An Anisotropic Visco-hyperelastic model for PET Behavior under ISBM Process Conditions

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Abstract. The mechanical behavior of Polyethylene Terephthalate (PET) under the severe loading conditions of the injection stretch blow molding (ISBM) process is strongly dependent on strain rate, strain and temperature. In this process, the PET near the glass transition temperature (Tg) shows a strongly non linear elastic and viscous behavior. In author's previous works, a non linear visco-hyperelastic model has been identified from equi-biaxial tensile experimental results. Despite the good agreement with biaxial test results, the model fails to reproduce the sequential biaxial test (with constant width first step) and the shape evolution during the free blowing of preforms. In this work, an anisotropic version of this visco-hyperelastic model is proposed and identified form both equi and constant width results. The new version of our non linear visco-hyperelastic model is then implemented into the Abaqus environment and used to simulate the free blowing process. The comparison with the experimental results managed in Queen's University Belfast validates the approach.

1. INTRODUCTION

The injection stretch blow molding (ISBM) process is managed at a temperature slightly above the glass transition temperature Tg. It involves multiaxial large strains at high strain rate. During the ISBM process, the PET behavior exhibits a high elasticity, a strain hardening effect and a strong viscous and temperature dependency. Therefore, much research has been conducted on the rheological behavior of PET. Essentially, the viscoelastic models which take into account the strain hardening and strain rate effects have been widely used for the ISBM process in literature. We have proposed a non linear incompressible visco-hyperelastic model to model the complex constitutive behavior of PET [1, 2]. Based on the experimental results of the equi-biaxial tensile test, we have identified the properties of this visco-hyperelastic behavior, but some improvements are needed to fit sequential biaxial tests or free blowing experiments.

In this work, an anisotropic version of the visco-hyperelastic model is proposed and detailed in the 2nd section. Starting from a recall of the isotropic version, we introduce the theoretical basements of the anisotropic version. This version uses, for the elastic part, an energy function W which depends on new invariants from I_4 to I_9. Derivation of the energy function W leads to a stress tensor that depends on structure tensor $\mathbf{A}_i$ built from the direction of anisotropy. A classical orthotropic formulation is chosen for the viscous part. In section 3, we identify this new version of the visco-elastic model using both equi-biaxial and constant width test results. Thanks to this identification, we can simulate a more industrial case: free blowing of PET preform. The model is implemented into the software ABAQUS / Explicit via a user- interface VUMAT to benefit from the opportunities of CAD and mesh construction software. The free blowing simulation, taking into account the anisotropy, is performed and is successfully compared to the experimental results.

2. VISCO-HYPERELASTIC MODEL FOR PET UNDER ISBM CONDITION

The strongly hyperelastic strain rate dependant and coupled with the temperature is modeled using a Maxwell like model in finite strain. The Cauchy stress tensor $\underline{\underline{\sigma}}$ can be written:

$$\begin{cases} \underline{\underline{\sigma}} = -P_e \underline{\underline{I}} + 2G \underline{\underline{\varepsilon_e}} \\ \underline{\underline{\sigma}} = -P_v \underline{\underline{I}} + 2\eta \underline{\underline{D_v}} \end{cases} \quad (1).$$

where $\underline{\underline{\varepsilon_e}}$ is an Eulerian strain tensor: $\underline{\underline{\varepsilon_e}} = \frac{1}{2}\left(\underline{\underline{B_e}} - \underline{\underline{I}}\right)$

$$G = G_0 \exp\left(\Lambda (I_1 - 3)^2\right),\ I_1 = trace\left(\underline{\underline{B_e}}\right),\ \eta\left(\overline{\varepsilon_v}, \dot{\overline{\varepsilon_v}}\right) = \eta_0 h\left(\overline{\varepsilon_v}\right) f\left(\dot{\overline{\varepsilon_v}}\right) \quad (2).$$

$$\eta_0 h\left(\overline{\varepsilon_v}\right) = \frac{\eta_0 \left(1 - \exp\left(-K\overline{\varepsilon_v}\right)\right)}{\left(1 - \overline{\varepsilon_v}/\varepsilon_{v\lim}\right)^N},\ f\left(\dot{\overline{\varepsilon_v}}\right) = \frac{1}{\left(1 + \left(\lambda\, \dot{\overline{\varepsilon_v}}/\dot{\varepsilon}_{ref}\right)^a\right)^{\frac{1-m}{a}}}$$

