Optimization by the C-NEM Method of the Stretch-Blow Molding Process of a PET Bottle Near T_g

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ABSTRACT: The stretch-blow molding process of poly(ethylene terephthalate) bottles generates some important modifications in the mechanical properties of the material. Considering, the range of temperature (T > T_g) that is usually used, the material has a very high viscosity and shows a strain hardening effect linked to the microstructure evolution. A simple visco-plastic model had been identified from experimental results of uniaxial and biaxial tensile tests [1]. In the present work, we use this model and a numerical technique to simulate the inflation of a preform under an internal pressure and also submitted to the elongation of a stretch rod. The finite elements method has a poor efficiency in the stretch-blow molding process because the final material strain is up to 300%. This strain level generates strong element distortions and necessitates to often re-mesh. In order to carry out simulations with strain higher than 300%, the constrained natural elements method (C-NEM [2]) is used. In fact, the C-NEM method allows simulation with high strain level without re-meshing. The original "mesh" can be use from the beginning to the end of the simulation. So the properties of the material can be recorded in each node, without loss of information. In a first approach C-NEM are applied to simulate and optimize stretch-blowing of a PET preform by using axis symmetric assumption, the mold is not taking into account.

KEYWORDS: PET, Stretch-Blowing, Simulation, C-NEM

1 INTRODUCTION

1.1 Nonlinear viscous model

From uniaxial and biaxial tensile tests managed on PET specimen at a temperature slightly higher (> 80°C) than the glass transition temperature T_g, Chevalier *et al.* [1] identified a simple nonlinear incompressible viscoplastic model, which represents macroscopically the strain hardening effect observed during tension for hight strain. This effect is related with the strain induced modification of the microstructure of PET [3, 4, 5]. The model (Eq.1) has been identified supposing the strain and stress fields uniformity in the PET specimen.

$$
\begin{aligned}
&\underline{\underline{\sigma}} = 2\eta \underline{\underline{D}} - p\underline{\underline{I}} \\
&\eta = K\dot{\overline{\gamma}}^{m-1} \\
&K = K_0 e^{(a\underline{\varepsilon}^3 + b\underline{\varepsilon}^2 + c\underline{\varepsilon})} \\
&\dot{\overline{\gamma}} = (2\underline{\underline{D}} : \underline{\underline{D}})^{\frac{1}{2}} \\
&\underline{\varepsilon} = \sup_i(\varepsilon_i) \quad i = 1, 2, 3
\end{aligned} \qquad (1)
$$

Where $\underline{\underline{D}}$ is the strain rate tensor, with the incompressibility condition $\mathrm{tr}(\underline{\underline{D}}) = 0$ on Ω. The hardening effect is related by the factor K, it varies exponentially with the equivalent strain $\underline{\varepsilon}$, the $\underline{\varepsilon}_i$ $(i = 1, 2, 3)$ are the eigen values of the logarithmic Eulerian strain tensor ($\underline{\underline{\varepsilon}} = 1/2 \log(\underline{\underline{B}})$, $\underline{\underline{B}}$ is the left Cauchy-Green tensor). The characteristics of the PET for this model are: $K_0 = 0.333 MPa.s^m$; $m = 0.4$; $a = 3.65$; $b = -7.6$; $c = 6.64$; $d = -0.099$. The model gives some good results for uniaxial and equi-biaxial nevertheless it is a bit inaccurate to represent 3D solicitations, the simulated behavior does not take into account the material anisotropy due to the macromolecular orientation. So, the model will be improved by adding an orthotropic viscosity.

1.2 Model improvement

The new anisotropic behavior can be written as the following manner:

$$\underline{\underline{\sigma}} = 2\underline{\underline{\underline{\underline{\eta}}}} : \underline{\underline{D}} - p\underline{\underline{I}} \qquad (2)$$

Where $\underline{\underline{\underline{\eta}}}$ is a fully symmetric forth order tensor, in the basis of the eigen values of the strain tensor all its components are empty except for the diagonal terms.

$$(\underline{\underline{\underline{\eta}}})_{ijij} = \begin{cases} \tilde{K}_i \dot{\overline{\gamma}}^{m-1} & \text{si} \quad i = j \\ \tilde{K}_k \dot{\overline{\gamma}}^{m-1} & \text{si} \quad i \neq j \end{cases}$$
$$\text{avec} \;\; k \neq i \neq j$$
$$\tilde{K}_i = \beta K_i + (1-\beta) \max_{j=1,2,3}(K_j) \tag{3}$$
$$i = 1,2,3 \quad \text{avec} \quad 0 \leq \beta \leq 1$$
$$K_i = K_0 e^{(a\varepsilon_i^3 + b\varepsilon_i^2 + c\varepsilon_i)} \quad i = 1,2,3$$

Where $\varepsilon_i, \dot{\overline{\gamma}}, a, b, c, d$ are even the same as defined before. And β is a parameter witch is used to adjust the degree of anisotropy. Taking into account the importance of geometrical transformations undergone by the preform during the stretch blow-molding process (strain up to 300%), we choose mesh-less method for the numerical simulations. So the Constrained-Natural Element Method [2] is choosen.

