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Finite element implementation including sensitivity analysis of a simple finite strain viscoelastic constitutive law

G. Rauchs *

Department of Advanced Materials and Structures, Centre de Recherche Public Henri Tudor, B.P.144, L-4002 Esch/Uelzecht, Luxembourg

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ABSTRACT

This article describes the implementation of a finite strain viscous hyper-elastic material law into a finite element code. The material model is made up of a Maxwell element in parallel with a spring. Both springs represent hyper-elastic material behaviour, and compressibility is taken into account. In addition to that, the sensitivity analysis using direct differentiation is described extensively. The implementation is verified by three test cases, uniaxial tension, pure shear and indentation testing. The sensitivity analysis by direct differentiation is validated by comparison against results obtained by a finite difference scheme.

1. Introduction

Polymers are an important class of materials with a large number of applications. For this reason, numerous constitutive models have been developed for accurately describing their deformation behaviour. Polymer materials may exhibit different characteristic constitutive features. On the one hand, many polymers exhibit a higher degree of viscous deformation at room temperature than metals, for example. Whereas some polymers exhibit a pronounced plastic deformation behaviour [1], other polymers, for example rubber-like materials, exhibit purely elastic behaviour over a wide range of deformations. In addition to that, they are nearly incompressible. A good overview of the general computation of viscosity is given in [2]. An important class of polymer materials is described by both viscous and hyper-elastic material behaviour. Rubber-like materials belong to this class of materials, and their mechanical properties are used in a large number of applications. Their low stiffness and large elastic deformations make them an ideal material for use in seals. Because of their pronounced viscosity, they are used for vibration and shock damping. All these properties, together with their high friction coefficient in combination with many surface materials have led to their use in tires. Because of the high practical relevance of rubber materials, several constitutive models for modelling them with a high degree of accuracy have been put forward, [3]. These material models are often developed in the framework of finite strain formulations, and their thermodynamic consistency has also been proved. Finite element implementations of such models have been presented by [4–6]. Cyclic loading of polymers may be affected by Mullins or Payne effect, the former altering the hyper-elastic behaviour with the number of cycles, whereas the latter alters viscous behaviour with the number of cycles.

In [4,5], the integration of the viscous hyper-elastic constitutive equation is performed by an exponential map, involving use of the principal directions and principal values, leading to a consistency condition with three unknowns. A similar formulation in principal directions for the case of elasto-plastic materials, like metals for example, may be found in [7]. In the present article, the integration of the constitutive equations, formulated in Oldroyd rates, is carried out with the Euler backward integration scheme [3], and the consistency condition is an equation involving second-order tensors, to be solved by tensorial calculus. The advantage of this numerical formulation lies in the fact that the consistent linearization is very straight-forward. In fact, in case an exponential map is used, either eigen-values and eigen-vectors have to be linearized, which is rather complex [4,5], and identical or near-identical eigen-values have to be accounted for, or the exponential map is approximated by a truncated Taylor series, see for example [8], which affects the accuracy in case of large time steps. A disadvantage of the formulation involving Oldroyd rates is that volume preservation of the inelastic deformation has to be enforced explicitly, as will be described below.

The equations necessary for a finite element implementation are first derived through a consistent linearization for use in a direct differentiation-based sensitivity analysis [9–15], from which the consistent linearization necessary for the solution of the equilibrium equation using the Newton–Raphson method can be re-

* Tel.: +352 54 55 80 508.
E-mail address: gaston.rauchs@tudor.lu

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trieved easily. The main application of direct differentiation is the calculation of sensitivities for use in gradient-based inverse methods, because direct differentiation, as well as the adjoint state method, enables the calculation of derivatives with respect to specific variables with a higher accuracy and much faster than with finite difference methods. It has been used in inverse methods relying on gradient-based numerical optimization, for the solution of inverse problems involving shape optimization in preform or die design in metal forming [10–12] or material parameter identification [9,16]. As the sensitivity analysis involves the calculation of derivatives by the solution of a system of linear equations – in opposition to the nonlinear equilibrium equations – a successful verification of the sensitivities, for example through comparison with results from the finite difference method, enables one to verify the correctness of the exact linearization.

As the viscous deformation is supposed to be volume-preserving, the inelastic corrector step in the stress calculation is performed using the volume-preserving integrator introduced by [17]. This integrator, developed with a constitutive law for metals, is used with a constitutive law for rubber in the present article. In order to show the ease with which this integrator may be introduced into a finite element implementation, the stress update and its linearization are first presented for the standard integrator, and subsequently complemented by the volume-preserving integrator.

In the following sections, matrix notation is preferably used. Index notation is used whenever doubts about the formulation may arise in matrix notation format. Tensors are written in boldface letters. Where Einstein's summation convention is used, repeated indices in a term should be read as summation over the spatial dimensions. This notation is extended to elemental indices as well, where repeated indices stand for summation over the directly connected nodes.

