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Finite Element Modeling of the Thermomechanical Behavior of Polyethylene

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Abstract*: This article presents a finite element study based on tests of characterizations to find the properties of the materials studied, the injection-blowing technique, chosen in this case, is characterized by the bi-axial of the material, and one benefits from the orientation of the macromolecules in the directions of use of the material. The objective of this work is to link all the mechanical and thermal parameters during the treatment of molten polymer materials subjected to high-stress rates that can lead to significant temperature increases due to viscous heating in the order of 200°C. Predicting the temperature range is essential for good temperature control and is a major factor in determining the quality of the final product. This forces us to choose an adequate law of behavior, capable of translating the mechanical evolution under the thermal effect while explaining the rheological response of the viscoelastic metal. So this process is usually accompanied by geometric defects resulting from the original residual stresses cooling speed and the process itself. In the packaging of food products, as in this case, the bottles require to have a stable filling and a certain storage capacity.*

Keywords*: finite elements, plastics, behavior law, viscoelastic, residual stress*

1.Introduction

Plastic products are present in many sectors, and to their performance, plastics and composites improve our quality of daily [1, 2]. Scientific research, and in particular the development of simulation tools in recent years, as well as the evolution of plastics processing techniques, are at the origin of this revolution [3]. The injection process raises several recurring questions, it is necessary to study the flow rate to avoid shearing and the heating rate to minimize and optimize the cooling speed and of course the relationship between thermal/stress [4,5]. Pressure must also be controlled to minimize shrinkage and improve dimensional retention or low to reduce residual stress and minimize mold clamping force, so it is important to monitor mold temperature to facilitate flow and relieve stress or low to minimize cycle time [7, 6] Given that the rheological properties of polymers depend on temperature, the use of numerical methods is almost unavoidable. However, none of the previous mathematical analyzes have taken into account the fluidity of the polymer, and only recently the difficulty of flowing through contractions. We see that many questions are related to residual stresses and strains [6, 8-10].

2. Materials and methods

2.1. Behavior law and thermomechanical characterization

The law of behavior $\sigma\ (\varepsilon, \dot{\varepsilon})$ constitutes the equation of the state of the material in so far as the deformation parameter ε adequately characterizes the structural state of the material. This property is only checked as a first approximation because, for a fixed value of ε, the polymer structure in the blown state evolves under the influence of the temperature by the creep phenomenon by the stress under the cooling effect to take the final form during plastic or hyper elastic deformation. This is confirmed by the relaxation after filling the shape of the mold, the deformation and the structure tend to return to their initial state, either quickly if the temperature is higher than T_g (melting), or very slowly if the temperature is lower than Tm (solidification), so here it must be said that our problem is always to solve the non-uniform parts or stresses after solidification. According to these hypotheses, it is possible to write the

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behavioral law of the studied polymers in a simplified form [11,12].

$$\sigma\ (\varepsilon, \dot{\varepsilon}) = \mathrm{K}.\,\mathrm{f}(\varepsilon).\,\mathrm{g}(\dot{\varepsilon}\ ) \qquad (1)$$

The parameters of this equation are respectively, or f(ε) is the effect of stress and $g(\dot{\varepsilon})$ the rate of deformation. More precisely, the function f(ε) groups the phenomena imposed on the piece can be written as follows:

$$f(\varepsilon) = V(\varepsilon).\,C(\varepsilon).\,H(\varepsilon) \qquad (2)$$

V(ε) defines viscoelastic behavior in the following form:

$$V(\varepsilon) = 1 - e^{\ (-w\varepsilon^{\vartheta})} \qquad (3)$$

H(ε) describes the progressive hardening behavior during large deformations:

$$H(\varepsilon) = e^{\ (h\varepsilon^{n})} \qquad (4)$$

C(ε) describes the stress of the material:

$$C(\varepsilon) = 1 + ae^{(-b\varepsilon)} \qquad (5)$$

The velocity of the instantaneous deformation is given by equation $g(\dot{\varepsilon})$ in the oozing form:

$$\mathrm{g}(\dot{\varepsilon}) = \dot{\varepsilon}^{m} \qquad (6)$$

where m and *n* are constants, the choice of the behavior law of the material studied depends on the transformation process used and the physical state of the material, as well as the response of the raw material to the melting temperature and the behavior during cooling periods. In all cases, in the case of the thermoforming of polymeric materials, a law of G'Sell-Jonas is used [13-15]:

$$\sigma_{\mathrm{eq}} = \mathrm{k(T)}\big[[1 - \mathrm{e}^{(-\omega\varepsilon_{\mathrm{ep}}}].\,[\mathrm{e}^{\left(\mathrm{h}\varepsilon_{\mathrm{eq}}^{2}\right)}]\,.\,\dot{\varepsilon}_{\mathrm{eq}}^{\mathrm{m}}\ \big] \qquad (7)$$

where (σ_{eq}) and ($\dot{\varepsilon}_{eq}$) indicate respectively the equivalent stress at the equivalent deformation and the equivalent deformation velocity at Von Mises. T denotes temperature while k depends on temperature. The sensitivity coefficients of strain rate (m), strain (h), and viscoelasticity (ω) vary only if the physical state of the material changes.

