



# An internal state variable material model for predicting the time, thermomechanical, and stress state dependence of amorphous glassy polymers under large deformation

J.L. Bouvard<sup>a,b,\*</sup>, D.K. Francis<sup>a</sup>, M.A. Tschopp<sup>b</sup>, E.B. Marin<sup>a</sup>, D.J. Bammann<sup>a</sup>, M.F. Horstemeyer<sup>a</sup>

<sup>a</sup> Center for Advanced Vehicular Systems, Mississippi State University, 200 Research Blvd, Mississippi State, MS 39762, United States

<sup>b</sup> Mines-ParisTech, CEMEF, UMR 7635, BP 207, 06904 Sophia Antipolis Cedex, France

## ARTICLE INFO

### Article history:

Received 15 February 2012

Received in final revised form 8 October 2012

Available online 23 October 2012

### Keywords:

B. Constitutive behavior

B. Polymeric material

B. Viscoplastic material

C. Finite elements

## ABSTRACT

This paper presents a complete theoretical accounting of the thermomechanical coupling within a viscoplastic model to predict the time, temperature, and stress state dependent mechanical behavior of amorphous glassy polymers. The foundational model formulation (Bouvard et al., 2010), developed to predict the time dependent behavior of amorphous glassy polymer, departed from the Haward and Thackray (1968) spring-dashpot representation widely used to model the mechanical behavior of polymers. Instead, the model equations were derived from within a large deformation kinematics and thermodynamics framework based upon the approach proposed by Coleman and Gurtin (1967) in which physically-based internal state variables (ISVs) were selected to accurately represent the underlying physics of the polymer deformation mechanisms. The updated model presented includes the distinction of temperature dependence. Hence, the present material model accounts for (i) the material strain softening induced by the polymer chain slippage; (ii) the material strain hardening at large strains induced by chain stretching between entanglement points; (iii) the time, temperature, and stress state dependence exhibited by polymers under deformation. The model also accounts for heat generation induced by plastic dissipation that leads to the thermal softening of the material under large deformation at medium strain rates. The material model response was compared to experimental data for an amorphous polycarbonate deformed at different strain rates, temperatures, and stress states. The simulations account for fully coupled thermomechanical applications. Good agreement was observed between the model correlation and the experimental data in compression (for both loading and unloading responses), creep, tension, and torsion for different strain rates and temperatures. Moreover, finite element simulations of a Split Hopkinson Pressure Bar compression device accurately captured the mechanical response of the material deformed under high strain rate conditions.

© 2012 Elsevier Ltd. All rights reserved.

## 1. Introduction

Major research efforts within the automotive industry are devoted to reducing the weight and, thereby, the greenhouse gas emissions of future vehicles. The ongoing development and application of new lightweight materials, such as polymers and composites, significantly contributes to green vehicle design and engineering, generating savings in fuel consumption as

\* Corresponding author at: Mines-ParisTech, CEMEF, UMR 7635, BP 207, 06904 Sophia Antipolis Cedex, France. Tel.: +33 (0) 4 93 67 89 59; fax: +33 (0) 4 92 38 97 52.

E-mail address: [jean-luc.bouvard@mines-paristech.fr](mailto:jean-luc.bouvard@mines-paristech.fr) (J.L. Bouvard).

well as reduced emissions and production costs. Amorphous polymers, in particular, are widely used in vehicle assembly due to their physical, optical (light transparency), and mechanical properties (toughness). Along with reducing vehicle weight, the reduction of expensive mechanical tests is also a priority for the automotive industry. Thus the demand for accurate and reliable numerical simulations that adequately represent the time, temperature, and stress state dependent material behavior of polymers under large deformation is of prime importance in the development of vehicular structural components designed to withstand impacts.

A large number of constitutive models were developed to predict the material response of glassy polymers (see Bouvard et al. (2009) for a review of the literature). Models initially developed for metals were used to reproduce the mechanical properties of polymers, such as the viscoplastic model based on overstress (VBO) (Krempf and Khan, 2003; Dusunceli and Colak, 2008; Khan and Yeakle, 2011), the material model based on a generalized yield criterion (following a parabolic Drucker and Prager formulation) developed by Ghorbel (2008), or more recently the model based on a generalized Frederick–Armstrong–Philips–Chaboche (FAPC) theory proposed by Voyiadjis et al. (2012) to capture the inelastic response of glassy polymers. Previous efforts also developed phenomenological models based on differential equations and combining linear and nonlinear springs with dashpots to predict the viscoelastic response of polymers (Ayoub et al. (2010, 2011), Zairi et al. (2011), among others).

