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Modeling, Simulation and Experimental Verification of Constitutive Models for Energetic Materials

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Simulation of the complete response of components and systems composed of energetic materials, such as PBX-9501(1) is important in the determination of the safety of various explosive systems. For example, predicting the correct state of stress, rate of deformation and temperature during penetration is essential in the prediction of ignition. Such simulation requires accurate constitutive models. These models must also be computationally efficient to enable analysis of large scale three dimensional problems using explicit lagrangian finite element codes such as DYNA3D(2). However, to be of maximum utility, these predictions must be validated against robust dynamic experiments. In this paper, we report comparisons between experimental and predicted displacement fields in PBX-9501 during dynamic deformation, and describe the modeling approach. The predictions used Visco-SCRAM and the Generalized Method of Cells which have been implemented into DYNA3D. The experimental data were obtained using laser-induced fluorescence speckle photography. Results from this study have lead to more accurate models and have also guided further experimental work.

INTRODUCTION

Finite element simulations are the preferred analysis tool used to predict the response of systems containing explosives. Predicting the correct state of stress, rate of deformation and temperature of a system under going dynamic loading is essential in the prediction of ignition. Thus, the constitutive model used to describe the mechanical behavior of the energetic material (explosive) must be accurate. Classical plasticity base constitutive models have been used, but with limited success due the fact that the microstructural mechanics producing inelastic behavior and ignition in the energetic material are vastly different from classical plasticity theory. Validating new proposed constitutive models requires robust dynamic experiments where the comparative information is much more than post mortum geometry. In this paper, we report the experimental verification methodology and the comparisons between experimental and predicted displacement fields in PBS-9501 during dynamic deformation.

CONSTITUTIVE MODELS

Visco-SCRAM

This model has been proposed by Johnson(3)(4) and combines Maxwell visco elasticity with

statistical crack mechanics(5). The result is an isotropic constitutive model that describes the behavior of a visco/brittle material. Statistical crack mechanics(5) is a physically based micromechanical description for the large deformation of brittle materials. During the process of deformation it is assumed that the crack distribution remains random and the size distribution of the cracks is exponential. The Visco-SCRAM approach provides a computational expedient constitutive model that can easily be implemented into a finite element code and exercised on a wide variety of three dimensional problems. Consider an n component Maxwell model, where G'' is the shear modulus and η'' is the time constant for the n th component. For a general visco-elastic solid let the strain rate be defined as,

$$\dot{\epsilon}_{ij} = \frac{1}{2} \left(\frac{\partial \dot{u}_j}{\partial x_i} + \frac{\partial \dot{u}_i}{\partial x_j} \right) \quad (1)$$

For an n component Maxwell model, the deviatoric strain rate is equal to the deviatoric strain rate in each component. The deviatoric state of stress is the sum of the deviatoric state of stress in each component.

The deviatoric stress rate in each Maxwell component is given by Equation 4,

$$\dot{s}_{ij}^n = 2G^n \dot{e}_{ij}^n - \frac{s_{ij}^n}{\tau^n} \quad (2)$$

By superposition of strains, the total deviatoric strain rate is the sum of the deviatoric viscoelastic strain rate and the deviatoric cracking strain rate.

$$\dot{e}_{ij} = \dot{e}_{ij}^{ve} + \dot{e}_{ij}^c \quad (3)$$

From Reference(4) the cracking strains are related to the deviatoric stress using,

$$e_{ij}^c = \beta^e c^3 s_{ij} \quad (4)$$

where c is the average crack radius. Thus from Reference(4) the relationship between the deviatoric cracking strains and the crack radius is,

$$2Ge_{ij}^c = \left(\frac{c}{a}\right)^3 s_{ij} \quad (5)$$

Or in rate form,

$$2G\dot{e}_{ij}^c = 3\left(\frac{c}{a}\right)^2 \frac{\dot{c}}{a} s_{ij} + \left(\frac{c}{a}\right)^3 \dot{s}_{ij} \quad (6)$$

Using Equations 6 and 2 an expression for the deviatoric stress rate in each Maxwell element may be obtained.

