Numerical Simulation of Thermoforming Process for a Lightly Cross-linked Poly (methyl methacrylate)

Ogura, Koji*1,*3/Tanifuji, Shin-ichiro*2/Takahashi, Masaoki*3

A straight vacuum-forming process is simulated by use of the commercial blow molding CAE system "SIMBLOW". The accuracy of numerically predicted values of thickness distributions are compared with experimental ones. Rheological properties of a lightly cross-linked poly (methyl methacrylate) (PMMA) are expressed using the Kaye-Bernstein-Kearsley-Zapas (K-BKZ) constitutive equation with the damping function of the Papanastasiou-Scriven-Macosko (PSM) model. The simulation conditions are based on an analysis of actual vacuum-forming behavior. The relaxation spectrum is obtained from dynamic moduli data, and the PSM model parameters are determined from experimental data of uniaxial extension by trial and error. The predicted thickness distributions along the center and corners of the mold agree very well with the experimental results. On the other hand, the accuracy of prediction decreases in the vicinity of large bending deformation, where deviation from the biaxial extension is expected.

Key words: Thermoforming/Poly (methyl methacrylate)/Numerical Simulation/K-BKZ model/CAE system

1. Introduction

Thermoforming is one of the simple polymer processing in which a flat sheet of softened thermoplastic resin is deformed over a mold by vacuum and/or air pressure with close contact of the mold. Due to its simplicity, thermforming is widely used for various products. Compared with other processes such as blow molding, injection blow molding, rotational molding and injection molding, thermoforming can be performed with lower molding pressure, lower mold costs and larger plastic part size. In many applications of thermoforming, sheet stretching is usually made at small draw ratio. Investigation on molding material properties and molding conditions are important to find optimum conditions and materials for plastic industrial products. Numerical simulations were made to find optimum thermoforming conditions and to investigate the effects of rheological properties on thermoforming behavior. Wang et al. proposed a new viscoplastic model for simulation, in which strain-hardening, strain-rate sensitivity of uniaxial extensional flow behavior and temperature effects were considered. The vacuum forming process of a square cup was simulated and results were compared with experiment. The simulated thickness distribution showed good agreement with the experimental results. In recent studies, viscoelastic constitutive equations were applied to describe...
rheological properties in thermoforming process. Lee et al. fitted experimental data of ABS polymer with predictions of Wagner model, which is a K-BKZ type single integral constitutive equation, and simulated the thermoforming performance using a commercial software to evaluate rheological behavior and initial sheet temperature distribution.

In the present study, straight vacuum-forming process is simulated by use of commercial blow molding CAE system SIMBLOW. The accuracy of numerically predicted values is checked by comparison with experimental data of a lightly cross-linked poly(methyl methacrylate). The rheological properties of the sample are described by a K-BKZ type constitutive equation, and necessary viscoelastic parameters are determined. The boundary conditions are based on the analysis of experimental vacuum-forming.

2. Experimental

2.1 Sample
A lightly cross-linked poly(methyl methacrylate) (PMMA) of 5 mm thickness was synthesized by casting polymerization. No anisotropy was observed in this casting sheet. Experimental data of dynamic viscoelasticity and extensional viscosity for the lightly cross-linked PMMA are shown in reference.

2.2 Vacuum forming conditions
Fig.1 shows a schematic diagram of the straight vacuum forming process. The straight vacuum forming experiments were performed using the thermoforming machine (Fuse Shinku Co., Ltd, CUPF 1015 PWB). The vacuum forming temperature was 200°C. Temperature distribution over the sheet just before vacuum forming was observed by thermography (Nippon Avionics Co., Ltd, TVS-2500 TE). As an example, Fig.2 shows the temperature distribution on the sheet just before vacuum forming. The temperature difference was observed below 5°C in surface direction. The dimensions of a female mold were 170 mm square, 70 mm depth with a slope of 1/30 and corner radius of 5 mm. The mold is made of ZAS alloy and the temperature was 80°C. Thickness distribution of the final product was measured by ultrasonic thickness gage (Panametrics, 25 DL).

3. Vacuum Forming Simulation
The commercial simulation software SIMBLOW (version 2003, Plamedia Corporation) was used to predict the thermforming behavior. This software estimates the deformation behavior from an analysis based on the mo-
momentum equation (1) and a viscoelastic constitutive equation (4) (shown later). Details of this analysis can be found in reference\(^7\).