2 Stretch-blowing of PET preform

In this section, we present the theoretical problem of incompressible viscous flow and the C-NEM formulation that we use to optimize the stretch-blowing process.

2.1 Governing equation and variational formulation

Taking into account the very high viscosity of PET, body and gravitational forces may be neglected. In the general 3D incompressible case, the researched solution is a mixed one, with a velocity field ($\underline{V}$) and a pressure field (p). $\underline{V}$ and p are respectively element of the space V_v and V_p with:

$$V_v = \left\{ \underline{V} \in H^1(\Omega) \, , \, \underline{V} = \underline{V}_d \text{ on } \partial\Omega_v \right\} \tag{4}$$
$$V_p = L^2(\Omega) \tag{5}$$

We consider variations of solution field such as

$$\underline{V}^* \in V_v^0 = \left\{ \underline{V} \in H^1(\Omega) \, , \, \underline{V} = \underline{0} \text{ on } \partial\Omega_v \right\} \tag{6}$$
$$p^* \in V_p \tag{7}$$

The problem consist to find the velocity field $\underline{V}$ and the pressure field p verifying the following balance equations and the constitutive model given by equation (1).

$$\int_\Omega \text{div}(\underline{V}) p^* dv = 0 \, , \; \forall p^* \in V_p \tag{8}$$
$$-\int_\Omega \underline{\underline{\sigma}} : \underline{\underline{D}}^* dv + \oint_{\partial\Omega} \underline{F}.\underline{V}^* ds = 0, \; \forall \underline{V}^* \in V_v^0 \tag{9}$$
$$\underline{\underline{D}}^* = \frac{1}{2}\left(\text{grad}(\underline{V}^*) + \text{grad}(\underline{V}^*)^\top\right)$$

The boundary conditions are:

$$\underline{V} = \underline{V}_d \quad \text{on } \partial\Omega_v \tag{10}$$
$$\underline{\underline{\sigma}}.\underline{n} = -\Delta p.\underline{n} \quad \text{on } \partial\Omega_p \tag{11}$$

Considering the constitutive model (Eq.1) and the previous boundary conditions (Eq.10-11), the equivalent variational formulation of balance equations is, in respect to $(\underline{V}, p) \in (V_v \times V_p)$ such as $\forall(\underline{V}^*, p^*) \in (V_v^0 \times V_p)$:

$$-\int_\Omega 2\underline{\underline{D}} : \underline{\underline{\underline{\eta}}} : \underline{\underline{D}}^* dv$$
$$+ \int_\Omega p \, \text{div}(\underline{V}^*) dv \; + \; \oint_{\partial\Omega} \underline{F}.\underline{V}^* ds = 0 \tag{12}$$
$$\int_\Omega \text{div}(\underline{V}) p^* dv = 0 \tag{13}$$

The stretch-blowing of a PET bottle is an axisymmetric problem. So, the 3D problem (Eq.12) can be reduced to a 2D axisymmetric problem using cylindrical coordinates (r, θ, z).

$$-\int_S 2r\underline{\underline{D}} : \underline{\underline{\underline{\eta}}} : \underline{\underline{D}}^* ds$$
$$+ \int_S rp \, \text{div}(\underline{V}^*) ds \; + \; \oint_{\partial\Omega} r\underline{F}.\underline{V}^* dl = 0 \tag{14}$$
$$\int_S r \, \text{div}(\underline{V}) p^* ds = 0 \tag{15}$$

In the problem of optimization, many simulations of stretch-blowing must be performed. In order to reduce the number of degrees of freedom (dof), currently 3 dof by nodes with the axisymmetric assumption, a pseudo-penalization method is computed. The hydrostatic pressure is replaced by a proportional term of the divergence of the velocity like in the following expression.

$$p = -\alpha \underline{\underline{I}} : \underline{\underline{\underline{\underline{\eta}}}} : \underline{\underline{D}} \quad \text{with} \quad \alpha = \frac{2\nu}{1-2\nu} \tag{16}$$