Initial material models were developed by Eyring (1936), Robertson (1966), Bauwens et al. (1969), Bauwens-Crowet (1973), and Argon (1973) to account for the intermolecular motion of the polymeric chains responsible for the time and temperature dependent yield behavior of these materials. In the sixties, Haward and Thackray (1968) initiated a new way of modeling the material behavior of glassy polymers by the use of a yield model (Eyring, 1936) combined in parallel with a hyperelastic model (three-chain model of James and Guth (1943)) to account for the strain hardening induced by the chain alignment at large deformations. This seminal work has been followed by many authors (e.g., Boyce et al. (1988), Govaert et al. (2000), Tomita (2000), Anand and Gurtin (2003), among others).

More recently, thermomechanical models have been developed to capture the time and temperature dependent behavior of amorphous polymers. Accordingly, Boyce et al. (1992) proposed a material model to study the complex thermomechanical coupling that evolves during the cold drawing process of glassy polymers. Arruda et al. (1995) developed a test setup and a three-dimensional constitutive model combined with a thermomechanically coupled finite element analysis to study the internal heat generation and its effect on the material behavior for compression tests performed at strain rates up to 0.1/s. Richeton et al. (2007) developed a three-dimensional constitutive model to describe the material response of amorphous polymers from the glassy to the rubbery state for a large range of strain rates. Recently, Anand et al. (2009) developed a thermomechanical model for amorphous glassy polymers based on the principle of virtual power that Srivastava et al. (2010) extended to capture the material deformation of these polymers above their glass transition temperature. Their thermodynamically-based model successfully captured the mechanical behavior of amorphous polymers when simulating complex processing operations (thermoforming, blow molding, and micro-hot-embossing).

In Bouvard et al. (2010), the formulation of a time-dependent material model for amorphous thermoplastics using a thermodynamic approach with physically-based internal state variables (ISVs) (Horstemeyer and Bammann (2010)) was proposed. The model formulation departed from the typical spring-dashpot representations widely used to model polymers. More specifically, it diverged from the Haward and Thackray (1968) approach, wherein an hyperelastic spring is coupled in parallel to an elastic-spring dashpot to account for the strain hardening at large deformation, nor did it follow subsequent models developed in that way (e.g., Boyce et al., 1988; Govaert et al., 2000; Tomita, 2000; Anand et al. (2003, 2009)). Instead, the Bouvard et al. model was based on the thermodynamic framework proposed by Coleman and Gurtin (1967) in which physically-based ISVs were selected to accurately represent the underlying physics of the polymer chain deformation. These ISVs, describing the current energetic state of the polymer network, were included in the Helmholtz free energy.

In Bouvard et al. (2010), the selection of the ISVs was made based on a hierarchical multiscale approach (Bouvard et al. (2009)). Molecular dynamics (MD) simulations were used to study deformation mechanisms during uniaxial tensile deformation of an amorphous polyethylene polymer (Hossain et al., 2010; Bouvard et al., 2010). Fig. 1 shows the multiscale strategy chosen to inform the continuum constitutive model. Changes in energy in the polymer atomic structure were analyzed to reveal the main micromechanisms of chain deformation and thereby provide qualitative information for the selection of the ISVs at the continuum level. Three ISVs were then introduced:

(i)  $\bar{\xi}_1$ , an internal strain-like quantity induced by entanglement points

It is well established that the entanglement density has a predominant effect on the mechanical behavior of polymers. Physical crosslinking such as entanglement points are considered as obstacles to chain motion. However as shown by Hossain et al. (2010), MD simulations performed on entangled polymers indicated that the number of entanglement points in the molecular chain changes with the deformation. As displayed in Fig. 1a, the change in the stress component associated to the Van der Waal's interaction ( $\sigma_{nb}$ ) shows that the chain entanglement slippage is a key mechanism leading to strain softening. At the continuum level, an internal strain quantity,  $\bar{\xi}_1$ , is introduced to account for the strain induced by entanglement points and further entanglement slippage (Fig. 1b).

(ii)  $\bar{\xi}_2$ , an internal strain-like scalar accounting for material hardening induced by chain alignment and chain coiling at large strains

Fig. 1a shows an increase in the non-bonded stress component beyond 40% strain. This increase may be correlated to groups of aligned chains that may induce additional strain hardening due to van der Waals interactions. Such an event was also observed in the atomic structure of a stretched polymer (Bouvard et al., 2010). This mechanism was introduced

Download English Version:

<https://daneshyari.com/en/article/786483>

Download Persian Version:

<https://daneshyari.com/article/786483>

[Daneshyari.com](https://daneshyari.com)