the time and cost of production of bottles with petaloid shaped base resistant to stress cracking.

PET is subject to environmental stress cracking (ESC) and a brittle failure initiated by "surface imperfection". ESC occurs when the glassy polymer is exposed to aggressive medium and loaded at low stress for long period of time^{5,6,7}. Since at least 15% of all plastic failures in service are caused by ESC^5 , the investigation of ESC phenomena is very important for the applications of all engineering plastics.

As the environmental stress cracking has been very big problem for manufacturers, some researchers⁸ focused on this issue and thought that this cracking problem was due to crsytallinity. The factors that affect the crystallinity have been identified as the processing temperature, pressure and environment⁹.

The temperature distribution on the preform during stretch blow molding¹⁰ and the packing pressure of the injection molded preform¹¹ are fairly important and affect the total processing time and crystallinity. The greatest base clearance is obtained by processing a light weight preform at a low reheat temperature or a heavy weight preform at high temperature¹². Zagorala et. al¹² have found that process conditions such as small cushion, low holding pressure and minimum holding times are needed for light weight preform and also reduce gate crystallinity and residual stresses.

Many reasons were given for ESC phenomena and a number of studies are still continuing on it. Fellers ascertained that the craze initiation is independent of molecular weight¹⁴. On the other hand, there are some researchers who regard that crystallinity is a very important parameter affecting the ESC behavior of PET material; and amorphous plastics are more susceptible to ESC than semi-crystalline plastics because of their poor permeation barrier⁵. It is also found that ESC resistance decreases as crystallinity increases for polyethylene¹⁵. Despite of all studies carried out, the results are controversial.

The studies conducted with homopolymer and copolymer PET at 30 $^{\circ}$ C indicated that the number of cracks increased with increasing exposure time; higher the copolymer concentration, higher the number of cracks. However, when no stress acts on the samples, no cracks are developed¹⁶.

Hanley et. al¹³ have said that the cracking phenomenon is directly related to the polymer morphology at the petaloid base and therefore the cracking is due to the phases of production process. The hoop extension differences in the inner and outer surfaces of the bottle affect the morphological properties¹⁷ as well. As the movement of the stretch rod affects the hoop extension, the stretch rod speed should be adjusted carefully¹⁸. In general, the central region of the petaloid base of bottle remains amorphous after the injection stretch blow molding¹³. The bottom area is hardly stretched because of its relatively low temperature (around 80°C). After stretching stops, the other regions continue to be stretched by the preblowing pressure and the middle-upper area is forced to move up. Consequently, since the bottom area is compressed and not stretched sufficiently by stretch rod, crystallization and orientation is less¹⁹.

Lyu et al.²¹ have studied the stress cracking problem of the petaloid shaped base by considering the geometry of the shape, while the other researchers²²⁻²⁴ have studied this problem without considering the geometric shape of the petaloid base. Compared to the present research, Lyu et al. have studied the same volume of the bottle except for its shape. They have assumed an even wall thickness distribution of the bottle. They have conducted the stress analysis of the bottle by using commercial software, namely Abaqus, at two different pressures: 0.4 MPa. 0.6 MPa.; and at three different thicknesses: 0.35, 2.0, 3.36 mm. which are the average values of the sidewall, the base and the preform respectively. According to their measurement of tensile yield stress of stretched PET material, they have concluded that for a PET bottle to have a high mechanical properties, its stretch ratio should be higher than the strain hardening point which corresponds to a ratio of initial wall thickness to final wall thickness between the center region and the region nearby.

In spite of these studies, reasons behind the stress cracking at the base of the bottles remain unresolved. Current research addresses stress cracking phenomenon by considering not only the geometry of the petaloid shaped base but also the process conditions used in the manufacturing of the bottles. The geometrical parameters that affect the stress cracking at the base of the bottles are identified as the foot length, valley width and clearance. On the other hand, as for processing of the bottles, blow pressure, temperature distribution of preform at the blowing stage, velocity of the stretch rod, and total time of both the stretch and the blowing stages are identified as the processing parameters.

In this study, firstly, the PET bottle to be studied was drawn by CATIA V5 R14 to comply with its actual dimensions. Three different wall thickness of the bottle was considered to be able to see the effects of the thickness on the petaloid shaped base of the bottle; and the thickness distribution throughout the bottle was also regarded as uniform. Two different internal pressure were applied to the inside surface of the bottle for each thickness. Von Mises stress values were recorded on each test conditions. Echip, which is a design of experiment and optimization software, was employed to determine the number of trials and consequently the optimum values of design parameters for the PET bottle.

There are generally two different cracking directions observed at the base of the bottle. The first is in the radial direction (Fig. 1a), which begins from the base center and goes towards the outside. The second is circumferential (Fig. 1b) where cracking appears at some distance from the base center and progresses circumferentially. However, circumferential cracking is phenomenon where the underlying causes are poorly understood¹⁰. Lyu et al.²¹ have said that there are three parameters at the base, which affect the stress cracking and they have optimized the petaloid shaped base by modifying

these three parameters, based on measurements of effective stresses at the base of the bottle. These parameters are foot length, valley width, clearance as seen in figure 2. They have found that the circumferential cracks are minimal at the valley in the case of large clearance, large foot length and narrow valley width.

As injection stretch blow molding (ISBM) is the preferred process for the production of carbonated soft drink bottles made out of PET, the current research aims to prevent stress cracking which occurs at the base of the bottle by optimizing the petaloid shaped base via the above mentioned ISBM process parameters.

Experimental

Setting the Material Properties

Material properties for virgin PET used in the stress analyses with CATIA V5 R14 are given in table1.

Bottle Design Used

The bottle design which was used for stress analyses is shown in figure 3. The bottle has a volume of 1.5 lt. and its thickness distribution is not even. The values of thickness are approximately 3mm and 0.3mm at the base of the bottle and sidewall of the bottle, respectively. However, as the thickness changes, depending on the process parameters of ISBM, temperature distribution of the preform becomes crucially important.

Results and Discussion

Thickness Distribution and Stresses in the Carbonated Soft-Drink Bottle

Thickness distribution of the PET carbonated soft-drink bottle used on this study is seen in figure 4. This distribution has been obtained through an injection stretch blow molding process simulation program. In order to be able to achieve this thickness distribution, the version of the above bottle that was optimized by obtaining minimum stress distribution at the bottle base, was used as mould. As can be seen in figure 4, the thickness distribution is not uniform all around the bottle. The thickest region is the petaloid shaped base, which is around 2-3 mm thick. The other regions except for the base of the bottle can be assumed to have uniform thickness between 0.3 and 0.4 mm and there is abrupt change in thickness between sidewalls and central region at the base, therefore, the fact that there is stress cracking problem at the base may be anticipated. At this region, it may not be possible to achieve a uniform thickness distribution because of its geometrical structure but, reducing the stresses in this region can be possible by modifying process parameters. Figure 6 and 7 show the simulated stresses in the petaloid shaped base for the current bottle and the optimized bottle design respectively.

According to the simulation results, it can be said that the maximum stress on the bottle is seen on the sidewall and the minimum stress is seen at the foot of the base. The reason why the minimum stress is at the foot of bottle is due to the fact that the stress analyzes were carried out where the bottle stands upright. However, at the valley region, the stress is relatively high compared to the other regions near the center of bottle base. The maximum stress is observed at the sidewall of the bottle, which is also the strongest section of the bottle. Although the stresses at the valley region near the center of the base seems to be less than that of the sidewall region, as the yield stress of the valley is less than that of the sidewall, which is around 50 MPa, the weakest region of the bottle is the valley²¹. So, the stresses at the valley should be lowered by modifying these three parameters mentioned above. For a bottle of 1.5 lt. whose thickness is 2mm, the maximum Von Mises Stresses are 9.86 MPa and 14.8 MPa at the internal gas pressure of 0.4 MPa and 0.6 MPa, respectively. According to these results, the maximum stresses at the petaloid shaped base for both gas pressures are lower than the yield stress of the material. Hereby, the base of the bottle seems to be sound against these internal pressures applied by the carbonated soft drinks on the bottle walls. Finally, to be able to see the effects of the wall thickness of the stress distribution, the thickness of the bottle was changed 1 mm and 2 mm. The stress distribution on the bottle was observed at these two values and the values resulted, are given in figure 11. As seen from these results, the maximum stress of the bottle increases.

Optimization of the petaloid shaped base

The optimization process of the petaloid bottom was carried out by modifying the three parameters: foot length, clearance, valley width as shown in figure 2. Trial numbers was determined by Echip7 design of experiment and optimization software program (table 2). Through the use of the same program, the optimum dimensions were obtained. As seen on figure 5, the optimum values are 22.45 mm, 12.95 mm, 1mm for foot length, valley width and clearance, respectively. As a result of these optimum dimensions, the maximum stress on the bottle is 8.2 MPa. The dimensions of the bottle currently used in industry are 29 mm, 16.17 mm, 7 mm for foot length, valley width and clearance, respectively and this bottle's maximum stress due to internal gas pressure is 9.88 MPa (Figure 6). The stress value of the optimized PET bottle whose dimensions were calculated by Echip7 is 8.61 MPa (Figure 7). This value is within the lower and higher limitations defined by Echip7. So the optimized bottle stress is 12.68 % less than the current bottle stress. Also, the thicker the wall thickness the lower stress values on the bottle. But, the fact that the thicker wall thickness causes higher material cost; the wall thickness value should therefore be optimized.



Figure 1. Cracks at the petaloid base of the bottle.

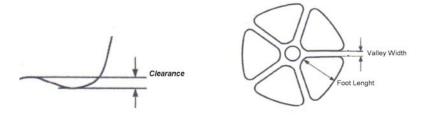


Figure 2. Design parameters of the petaloid base

Table 1. Material properties for Virgin PET

Young Modulus	2.9e+009N/m2
Poisson Ratio	0.4
Density	1200kg/m3
Yield Strength	5.5e+007N/m2

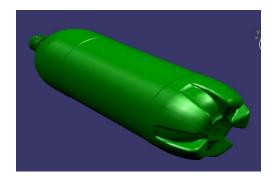


Figure 3. The bottle of 1.5 lt. modified in this study

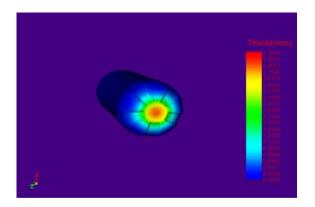


Figure 4. Thickness distribution on the bottle after Processing of ISBM

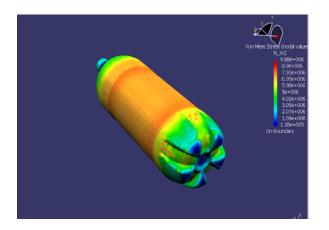


Figure 6. The Von Mises stress distribution of the current bottle

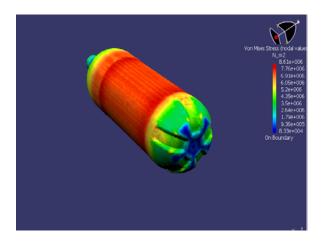


Figure 7. The Von Mises stress distribution of the optimized bottle

Table2. Design variables and values

TRIAL	Foot_length	Clearance	Valey_width	
2	41.0	12.0	3.0	
11	28.5	6.5	17.0	
1	16.0	1.0	3.0	
4	16.0	12.0	17.0	
7	41.0	1.0	10.0	
15	28.5	6.5	10.0	
12	28.5	12.0	10.0	
3	41.0	1.0	17.0	
6	41.0	6.5	3.0	
5	28.5	1.0	3.0	
13	41.0	1.0	3.0	
14	41.0	12.0	17.0	
10	16.0	6.5	10.0	
8	16.0	12.0	3.0	
9	16.0	1.0	17.0	

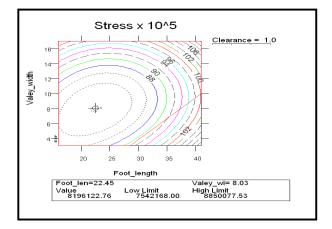
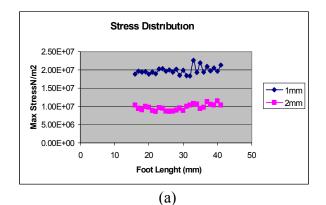
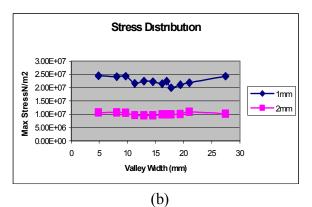


Figure 5. Optimization results with Echip program.





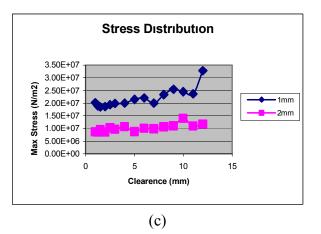


Figure 8. Max Stress distribution at two different wall thickness with respect to the three parameters of petaloid shaped base: (a) Foot length, (b) Valley width, (c) Clearance.

Clearance (mm)	Max Von Mises Stress (N/m2)
1	8.64e+6
6	1.01e+7
12	1.17e+7

(a)

Valley width (mm)	Max Von Mises Stress (N/m2)
4.85	1.06e+7
16.17	9.86e+6
27.49	1.02e+7

(b)

Max Von Mises Stress (N/m2)
1.03e+7
8.90e+6
1.03e+7

(c)

Figure 9. The Highest Max Von Mises Stress values for some parameters.

Conclusion

In this study we optimized the petaloid shaped base of the CSD bottle in order to prevent stress cracking since the cracking problem has occurred in this section of the bottle. In the previous studies, it has been identified that there are three parameters which affect the cracking at the base of the bottle most; these are foot length, clearance and valley width. These three parameters were therefore modified by changing their numerical values through the Echip 7 software. The optimization process was carried out by measuring Von Mises stress values at the base of the bottle by means of Catia V5 R14 program and concluded that the highest maximum stress occurred at the sidewalls and where it joins the sidewalls. As a result, the optimum dimensions of these three parameters were found by the Echip 7 software and the bottle was redesigned. The stress distributions with respect to various design parameters are shown in figure 9. It can be said that small foot length, small clearance and medium valley width are the best combination for a sound petaloid shaped base design. On the other hand, valley width does not have any considerable effect on the stress occurrence at the petaloid base of the bottle. While the higher wall thickness results in the lower the stress distribution on the bottle as shown in figure 8, wall thickness needs to be optimized to reduce the higher material cost resulting from thicker wall thicknesses.

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