where Λ and G_0 are constant. λ, m, a are parameters in the Carreau type law $f\left(\dot{\overline{\varepsilon_v}}\right)$ and $\dot{\varepsilon}_{ref}$ is a reference strain rate that can be taken equal to 1 s^{-1} for sake of simplicity. η_0, K, N and $\varepsilon_{v\lim}$ are parameters in h function which can be identified from biaxial elongation tests [1,2]. P_e and P_v are hydrostatic pressures associated to incompressibility conditions. $\underline{\underline{B_e}}$ is the elastic part of the left Cauchy deformation tensor. From the assumption of additivity of the elastic deformation rates and viscous, assumption of the pure elastic spin rate and the Oldroyd equation of $\underline{\underline{B_e}}$, the constitutive equation can be obtained:

$$\frac{\delta \underline{\underline{B_e}}}{\delta t} = -\left(\underline{\underline{D_v B_e}} + \underline{\underline{B_e D_v}}\right) \Rightarrow \frac{\delta \underline{\underline{B_e}}}{\delta t} + \frac{G}{\eta} \underline{\underline{B_e}}\, \underline{\underline{\widehat{B}_e}} = 0 \quad (3).$$

This model reproduces nicely the equi-biaxial elongation results obtained from experimental tests managed à QUB [3] even if our visco-elastic model is quite different from the one used at QUB [4]. Figure 1 shows the stress-strain curves at 90°C for different strain rates on left graph and for 8 s^{-1} strain rates at different temperature on the right. This large range of strain, strain rate and temperature is near ISBM conditions and the mean difference on the entire set of results is less than 5%.

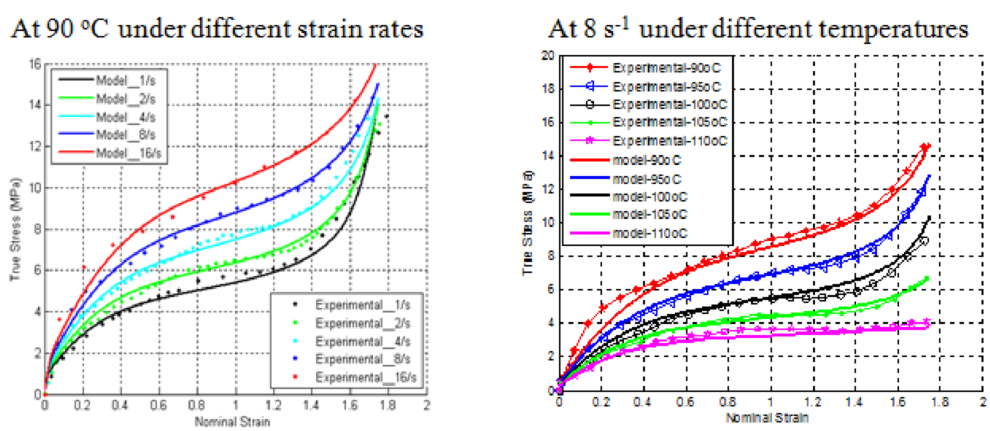

FIGURE 1. Comparison between experimental results and model simulations

To obtain the correct aspect ratio between length and radius during the free blowing simulation or to reproduce accurately the constant width test, one needs to introduce anisotropy in both viscous and elastic parts of the model. The deviatoric part of the stress tensor $\underline{\underline{\hat{\sigma}}}$ can be written in equation 6 in our case:

$$\hat{\underline{\underline{\sigma}}} = 2\eta \underline{\underline{D_v}} \text{ that also writes: } \begin{pmatrix} \hat{\sigma}_{11} \\ \hat{\sigma}_{22} \\ \sqrt{2}\sigma_{12} \end{pmatrix} = 2\begin{bmatrix} \eta_{11} & \eta_{12} & 0 \\ \eta_{12} & \eta_{22} & 0 \\ 0 & 0 & \eta_{44} \end{bmatrix} \begin{pmatrix} D_{v11} \\ D_{v22} \\ \sqrt{2}D_{v12} \end{pmatrix} \tag{4.}$$