2.3. Finite element resolution method

About polymer fusion, different laws of viscoelasticity apply. This is an expression of the Maxwell model, the treatment of flow problems is based on the resolution of equations derived from conservation principles [16, 17]:

* Preservation of the mass: $\frac{\partial\rho}{\partial t} + \vec{\nabla}\ .\,(\rho\ \vec{V}\ ) = 0$ (8)

with $\vec{V}$ the velocity field in the fluid and ρ the density of the fluid.

* Conservation of the quantity of movement: $\rho\left(\frac{\partial V}{\partial t} + V.\nabla \mathrm{V}\ \ \right) = \nabla.\sigma + \rho \mathrm{f}$ (9)

where the Cauchy stress tensor and f are the force vector per unit volume, as appropriate. The Cauchy strain tensor may break down as follows:

$$\sigma = -pI + S \tag{10}$$

with p the hydrostatic pressure, ***I*** the identity tensor, and S the tensor depend on the rheological model used to represent the behavior of the fluid «viscous stress», Finally, thermodynamics gives the heat conservation equations and a state relationship between density (ρ) and pressure (P) with the strain velocity tensor:

$$\rho C_p\left(\frac{\partial T}{\partial t}+\vec{\nabla}T.\vec{V}\right)-\beta T\left(\frac{\partial P}{\partial t}+\vec{\nabla}P.\vec{V}\right)=S\dot{\mathcal{E}}+\vec{\nabla}.(k\vec{\nabla}\mathrm{T}) \tag{11}$$

β the coefficient of thermal expansion of the fluid defined by:

$$\beta = -\frac{1}{\rho}\left(\frac{\partial\rho}{\partial T}\right)_P \tag{12}$$

Avrami's equation is generally applicable to any type of crystallization, its simplicity of application still makes it the most widely used method today to obtain quantitative information on the crystallization kinetics of polymers, therefore the Avrami model can be used to identify the change in relative crystallinity over time [18, 19]:

$$\alpha = 1 - e^{-kt^n} \tag{13}$$

with *k* it is a constant that contains nucleation and growth factors *n* It is the exponent Avrami depending on the nucleation mechanism and crystal growth form [20].

2.4. Numerical model

Our study is based on a real problem, the case of the injection blow molding process essentially dedicated to the manufacture of the bottles for the packaging of food products (milk), the experimental data taken will be used later in numerical resolution. The boundary conditions and the thermal and mechanical characteristics of the high-density polyethylene part are as follows (Table 1) [21, 22] and the mechanical and thermal characteristics of the Duralumin mold are shown in (Table 2) [23-25].

Table 1. Mechanical characteristics of high-density polyethylene

Properties	PE-HD
Density ρ (ton·mm^{-3})	9.5e-10
Poisson's ratio **ν** (-)	0.41
Young modulus E (MPa)	800
Specific heat Cp (mJ .kg -1C^{-1})	1,750
Thermal conductivity k (Wm^{-1}K^{-1})	0.5
Thermal expansion coefficient, α /°C	155. 10^{-6}

Table 2. Thermo-mechanical characteristics of the Duralumin mold

Properties	Duralumin
Density ρ (ton·mm^{-3})	2.7e-10
Poisson's ratio ν (-)	0.33
Young modulus E (MPa)	690
Specific heat Cp (mJ ·kg $^{-1}$·C^{-1})	896
Thermal expansion coefficient, α / °C	23.6. 10^{-6}
Thermal conductivity k (Wm^{-1}K^{-1})	204
Melting point °C	550—630

Knowing the shape of the molded part, the thermal properties of the plastics, and the manufacturing conditions, it is possible to make a good approximation of the cooling time for several years, the following equation for the calculation of t_c (equation 14) [26, 27].

$$tc = (\frac{S^2}{a\,\alpha}) ln \left\{ k(\frac{T_M - T_C}{T_D - T_C}) \right\} \tag{14}$$

