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Enhancements on a micromechanical constitutive model of solid propellant

Junyoung Hur[a], Jae-Beom Park[b], Gyoo-Dong Jung[b], Sung-Kie Youn[a,*]

[a] Department of Mechanical Engineering, KAIST, 291 Daehak-ro, Yuseong-gu, Daejeon 305-701, Republic of Korea
[b] Agency for Defense Development, Advanced Propulsion Technology Center, Republic of Korea

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ABSTRACT

A constitutive model of solid propellant based on the micromechanical approach is presented. Proposed model includes the effects of temperature and strain rate dependency, and severe nonlinearities under cyclic loading. Damage is represented by the reduced elastic moduli which is the function of the void volume fraction. Dependency of the material properties on temperature and strain rate is incorporated in the shear modulus of the binder matrix. Using the test data from the uniaxial tests, it is expressed as a function of temperature and strain rate. Using the function, homogenized elastic tensor represents the effects of temperature and strain rate. The cyclic loading behaviors are controlled by introducing artificial strain rate and modified stress based on the unloading and reloading curves. Proposed constitutive model is implemented into the user subroutine of ABAQUS. Finally, accuracy of the constitutive model is verified under various loading conditions.

1. Introduction

Solid propellant is a highly filled composite material with particles and binder matrix to improve combustion performance. The particles include the fuel, oxidizer and other additives and display elastic behavior, whereas the binder matrices such as HTPB (hydroxyl-terminated polybutadiene) or PBAN (polybutadiene–acrylonitrile–acrylic acid) which are used to be the cushion of oxidizer particles behave as a viscoelastic material. The accurate stress analysis of solid propellant is necessary to ensure the performance and safety of rocket.

However, constitutive modeling of solid propellant is quiet a complex process since both elastic and viscoelastic behaviors should be considered. Also, degradation of mechanical properties so called 'damage' makes the response of solid propellant highly nonlinear under various loading conditions. In the microscopic aspects, creation and expansion of voids occur at the interface between oxidizer particles and polymeric binder matrix. This phenomenon is called 'dewetting' (Farris, 1968). It causes the softening of the material. In addition to dewetting phenomenon, severe nonlinearity of solid propellant is observed during cyclic loading which includes drastic decrease of stress during unloading. Furthermore, Dependency of softening behavior on the maximum loading of the previous steps is also observed. This behavior is known as Mullins effect (Ogden and Roxburgh, 1999). Modeling of these phenomena is complicated since they are dependent on the temperature, strain rate and strain level.

Over the last few decades, many studies on the constitutive model of particulate viscoelastic material have been reported. Schapery proposed the *J* integral theory in viscoelastic material (Schapery, 1984) and damage prediction using internal state variables with potential (Schapery, 1991). Later, Park and Schapery developed a constitutive model of damaged viscoelastic material with two internal variables (Park and Schapery, 1997) and it is extended to the three dimensional stress state (Ha and Schapery, 1998). Hinterhoelzl and Schapery addressed the constitutive model by describing anisotropic effects caused by damage (Hinterhoelzl and Schapery, 2004).

In addition to the Schapery and his co-workers' study, constitutive models of solid propellant including damage effect have been developed by many researchers. Swanson and Christensen introduced a softening function into heredity integral (Swanson and Christensen, 1983). Simo addressed a generalized three dimensional constitutive model using free energy with deviatoric and volumetric parts (Simo, 1987). Ozupek and Becker enhanced Simo's model by combining softening function and deviatoric free energy (Ozupek and Becker, 1992). Later, this model is modified by considering pressure, strain rate and cyclic loading (Ozupek and Becker, 1997), and it is effectively implemented into the finite element code (Canga et al., 2001). Jung and Youn developed a

* Corresponding author. Tel.: +8242 350 3034.
E-mail address: skyoun@kaist.ac.kr (S.-K. Youn).

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constitutive model using Simo's model and proposed dewetting criteria (Jung and Youn, 1999). Then it is extended to cyclic loading condition and three dimensional stress state (Jung et al., 2000). Mathous and Geubelle studied multiscale modeling using Mori–Tanaka homogenization (Mori and Tanaka, 1973) and dewetting modeling based on the cohesive law (Matouš and Geubelle, 2006).

The constitutive models stated above can be categorized as 'phenomenological models' which use internal variables to describe damage in macroscopic aspects. In contrast to these models, Xu et al. proposed a 'Micromechanical approach' (Xu et al., 2007) starting from the unit cell of viscoelastic material with spherical void under small deformation. Then it is extended to the large deformation (Xu et al., 2008) using Hashin–Shrikman homogenization theory (Hashin and Shtrikman, 1963). However, these models are not verified under cyclic loading and varying temperature.

The scope of this paper is to enhance the micromechanical constitutive modeling of Xu et al. (2008) to include the effects of strain rate, temperature and cyclic loading. During the homogenization process, behavior of binder matrix is expressed as a function of strain rate and temperature. Cyclic loading effects are implemented by introducing unloading/reloading curves and artificial strain increment. This paper is organized as follows. Constitutive modeling of solid propellants with micromechanical approach is addressed in Section 2. Section 3 explains the numerical implementation scheme of constitutive model into the finite element program. Calibration procedures and results of specimen tests are shown in Section 4, and conclusions are presented in Section 5 .