The momentum equation is expressed as

\[
\int \nabla \Phi \cdot \sigma^{\text{st}} \, dV = \int \Phi f^{\text{st}} \cdot ndS \tag{1}
\]

where \( \Phi \) is the vector form of the membrane finite element basis functions, \( \sigma \) is the extra stress tensor, \( f^{\text{st}} \) is an external force corresponding to the vacuum suction force and \( n \) is the unit normal vector. The volume integration and area integration are evaluated in the known region (region of element volume \( \Omega \) and region of area \( S' \)) at time \( t \). At each discrete computational time \( n \Delta t \), the thickness of PMMA sheet \( H^t \) is renovated according to the following equation.

\[
H^{t+1} = H^t / (1 + \nabla \cdot \Phi \Delta t) \tag{2}
\]

Here, \( \nabla \cdot \Phi \) is the flow velocity vector.

Analysis of energy equation considers the heat conduction in thickness direction and the heat transfer coefficient between sheet and air or mold by use of finite difference mesh attached to membrane element.

\[
\rho C_v \frac{DT}{Dt} = \nabla \cdot (\kappa \nabla T) \tag{3}
\]

Here, \( \rho \) is the density, \( C_v \) the specific heat, \( T \) the temperature, and \( \kappa \) is the heat conductivity. We assume that the heat transfer coefficient is constant in vacuum forming process.

The three-dimensional computation is very elaborate, so it is assumed that the deformation can be modeled in terms of the biaxial extension. The viscoelastic stress is approximately calculated by

\[
\sigma_{ij} - \sigma_{ij}^{(r)} = \sum_{r' \neq r} \int_{\tau_{t'} = 0}^{\tau_t} \left[ \sum_i G_i \exp \left( -\frac{n \Delta t - t'}{\tau_i} \right) \right] B_i(t') B_{r'}(t') dt' + \left[ \sum_i G_i \exp \left( -\frac{n \Delta t}{\tau_i} \right) \right] h(t') B_{r'}(0) \tag{4}
\]

where, the component of the strain tensor \( B \) is calculated using the area \( S(t) \) of the membrane element:

\[
B_i(t') = \frac{S(t)}{S(t')} - \left( \frac{S(t')}{S(t)} \right)^2 \tag{5}
\]

The damping function \( h \) is given by the following expression proposed by Papanastasiou et al.\(^7\):

\[
h = \frac{\alpha}{\alpha - 3 + \beta I_{c-1} + (1 - \beta) I_c} \tag{6}
\]

where \( \alpha \) and \( \beta \) are parameters in the range of \( \alpha > 1 \) and \( 0 < \beta < 1 \), and \( I_{c-1} \) and \( I_c \) are the first invariants of the Finger \( C_{1-1}^{c-1}(t') \) and the Cauchy strain tensors \( C(t') \), respectively.

The temperature dependence of the relaxation time is expressed by

\[
\tau_r(T) = a_r \tau_r(T_{ref}) \tag{7}
\]

with the Arrhenius equation for the shift factor \( a_r \):

\[
\log a_r = \frac{\Delta H}{2.303 R \left( \frac{1}{T} - \frac{1}{T_{ref}} \right)} \tag{8}
\]

where \( T_{ref} \) is the reference temperature, \( R \) is the gas constant and \( \Delta H \) is the activation energy (\( T_{ref} = 200^\circ C \) and \( \Delta H = 222 \text{ KJ/mol} \) for this system).

The simulation is performed for 1/4 of the sheet in consideration of symmetry of the vacuum forming mold. Fig.3 shows a schematic diagram of initial mesh configuration of the mold and sheet. The sheet is divided into 4900 elements with 5041 nodes. The initial temperature of PMMA sheet is 200°C. The surrounding air temperature is constant at 20°C. Table 1 summarizes computational condition for the vacuum forming analysis.

