Rheological Modeling of Fracture in Plug-Assisted Vacuum Thermoforming

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ABSTRACT: The fracture of polymeric sheets is one of the practical problems occurring during plug-assisted vacuum thermoforming. This defect can occur during both the plug-assist and vacuum-forming stages. This article focuses on two issues: (1) the origins of fracture creation and (2) the determination of the process parameters needed for removal of the defect. The results of our work not only lead to an understanding of the cause of this problem but also enable us to calculate the parameters that affect the fracture of polymeric sheets during plug-assisted vacuum thermoforming. © 2010 Wiley Periodicals, Inc. J Appl Polym Sci 117: 171–177, 2010

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INTRODUCTION

Polymer processing, that is, the production of all forms of polymeric articles, has found a great place in chemical industries. Thermoforming is one of the most popular techniques in this field and applies to thermoplastic sheets and plastic films. This forming technique is mainly used for various packaging applications such as medical devices, consumer electronics, food containers, and pharmaceuticals.[1–3] The reasons for the widespread application of thermoforming are its high performance, simplicity, compactness, and relatively low-cost equipment. These specifications make it possible to produce complex, large-scale configurations and free-form shapes. In thermoforming, a heated plastic sheet is stretched into a mold cavity by the application of pressure, and it is eventually assisted by direct mechanical loading.

Products of plug-assisted vacuum thermoforming, especially at high temperatures, can contain two types of imperfections: fracture of the polymeric sheet during the deformation process and warpage. The main reason for these defects can be found in the nature of the thermoforming process. Initially, it seems that these defects can be eliminated by the simple control of the state parameters of the thermoforming process. However, this is not a straightforward operation. For the removal of the defects, as the first step, the origins of the imperfections must be identified. Then, for eliminating the situations in which these defects occur, the parameters of the deformation process must be modified. To make these steps operational, it is necessary to provide a complete image of all possible reasons for the defects. Through systematic reasoning, the process parameters can be determined for the removal of the defects.[4,5]

This article focuses on two issues: (1) the origins of fracture creation and (2) the determination of the process parameters needed for the removal of the fracture. However, the mathematical calculation of the parameters that affect this defect has attracted little attention. The results of our work not only lead us to an understanding of the cause of this problem but also enable us to work out a method for calculating the related parameters affecting polymeric sheet fracture during plug-assisted vacuum thermoforming. This enables us to eliminate the defect during the deformation process.

RHEOLOGICAL MODEL AND DESCRIPTION OF THE PROCESS

The phenomenon of polymeric sheet fracture is a practical problem of plug-assisted thermoforming for the production of hollow, symmetrical products. This defect can be created during both the plug-assist and vacuum-forming stages. A sketch of the plug-assisted thermoforming process is shown in Figure 1.

One sample of polymeric sheet fracture can be viewed in Figure 2.

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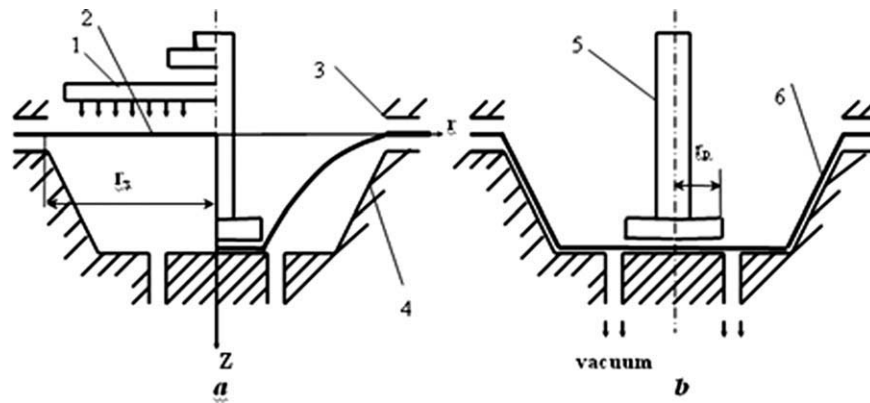
Figure 1 Representation of the sections in the two stages of plug-assisted thermoforming: (a) plug-assist stage and (b) vacuum stage [(1) heater, (2) forming sheet, (3) clamp frame, (4) mold, (5) plug, and (6) deformed sheet].