In the next sections, the constitutive equations for viscous hyper-elastic material behaviour for rubber and the numerical implementation of the stress and internal variable update equations are presented. In fact, the model used is model A from [3], which has been derived for incompressible material behaviour, and will be complemented with bulk terms for the case of compressible or near-incompressible behaviour. As no radial return algorithm with a single scalar consistency parameter is possible for this material law, a tensorial equation has to be solved through a local Newton–Raphson scheme, which requires the inversion of a fourth-order tensor, described in a separate section. After that, these update equations are linearized, in a way that the material stiffness part and the explicit parts required for sensitivity analysis can be easily obtained. The subsequent section shows the determination of the global stiffness matrix. Whereas in [15], the sensitivity analysis of a mixed method for use in frame elements is described, in this paper, both the sensitivity analysis and the calculation of the stiffness matrix are performed in the framework of a mixed displacement–pressure finite element formulation, necessary because of the near-incompressibility of the rubber-like materials. In the last section, the sensitivity analysis is assessed by comparing finite difference gradient results to direct differentiation results, first for the simple test cases of uniaxial tension and pure shear, subsequently for an indentation test of rubber, characterized by a highly multiaxial and inhomogeneous stress field. A practical application of the sensitivity analysis, e.g. the determination of material parameters of rubber by indentation testing and gradient-based numerical optimization using a finite element model of the indentation test, will be presented elsewhere [18]. This application also motivates the selection of the rather simple constitutive law involving a small number of material parameters, developed in [3], in order to keep the number of material parameters to be identified reasonably low.

2. Constitutive formulations

2.1. Hyper-elasticity using Mooney–Rivlin potential

In finite deformation hyper-elastic constitutive modelling, extensive use is made of the invariants of a second-order tensor

$$I_{\mathbf{b}} = \mathbf{I} : \mathbf{b}, \tag{1}$$

$$II_{\mathbf{b}} = \frac{1}{2}\left((\mathbf{I} : \mathbf{b})^2 - \mathbf{b} : \mathbf{b}\right), \tag{2}$$

$$III_{\mathbf{b}} = det\,\mathbf{b}, \tag{3}$$

where $I_{\mathbf{b}}$, $II_{\mathbf{b}}$ and $III_{\mathbf{b}}$ are the invariants of the left Cauchy–Green tensor $\mathbf{b}$:

$$\mathbf{b} = \mathbf{F}\mathbf{F}^{\mathbf{T}}. \tag{4}$$

The deformation gradient $\mathbf{F}$ is defined from the current geometric configuration $\mathbf{x}$ and the reference configuration $\mathbf{X}$ by

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}. \tag{5}$$

These definitions are often altered in order to remove the volume change

$$\bar{I}_{\mathbf{b}} = III_{\mathbf{b}}^{-\frac{1}{3}} I_{\mathbf{b}}, \tag{6}$$

$$\bar{II}_{\mathbf{b}} = III_{\mathbf{b}}^{-\frac{2}{3}} II_{\mathbf{b}}. \tag{7}$$

The hyper-elastic Mooney–Rivlin potential has the form

$$\boldsymbol{\Psi} = a(\bar{I}_{\mathbf{b}} - 3) + b(\bar{II}_{\mathbf{b}} - 3) + \frac{c}{2}(\sqrt{III_{\mathbf{b}}} - 1)^2, \tag{8}$$

Including Eqs. (6) and (7) into the definition of the Mooney–Rivlin potential yields

$$\boldsymbol{\Psi} = a(I_{\mathbf{b}} III_{\mathbf{b}}^{-\frac{1}{3}} - 3) + b\left(II_{\mathbf{b}} III_{\mathbf{b}}^{-\frac{2}{3}} - 3\right) + \frac{c}{2}(\sqrt{III_{\mathbf{b}}} - 1)^2, \tag{9}$$

The Kirchhoff stress $\boldsymbol{\tau}$ is related to the left Cauchy–Green deformation tensor $\mathbf{b}$ through

$$\boldsymbol{\tau} = 2\mathbf{b}\left(\frac{\partial \Psi}{\partial I_{\mathbf{b}}}\frac{\partial I_{\mathbf{b}}}{\partial \mathbf{b}} + \frac{\partial \Psi}{\partial II_{\mathbf{b}}}\frac{\partial II_{\mathbf{b}}}{\partial \mathbf{b}} + \frac{\partial \Psi}{\partial III_{\mathbf{b}}}\frac{\partial III_{\mathbf{b}}}{\partial \mathbf{b}}\right) \tag{10}$$

with

$$\frac{\partial I_{\mathbf{b}}}{\partial \mathbf{b}} = \mathbf{I}, \tag{11}$$

$$\frac{\partial II_{\mathbf{b}}}{\partial \mathbf{b}} = I_{\mathbf{b}}\mathbf{I} - \mathbf{b}, \tag{12}$$

$$\frac{\partial III_{\mathbf{b}}}{\partial \mathbf{b}} = III_{\mathbf{b}}\mathbf{b}^{-1}, \tag{13}$$

which gives

$$\boldsymbol{\tau} = 2\left(\frac{\partial \Psi}{\partial I_{\mathbf{b}}}\mathbf{b} - \frac{\partial \Psi}{\partial II_{\mathbf{b}}} III_{\mathbf{b}}\mathbf{b}^{-1} + \left(\frac{\partial \Psi}{\partial II_{\mathbf{b}}} II_{\mathbf{b}} + \frac{\partial \Psi}{\partial III_{\mathbf{b}}} III_{\mathbf{b}}\right)\mathbf{I}\right). \tag{14}$$

It should be noted that use is made of the Cayley–Hamilton theorem,

$$\mathbf{bbb} - I_{\mathbf{b}}\mathbf{bb} + II_{\mathbf{b}}\mathbf{b} - III_{\mathbf{b}}\mathbf{I} = \mathbf{0}. \tag{15}$$

The coefficients of Eq. (9) are subjected to some restrictions: vanishing internal energy and stress in the unstrained state, positive bulk and shear moduli at the unstressed state. It can easily be shown that these conditions are met with the Mooney–Rivlin potential.

2.2. Viscoelasticity

The viscoelasticity model used in the current implementation is a Maxwell element in parallel with a spring, called model A in [3], and its rheological model is sketched in Fig. 1.