We choose specific h_i functions [5] for each orthotropic direction (i=1 the longitudinal direction and i=2 hoop direction):

$$\begin{cases} \eta_{11} = \eta_0 h_1 f\left(\overline{\dot{\varepsilon}_v}\right) \\ \eta_{12} = \beta\eta_0 \max(h_1, h_2) f\left(\overline{\dot{\varepsilon}_v}\right) \\ \eta_{22} = \eta_0 h_2 f\left(\overline{\dot{\varepsilon}_v}\right) \\ \eta_{44} = \eta_0 h\left(\overline{\varepsilon_v}\right) f\left(\overline{\dot{\varepsilon}_v}\right) \end{cases}, \quad \begin{cases} h_1 = \dfrac{\left(1-\exp\left(-K\overline{\varepsilon_v}\right)\right)}{\left(1-2\varepsilon_{v1}/\varepsilon_{v\lim}\right)^N} \\ h_2 = \dfrac{\left(1-\exp\left(-K\overline{\varepsilon_v}\right)\right)}{\left(1-2\varepsilon_{v2}/\varepsilon_{v\lim}\right)^N} \end{cases} \tag{5.}$$

Expressions of the functions h_i assure to give the same model than the isotropic one when the strain is purely equi-biaxial.

In order to build the elastic part of the model we need new invariants, namely:

$$\begin{aligned} &I_4 = \underline{n_1} \cdot \underline{\underline{B}} \cdot \underline{n_1}, \quad I_6 = \underline{n_2} \cdot \underline{\underline{B}} \cdot \underline{n_2}, \quad I_8 = \underline{n_3} \cdot \underline{\underline{B}} \cdot \underline{n_3}, \\ &I_5 = \underline{n_1} \cdot \underline{\underline{B}}^2 \cdot \underline{n_1}, \quad I_7 = \underline{n_2} \cdot \underline{\underline{B}}^2 \cdot \underline{n_2}, \quad I_9 = \underline{n_3} \cdot \underline{\underline{B}}^2 \cdot \underline{n_3} \end{aligned} \tag{6.}$$

where $\underline{n_1}$, $\underline{n_2}$ et $\underline{n_3}$ are the privileged directions. Three second order tensors can be introduced:

$$\underline{\underline{A_1}} = \underline{n_1} \otimes \underline{n_1}, \quad \underline{\underline{A_2}} = \underline{n_2} \otimes \underline{n_2}, \quad \underline{\underline{A_3}} = \underline{n_3} \otimes \underline{n_3} \tag{7.}$$

The stored energy function W is then decomposed into two parts W_{iso} and W_{ani} such that

$$W\left(\underline{\underline{B}}, \underline{\underline{A_1}}, \underline{\underline{A_2}}, \underline{\underline{A_3}}\right) = W_{iso}\left(\underline{\underline{B}}\right) + W_{ani}\left(\underline{\underline{B}}, \underline{\underline{A_1}}, \underline{\underline{A_2}}, \underline{\underline{A_3}}\right) \tag{8.}$$

Due to the representation theorem, W can be rewritten as

$$W\left(\underline{\underline{B}}, \underline{\underline{A_1}}, \underline{\underline{A_2}}, \underline{\underline{A_3}}\right) = W_{iso}\left(I_1, I_2\right) + W_{ani}\left(I_4, I_5, I_6, I_7, I_8, I_9\right) \tag{9.}$$

where W_{iso} and W_{ani} are isotropic convex functions of their arguments. Hence, the Cauchy stress writes:

$$\begin{aligned} \underline{\underline{\sigma}} = 2\frac{\partial W}{\partial B} &= -p\underline{\underline{I}} + 2\left(W_1 + I_1 W_2\right)\underline{\underline{B}} - 2W_2 \underline{\underline{B}}^2 \\ &+ 2I_4 W_4 \underline{\underline{A_1}} + 2I_4 W_5\left(\underline{n_1} \otimes \underline{\underline{B}}\underline{n_1} + \underline{n_1}\underline{\underline{B}} \otimes \underline{n_1}\right) \\ &+ 2I_6 W_6 \underline{\underline{A_2}} + 2I_6 W_7\left(\underline{n_2} \otimes \underline{\underline{B}}\underline{n_2} + \underline{n_2}\underline{\underline{B}} \otimes \underline{n_2}\right) \\ &+ 2I_8 W_8 \underline{\underline{A_3}} + 2I_8 W_9\left(\underline{n_3} \otimes \underline{\underline{B}}\underline{n_3} + \underline{n_3}\underline{\underline{B}} \otimes \underline{n_3}\right) \end{aligned} \tag{10.}$$

where $W_i = \partial W / \partial I_i$

We choose the Hart Smith model, so W can be written as the following form:

$$W\left(\underline{\underline{B}},\underline{\underline{A_1}},\underline{\underline{A_2}},\underline{\underline{A_3}}\right)=G_1\int_0^{I_1-3}e^{\Lambda_1X^2}dX+G_2\left(\int_0^{I_4-1}e^{\Lambda_2X^2}dX+\int_0^{I_6-1}e^{\Lambda_2X^2}dX\right) \quad (11).$$