ν is the equivalent of the Poisson ration in elasticity. To reproduce a behavior close to the incompressibility, authors usually take $\nu = 0.49$ (0.5 being for the incompressibility case). By using this method, the number of dof is 2 by node and the constitutive model (Eq.1) and the variational formulation (Eq.14) become:

$$\underline{\underline{\sigma}} = 2\underline{\underline{\underline{\underline{\eta}}}} : \underline{\underline{D}} + \alpha(\underline{\underline{I}} : \underline{\underline{\underline{\underline{\eta}}}} : \underline{\underline{D}})\underline{\underline{I}} \tag{17}$$

$$-\int_S 2r\underline{\underline{D}} : \underline{\underline{\underline{\underline{\eta}}}} : \underline{\underline{D}}^* ds - \int_S r\alpha(\underline{\underline{I}} : \underline{\underline{\underline{\underline{\eta}}}} : \underline{\underline{D}}) \operatorname{div}(\underline{V}^*) ds + \oint_{\partial\Omega} r\underline{F}.\underline{V}^* dl = 0 \tag{18}$$

In order to simplify the notation of the equation(18), we introduce a new forth order tensor $\underline{\underline{\underline{\underline{\tilde{\eta}}}}}$ as the stiffness tensor in elasticity. Its non-null components are given by the following:

$$(\underline{\underline{\underline{\underline{\tilde{\eta}}}}})_{iijj} = \begin{cases} (1+\frac{\alpha}{2})\tilde{K}_i \dot{\overline{\gamma}}^{m-1} & \text{si} \quad i = j \\ \frac{\alpha}{2}\tilde{K}_k \dot{\overline{\gamma}}^{m-1} & \text{si} \quad i \neq j \\ \text{avec } k \neq i \neq j & \end{cases}$$

$$(\underline{\underline{\underline{\underline{\tilde{\eta}}}}})_{ijij} = \tilde{K}_k \dot{\overline{\gamma}}^{m-1} \quad \text{si} \quad i \neq j \quad \text{avec} \quad k \neq i \neq j \tag{19}$$

$$\tilde{K}_i = \beta K_i + (1-\beta) \max_{j=1,2,3}(K_j)$$

$$i = 1,2,3 \quad \text{avec} \quad 0 \leq \beta \leq 1 \tag{20}$$

$$K_i = K_0 e^{(a\varepsilon_i^3 + b\varepsilon_i^2 + c\varepsilon_i)} \quad i = 1,2,3 \tag{21}$$

with this new tensor, we can write the equation(18) in a simple manner easer to compute (Eq.22).

$$-\int_S 2r\underline{\underline{D}} : \underline{\underline{\underline{\underline{\tilde{\eta}}}}} : \underline{\underline{D}}^* ds + \oint_{\partial\Omega} r\underline{F}.\underline{V}^* dl = 0 \tag{22}$$

2.2 *Optimization of the process*

In this work, the mold is not take into account. The optimization is realized on two operating parameters: the speed of the stretch rod (V_r) and the moment where the blow pressure is applied (t_p). The blow pressure is activated when the stretch rod has a given length, so t_p is in millimeter. In all simulations the same profile of temperature is applied. The process conditions are shown in figure 1 and figure 2.

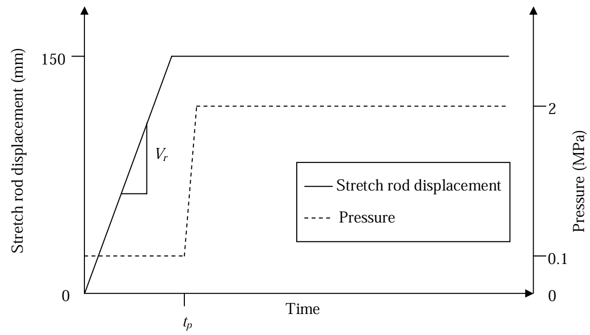

Figure 1: Simulated operating conditions

The geometry of the preform is simplify. We choose a preform with an uniform thickness. Simulations are stopped when the volume of the bottle reaches 0.5 L.