2. Constitutive modeling

2.1. Preliminaries

Micromechanical constitutive modeling of solid propellant (Xu et al., 2008) assumes that solid propellant is a three-phase composite material with the binder matrix, the particles (fuel and oxidizer) and the voids. To perform the homogenization, a "representative volume element" (RVE) of the solid propellant with total volume V is introduced as follows:

$$c_m = \frac{V_m}{V}, c_p = \rho = \frac{V_p}{V}, c_v = f = \frac{V_v}{V}, c_m + \rho + f = 1, \tag{1}$$

where V_m, V_p and V_v represent the volume of matrix, particle and void, respectively, and c_m, ρ and f define the volume fraction of each phase. The total deformation rate $\mathbf{D}$ is expressed as the summation of elastic part $\mathbf{D}^e$ and a viscous part $\mathbf{D}^v$:

$$\mathbf{D} = \mathbf{D}^e + \mathbf{D}^v. \tag{2}$$

2.2. Elastic response

The homogenization process of the solid propellant with three phases (binder, particle and voids) is performed with the following two steps (Bonnenfant et al., 1998).

Effective moduli with matrix and particles by applying Hashin–Shtrikman lower bounds (Hashin and Shtrikman, 1963) . This estimates the most compliant behavior of particle-reinforced composite. Let the phases '1' and '2' denote the binder matrix and particles, then the effective shear modulus μ_{hom} and bulk modulus κ_{hom} are represented as:

$$\mu_{\text{hom}} = \frac{\sum_{i=1}^{2} (c_i\mu_i)/(6\mu_i(\kappa_1 + 2\mu_1) + \mu_1(9\kappa_1 + 8\mu_1))}{\sum_{j=1}^{2} \left(c_j\right)/\left(6\mu_j(\kappa_1 + 2\mu_1) + \mu_1(9\kappa_1 + 8\mu_1)\right)},$$
$$\kappa_{\text{hom}} = \frac{\sum_{i=1}^{2} (c_i\kappa_i)/\left(3\kappa_j + 4\mu_1\right)}{\sum_{j=1}^{2} c_j/\left(3\kappa_j + 4\mu_1\right)}, \tag{3}$$

where c_i, μ_i and κ_i are the volume fraction, shear and bulk modulus of each phase. In this work, binder is assumed to be incompressible material and particles shows rigid behavior. Then moduli of each phase are expressed as follows:

$$\begin{aligned} &\mu_1 = \mu_m, \kappa_1 = \infty \\ &\mu_2 = \kappa_2 = \infty, \end{aligned} \tag{4}$$

where μ_m represents the shear modulus of binder. The volume fractions of binder and particles excepting void are represented as:

$$c_1 = \frac{1 - f - \rho}{1 - f}, c_2 = \frac{\rho}{1 - f}. \tag{5}$$

Using Eqs. (4) and (5), effective moduli are expressed as:

$$\mu_{\text{hom}} = \frac{2 - 2f + 3\rho}{2(1 - f - \rho)}\mu_m, \kappa_{\text{hom}} = \infty. \tag{6}$$

Effective moduli including void by applying Hashin–Strikman upper bound (Hashin and Shtrikman, 1963) which represents the stiffest behavior. Let the phases '1' and '2' are the void and effective moduli of the previous step, respectively, then the effective moduli are expressed as:

$$\bar{\mu} = \frac{\sum_{i=1}^{2} (c_i\mu_i)/(6\mu_i(\kappa_2 + 2\mu_2) + \mu_2(9\kappa_2 + 8\mu_2))}{\sum_{j=1}^{2} \left(c_j\right)/\left(6\mu_j(\kappa_2 + 2\mu_2) + \mu_2(9\kappa_2 + 8\mu_2)\right)},$$
$$\bar{\kappa} = \frac{\sum_{i=1}^{2} (c_i\kappa_i)/\left(3\kappa_j + 4\mu_2\right)}{\sum_{j=1}^{2} c_j/\left(3\kappa_j + 4\mu_2\right)}. \tag{7}$$

In this work, void is assumed to have zero-moduli, then homogenized moduli take the form:

$$\bar{\kappa} = a\mu_m \text{ where } a = \frac{2(1 - f)(2 - 2f + 3\rho)}{3f(1 - f - \rho)}$$
$$\bar{\mu} = b\mu_m \text{ where } b = \frac{9f}{4(3 + 2f)}a. \tag{8}$$

With the homogenized moduli, elastic part of the constitutive law is expressed with the following hypoelastic form:

$$\mathbf{D}^e = \mathbf{M}^e : \overset{\nabla}{\boldsymbol{\sigma}} = \left(\frac{1}{2\bar{\mu}}\mathbf{K} + \frac{1}{3\bar{\kappa}}\mathbf{J}\right) : \overset{\nabla}{\boldsymbol{\sigma}}, \tag{9}$$

where $\boldsymbol{\sigma}^\nabla$ is the Jaumann rate of the Cauchy stress, $\mathbf{K}$ and $\mathbf{J}$ are the fourth-order tensors with the following components:

$$J_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl}, K_{ijkl} = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right). \tag{10}$$

2.3. Representation of temperature and strain rate effects

In the previous research on micro-mechanical modeling of solid propellant (Xu et al., 2008), the shear modulus of binder μ_m is assumed to be a constant value. However, polymeric structure of the binder matrix shows severe temperature and strain rate dependencies. Therefore, elastic response described in Section 2.2 needs to include these effects. One of the treatments is to utilize a generalized Maxwell model of binder (Clements and Mas, 2004). However this approach is not suitable for the hypoelastic constitutive law.

In this work, polymeric binder matrix is assumed to show temperature and strain rate dependent behaviors. From the test data of solid propellant under various temperatures and strain rates, which are discussed on Section 4.1, the measured shear modulus of binder decays exponentially with respect to temperature. Also, after temperature dependency is represented by an exponential function, there exists vertical shift of the curves when strain rates vary. From these observations, shear modulus of binder is represented by a function with temperature and strain rate dependencies as follows:

$$\mu_m(T, \dot{\varepsilon}) = g_T(T) \cdot g_{\dot{\varepsilon}}(\dot{\varepsilon}), \tag{11}$$