So the elastic stress yields to:

$$\underline{\underline{\sigma}}=-p\underline{\underline{I}}+2G_1e^{\Lambda_1(I_1-3)^2}\underline{\underline{B}}+2I_4G_2e^{\Lambda_2(I_4-1)^2}\underline{\underline{A_1}}+2I_6G_2e^{\Lambda_2(I_6-1)^2}\underline{\underline{A_2}} \quad (12).$$

Therefore, the equation 3 in 2D plane stress case can be modified as:

$$2\underline{\underline{\eta}}\underline{\underline{D_v}}=2G_1e^{\Lambda_1(I_1-3)^2}\underline{\underline{\hat{B}}}+2I_4G_2e^{\Lambda_2(I_4-1)^2}\underline{\underline{\hat{A_1}}}+2I_6G_2e^{\Lambda_2(I_6-1)^2}\underline{\underline{\hat{A_2}}}$$

$$\Rightarrow\begin{pmatrix}D_{v11}\\D_{v22}\\D_{v12}\end{pmatrix}=\begin{bmatrix}\dfrac{\eta_{22}}{\eta_{11}\eta_{22}-\eta_{12}^2} & \dfrac{-\eta_{12}}{\eta_{11}\eta_{22}-\eta_{12}^2} & 0\\ \dfrac{-\eta_{12}}{\eta_{11}\eta_{22}-\eta_{12}^2} & \dfrac{\eta_{22}}{\eta_{11}\eta_{22}-\eta_{12}^2} & 0\\ 0 & 0 & \dfrac{1}{\eta_{44}}\end{bmatrix}\begin{pmatrix}\tilde{d}_{11}\\\tilde{d}_{22}\\\tilde{d}_{12}\end{pmatrix} \quad (13).$$

3. IDENTIFICATION AND BLOWING SIMULATION OF A PET PREFORM

The identification process, minimizing the square difference between model and experimental values of both equi-biaxial and constant width tests, leads to the coefficient values shown in Table 1. The mean differences highlighted on the curves shown on Figure 2 are 12.8% for constant width in the elongation direction and 6.2% in the blocked direction. For equi-biaxial test, the error is 6.3%.