$$\dot{s}_{ij}^n = 2G^n \dot{e}_{ij}^n - \frac{s_{ij}^n}{\tau^n} - \frac{G^n}{G} \left[3\left(\frac{c}{a}\right)^2 \frac{\dot{c}}{a} s_{ij} + \left(\frac{c}{a}\right)^3 \dot{s}_{ij} \right]$$

Where,

$$\dot{s}_{ij} = \frac{2G\dot{e}_{ij} - \sum_{n=1}^n \frac{s_{ij}^n}{\tau^n} - 3\left(\frac{c}{a}\right)^2 \frac{\dot{c}}{a} s_{ij}}{1 + \left(\frac{c}{a}\right)^3}$$

The crack radius growth rate is determined as a function of K , where

$$K < K' \quad \dot{c} = v_{\max} \left(\frac{K}{K_1} \right)^m \quad (7)$$

$$K \geq K' \quad \dot{c} = v_{\max} \left[1 - \left(\frac{K_o}{K} \right)^2 \right]^m \quad (8)$$

Where, $K' = K_o \sqrt{1 + \left(\frac{2}{m}\right)}$, and

$$K_1 = K_o \sqrt{1 + \left(\frac{2}{m}\right)} \left[1 + \frac{m}{2} \right]^{\frac{1}{m}}, K = \sqrt{\pi c} \sigma_{eff}$$

The parameters, $a=0.001$ m, $\nu = 0.3$, $m = 10$,

$K_o = 5 \times 10^5$ Pa $\sqrt{m}$, $c_o = 0.00003$ m, $v_{\max} = 300$ m/s, have been determined using hopkinson bar data.

Generalized Method of Cells

The Generalized Method of Cells(6) is a physically based unified micromechanical modeling approach to describing the elastic and inelastic macroscopic behavior of a heterogeneous materials. The method of cells approach allows for the material description of the constituents and the interfaces that exist between the constituents. The microstructure of the composite material is idealized by a representative volume element (RVE). The RVE is representative of the microstructure of the aggregate heterogeneous material. The constitutive behavior of the constituents is defined along with constitutive behavior of the constituent interfaces. Continuity of displacements and continuity of tractions are imposed across the interfaces in the RVE. The macromechanical behavior is obtained from appropriate averages of the behavior of the constituents and the behavior of the constituent interfaces. In addition to being able to represent the microscopic behavior of the material this approach is also sufficiently computationally efficient to be implemented into a three dimensional finite element code for structural analysis. The following development has been presented in detail in Reference(6), and will be briefly presented here for continuity. A general heterogeneous particulate material may be represented by an idealized RVE shown in Figure 1.

The RVE in Figure 1 has 27 subcells, however the number of subcell in any of the three coordinate directions is arbitrary. Consider the

material to have periodic structure whose repeating volume element consists of rectangular parallelepiped subcells. Each subcell can be filled, by an arbitrary constitutive model,

$$\dot{\sigma}_{ij}^{(\alpha\beta\gamma)} = C_{ijkl}^{(\alpha\beta\gamma)} \dot{\epsilon}_{kl}^{(\alpha\beta\gamma)} - \dot{\Gamma}_{ij}^{(\alpha\beta\gamma)} \quad (9)$$

FIGURE 1. Representative Volume Element, RVE

Since the average behavior of the heterogeneous material is sought, it is sufficient to consider a first order theory in which the velocities in each subcell are expanded linearly in terms of the distances from the center of the subcell. Introducing a local coordinate system $\bar{x}$ whose origin is located at the center of the subcell $(\alpha\beta\gamma)$.

$$\dot{u}_i^{(\alpha\beta\gamma)} = \dot{w}_i^{(\alpha\beta\gamma)}(x) + \bar{x}_i \dot{\phi}_i^{(\alpha\beta\gamma)} + \bar{x}_2 \dot{\chi}_i^{(\alpha\beta\gamma)} + \bar{x}_3 \dot{\psi}_i^{(\alpha\beta\gamma)} \quad (10)$$

With the strain rate in each subcell given by Equation 10,

$$\dot{\epsilon}_{ij}^{(\alpha\beta\gamma)} = \frac{1}{2} \left(\frac{\partial \dot{u}_j^{(\alpha\beta\gamma)}}{\partial \bar{x}_i} + \frac{\partial \dot{u}_i^{(\alpha\beta\gamma)}}{\partial \bar{x}_j} \right) \quad (11)$$