A similar relationship has been established which defines the cycle time reduction (CTR expressed in %) as a function of the temperature coefficient (Tc) containing these temperatures according to the following equation (15) [26]:

$$CRT = f(TC) = f((\frac{T_M - T_C}{T_D - T_C}) \tag{15}$$

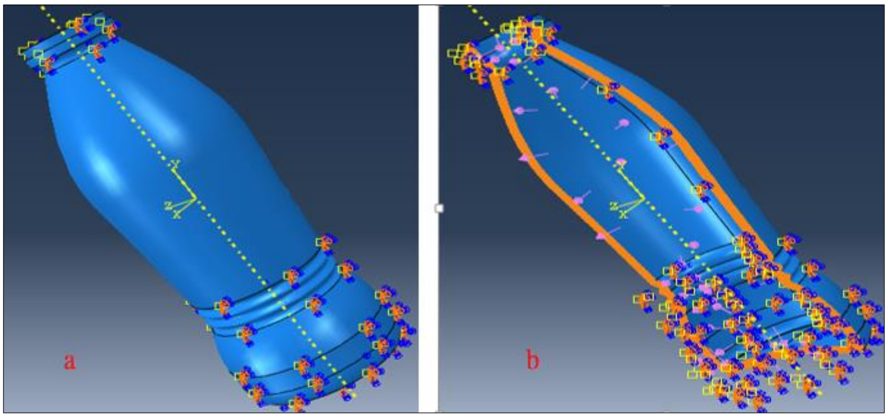

Figure 1. a. Fixing the part in contact with the mold,
b. Blowing pressure applied inside the bottle

where tc = cooling time, S = thickness of the part (m^2) The plane in the case of the cylinder is we replace S by D diameter of the cylinder D(m), α = effective thermal diffusivity [m²/s], and a=case of cylinder geometries is π^2 and for plan geometrics, the constant a=23.1, which is the ratio of the averaged values of the thermal conductivity divided by the product of density and specific heat capacity (mm²/s). When TM= melting temperature (°C), Tc = injection temperature (°C), TD = temperature of the part when the mold opens, usually replaced by the deflection temperature,TD=TE demolding temperature [°C], and K = coefficient related to the thickness molding (case geometries cylinder is $4/\pi$ and for strip geometrics, the constant a is 0.692) [28].

3. Resultats and discussions

The design of the mold must estimate on average the time required for stiffening, as well as the time required for solidification since the cylinder studied has a cylindrical lower part, with particular singularities, a semi-infinite part of the body or the neck of the bottle with a greater thickness (Table 3).

Table 3. Control of cooling temperature t_c (by experimental measurements) of bottle geometry

S or D	a	K	α	TM	Tc	TD	T(s)	T(mn)
3.00E-04	9.8596	1.2738	2.26E-07	226	73.5	132	0.048474	0.000808
5.00E-04	9.8596	1.2738	2.26E-07	226	73.5	132	0.13465	0.002244
1.00E-03	9.8596	1.2738	2.26E-07	226	73.5	132	0.538598	0.008977
1.20E-02	23.1	6.92	2.26E-07	226	73.5	132	79.78541	1.329757
1.25E-02	23.1	6.92	2.26E-07	226	73.5	132	86.57271	1.442879
1.50E-03	23.1	6.92	2.26E-07	226	73.5	132	1.246647	0.020777
2.00E-03	23.1	6.92	2.26E-07	226	73.5	132	2.216261	0.036938

We have chosen to create a model with these given or conclusive, so the cause of the residual stresses is major and present (Figure 2), If the cooling time of the feed system far exceeds the cooling time in a single mold, the designer should rethink the feed system to avoid increasing the mold cycle time.

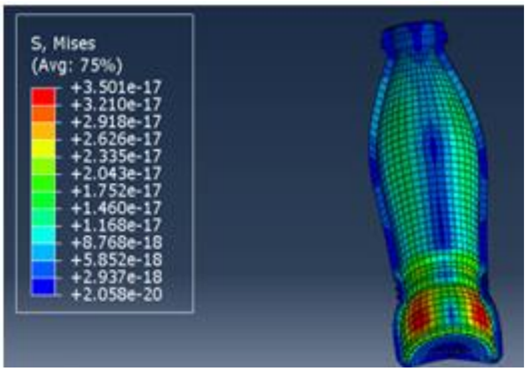

Figure 2. Von Mises constraint result

In this Figure 2, notice that the maximum stress is localized to the lower part of the cylinder because time has cooled.