Unfortunately, as mentioned previously, this problem is an overlooked area in thermoforming research. Its successful solution is directly dependent on the selection of the proper rheological model.

One of the theoretical models in this area was developed by Leonov:[6]

$$\bar{\sigma} + p\bar{\delta} = 2\bar{c}W_1 - 2\bar{c}^{-1}W_2$$

$$\bar{e}_f = 1/\theta_0 G_0(T)\exp[-\beta W^s/G_0(T)] \cdot [(\bar{c} - I_1\bar{\delta}/3)W_1{}^s$$
$$- (\bar{c}^{-1} - I_2\bar{\delta}/3)W_2{}^s] \quad (1)$$

$$\frac{d\bar{c}}{dt} + \bar{\omega}\bar{c} - \bar{c}\bar{\omega} - \bar{c}(\bar{e} - \bar{e}_f) - (\bar{e} - \bar{e}_f)\,\bar{c} = 0$$

where $\bar{\sigma}$ is the stress tensor, p is the Lagrange multiplier determined by the boundary condition, $\bar{\delta}$ is the identity tensor, $\bar{c}$ is the Cauchy strain tensor, $\bar{e}_f$ is the flow strain rate tensor, $\bar{\omega}$ is the vortex tensor, $\bar{e}$ is the strain rate tensor, $\theta_0(T)$ is the relaxation time at temperature T, $G_0(T)$ is the tensile modulus at temperature T, W is the strain energy function [$W = W(I_1,I_2)$], β is the flexibility parameter of the macromolecular chains, I_1 and I_2 are the primary and secondary strain tensor invariants, and $2W^s = W(I_1,I_2) + W(I_2,I_1)$ is the symmetric function of W.

The last can be shown as follows:

$$W_1 = \frac{\partial W}{\partial I_1}, W_2 = \frac{\partial W}{\partial I_2}$$

$$W_1^s = \frac{\partial W^s}{\partial I_1}, W_2^s = \frac{\partial W^s}{\partial I_2}$$

MEASUREMENT OF THE RHEOLOGICAL AND MATERIAL PARAMETERS

Consider a polymeric sheet with radius r_3 heated for the production of an axisymmetric article. It is deformed by the movement of a plug with radius r_p at constant velocity V_p in the direction of the z axis. The implemented material is assumed to be incompressible and isotropic. The deformation process is carried out under isothermal conditions. The deformed sheet can be considered a thin shell, so the hot polymer can be modeled as a membrane. Therefore, the bending resistance of the hot sheet is ignored, and the material thickness is assumed to be small in comparison with the dimensions of the material. Three different stretch ratios involved in the deformation process are as follows:

$$\lambda_1 = \frac{d\xi}{d\xi_0}; \lambda_2 = \frac{r}{r_0}; \lambda_3 = \frac{h}{h_0} \quad (2)$$

where λ_1, λ_2, and λ_3 are the principal stretch ratios in the meridional, radial, and thickness directions of the membrane, respectively (they are related together by the incompressibility condition $\lambda_1 \lambda_2 \lambda_3 = 1$); ξ and ξ_0 are the lengths of the meridians in the deformed and strainless sheets, respectively; r and r_0 are the radii of the deformed and strainless sheets, respectively; and h and h_0 are the thicknesses of the

Figure 2 Fracture of the polymeric sheet during plug-assisted vacuum thermoforming. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

sheet after and before deformation, respectively. The mechanical prestretching is planar stretching (pure shear). Therefore, the following conditions exist:

$$\lambda_2 = 1, \sigma_3 = 0, \lambda_3 = \lambda_1^{-1} \quad (3)$$

where σ_3 is stress in thickness direction. With respect to the conditions and the tensors in eq. (1), the following expression can be written:

$$\bar{e} = \dot{\varepsilon} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}_{,\bar{\omega}=0,}$$

$$\bar{c} = \begin{pmatrix} c & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & c^{-1} \end{pmatrix}, \quad \bar{c}^{-1} = \begin{pmatrix} c^{-1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & c \end{pmatrix} \quad (4)$$

where $\dot{\varepsilon} ::$ is the rate of deformation in the longitudinal direction.

