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The Use of Elasto-Visco-Plastic Material Model Coupled with Pressure-Volume Thermodynamic Relationship to Simulate the Stretch Blow Molding of Polyethylene Terephthalate

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Abstract. The use of polyethylene terephthalate (PET) in the stretch blow molding process presents several challenging issues due to various processing parameters and complex behavior of the material, which is both temperature and strain-rate dependent. In this paper, we generalize the G'Sell-Jonas law in 3D to model and simulate the elasto-visco-plastic (EVP) behavior of PET, taking into account strain-hardening and strain-softening. It is observed that the internal pressure (inside the preform) is significantly different from the nominal pressure (imposed in the blowing device upstream) since the internal pressure and the enclosed volume of the preform are fully coupled. In order to accurately simulate this phenomenon, a thermodynamic model was used to characterize the pressure-volume relationship (PVR). The predicted pressure evolution is thus more realistic when imposing only the machine power of the blowing device (air compressor or vacuum pump). Mechanical and temperature equilibrium equations are fully nonlinear and solved separately with implicit schemes on the current deformed configuration, which is updated at each time step. Biaxial characterization tests were used to determine the model parameters in order to simulate the stretch blow molding process using the pressure-volume thermodynamic relationship. To validate this model, thickness predictions for three industrial cases will be presented and compared to experimental measurements.

Keywords: Stretch blow molding, modeling, finite element, PET material, material model, thickness predictions, industrial cases.

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INTRODUCTION

Stretch blow molding (SBM) is the process of choice for the production of PET containers, in particular for the food and beverage industry as well as the pharmaceutical sector. The SBM process is a high volume process with costly tooling for both the preform and the container. For example, an injection-molding machine can have a 144-cavity preform configuration and a stretch blow-molding machine a 16-cavity blow molds. Therefore, it is critical in the prototype phase, to efficiently model the whole process especially in the preform stretching and blowing phases in order to minimize tooling modifications, which can be quite costly.

The objective of this work is to propose a thermomechanical approach coupled with an adequate

material model to model the preform PET deformation during the process.

ELASTO-VISCO-PLASTIC MODEL OF PET

The behavior of PET depends essentially on strain level, strain rate and temperature [1]. In the stretch blow molding process, the elastic strain part of strain is negligible compared to the plastic part and is modeled by a linear law. Two parameters are used to define the material's elastic behavior: Young's modulus, E , and Poisson's ratio, ν , which depend only on temperature. The plastic strain starts with the preform stretch loading and is strain rate dependent. To model this visco-plastic part, we generalize the G'Sell-Jonas law [2] in 3D by taking into account both hardening and softening phenomena. After studying

the behavior of several polymers in unidirectional tension, G'Sell and Jonas [2] presented the following model for a uniaxial deformation:

$$\sigma_0(\varepsilon, \dot{\varepsilon}, T) = K e^{\frac{a}{T}} (1 - e^{-w\varepsilon}) e^{(h_g \varepsilon^2)} \dot{\varepsilon}^m \quad (1)$$

Where K , a , w , h_g and m are the constant parameters of the model and T , ε denote the temperature and total axial strain, respectively. The point indicates the derivative with respect to time. h_g is the hardening modulus since it controls the strain hardening of the polymer. However, softening phenomenon, which is also observed in PET, is not taken into account by the G'Sell-Jonas's law [3]. In 3D cases, the generalized model proposed in this paper, is based on the Von Mises criterion and does not take into account the hydrostatic pressure nor the material orientation. This law is written as follows:

$$J_2(p, \dot{p}, T) = K e^{\frac{a}{T}} (1 - e^{-wp}) e^{(h_g p^2 - h_f p)} \dot{p}^m \quad (2)$$

Where J_2 is the Von Mises stress, and p is the equivalent visco-plastic strain. To model the softening phenomenon, we have introduced the h_f parameter which is called the softening modulus. The state laws describing the stress-strain relationship are given as follows:

$$\begin{aligned} \mathbf{S} &= \mathbf{H} \mathbf{E}^e = \mathbf{H}(\mathbf{E} - \mathbf{E}^{vp}) \\ \dot{\mathbf{E}}^{vp} &= \frac{3}{2J_2} \dot{p} \mathbf{S} \end{aligned} \quad (3)$$

Where $\mathbf{S}$, $\mathbf{E}^e$, $\mathbf{E}^{vp}$ are the second-order stress, elastic strain and visco-plastic strain tensors, respectively, and $\mathbf{H}$ is the fourth-order elasticity tensor (Hooke's law).

Material characterization

Biaxial stretching experiments of the PET materials were performed on the Bruckner stretcher as shown in Figure 1. This biaxial tester allows the mechanical behavior of the PET sheets to be studied by stretching them in both directions of the sheet plane. It is equipped with a special mechanism that allows the sample to be clamped and then stretched smoothly in the sheet plane [4-5]. The material is heated to the desired temperature before testing by hot air circulating in the conditioning chamber of the tester. The sample can be stretched either simultaneously in the machine direction and the transverse direction or sequentially, i.e., one after the other. Additionally, the

test can be performed at either constant velocity or constant strain rate. The dimensions of the samples are 85mm x 85mm x 1.5mm. The samples were heated up to three set-up temperatures (90, 105 and 115 °C) and simultaneously stretched in both directions (at three constant strain rates: 10, 50 and 100% s^{-1}) so that the strain hardening in the stress-strain curve could be observed. The model parameters are obtained by fitting biaxial stretching data at different temperatures. K and a are temperature independent, whereas the temperature dependency of w , h_f , h_g and m is given by a linear interpolation between two temperature values. Figures 2a-c depict the experimental data and the fitting curves of PET at 90°C, 105°C and 120°C. Table 1 gives the EVP model constants for PET.