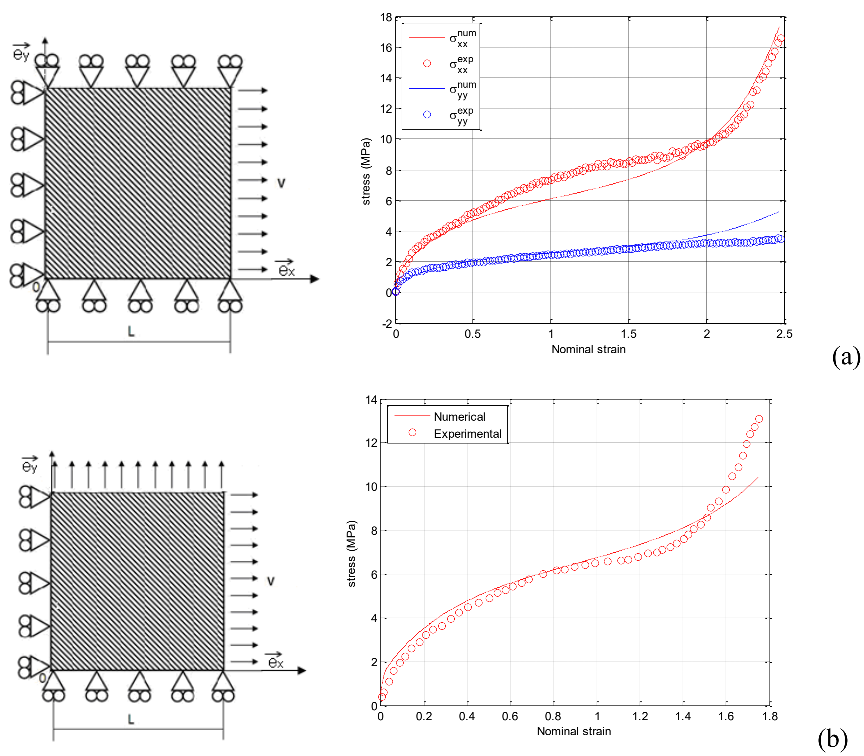

FIGURE 2. Comparison between experimental results and model simulations at 2 s^{-1} and 90°C: (a) Constant Width; (b) Equi-biaxial

TABLE 1. Model coefficient values

G_1	Λ_1	G_2	Λ_2	β
3 MPa	1	5 MPa	1	-0.05

The model is implemented into the software ABAQUS / Explicit via a user interface VUMAT. We now focus on the simulation of a preform stretched by an internal rod and blown with internal pressure. The preform geometry is meshed and the longitudinal stretch rod by shell elements in ABAQUS environment. The geometry of revolution of the preform and the rod has been exploited to reduce the simulation time by using an axisymmetric model. The model air mass flow which is injected into the preform / bottle is incorporated by exchange of fluid between components (fluid structure interaction implanted in ABAQUS).

CPU time (2.66 GHz Pentium 4) for one free blow simulation is about 6 hours. Figure 3 shows the first free blow and stretch blow simulation results obtained with the isotropic version of the visco-elastic model. We can see that the elements in the center area of the bottle are not enough stretched in the longitudinal direction. The comparison of the final shape of the PET bottle with typical shapes obtained during real free blowing of perform is not satisfactory. The reason is that once the elements are stretched along the hoop direction, the behavior of PET reached the state of the strain hardening also in the longitudinal direction.

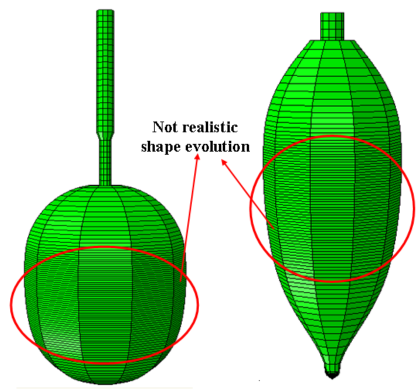

FIGURE 3. First free blow and stretch blow simulation using the isotropic model

Using the anisotropic version of the model, one can see on Figure 3 that the evolution of the bottle shape is in good agreement in comparison with the real blown bottle.

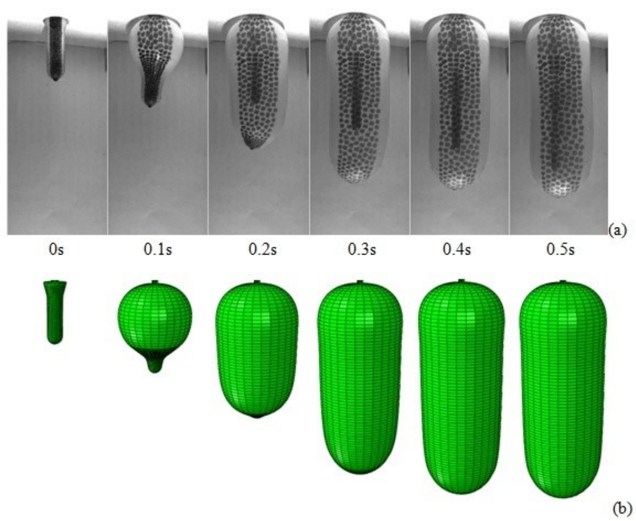

FIGURE 4. (a) Stretch and free blowing of a preform; (b) Abaqus simulation with anisotropic model

CONCLUSIONS

An orthotropic visco-hyperelastic model has been developed for the strain-rates and temperatures range near of the stretch-blow molding process. Both elastic and viscous parts are developed has an orthotropic behavior and the complex form of the model is provided.

Thanks to data provided from equi-biaxial and constant width elongation tests, the identification procedure can be achieved and gives the coefficient values of the model. The mean difference between model and experiments is about 10%.

The model is implemented in ABAQUS and used to simulate free blowing of PET perform. The comparison with a real free blowing test validates the anisotropic version of the visco-elastic model for PET near Tg.

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