The primary and secondary invariants of tensor $\bar{c}$ can be derived from eq. (4) as follows:

$$I_1 = I_2 = c + 1 + c^{-1} \quad (5)$$

With eqs. (4) and (5), the following form of eq. (1) can be developed:

$$\bar{\sigma} + p\bar{\delta} = 0.5\, G_0(T) \cdot \begin{pmatrix} c - c^{-1} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & c^{-1} - c \end{pmatrix} \quad (6)$$

$$\bar{e}_f = \frac{1}{4\theta_0(T)} exp\left[-\beta\left(c + c^{-1} - 2\right)\right]$$
$$\cdot \begin{pmatrix} c - c^{-1} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & c^{-1} - c \end{pmatrix} \quad (7)$$

Parameter p results from eq. (3): $\sigma_3 = 0$. By the substitution of eqs. (4) and (7) into eq. (1), we can obtain the following:

$$\frac{dc}{dt} = 2\left[\dot{\varepsilon} \cdot c - (c^2 - 1)\frac{1}{4\theta_0(T)}exp\left[-\beta(c + c^{-1} - 2)\right]\right] \quad (8)$$

This differential equation defines the kinetics of elastic strain during the deformation process of viscoelastic media. The deformation rate is defined as follows:

$$\dot{\varepsilon} = \frac{d\varepsilon^H}{dt} = \frac{d\ln\lambda}{dt} = \frac{1}{\lambda}\frac{d\lambda}{dt} \quad (9)$$

where ε^H is the Hencky strain.

The previous equation can be represented in a dimensionless state form:

$$E(\tilde{t}) \equiv \dot{\varepsilon}(t) \cdot \theta_0(T) = \frac{\tilde{t}}{\tilde{t}^2 + a^2} \quad (10)$$

where

$$\tilde{t} \equiv \frac{t}{\theta_0(T)}$$

$$a \equiv \tilde{r}^2 \frac{r_3}{V_p\theta_0(T)} \cdot \frac{1 - \tilde{r}_p}{\tilde{r}_p}$$

$\tilde{r} = r/r_3$ is the dimensionless radius of the sheet, and $\tilde{r}_p = r_p/r_3$ is the dimensionless radius of the plug. Finally, from eq. (6) and the condition shown by eq. (3), the following relationship can be derived:

$$\sigma_1 \equiv \sigma = G_0(T) \cdot \left(c - c^{-1}\right) \quad (11)$$

where σ_1 is the meridional stress.

MODELING OF FRACTURE

It can be easily determined that one reason for the fracture of polymeric sheets is σ_1 reaching its critical value. The critical level depends on the strength limit of the polymer at its deformation temperature. The fracture of a polymeric sheet occurs under the following condition:

$$\sigma_1 \equiv \sigma_* = [\sigma(T)] \quad (12)$$

where $\sigma(T)$ is the strength limit of the polymer at processing temperature T and σ_* is the critical value of the stress.

Polymeric sheets during the deformation process experience an accumulation of elastic deformation.[7] The kinetics of this process can be specified on the basis of the parameters of the deformation process. This accumulation can be a reason for the destruction of the sheet during this process. With eqs. (11) and (12), the following condition for the destruction of the sheet in the plug-assist stage can be derived:

$$\sigma_1 \equiv \sigma_* = G_0(T) \cdot \left(c_* - c_*^{-1}\right) = [\sigma(T)] \quad (13)$$

where σ_* and c_* are the critical stress and elastic deformation in the meridional direction, respectively.