FIGURE 1. Bruckner biaxial stretcher.

TABLE 1. EVP model constants for PET.

Temperature (°C)	90	105	115
h_f	0.17764	0.23095	0.3521
h_g	0.00979	0.01282	0.015744
m	0.2264	0.2759	0.5
K (MPa s^m)	3.1858 10^{-10}		
a (°K)	8170.547		
w	5000		

PRESSURE-VOLUME RELATIONSHIP

Thermodynamic Model

In practice, the inflation pressure is imposed and measured in the blowing device upstream and not inside the preform. There are, however, large differences between these two pressures since the enclosed volume of the preform and the internal pressure are fully coupled. In the literature, a few studies have been developed [6-7] in order to better understand and represent the pressure-volume relationship (PVR). In this paper, we present a mathematical model based on a thermodynamic approach [8]. Two main hypotheses are considered:

- during inflation, the air mass inside the preform varies and its derivative with respect to time

defines the flow-rate of the air compressor. The thermodynamic state remains uniform during this time;

- b) kinetic and potential energy variation is assumed to be negligible inside the control volume (preform).

$$\gamma P \frac{dV}{dt} + V \frac{dP}{dt} = W_{net} \quad (4)$$

where P is the internal pressure, V the volume of the preform, $\gamma=1.4$ for the air and W_{net} represents the air compressor power.

Numerical Implementation

Pressure-volume relationship (Eq 4) has been implemented in the BlowSim finite element code. The numerical integration is done by discretizing the loading. The algorithm can be described as follows:

1. Initially, pressure is set to a value (one atmosphere), the initial volume of the preform is calculated, and the machine power is imposed;
2. at a discrete time t_n , the new volume is calculated from the nodal displacements;
3. equation (4) is solved with implicit scheme to calculate the internal pressure;
4. the external loads are known from the pressure value found in step 3 and the resolution of finite element problem allows to update the nodal displacements;
5. finally, steps 2 to 4 are re-executed until the final time step.

The predicted pressure evolution is thus more realistic when imposing the air compressor power instead of pressure. Mechanical and temperature equilibrium equations are fully nonlinear and solved separately with implicit schemes on the current deformed configuration, which is updated at each time step.

INDUSTRIAL SIMULATION CASES

Three industrial cases were studied to validate the EVP material model and the PVR implemented in the BlowSim software technology from National Research Council of Canada. The numerical predictions were compared with the experimental measurements in the case of two stretch blow molded PET bottles and in a biomedical balloon forming application.

Oval and 20oz Hot Fill Bottles

It is to be noted that these two industrial cases have been performed in co-ordination with Graham Packaging Company. Figures 3 and 4 show the preform deformation for the two bottles during stretching and blowing into the mold. Preforms have been meshed using irregular triangular elements. The preform surface temperature was obtained from

FIGURE 2. Experimental data and fitting curves of PET at: a) 90 °C, b) 105 °C, c) 115 °C.

The energy balance may be simplified as follows:

experiments and is considered uniform for the oval bottle (112°C) and varies from 80°C to 110°C for the 20oz Hot Fill bottle. From the initial state, preforms are simultaneously stretched and/or pre-blown with a low air compressor power (0.1 and 0.04 HP for oval and 20oz Hot Fill bottles respectively). Then, they are blown using a higher machine power (3 HP) to take the final shape in the mold.

The simulated inflation pressure history for the oval bottle is plotted in Figure 5. One can notice that the pressure increases in the pre-blow or stretching phase and suddenly decreases when the preform starts to inflate. The pressure will finally flatten out at a maximum pressure since the preform reaches the cavity wall and no air is entering inside the cavity at that time.

The comparison between predicted and measured wall thickness distributions of the bottles are shown in Figures 6 and 7. From these figures, it can be observed that the thickness prediction using the EVP material model is in good agreement with the experimental thickness measurements. Although, slight differences between these results are observed, they are not substantial in spite of the bottle's complex geometry, particularly in the case of the 20oz Hot Fill bottle.

Balloon Forming for a Biomedical Application

Figure 8 shows the mould dimensions. The preform deformations for a balloon during stretching and blowing into the mold are shown in Figure 9. Table 2 resumes the comparison between predicted and measured thickness distributions of the balloon. A good agreement is found, particularly in center area of balloon.

FIGURE 3. Stretch/Blow molding of the Oval Bottle.

FIGURE 4. Stretch/blow molding of the 20oz Hot Fill Bottle.

CONCLUSION

In this work, an elasto-visco-plastic model for the PET was presented which takes into account the hardening and the softening of the material. All unknown parameters have been identified by fitting biaxial stretching data at different temperatures. Moreover, a thermodynamic model to represent the pressure-volume relationship during the blow molding process has been used. After implementation of the model in a finite element code, simulations of the stretching and inflation stage, using measured temperature distributions, were also presented. The predicted container thickness distributions were found to be in good agreement with experimental results. The EVP model is then appropriate to represent the PET behavior deformation and the use of a pressure-volume thermodynamic relationship with this model confirm the ability to better simulate non-isothermal stretch blow molding.

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FIGURE 5. Pressure versus Time for Oval Bottle.

FIGURE 6. Thickness Distribution along Oval Bottle.

FIGURE 7. Thickness Distribution of the 20oz Hot Fill Bottle.

TABLE 2. Thickness comparison for balloon forming (mm).

	EXPERIMENTAL	SIMULATION
CONE AREA THICKNESS (mm)	0.0175	0.0196
CENTER THICKNESS (mm)	0.0180	0.0176

FIGURE 8. Mould Dimensions for Balloon Forming.

FIGURE 9. Balloon Forming Simulation Validation.

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