A CONSTITUTIVE MODEL FOR POLYCARBONATES

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ABSTRACT: This paper presents a set of constitutive equations to model cold-drawing (necking) in polycarbonates (PC). The model is based on hyperelastic extension of the $J_2$-flow theory to the finite strain range. Accordingly, an appropriate yield surface and an associative flow rule are presented. The ensuing numerical constitutive integration algorithm is based on the operator splitting technique. Numerical results are presented to show correlation with the experimental data.

INTRODUCTION: The understanding of physical behavior of engineering thermoplastics and development of appropriate constitutive equations for analysis and design continues to be of considerable interest for engineering applications. Polycarbonate (PC), a transparent amorphous thermoplastic, has received considerable attention because of its high impact resistance and its recognition as a load bearing material due to sufficiently high glass transition temperature. The characteristics of deformation around a notch in polycarbonate, shear banding at short times and high loads, and micro-cracking at low stresses and long times has been reported by various investigators. [see e.g., 1,2,4,6 and references therein]. The objective of this paper is to develop a set of constitutive equations that models the “double” glass transition phenomena in polycarbonates and examine the model by comparing its predictions with experimentally observed neck propagation under uniaxial tension.

CONSTITUTIVE MODEL: We now present the constitutive model in the spatial framework. We assume that the thermodynamic state is characterized by the variables $\{g, b^{-1}, q, F\}$, where $g$ is the spatial metric tensor, $b$ is the elastic left Cauchy-Green tensor, and $q$ is a set of internal state variables characterizing the inelastic transition. For simplicity, we assume an uncoupled free energy potential in the internal variables $q$ of the form

$$\phi(g, b^{-1}, q, F) = \tilde{\phi}(g, b^{-1}, F) + \chi(q)$$  \hspace{1cm} (1)

The consistency and persistency conditions can be expressed as

$$\dot{\gamma} \geq 0; \quad \tilde{\varphi}(g, b^{-1}, q, F) \leq 0; \quad \gamma \tilde{\varphi}(g, b^{-1}, q, F) = 0$$  \hspace{1cm} (2)

where $\gamma$ is the consistency parameter and $\varphi$ is the yield condition.
We consider the following uncoupled hyper-elastic stored energy function with uncoupled pressure relative to the unloaded configuration.

$$\bar{\phi}(g, b^{e^{-1}}, F) = \frac{1}{2} K (\log J)^2 + \frac{1}{2} \mu (I_{\text{b}} - n_{sd})$$  \hspace{1cm} (3)

where $I_{\text{b}} = \bar{J}^{-\frac{2}{3}} b^e : g = b^e \circ \tilde{g}_{ij}$, $K$ is the bulk modulus and $\mu > 0$ is the shear modulus. The Kirchhoff stress tensor can then be obtained via

$$\tau = 2 \rho_0 \frac{\partial \bar{\phi}(g, b^{e^{-1}}, F)}{\partial g} = K \log J g + \bar{J}^{-\frac{2}{3}} \mu \text{dev}[b^e]$$  \hspace{1cm} (4)

We now present the Von Mises yield condition

$$\bar{\varphi}(g, b^{e^{-1}}, q, F) := \|s\| - \sqrt{2/3} \kappa (\bar{\varepsilon}^p) \leq 0$$  \hspace{1cm} (5)

where $q = \{\bar{\varepsilon}^p\}$; $\bar{\varepsilon}^p$ is the equivalent inelastic (or plastic) flow, $s = \text{dev}[\tau]$, and $\|s\| = \sqrt{s : s}$. The associative flow rule obtained from maximum plastic dissipation (see e.g., Lubliner [3]) can be expressed as

$$\bar{J}^{-\frac{2}{3}} \mu \text{dev} [L_\sigma b^e] = -\frac{2}{3} \mu J^{-\frac{2}{3}} \text{tr} [b^e] \dot{\gamma} n$$  \hspace{1cm} (6)

where $n = s/\|s\|$ is the normal to the yield surface and trace of the Lie derivative of $b^e$ i.e., $\text{tr}[L_\sigma b^e] = 0$.