The amount of critical elastic deformation can be specified easily on the basis of eq. (13):

$$c_* = \frac{1}{2}\left(\frac{[\sigma(T)]}{G_0(T)} + \sqrt{\left(\frac{[\sigma(T)]}{G_0(T)}\right)^2 + 4}\right) \quad (14)$$

It should be mentioned that previously in this article, an assessment of the variation of the elastic deformation with time (dC/dt) is presented.

During deformation of the sheet, the following zone is at high risk of destruction:

$$\tilde{r} = \tilde{r}_p$$

Exactly in this cross-section area, dimensionless parameter a has its lowest value. Thus, on the basis of the previous equations, $\dot{\varepsilon}$ and the accumulated elastic deformation are at their highest values. It is clear that no destruction of the sheet occurs while the accumulated elastic deformation anywhere on its cross-section area is less than its critical limit.

The processing time for the plug-assist process can be obtained on the basis of the following relationship:

$$t_{\text{plug}} = \frac{H}{V_P} \tag{15}$$

where H is the depth of the sheet and t_{plug} is the time of mechanical stretching with the plug.

Parameter a at the critical cross section of the sheet can be shown in the following form:

$$a = r_3 \frac{\tilde{r}_p(1 - \tilde{r}_p)}{V_p \theta_0(T)} \tag{16}$$

Through the combination of the previous two equations, we can obtain the following:

$$\tilde{t}_{\text{plug}} = a \frac{H}{r_3 \tilde{r}_p(1 - \tilde{r}_p)} = \frac{H}{V_p \theta_0(T)} \tag{17}$$

where

$$\tilde{t}_{\text{plug}} = t_{\text{plug}}/\theta_0(T)$$

RESULTS AND DISCUSSION

Now, the critical dimensionless parameters $(a = a_*)$ can be obtained with dC/dt. Under this condition, the amount of elastic deformation reaches its critical value $(c = c_* = \text{maximum})$ but not more than that. In other words, under critical conditions (i.e., the critical value of $a = a_*$), the elastic deformation reaches its critical level (c_*). The value of this parameter is obtained through the solution of the dC/dt differential equation with various guesses for a. The critical velocity of the plug (V_{*p}) can be obtained with the evaluated critical value of a:

$$a = r_3 \frac{\tilde{r}_p(1 - \tilde{r}_p)}{V_p \theta_0(T)}$$

Deformation of the polymeric sheet by a plug with this velocity results in its destruction. Thus, the condition for avoiding fracture in a sheet is as follows:

$$V_p < V_{*p} = \frac{r_3}{a_* \theta_0(T)} \tilde{r}_p(1 - \tilde{r}_p) \tag{18}$$

By considering the presented formula for parameter a, we can conclude that its amount can be altered not only by a change in the plug velocity but also by the tuning of other process parameters. The adjustment of parameter a can be achieved by the setting of the relaxation time parameter for the implemented polymeric material. This parameter is temperature-dependent. Thus, through the suitable selection of thermal regimens, the occurrence of polymeric sheet fracture can be eliminated. Basically, the deformation process has a physical nature. The effects of this deformation on a polymeric sheet are (1) the development of a macromolecule mixing process and (2) the adjustment of the macromolecular structure direction with the direction of the applied force field. This results in an accumulation of elastic deformation within the polymer. In addition, the movement of the polymer structure due to heating results in a reduction of the accumulated elastic deformation level. The rate of this process is defined by the relaxation time. Thus, the accumulation of a certain amount of elastic deformation in a polymeric sheet is the result of two competitive processes. As the rate of the process of polymer structure alteration under deformation is temperature-dependent, its increase means a reduction of the relaxation time and consequently an increase in this process diffusivity rate. This issue reduces the level of the accumulated elastic deformation. The adequacy of eq. (8) has been verified through the comparison of experimental values in the fixed section of the deformed sheet with the theoretical results from eq. (11). A comparison of the results for meridional stress at 140°C is presented in Figure 3.

