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Constitutive modeling of solid propellants for three dimensional nonlinear finite element analysis

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A R T I C L E I N F O

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A B S T R A C T

A three dimensional constitutive model for solid propellants is proposed and implemented in a finite element software. The effects of viscoelasticity, large deformation, temperature, pressure, softening in monotonic and cyclic loadings are represented. Damage is assumed to initiate by failure of the particle-binder bond or failure in the binder itself. Opening of the micro-cracks resulting from either failure is associated with the evolution of damage. Stress softening during unloading and reloading is captured via a cyclic function modifying the viscoelastic stress. The implementation algorithm is stable and robust, therefore analysis of general geometries and loadings are possible. The model may be calibrated with a small number of test data, therefore is suitable for practical use in the industry.

1. Introduction

Composite solid propellants exhibit highly nonlinear mechanical behavior due to large deformation, temperature, loading rate, superimposed pressure, cyclic loading and damage. A constitutive model that accounts for the effect of these factors may be quite complex and need a large number of test data to calibrate model parameters. On the other hand, prediction of structural integrity of a rocket motor grain and reliable determination of its service life typically require accurate, three-dimensional stress analysis. A constitutive model developed as part of a computational procedure, such as finite element analysis, needs not only to realistically predict the behavior of the propellant under various loading conditions, but also be well suited for numerical implementation. To be of practical use in the industry, the amount of test data required should be minimized. Furthermore, a robust and numerically stable implementation algorithm should be developed in order to minimize convergence difficulties that may result from mathematical nonlinearities.

In the following, recent literature on propellant constitutive modeling is reviewed in terms of model development, computational implementation, verification–validation and application to stress analysis.

Several of the following constitutive models aim to represent the nonlinearity due to damage within the linear viscoelastic framework. Park and Schapery's [1] viscoelastic constitutive model with growing damage is based on thermodynamics framework and internal state variables [2]. The model was initially proposed as one-dimensional and later extended to three dimensions by Ha and Schapery [3]. Simulation results for uniaxial and biaxial loading cases were presented. A variation of the model was proposed by Jinseng et al. [4] where damage was assumed to evolve as a function of temperature. The validation was based on uniaxial test data and homogeneous deformation. Also based on Park and Schapery's framework, Wang et al. [5] investigated the behavior of propellants at low temperature and high strain rate and accurately predicted uniaxial homogeneous deformations.

Xu et al.'s [6] model accounted for propellant porosity. Uniaxial monotonic loading was well represented, however the nonlinear effects during unloading were not captured. The predictive capability for three dimensional analysis was not provided. Chyuan [7] conducted linear viscoelastic stress analysis of a rocket motor grain to study the effect of thermal loading. Propellant non-linearity was included [8] by varying the bulk modulus as a function of compressive stresses. The study showed that for compressive thermal stress states, non-linear bulk modulus modeling significantly affects the response as compared to linear analysis with constant bulk modulus. Hur et al.'s [9] constitutive model is based on the calculation of effective shear and bulk modulus of the propellant including the effect of voids, in addition to the binder and the particles. The moduli of the binder were assumed to depend on temperature and strain rate. Damage evolution was modeled as strain-controlled nucleation of voids. The model was implemented in a finite element code. Uniaxial and biaxial loading simulations

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were given, however, the robustness of the algorithm under more complex loading states was not discussed. Huiru et al. [10] presented a three dimensional constitutive model for solid propellant which assumes the Poisson's ratio to depend on time and temperature. The model was implemented into a commercial finite element code, however validation against test data was not provided. Three dimensional thermal cyclic and ignition pressurization analyses showed that Von Mises stress predictions with viscoelastic Poisson's ratio are significantly higher than those with constant Poisson's ratio. Liu et al. [11] presented experimental results for a high performance propellant at various strain rates and temperatures. Based on dilatation measurements, it was concluded that for the initial linear portion of the deformation the material was almost incompressible, while at higher strain volume change increased due to the formation of voids following interface debonding. Test data was conclusive regarding the dependence of the shear modulus on the strain rate and temperature, while that of the bulk modulus was found to be quite complex, partly due to difficulties involved in accurate measurement of the bulk behavior. Bin et al.'s [12] viscoelastic model accounted for damage through the definition of an effective stress. The model was implemented in a finite element code and the algorithm was validated with respect to analytical results for uniaxial creep. A three dimensional analysis of an internally pressurized solid rocket motor was presented.