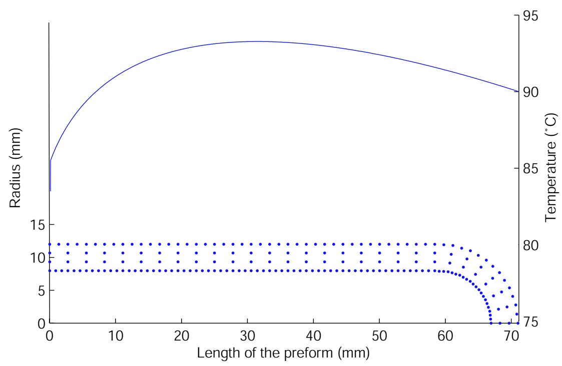

Figure 2: Profile of temperature along the preform

The results of the optimization are given in the figure 3. We can see the standard deviation ($\sigma^{1/2}$) of the thickness as a function of V_r and t_p. V_r goes from 500 mm.s^{-1} to 1625 mm.s^{-1} and t_p goes from 80 mm to 130 mm. $\sigma^{1/2}$ has not got minimum, but the best bottle is given for $t_p = 80$ mm and $V_r = 500$ mm.s^{-1}. In this case the stretch rod can not push the bottom of the bottle, during all the process, because the strain rate due to the pressure is higher than the strain rate caused by the stretch rod.

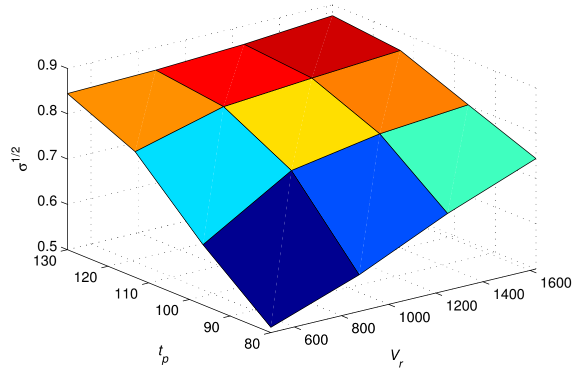

Figure 3: Standard deviation ($\sigma^{1/2}$) of the thickness after stretch blowing

The evolution of two different bottles is shown in the figure 4, one for $t_p = 80$ mm and $V_r = 500$ mm.s^{-1} and one for $t_p = 130$ mm and $V_r = 1625$ mm.s^{-1}. In the figure 5, we plot the thickness, of the two final bottles, versus ξ. ξ is defined by the ratio between the curvilinear abscissa (length travel from the neck of the bottle) and the maximum of the curvilinear abscissa.

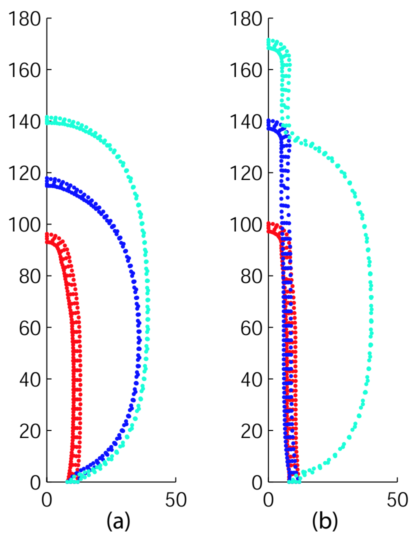

Figure 4: Evolution of the bottle (a) $t_p = 80$ mm and $V_r = 500$ mm.s^{-1} (b) $t_p = 130$ mm and $V_r = 1625$ mm.s^{-1}

3 Conclusion

The constitutive model proposed by Chevalier *et al.* [1] has been enriched by introducing a parameter of anisotropy (β), which allows to take into account the effect of the molecular orientation of the PET for complex loads. Using the meshless method (C-NEM) permits the simulation and optimization of forming processes involving high strains without "remeshing" and degradation of the solution. We have highlighted the influence of the parameters V_r and t_p in the process of deformation of the bottle.
In order to improve this work, it is necessary to take into account the mold and thermodynamic effects [6] and compare our results with experiments [7].

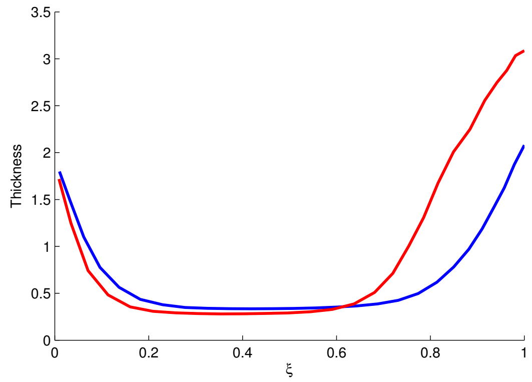

Figure 5: Thickness of bottle (–) $t_p = 80$ mm and $V_r = 500$ mm.s^{-1} (–) $t_p = 130$ mm and $V_r = 1625$ mm.s^{-1}

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