The strain rate in each subcell may be established.

$$\begin{aligned} \dot{\epsilon}_{11j}^{(\alpha\beta\gamma)} &= \dot{\phi}_1^{(\alpha\beta\gamma)}, \quad \dot{\epsilon}_{22j}^{(\alpha\beta\gamma)} = \dot{\chi}_2^{(\alpha\beta\gamma)}, \quad \dot{\epsilon}_{33j}^{(\alpha\beta\gamma)} = \dot{\psi}_3^{(\alpha\beta\gamma)} \\ 2\dot{\epsilon}_{23}^{(\alpha\beta\gamma)} &= \dot{\chi}_3^{(\alpha\beta\gamma)} + \dot{\psi}_3^{(\alpha\beta\gamma)} \\ 2\dot{\epsilon}_{13}^{(\alpha\beta\gamma)} &= \dot{\psi}_1^{(\alpha\beta\gamma)} + \dot{\phi}_3^{(\alpha\beta\gamma)} \\ 2\dot{\epsilon}_{12}^{(\alpha\beta\gamma)} &= \dot{\chi}_1^{(\alpha\beta\gamma)} + \dot{\phi}_2^{(\alpha\beta\gamma)} \end{aligned} \quad (12)$$

Each subcell interface may be described using an interface constitutive law similar to the decohesion laws proposed by Needleman(7).

Employing continuity of displacements and continuity of tractions conditions at the interfaces between the subcells of the RVE, and at the interfaces between the neighboring RVE, results in a set of linear algebraic equations which may be solved for the microvariables,

$$\dot{\phi}, \dot{\psi}, \dot{\chi}$$

Once the microvariables have been determined, the strain rate in each subcell may be determined using Equation 11. The stress rate in each subcell is determined using the subcell strain rate and the appropriate subcell constitutive law, Equation 12. The subcell stresses are integrated to determine the subcell stress. The macroscopic stress is determined using volume averaging.

IMPLEMENTATION INTO DYNA3D

A continuum finite element code is the preferred analysis tool used to simulate the complete response of engineering structures. In this case both constitutive models will be implemented into the three dimensional explicit lagrangian finite element code DYNA3D(2).

PREDICTION OF IGNITION

It is well known that the bulk heating which occurs when an explosive is impacted is insufficient to cause a reaction. Then energy deposited must be localized, raising the temperatures of these regions to temperatures in excess of the ignition temperature. These localized regions are called "hot spots" and can arise from many mechanisms. A "hot spot" model using modified Frank - Kamenetskii(8) equations has been implemented into DYNA3D. The details of this model are presented in Reference(9).

EXPERIMENTAL VERIFICATION

The dynamic impact experiments were conducted and reported elsewhere(10) in which a projectile was fired at the nominal velocity of 185 m/s at pushers of various geometry. The pushers induce deformation in the high explosive based on their geometry. The in plane displacement field on the surface of the explosive is measured using laser-induced fluorescence speckle photography(11). The measure displacement field can be directly compared with displacement field predicted using the DYNA3D simulation. Constitutive model validation and modification is based on the ability of the constitutive model to reproduce the experimental displacement field. Figure 2 shows the impact test geometry. Figure 3 shows DYNA3D finite element model that faithfully

reproduces the geometry of the impact experiment.

FIGURE 2. Impact test geometry

FIGURE 3. DYNA3D Finite element model of the Asay impact test

FIGURE 4. Experimental displacement field obtained using laser-induced fluorescence speckle photography(9).

Figure 4, show the experimental displacement field for PBS-9501(Sugar Mock). Figure 5 shows the predicted displacement field using

DYNA3D with the Visco-SCRAM constitutive model at the same point in time. The comparison is both qualitatively and quantitatively good. The Generalized Method of cells has been implemented into DYNA3D in the form of a 2X2X2 and a 3X3X3 RVE. The predicted results are very promising and will appear in a later publication.

FIGURE 5. Predicted displacement field, obtained using DYNA3D and VISCO-SCRAM

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