4. Results and Discussion

4.1 Material Characterization

A relaxation spectrum is determined from the experimental data of the storage and loss moduli by using Tschogl’s second order approximation equation\(^7\). The experimental data of storage and loss moduli for a lightly cross-linked PMMA at 200°C are reproduced in Fig.4\(^7\). A tentative discrete relaxation spectrum \( G(t) \) corresponding to seven relaxation times \( \tau_r = 10^{-3} \sim 10^5 \) are determined. Then, a final set of \( (\tau_r, G) \) is obtained by trial and error method by fitting to \( G' \), \( G'' \) master curves according to the following equations.
Introducing a long relaxation time ($r = 10^{5}$s) and corresponding $G_s$, it is possible to fit $G'$ and $G''$ data over 6 and 5 decades of frequency respectively. Table 2 summarizes a final set of $(r, G_s)$ for the lightly cross-linked PMMA.

In this study, the PSM model parameters $\alpha$ and $\beta$ are determined from uniaxial extension data by trial and error method. The PSM model cannot accurately describe the biaxial extension data in which strain-softening followed by upturn behavior was observed. The characteristic behaviors of the lightly cross-linked PMMA in nonlinear region of uniaxial and biaxial extensions are prominent strain-hardening behavior in the uniaxial stress growth coefficient $r_{\varepsilon} (t, \varepsilon)$ and weak strain-softening followed by upturn in the biaxial stress growth coefficient $\eta_s (t, \varepsilon)$.

Fig. 5 compares the uniaxial extension data with the PSM model prediction for $\alpha = 30.0$ and $\beta = 0.01$. The predicted values show good agreement with the experimental data in the range of strain rate measured.

### Table 1 Computational condition for the vacuum forming analysis

<table>
<thead>
<tr>
<th>Material properties of PMMA melt</th>
<th>Density $\rho$</th>
<th>$1100 \text{ kg/m}^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific heat $C_v$</td>
<td></td>
<td>$3.62 \text{ kJ/kg} \cdot \text{K}$</td>
</tr>
<tr>
<td>Thermal conductivity $\kappa$</td>
<td></td>
<td>$0.19 \text{ W/m} \cdot \text{K}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time profile vacuuming pressure</th>
<th>Inflation time (s)</th>
<th>Vacuuming pressure (KPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>8.0</td>
<td>40.0</td>
</tr>
<tr>
<td></td>
<td>15.0</td>
<td>40.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Thermal condition</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambient air temperature</td>
<td>20°C</td>
</tr>
<tr>
<td>Mold temperature</td>
<td>80°C</td>
</tr>
<tr>
<td>Heat transfer coefficient between sheet and air</td>
<td>10.0 $\text{ W/m}^2 \cdot \text{K}$</td>
</tr>
<tr>
<td>Heat transfer coefficient between sheet and mold</td>
<td>800.0 $\text{ W/m}^2 \cdot \text{K}$</td>
</tr>
</tbody>
</table>

(Activation energy $\Delta H (T_{m} = 200^\circ \text{C}) : 222 \text{ KJ/mol}$)

### Table 2 Discrete relaxation spectrum of a PMMA at 200°C

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\tau_s$</th>
<th>$G_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1.00 \times 10^4$</td>
<td>$4.00 \times 10^4$</td>
</tr>
<tr>
<td>2</td>
<td>$1.00 \times 10^5$</td>
<td>$1.61 \times 10^4$</td>
</tr>
<tr>
<td>3</td>
<td>$1.00 \times 10^6$</td>
<td>$5.47 \times 10^4$</td>
</tr>
<tr>
<td>4</td>
<td>$1.00 \times 10^7$</td>
<td>$6.74 \times 10^4$</td>
</tr>
<tr>
<td>5</td>
<td>$1.00 \times 10^8$</td>
<td>$8.96 \times 10^4$</td>
</tr>
<tr>
<td>6</td>
<td>$1.00 \times 10^{-1}$</td>
<td>$1.01 \times 10^5$</td>
</tr>
<tr>
<td>7</td>
<td>$1.00 \times 10^{-2}$</td>
<td>$1.80 \times 10^5$</td>
</tr>
<tr>
<td>8</td>
<td>$1.00 \times 10^{-3}$</td>
<td>$1.34 \times 10^5$</td>
</tr>
</tbody>
</table>

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Fig. 6 Time dependence of the biaxial stress growth coefficient \( \eta_\sigma (t, \dot{\varepsilon}_s) \) for a lightly cross-linked PMMA at 200°C obtained at various \( \dot{\varepsilon}_s \). The solid lines are calculated by the K-BKZ equation using the damping function of the PSM model.

Fig. 6 shows similar comparison in biaxial extension. Here the same values of parameters as in the uniaxial extension are used. In the nonlinear viscoelastic region, the PSM model predicts only the strain-softening behavior. It is considered that the PSM model underestimates the deformation of lightly cross-linked polymer chain in biaxial extension as suggested for branched polymers. On the other hand, the biaxial stress growth coefficient at constant strain rate does not show upturn in most of the strain range in this vacuum-forming experiment. Therefore it is considered that the PSM model can be used for this numerical simulation.

4.2 Vacuum-forming Analysis

Fig. 7 shows predicted time sequence of sheet shape and temperature distribution in the inflation process. At first, center and vicinity of flange of sheet contact to mold, and the contact of sheet to mold is proceeded with inflation of sheet successively. Depression of sheet temperature is so small in the inflation process that temperature effect for free inflation behavior is small. As compared with isothermal results, no apparent difference between both results is predicted in the thickness distribution of final molding product. The sheet temperature decreases rapidly after contacting to mold, although this analysis is assumed that deformation of sheet is stopped at the inflating sheet contact of mold and that the heat conduction in the sheet plane direction can be neglected. Therefore the sheet temperature condition in free inflation process has weak influence on thickness distribution of final molding product. It is considered that the influence of initial temperature distribution on final thickness distribution is larger than the variation of temperature during the inflation process. In this study, initial sheet temperature distribution is less than 5°C (see Fig. 2), which was measured by an infrared ray thermometer in experimental straight vacuum-forming. Further study is necessary to evaluate the non-uniformity in temperature distribution of thermoforming sheet.

Figs. 8 and 9 compare experimental and predicted thickness distribution of the final product. The experimental data were obtained using an ultrasonic measuring device at 10 mm pitch.

The thinnest thickness point of the experimental data was a corner of the mold which corresponds to the most delayed point of contact to the mold. In Fig. 8, along the line ABC between the bottom of center (A) and a corner (B), the predicted thickness values show remarkable agreement with the experimental data. On the other hand, between a corner (B) and a flange (C), the predicted thickness deviates from the experimental results. In the vicinity of the corner, the predicted values underestimate the experimental ones, while overestimation is observed in the vicinity of the flange.

In Fig. 9, along the line AB'C', good agreement is ob-
tained between the predicted values and experimental data. Although much smaller but similar discrepancy between the predicted and the measured thickness appears along the line B'C'. These discrepancies may be due to (1) modeling by membrane elements and/or (2) simplified deformation mode of biaxial extension. A membrane element does not produce the resistant force against the bending deformation. It is considered that membrane element may not be suitable to actual molding behavior at a part of large bending deformation. The simplified membrane deformation as biaxial extension may not be a good assumption in the vicinity of flange. In order to solve these problems, a further study is necessary to develop viscoelastic analysis tools for treatment of general deformation mode.

5. Conclusions

In this study, a straight vacuum-forming process is simulated by use of the commercial blow molding CAE system "SIMBLOW". Uniaxial and biaxial extension data of a lightly cross-linked PMMA are expressed by the K-BKZ type constitutive model (Papanastasiou-Scriven-Macosko). It is found that the predicted thickness distributions along the center and corners of mold agree very well with experimental results. The accuracy of predicted thickness values decreases in the vicinity of large bending deformation.
References

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和文要旨
ストレート真空成形現象を市販のプロー解析システム“SIMBLOW”を用いてシミュレートし、実際のストレート真空成形品の厚み分布測定結果との比較解析を通じて数値シミュレーションの予測精度について検証した。シミュレーションにおいては樹脂のレオロジー特性をK−BKZ型構成方程式により表現するとともに、成形現象解析から与えられる解析条件をもとに解析を行った。樹脂のキャラクタリゼーションでは、動的粘弾性測定結果から緩和スペクトルを求めるとともに、K−BKZ構成方程式の物質パラメーターは一軸伸長挙動にフィットする値を試行錯誤的に求めた。ストレート真空成形の数値解析の結果、成形上重要される成形型コーナーの最薄部位から成形形体中央部までの間の肉厚を定量的に捉えることが可能であったが、大きな曲げ変形を伴ってシートが金型と接触する部位では肉厚予測精度が低下した。