We present the following hardening law which mimics the behavior of stress at a material particle during change of phase from one stable state to the other.

$$\kappa (\bar{\varepsilon}^p) = \sigma_{dr} + (\sigma_\infty - \sigma_{dr}) (1 - \exp(-\delta_1 \bar{\varepsilon}^p)) + (\sigma_\infty - \sigma_{dr}) \exp(\delta_2 (\bar{\varepsilon}^p - \lambda))$$  \hspace{1cm} (7)

$$\dot{\bar{\varepsilon}}^p = \sqrt{2/3} \dot{\gamma}$$  \hspace{1cm} (8)

where $\sigma_{dr}$, $\sigma_\infty$, $\delta_1$, $\delta_2$ and $\lambda$ are material specific constants. $\lambda$ is related to the so-called maximum residual strain under uniaxial state and is termed as the draw-ratio. It has been shown experimentally [6] that under uniaxial loading conditions, neck formation in the physical specimen occurs at an appropriate initiating stress called the draw-stress $\sigma_{dr}$. Furthermore, $\sigma_\infty$ represents the stress that a material particle can develop once the neck has propagated over the entire specimen and further straining takes place only with a further increase in applied stress. $\delta_1$ and $\delta_2$ are the constitutive parameters that help in mapping the hardening law precisely and accurately onto the actual transformation surface for polycarbonates.

**Remark:** It is important to note that $\delta_1$ and $\delta_2$ are functions of $E_1$, $E_2$ and the slope of the transformation surface.

**OPERATOR SPLITTING METHODOLOGY** We adopt an operator splitting methodology and an updated Lagrangian framework to develop the numerical solution procedure [5].
Part I: Elastic Predictor: In the elastic problem the inelastic (or plastic) flow is assumed frozen. Furthermore the rate of deformation tensor in the spatial configuration is obtained as the Lie derivative of the total spatial strain tensor \( e \) relative to the flow associated with the spatial velocity field \( v \). Consequently,

\[
L_v e = d
\]

\[
L_v e^i = 0
\]

\[
L_v q = 0
\]

At this point it is checked that the stress state is admissible. In case the state is inadmissible, i.e., it violates the Kuhn-Tucker complementary conditions, then a correction to the stress needs to be applied as follows.

Part II: Plastic Corrector (return mapping): The plastic corrector is often referred to as return mapping because it enforces the yield conditions in a manner consistent with the assumed flow rule. In the inelastic (or plastic) corrector phase \( L_v e \equiv 0 \), i.e., the elastic deformation is frozen and the inelastic corrector takes place at a fixed current configuration. Consequently, the Lie derivative reduces to ordinary time differentiation. The inelastic/plastic problem can be written as

\[
L_v e = 0
\]

\[
L_v e^i = \dot{\gamma} \bar{n}(g, b^{c^{-1}}, q, F)
\]

\[
L_v q = \dot{\gamma} \bar{h}(g, b^{c^{-1}}, q, F)
\]

\[
\bar{\varphi}(g, b^{c^{-1}}, q, F) = 0
\]

Once we obtain the stress state compatible with the proposed model, we can solve the resulting nonlinear system of equations via the Newton Raphson method or with any of its variants. After obtaining the converged solution for the current load level we update the state variables and go to the next load level.

Numerical Results: We have performed a simulation of neck propagation under displacement control. The material properties are: Young’s Modulus \( E = 2.2 \) GPa, yield stress \( \sigma_y = 60 \) MPa, draw stress \( \sigma_{dr} = 40 \) MPa, draw ratio \( \lambda = 1.7 \), density \( \rho = 1200 \text{kg/m}^3 \), Poisson ratio \( \nu = 0.3 \). Figure 1a shows the initial undeformed mesh, Fig. 1b shows the deformed mesh (during the process of neck propagation), and Fig. 1c shows the axial stress in the deformed configuration.

Conclusions: We have presented a finite strain constitutive model for phase transition in polycarbonates. We have defined a yield surface that mimics very closely the stress state at a material particle during the phase transition. The nonlinear constitutive equations have been implemented in a finite element framework using 4-node isoparametric elements. Furthermore, we have used a backward Euler implicit formula for numerical integration of (12) - (15).
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REFERENCES