Only few contributions address damage within the finite deformation framework. Jung and Youn's [13] constitutive model is based on a viscoelastic dewetting criterion which is an extension of the elastic dewetting criterion proposed by Vratsanos and Farris [14]. Based on this criterion, a critical stress for particle debonding was determined and the softening of the modulus, hence the softening in stress was calculated. The model compared well with test results for uniaxial straining at various strain rates and temperatures. Calibration of the damaging model parameters such as adhesion energy and particle size distribution does not appear to be straightforward. A computational algorithm of the model was proposed by Jung et al. [15] and was implemented in ABAQUS software. Yun et al. [16] proposed an alternative damage function to that of [15] and also provided the three dimensional computational algorithm for finite element implementation. Simulations of either implementation agree reasonably well with test data for uniaxial and biaxial loading at various rates and temperatures. Simulations of non-homogeneous deformations were not provided in neither publication.

In summary, although the propellant constitutive models available in the literature represent non-linearity due to damage, most of them are valid for small displacements and rotations only. Few of these models were implemented in a computational software and the verification was carried out only for homogeneous deformation states. The first aim of the constitutive model proposed in this work is to represent the effects of viscoelasticity and damage within the finite deformation framework. Model parameters are to be determined effectively with a moderate amount of test data. The next objective is to implement the model in a general purpose, finite element software so that it can be readily used for stress analysis of a rocket motor subjected to general loadings. As part of this goal, the verification and validation of the model aims to include homogeneous as well as inhomogeneous deformation states.

The formulation described in this paper is the modified and enhanced version of a previously developed model [17]. New damage initiation and evolution criteria are proposed. Softening during unloading–reloading is accounted for by introducing a cyclic function which multiplies viscoelastic stress. The constitutive model was implemented in commercial finite element software ABAQUS [18] as a user material. The basic three dimensional viscoelastic model, and enhancements to the model are described in Section 2. Identification of model parameters and functions are presented Section 3. In Section 4 predictions with the implemented model are compared with experimental data. Conclusions and future work are presented in Section 5.

2. Constitutive model

The three dimensional nonlinear viscoelastic constitutive model described in this section represents the effects of strain rate, temperature, superimposed pressure and cyclic loading on the stress and dilatational response of the propellant. The basic finite strain model uses the framework of Simo [19], the pioneering work in setting the computational framework for constitutive modeling of finitely deforming, nearly incompressible materials. The damage model uses the dilatation model of Özüpek and Becker [20]. Damage initiation and damage evolution criteria are proposed to account for the softening of the stress response due to microstructural changes. Damage is assumed to initiate by failure of the particle-binder bond or failure in the binder itself. Opening of the micro-cracks resulting from either failure is associated with the evolution of damage.

2.1. Viscoelastic constitutive model

The proposed three dimensional viscoelastic constitutive model is characterized by uncoupled deviatoric and volumetric responses. The separation of the response allows efficient formulation for nearly incompressible materials such as solid propellants and is suitable for the development of separate damage models for volumetric and deviatoric responses.

2.1.1. Elastic response

Elastic response of the material model is derived from a strain energy density function which is expressed as an additive decomposition of volumetric and deviatoric parts as

$$\psi^0 = U^0(J) + g(s_g)\bar{\psi}^0(\bar{I}_1, \bar{I}_2) \tag{1}$$

where $g(s_g)$ accounts for the effect of damage on the distortional response as described in Section 2.2.1, J is the volume ratio, and $\bar{I}_1$, $\bar{I}_2$ are the deviatoric invariants of right Cauchy–Green deformation tensor $\mathbf{C}$. The volumetric and deviatoric elastic stresses calculated from Equation (1) are, respectively

$$\bar{P} = \frac{\partial U^0}{\partial J} \qquad \text{and} \qquad \mathbf{\Pi} = g(s_g)J^{-2/3}DEV\left(\frac{\partial \bar{\psi}^0}{\partial \bar{\mathbf{E}}}\right) \tag{2}$$

where $DEV(\bullet) = (\bullet) - \frac{1}{3}[\mathbf{C} : (\bullet)]\mathbf{C}^{-1}$.

Volumetric part of the strain energy function used in this study is of the form

$$U^0 = \frac{1}{2}K(J_e - 1)^2 \tag{3}$$

with

$$J_e = \frac{J}{J_{th}J_c}, \quad J_{th} = [1 + \alpha_{th}(T - T_0)]^3 \quad \text{and} \quad J_c = 1 + c(t) \tag{4}$$

where $c(t)$ represents the volume change due to damage. K is bulk modulus, α_{th} is coefficient of thermal expansion, and J_e, J_c, J_{th} are the volume ratios due to elastic, inelastic and thermal effects, respectively.

The distortional part of the elastic strain energy density is represented with a Neo-Hookean polynomial

$$\bar{\psi}^0 = c_{10}(\bar{I}_1 - 3) \tag{5}$$