At a certain plug velocity, an evaluation of the relaxation state without the occurrence of the fracture phenomenon can be obtained with eq. (16):

$$\theta_0(T) < \frac{r_3}{a_* V_p} \tilde{r}_p(1 - \tilde{r}_p) \tag{19}$$

Theoretical and experimental information for specifying quantitative relations between the relaxation time and temperature of different polymers does not exist at present. Thus, the definition of the thermal regimen for polymeric sheets is only possible on the basis of a nonlinear regression analysis of the following equation:

$$\dot{\gamma} = \frac{1}{\theta_0(T) \cdot F(c_{12})} \cdot \frac{c_{12}}{1 - c_{12}^2} \tag{20}$$
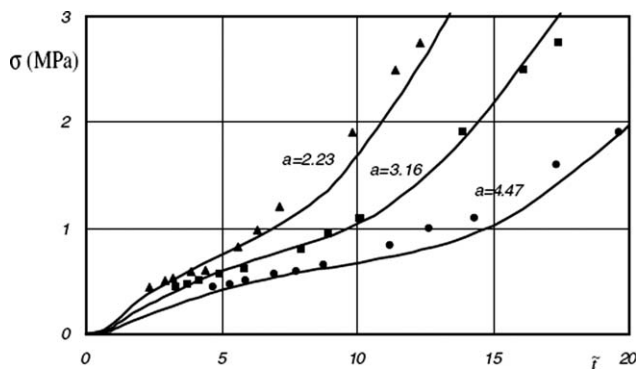
Figure 3 Stress (σ) versus the deformation time $(\tilde{t})$ for acrylonitrile–butadiene–styrene sheets at different plug velocities. The lines represent the theoretical equation [eq. (11)], and the points represent the experimental data.

where

$$\dot{\gamma} \equiv \frac{d\gamma}{dt}$$

$$F(c_{12}) = \exp\left[(\beta - 7.8\sqrt{1 - c_{12}^2})\left(\frac{1}{\sqrt{1 - c_{12}^2}} - 1\right)\right]$$

γ is the shear rate, and c_{ij} is a component of the tensor of elastic deformation at an arbitrary coordinate.

The experimental basis for performing such an analysis is the curves of the polymer flows at different temperatures. This information is obtained on the basis of viscometer experiments. In the next step, the relaxation times at different temperatures are compared with the critical levels [eq. (19)]. This results in the identification of a suitable thermal regimen for the deformation process. The defect can be removed by the specification of the regimen throughout the process. The study of the formula obtained for parameter a reveals that this parameter depends on technical–structural parameters such as r_3 and r_p. The possibility of implementing these parameters for solving the problem of sheet fracture is a theoretical issue rather than a practical one because these two parameters depend on the geometrical shapes of polymeric products.

It must be mentioned that a practical solution to sheet destruction during the plug-assist stage can be obtained by the adjustment of the parameter $\tilde{r}_p$ to its optimum value. This value can be easily obtained with eq. (16):

$$\tilde{r}_{p\ \text{opt}} = 0.5 \tag{21}$$

The destruction of a polymeric sheet can occur not only in the plug-assist stage but also in the stage

of vacuum thermoforming. In the latter stage, the reason for the destruction is the same as that in the other stage: the stress reaches its critical level. This parameter depends on the polymer strength level at a certain temperature. In other words, the occurrence of plate destruction in this stage is the same as that the other stage, and this validates eq. (12).

From eq. (12), the following equation can be derived:[8]

$$\sigma_1 = \frac{G_0(T)}{2}\left(c\lambda_1^2 - \frac{1}{c\lambda_1^2} - c^{-1}\lambda_1^{-2}\lambda_2^{-2} + c\lambda_1^2\lambda_2^2\right) - \Delta p \tag{22}$$

where ΔP is the pressure drop.

