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Coupled viscoelastic–viscoplastic modeling of homogeneous and isotropic polymers: Numerical algorithm and analytical solutions

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ABSTRACT

A coupled viscoelastic–viscoplastic (VE–VP) model is implemented and studied. The total strain is the sum of VE and VP parts, and the Cauchy stress is given by a linear VE model as a Boltzmann integral of the history of VE strains. The proposed computational algorithm features fully implicit integration, return mapping based on a two-step VE predictor/VP corrector strategy, and a consistent tangent operator. The algorithm is applied to J_2 VP coupled with VE. Very compact expressions are obtained which are form-identical to classical elasto-viscoplasticity (EVP) provided that the constant linear elastic shear and bulk moduli are replaced with incremental relaxation moduli which are appropriate functions of the time increment. Two different integration methods to obtain the incremental moduli are proposed and assessed. Closed-form solutions for uniaxial tension and simple shear are developed, based on an original solution method for integro-differential equations. The analytical results enable to illustrate the constitutive model and provide unambiguous benchmarks for numerical algorithms. Model predictions are compared with experimental data and reasonable correlation is obtained.

1. Introduction

Polymer materials exhibit rate and time-dependent responses which are usually described by viscoelastic (VE) or elasto-viscoplastic (EVP) constitutive models. The difference between the two classes of models can be illustrated by a uniaxial tension test which comprises a monotonic loading phase followed by unloading to zero stress. In a VE model, the response is rate-dependent in both phases, which implies that the stress–strain slope (Young's modulus) is not constant, but increases with the strain rate. Also, even in linear VE, the relation between stress and strain may be non-linear. Finally, upon unloading to zero stress, the material can retrieve its initial state of zero strain, not immediately, but after a long time. Complete description of VE behavior is available in [9,18,40,47].

During the same uniaxial load/unload test, an EVP material will behave differently. If the stress is below an initial yield stress (σ_y), then the response is rate-independent linear elastic (thus Young's modulus is constant). Beyond σ_y the stress–strain response is both nonlinear and rate-dependent, with the stress increasing with the strain rate. Unloading is linear elastic, and therefore rate-independent. After unloading to zero stress, there remains an irreversible strain which does not disappear even after a long time. For a description of EVP models, see [35,30] and the review in [7].

Note that VE and EVP models are written a priori in very different manners, however a link between the two classes of models does exist. Indeed, it is shown in [6] that an EVP model possessing several back stresses may behave like a VE model written in spectral form (i.e., decomposing the VE strain into an elastic one and a spectrum of viscous strains each having its own relaxation time).

The behavior of numerous polymer materials such as thermoplastics in general is time and rate-dependent at all stages of deformation. This means that the stress–strain response will depend on the strain rate both below and above σ_y. Upon unloading, the slope is rate-dependent and may be non-linear, even strongly so. Unloading to zero stress leads to a permanent strain which might diminish with time but does not disappear completely even after a long waiting time. All those features can be described by *coupled* viscoelastic–viscoplastic (VE–VP) constitutive models. Most models suppose a decomposition of the total strain into a sum of VE and VP parts, and relate the Cauchy stress to the history of VE strains via a VE model, which can be linear, nonlinear, isothermal or thermally coupled.

A first approach is to write the VE response in hereditary integral form, which is Boltzmann's form if the VE model is linear, and usually of Schapery-type for nonlinear VE models. Linear and isothermal VE is considered in [31,39,38]. The VE response is nonlinear and coupled with thermal strains in [8,17,26].

A second class of models write the VE part of the response not in an integral form, but in a differential (or rate) one. Such VE–VP

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models can be found in [20,10]. In the latter reference, the VE part is actually a modified elasticity model. Indeed, the classical linear elastic expression linking the elastic strain rate to the stress rate is modified by introducing a stress-dependent coefficient which introduces nonlinearity.

In the present work, a coupled VE–VP model is implemented and studied. The total strain is supposed to be the sum of VE and VP parts, and the Cauchy stress is related to the history of VE strains via a linear VE model written as a Boltzmann integral. The proposed computational algorithm features fully implicit integration, return mapping based on a two-step VE predictor/VP corrector strategy, and a consistent tangent operator. Analytical solutions are developed in uniaxial tension or simple shear. With respect to the existing literature on coupled VE–VP models, the main contributions of the present article are summarized hereafter and will be detailed in the remainder of the text.

Compared to the numerical algorithms proposed by Saleeb et al. [39], Kim and Muliana [26], Ryou and Chung [38], our results are much more *compact* and shown to be *form-identical* to classical EVP provided that the constant linear elastic shear and bulk moduli G and K are replaced with incremental relaxation moduli. The latter are appropriate functions $\widetilde{G}(\Delta t)$ and $\widetilde{K}(\Delta t)$ of the time increment Δt. Two different integration methods to obtain the incremental moduli are proposed and compared against each other, theoretically and numerically, both for finite and small time increments.

Another important contribution is the development of closed-form solutions for uniaxial tension and simple shear. The mathematical developments are rather elaborate, as one arrives to integro-differential equations which are difficult to solve and for which we propose an original solution method. The analytical results enable us to illustrate the constitutive model and provide unambiguous benchmarks for numerical algorithms.

This paper is restricted to the regime of small perturbations (small strains, displacements and rotations). The VE part of the model is linear and isothermal. Thermal strain coupling and/or Schapery-type nonlinear VE [41–44] can be developed and implemented, as has already been proposed in some of the previously cited references. An extension to the large deformation regime can be developed based on the constitutive models of [3,4,27], for instance, and the numerical algorithms of [34,24].