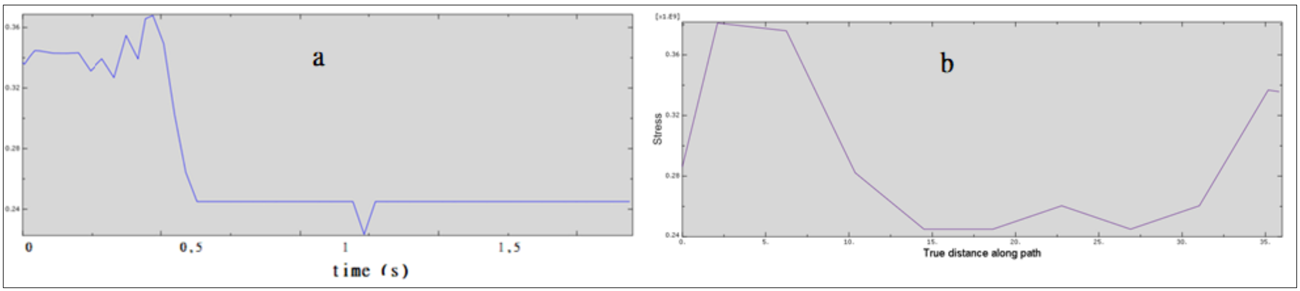

Figure 3. a. Evolution of stress (relaxation) as a function of time imposed on the bottle, b. Evolution of the pressure according to the base radius

The propagation of the heat flux on the surface of the bottle results from linearity (Figure 4a) of the wall, so the problem arises at the level of the base, mainly and of the cavity (Figure 4b).

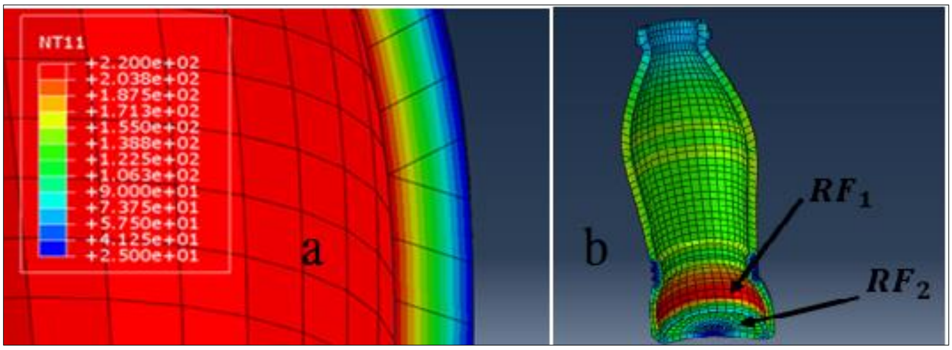

Figure 4. Effect of temperature just after blowing (at t = 0S)

From these figures, one can study the effect of the reaction force and the relation between the two parts in contact with the basic contour of the bottle studied previously, as result of TRF1>TRF2, it can be concluded from this curve (Figure 5a) that the reaction force reaches its maximum value in the area whose shape is flat. On this curve (Figure 5b), we will identify the maximum value of the reaction force in the base to compare it with the results found previously.

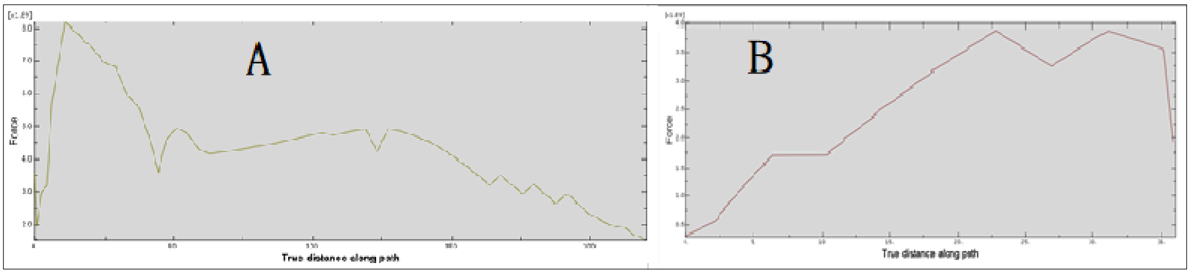

Figure 5. a. Evolution of the reaction force as a function of the length of the bottle, b. Evolution of the reaction force as a function of the base radius of the bottle

4. Conclusions

If we compare the results found on the model with those previously found in the theoretical study and experimental observation, we can conclude that the defect still exists in the lower area of the bottle, by comparing the results:

-The shape of the bottle has a significant effect on the distribution of blowing pressure, heat flow and reaction force, the time interval between the parts of the studied part, large enough and therefore these results can lead to important deformations, these defects must be solved and their impact on the stability of the bottle must be avoided.

- Adding an additional dedicated cooling circuit to further cool the bottom contour of the bottle which is the main cause of our problem presents a solution.

- Modification on the mold at the level of the basic outline of the bottle in order to catch up with the already existing deformation.

-Modification on the shape of the bottle, in particular the lower part, so these results valid for these processes always these claims present a saving of time and material.

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