One can conclude that sheet destruction during the vacuum stage occurs under the following condition:

$$\sigma_1 \equiv \sigma_* = \frac{1}{2}G_0(T) \cdot \left[c_*c_{*1} - (c_*c_{*1})^{-1}\right.$$
$$\left. + c_*c_{*1}c_{*2} - (c_*c_{*1}c_{*2})^{-1}\right] = [\sigma(T)] \tag{23}$$

where c_{*1} and c_{*2} are the amounts of critical elastic deformation in the meridional and radial directions during the vacuum stage, respectively.

Let us consider that during the destruction of the polymeric sheet, the following relation must be satisfied:[8]

$$cc_1(1 + c_2) >> (cc_1)^{-1}(1 + c_2^{-1}) \tag{24}$$

It can be easily understood that the stress–strain state of the sheet during the vacuum stage, which is a nonsymmetrical biaxial expansion/contraction, can be assumed to be uniaxial strain with a low level of error. In other words, we find the following:

$$cc_1(1 + c_2) \approx c_{\text{uniaxial}} \tag{25}$$

This provides the ability to carry out a practical evaluation of the critical state in a polymeric sheet through the implementation of eqs. (14) and (23). This results in the following relationship:

$$[\sigma(T)] \approx [\sigma_p(T)] \tag{26}$$

On the basis of eq. (23), the following relation can be derived for the accumulation of the critical values of elastic deformation during the first stage (plug assist) and the second stage (vacuum):

$$c_* = \left(\frac{[\sigma_p(T)]}{G_0(T)} c_{*2} + \sqrt{\left(\frac{[\sigma_p(T)]}{G_0(T)} c_{*2}\right)^2 + c_{*2}(c_{*2}+1)^2} \right)$$
$$\cdot [c_{*1}c_{*2}(c_{*2}+1)]^{-1} \quad (27)$$

On the basis of an analysis of eq. (23) and with consideration of eq. (27) during the vacuum stage, a polymeric sheet is destroyed under the following conditions:

$$cc_1(c_2+1) \geq c_* c_{*1}(c_{*2}+1)$$
$$= \left(\frac{[\sigma_p(T)]}{G_0(T)} + \sqrt{\left(\frac{[\sigma_p(T)]}{G_0(T)}\right)^2 + c_{*2}\left(1 + c_{*2}^{-1}\right)^2} \right)$$
$$(28)$$

It is clear that during the vacuum stage, the destruction of the polymeric sheet occurs on a cross-section surface that satisfies the following condition:

$$cc_1(1+c_2) = \text{maximum} \quad (29)$$

During this stage, to prevent sheet destruction, the deformation process must be managed in a way that guarantees the following:

$$cc_1(1+c_2) = \text{maximum} < c_* c_{*1}(1+c_{*2}) \quad (30)$$

It is well known that because of the speed of the deformation process, there is no relaxation process during the vacuum stage. Thus, in this stage, there is an elastic accumulation. This implies that there is no possibility of managing elastic deformation. Therefore, during this stage, critical conditions exist for the accumulation of elastic deformation within a polymeric sheet [eq. (29)]:

$$c_1 c_2 = c_{*1} c_{*2} \quad (31)$$

Now, with eq. (27), c_* can be specified. This must not be misused with the critical deformation [eq. (14)], which supports the first stage. The value of c_* during the second stage must not reach its value during the first stage.

During polymeric sheet fracture, the order of the first term in the square-root section of eq. (28) is several times larger than that of the second term. Thus, the amount of critical deformation can be determined with the following relationship:

$$c_* c_{*1}(c_{*2}+1) \approx 2 \frac{[\sigma_p(T)]}{G_0(T)} \quad (32)$$

Two parameters, the tensile modulus and strength limit, for various materials at different temperatures are required to use the last equation.

The amount of tensile modulus is obtained through rheological experiments; there is enough information on this in various references.[9] The information required for the polymer strength limit at various temperatures can be found in the literature.[10] If this information is unavailable, the following theoretical method can be used:

$$\frac{[\sigma_p(T)]}{[\sigma_p(T = 293K)]} \approx 1 - B \cdot \frac{T - 293}{T_B - 293} \quad (33)$$

where $\sigma_p(T)$ is the polymer strength limit at a specific temperature and T_B is the mean softening temperature that specifies the stability of a polymer shape. Parameter B is a dimensionless coefficient. It shows the relative variation of the polymer strength limit with respect to the temperature variation.[10]

As can be seen, the worst destructive zone is the tinniest section of the throat. Within this zone, eq. (29) becomes the following:

$$cc_1(1+c_2) \approx c \cdot 59 \cdot (1 + 0.25) = \text{maximum} \quad (34)$$

Through the substitution of relations (33) and (34) into eq. (32), the following relationship for the evaluation of the amount of critical elastic deformation can be derived:

$$c_* \approx 2 \frac{[\sigma_p(T = 293 \text{ K})]}{59 \cdot (1 + 0.25) \cdot G_0(T)} \left(1 - B \cdot \frac{T - 293}{T_B - 293}\right) \quad (35)$$

Now the thermal zone can be specified through the comparison of the derived amount based on this relation with the accumulated elastic deformation in a certain cross-section area during the plug-assist process at different temperatures {i.e., for various values of dimensionless parameter $a = f[\theta_0(T)]$ and at constant plug velocities}. Performing the deformation process within this thermal zone results in the production of a polymeric article without any fracture. A comparison of the results is shown in Table I.

The amount of accumulated elastic deformation in a certain cross-section area at the end of the plug-

TABLE I
Presentation of Elastic Deformation at Different Sheet Temperatures

	Sheet temperature			
	393 K	398 K	403 K	408 K
θ_0 (s)	1	0.6	0.36	0.2
a	2	3.33	5.56	10
c/c_*	1.27	1.1	0.98	0.9
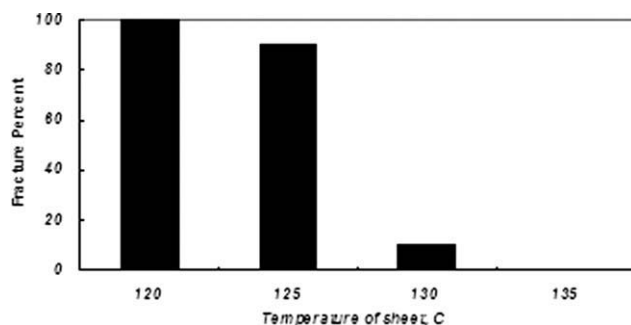
Figure 4 Fracture percentage of high-impact polystyrene sheets during vacuum thermoforming.

assist process is obtained by the solution of the differential equation dC/dt with various amounts for $a = f[\theta_0(T)]$.

The relaxation time for high-impact polystyrene is shown in Table I. For this polymer, β is approximately 2.5, and $G_0(T = 393 \text{ K} \Longleftrightarrow 408 \text{ K})$ is approximately 0.5 MPa. These rheological parameters were obtained by various tests with a viscometer. On the basis of the derived results in Table I, within the thermal range of 398–405 K, one can forecast that the produced polymeric articles can be divided into two classes: perfect and defective (with fracture). Tests were performed with plug-assisted vacuum thermoforming equipment at different temperatures. To have a statistical form for the destruction process, 10 tests at each temperature were performed. The percentage of products with fracture at each temperature is shown in Figure 4.

CONCLUSIONS

The experimental results confirm our presented model closely. An analysis of the results shows that the occurrence of fracture during plug-assisted vacuum thermoforming is due to the following processing factors:

- A reduction in the deformation temperature results in an increase in the polymer relaxation time; consequently, there is a high level of accumulation of elastic deformation during the plug-assist stage.
- Increases in the plug velocity result in an accumulation of elastic deformation to a high level.
- The mechanical properties [$\sigma_p(T)$] and rheological parameters [$G_0(T)$, β, and $\theta_0(T)$] vary throughout the process.
- Frozen-in elastic deformation forms during the cooling of the sheet.
- The value of the radius of the used plug is not optimal.

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