The paper has the following outline. The VE–VP constitutive equations are summarized in Section 2. The computational algorithm is detailed and studied in Section 3. Analytical solutions for uniaxial tension and simple shear are developed in Section 4. The model and its predictions are verified and validated in Section 5. Numerical predictions are assessed against analytical results in Section 5.1. Model predictions are compared to experimental data collected from Zhang and Moore [48] in Section 5.2. Finite element simulations are reported in Section 5.3. A discussion regarding both the constitutive modeling and the numerical algorithms is conducted in Section 6. Conclusions are drawn in Section 7. The paper closes with two appendices. Appendix A develops the computation of the consistent tangent operator, and Appendix B details the derivation of the closed-form solution in uniaxial tension.

The following abbreviations are used throughout the text. VE: viscoelastic(ity), VP: viscoplastic(ity), EVP: elasto-viscoplastic(ity), and VE–VP: viscoelastic(ity)-viscoplastic(ity).

Boldface symbols designate second or fourth-rank tensors, as indicated by the context. Dyadic and inner products are expressed as:

$$(\boldsymbol{a} \otimes \boldsymbol{b})_{ijkl} = a_{ij} b_{kl}, \quad \mathbf{a} : \mathbf{b} = a_{ij} b_{ji}, \quad (\mathbf{A} : \boldsymbol{b})_{ij} = A_{ijkl} b_{lk},$$

where summation over a repeated index is supposed. The symbols $\mathbf{1}$ and $\mathbf{I}$ designate the second- and fourth-rank symmetric identity tensors, respectively. Finally, the spherical and deviatoric operators $\mathbf{I}^{vol}$ and $\mathbf{I}^{dev}$ are given by:

$$\mathbf{I}^{vol} \equiv \frac{1}{3} \mathbf{1} \otimes \mathbf{1} \quad \text{and} \quad \mathbf{I}^{dev} \equiv \mathbf{I} - \mathbf{I}^{vol}.$$

2. Constitutive equations

The constitutive model is based on the assumption that the total strain is subdivided into VE and VP parts:

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^{ve} + \boldsymbol{\epsilon}^{vp}. \tag{1}$$

This strain decomposition has some physical basis. Indeed, for semi-crystalline polymers, several micromechanical models suppose that cyrstalline lamellae and amorphous polymer chains obey VP and VE models, respectively, and are assembled in series (and thus follow a Reuss model); e.g. Nikolov et al. [32].

2.1. Linear viscoelastic part

The Cauchy stress $\boldsymbol{\sigma}(t)$ is related to the history of VE strains $\boldsymbol{\epsilon}^{ve}(\tau)$ for $\tau \leqslant t$ via a linear VE model expressed by Boltzmann's hereditary integral [5]:

$$\boldsymbol{\sigma}(t) = \int_{-\infty}^{t} \mathbf{E}(t-\tau) : \frac{\partial \boldsymbol{\epsilon}^{ve}}{\partial \tau} \, d\tau. \tag{2}$$

For an isotropic material, the fourth-rank relaxation tensor is written as:

$$\mathbf{E}(t) = 2G(t)\mathbf{I}^{dev} + 3K(t)\mathbf{I}^{vol}, \tag{3}$$

where $G(t)$ and $K(t)$ are shear and bulk relaxation functions, respectively, that can be expressed in the form of Prony series:

$$G(t) = G_\infty + \sum_{i=1}^{I} G_i \exp\left(-\frac{t}{g_i}\right) \quad \text{and}$$
$$K(t) = K_\infty + \sum_{j=1}^{J} K_j \exp\left(-\frac{t}{k_j}\right). \tag{4}$$

Here, g_i ($i = 1,\ldots,I$) and k_j ($j = 1,\ldots,J$) are the deviatoric and volumetric relaxation times, respectively, G_i ($i = 1,\ldots,I$) and K_j ($j = 1,\ldots,J$) are the corresponding moduli or weights, and G_∞ and K_∞ are the long-term elastic shear and bulk moduli.

Then, by substituting Eqs. (3) and (4) into Eq. (2), the deviatoric ($\mathbf{s}(t)$) and dilatational ($\sigma_H(t)$) parts of the stress tensor may be expressed in function of the deviatoric ($\xi(t)$) and dilatational ($\epsilon_H(t)$) parts of the strain tensor:

$$\begin{cases} \mathbf{s}(t) = 2G_\infty \boldsymbol{\xi}^{ve}(t) + \sum\limits_{i=1}^{I} \mathbf{s}_i(t), \\ \sigma_H(t) = 3K_\infty \epsilon_H^{ve}(t) + \sum\limits_{j=1}^{J} \sigma_{H_j}(t), \end{cases} \tag{5}$$

where viscous components are defined by:

$$\begin{cases} \mathbf{s}_i(t) \equiv 2G_i \exp\left(-\frac{t}{g_i}\right) \int_{-\infty}^{t} \exp\left(\frac{\tau}{g_i}\right) \frac{\partial \boldsymbol{\xi}^{ve}}{\partial \tau} \, d\tau, \\ \sigma_{H_j}(t) \equiv 3K_j \exp\left(-\frac{t}{k_j}\right) \int_{-\infty}^{t} \exp\left(\frac{\tau}{k_j}\right) \frac{\partial \epsilon_H^{ve}}{\partial \tau} \, d\tau. \end{cases} \tag{6}$$

2.2. Viscoplastic part

In the present work, only the rate-dependent J_2 VP model was implemented. However, some results of the proposed algorithm are general and valid for other VP models, as discussed in Section 6.1. For J_2 VP with isotropic hardening, the yield function is given as follows: