INFLUENCE OF MECHANICAL PROPERTIES ON NON-SHOCK IGNITION

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Modeling non-shock ignition as seen in safety related tests such as the Steven, Susan and drop-skid tests is still a very difficult task. Explosives formulations based on plastic bonded granular materials (PBXs) display complex mechanical behaviors including temperature and strain rate sensitivity, strain localization at several different length scales and unusual fracture behavior. Some recent experiments done in the Steven test configuration involve small changes in the geometry of the experiment and also small changes in the PBX formulation providing a set of experiments that can be used to evaluate various ignition models. We began a study of the influence of small changes in the mechanical properties and ignition models from several different constitutive models including Scram, Viscoscram and viscoelastic plastic models, their integrated numerical heat transfer ignition models, and two separable models Ignition and Growth and recently developed linear operator based approximation. The Steven experiments provide a computationally tractable geometry, reproducible ignition conditions, and additional information such as measured back plate strain histories that provide checks on the mechanical models. The mechanical constitutive models can influence ignition behavior if the models allow for strain localization. We compare the behavior of the different mechanical and ignition models in the Steven and other experimental configurations. We explore the possible effects of grit at the boundaries of the explosive on ignition conditions. This is clearly important in the standard drop skid test with sand coated targets. Most ignition models lack a method for treating this type of boundary condition except through friction at the boundary.

INTRODUCTION

Several mechanical constitutive models specifically adapted for explosive materials have recently been incorporated into the Dyna3D finite element computer program. Frequently elastic-plastic types of models, designed for metals, are used to model explosives even though they are known to lack many characteristics exhibited by PBX explosives such as viscoelastic behavior. The more recent models, Scram and Viscoscram, are now available in versions of the Dyna3D code and we attempt to compare their features on a variety of test problems. Some of the problems are idealized to bring out the inherent differences. The Steven experiments are used for their extensive ignition results. Non-shock ignition is the specific goal here so the mechanical models are compared at fairly high strain rates and strain levels.

CONSTITUTIVE AND IGNITION MODELS

The SCRAM model was developed by Dienes,[1,2,3,4] and implemented in Dyna3D by Middleditch. This model is based on the concept of a statistical distribution of cracks, and evolution equations describing their growth, intersection, and rate effects. Most development work was done in the Pronto code, and only recently has the model been implemented in Dyna3D. This is a complex model, requiring 96 parameters to define the characteristics of a particular material. We use parameters supplied by the authors. In addition to the mechanical constitutive model SCRAM features an embedded ignition model based on a one-dimensional reactive heat transfer model with single term Arrehenius kinetics.

ViscoSCRAM was originated by Johnson and Bennett,[5,6] with continued development and implementation by Bennett. This model uses a more traditional viscoelastic formulation to handle rate effects coupled with a simplified version of SCRAM fracture mechanics. In SCRAM, the initial distribution of fractures includes a specified number of fracture orientations in addition to a distribution of fracture sizes. In ViscoSCRAM the fracture behavior is integrated over all orientations reducing the complexity of the model, but also reducing its accuracy and flexibility to some extent.

Traditional elastic-plastic models, possibly with a jwl equation of state for the bulk response is used as a reference. The authors have used this type of model for all previous modeling of Steven experiments. There is no explicit rate-dependence or coupling of pressure and shear modulus in this formulation. We select moduli for the expected loading rate and pressure conditions, and use eos values from shock loading experiments, giving a model that captures the basic response but misses many details in the time dependent response. The Steven experiment approximates a ramp loading and unloading condition, without long time dwells to allow for the creep or relaxation response that a viscoelastic model provides, so this is not a totally unreasonable assumption. DePiero also uses an elastic-plastic model in his adaptation of the Tarver Ignition and Growth shock ignition model to non-shock conditions. To evaluate pressure dependent models we did some calculations with a cap model.

LOCALIZATION AND FRACTURE

Localization is the essential feature of initiation in explosives. The linear operator based ignition model[7,8,9] that we usually use is based on the localization caused by inter-granular friction between HE crystals. The embedded ignition models in SCRAM and ViscoSCRAM take shear crack sliding as the thermal source for the ignition model. In either case, increasing the shear strain rate will increase the dissipation rate and drive ignition. The gross mechanical behavior of grain beds is known to exhibit shear band like modes, resulting in strong localization of the shear strain rate. Materials that exhibit this behavior can exhibit highly non-linear behavior if the deformation mode changes as a function of impact velocity in a given structural configuration. Plasticity models with small or zero amounts of strain hardening, or cap models, easily generate this localization behavior. It is not clear from the formulation of SCRAM and ViscoSCRAM if they will exhibit this behavior.

Gross fracture is also an important structural behavior. In the Steven tests recovered explosive discs show extensive fracturing both near the projectile and at the outer rim of the explosive disc as a result of radial flow. Both SCRAM and ViscoSCRAM use a statistical distribution of Griffith cracks as part of the underlying theory, but it is not obvious how well these will approximate discrete cracks.

TEST PROBLEMS

A series of test problems were defined when we began this study. Simple tension and compression tests, as used in the basic calibration process, provide a first check. A series of punch problems are used to investigate the strain localization behavior of the different constitutive equations. Taylor impact test simulations are also done. A Brazil test configuration is used to evaluate fracture characteristics with transverse compressive stresses as a comparison to the ordinary tension test. Finally Steven tests include several precisely defined similar configurations with ignition data available. Originally this was envisioned as a direct comparison between the models under a variety of test configurations.

A few problems arose in trying to carry out this program. The models were implemented in different and incompatible ways. For example, each model has some features that involve a specific set of units. The native implementation of Scram is built on cgs units, Viscoscram uses mks, while the Tarver ignition and growth model uses Mb-microsecond units. Even our linear operator ignition model that appears to have only a single dimensional constant turned out to have two additional constants that depend on the units of time buried in the post-processor. Although there is some flexibility in choice of units there was no single set of units that could be used for all the models. The ideal solution would be to modify the implementations so that all dimensioned constants are brought out to the user interface, however this option was not practical on the time scale of this project. Our solution was to generate problem definitions in each of the preferred units, then convert the output variables back to a common set of units. In addition we had minor but time consuming problems with the pre- and post-processing tools for Dyna3D, the result being that only a subset of the problems are analyzed and summarized.

Most of the test problems have very simple geometric configurations. The tension and compression tests were done with one-element cubes, of 1 mm size, although the size should not matter. The punch problems were done with 100x100x1 blocks of explosive supported with non-frictional boundary conditions, that is symmetry-planes, at the sides and bottom, effectively creating a two-dimensional problem. Punches of various sizes were used, narrower, equal and wider than the explosive block. The

Taylor impact problem is a right circular cylinder with diameter 16 mm and length 76 mm, impacting a cylindrical steel target with 50 mm diameter and length. The Brazil test is a cylinder of 25 mm diameter, loaded laterally between two rigid flat platens.

The Steven experiments come in a variety of configurations as done at Los Alamos by Idar[10,11] and co-workers and at LLNL by Chidester[12,13] and co-workers. In this report we primarily discuss the original LANL design with 25 mm thick explosive, and a modified design with 12.5 mm thick explosive. We have also analyzed Steven configurations with a Teflon ring surrounding the HE cylinder and several shapes of projectiles done by Chidester. Note that in the Taylor and Steven experiments interfacial friction can be an important variable. The cover plate in the Steven experiment is believed to play an important role in the results and is always made from 304 SS, a controlled alloy. The other parts, and the target in the Taylor test, are made from 304 SS in some cases and A36 or 4330 steel alloys. These changes likely influence the back plate strain histories used in the LANL experiments as a check on the calculations. Modeling of the Sylgard layer and the Teflon ring was consistent in all our calculations, but not necessarily accurate. The Sylgard was usually taken as a Blatz -Ko rubber with a shear modulus of 800 MPa, a very high value but chosen to give a reasonable bulk modulus.

COMPUTATIONAL RESULTS

We began the constitutive tests with one-element problems in uniaxial stress, tension and compression. Some uniaxial strain problems in tension and compression using 100x100 blocks were also done. The single element problems should replicate the calibration data and in the case of ViscoSCRAM and the elastic-plastic models did so. SCRAM needed at least 100 elements to work correctly so this check problem was passed. Viscoscram shows a remarkable ability to capture the long unloading tail observed in compression tests on PBX 9501, even in a one-element test problem. This is a highly unstable material behavior and might lead to strong localization in problems with refined meshing.

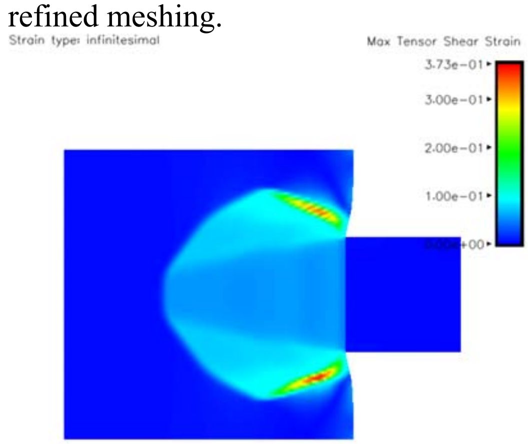

Figure 1 Cap model shows strong localization in this punch problem.

The punch problems, done with fixed punch velocities of 20 m/s, showed some of the most interesting differences in behavior among the models. The results of some punch problems are shown in Figures 1 and 2. Figure 1 shows a problem run with a cap type constitutive equation displaying the effects of localization that occurs in this type of model. The localization with Scram is much less pronounced, as seen in Fig. 2. Scram has rate dependent terms in the crack growth models that can affect stability and evidently suppress localization. The shape of the deformation region resembles results seen in cylindrical samples.

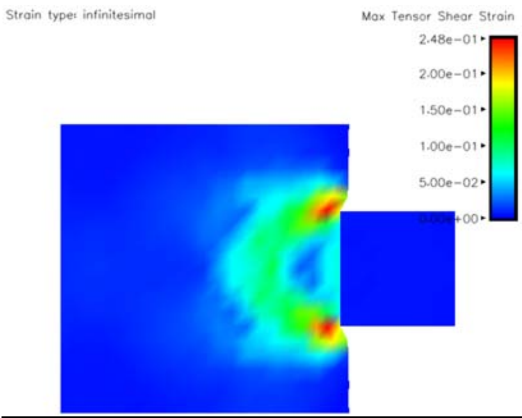

Figure 2 This punch problem done with the SCRAM model shows less localization than in Fig. 1.

Only a few Brazil test calculations are done. One interesting comparison is shown in Figs. 3 and 4 of a calculation using ViscoSCRAM as implemented in ABAQUS. The agreement with the measured load history is quite good, much better than a calculation with our elastic-plastic model. However the strain distribution shown in Figure 4 does not resemble the observed fracture that should run between the loading points, but not go all the way to the loading points. The wedge at the loading point is accurate though.

Our experience to date in Steven experiments revolves around the elastic-plastic models, primarily because of the large number of elements needed in 3-D models to obtain reasonable spatial resolution. Both SCRAM and ViscoSCRAM are slow compared with traditional models.

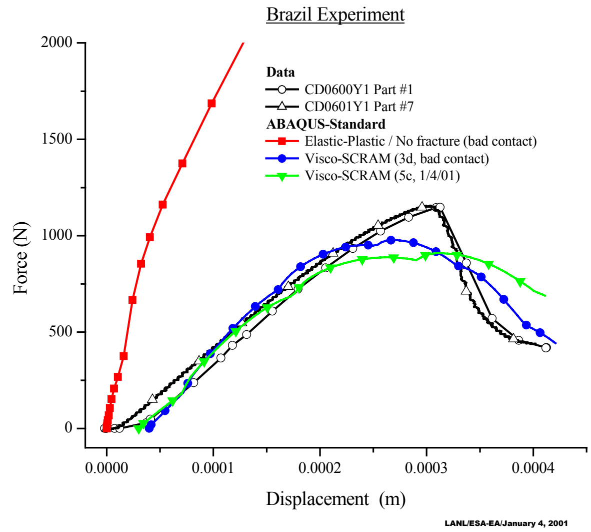

Figure 3 Load deflection for Brazil test is a difficult test. Note that elastic plastic model simply dies, while ViscoSCRAM follows post peak unloading.

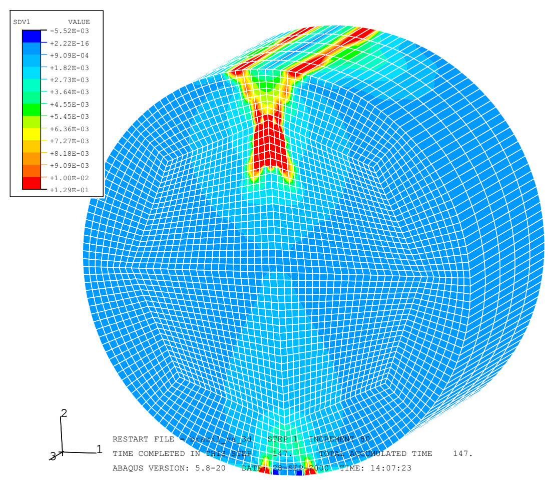

Figure 4 The strain distribution calculated with ViscoSCRAM does not match experiments though.

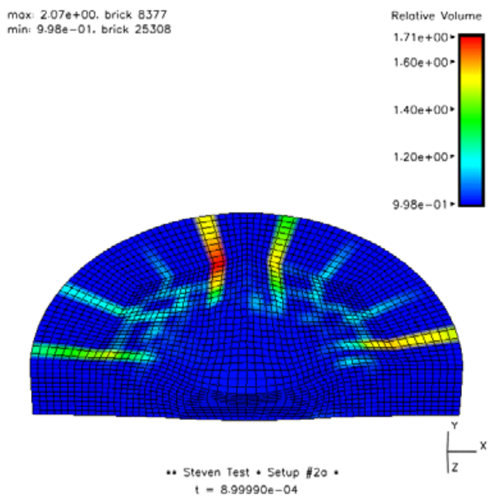

Figure 5 Shows strain localization from fracture behavior in the elastic-plastic explosive model.

In doing the elastic-plastic calculations we observed some differences between our previous 2-d models and the 3-d models we are trying to use for comparison purposes. In some cases the time and location of ignition moved around in a previously unobserved manner. We currently believe this is partly due to differences in the mesh density, but also found a large sensitivity to the coefficient of friction values used in the models.

The original calculations were all done with a coefficient of friction of 0.2 between metal parts, 0.3 between the Sylgard and metal, and 0.5 on any explosive surface. Some of the 3-d models omitted the Sylgard layer because it is thin, only 0.5 mm. If the mesh is done with cubical elements, then most are in the Sylgard, rather than the HE unless 0.25 mm elements are used in the HE as well. This leads to millions of elements in the HE, and impractical run times even with large parallel systems. We hope to do a few calculations of this sort eventually, but not at the beginning. A mesh using about 150000 elements required 18 days to run on a single processor system. When done, we noticed a problem with the slide line arrangement that makes the results useless. Exploration of behavior is not practical with these large problems.

Figure 5 illustrates a localization mode that occurs with the elastic plastic model in highly resolved 3-D simulations. The lines show irregular regions where the elements have fractured relieving the hoop stress at the outer boundary and the radial stress near the projectile caused lip. This type of localization is not observed in 2-D simulations because of the assumed axi-symmetry. The localization is strikingly similar to the observed fracture pattern in un-reacting Steven experiments that have been disassembled. The resolution of the pattern is clearly limited by the mesh density.

GRIT BEHAVIOR

When grit is involved in an experiment then a different type of ignition model is usually needed. In some cases it is possible that the grit just provide a very high effective coefficient of friction and that ignition actually takes place in the interior of the explosive, but this is not the only situation. There are three materials involved in a grit problem, the explosive, the grit particles and another surface. The grit particles are glued to the other surface in the large scale drop skid test, while in the case of the drop weight impact test the grit is actually glued to paper and the explosive is in the form of a loose powder – an extremely complex situation to model. Experiments done with one or a few grit particles by Dyer and Taylor[14] show sensitization even in situations where the change in overall friction values must be negligible. They attributed this to the grit particle acting as a local hot spot after becoming embedded in the explosive surface and then friction heats the grit. The interaction of the grit with the two adjacent surfaces depends on the relative hardness of the materials, their heat capacity, melting temperature, and thermal conductivity. The case of a hard, high melting point, particle like common sand proved very sensitizing in the Dyer and Taylor experiments. In addition to the frictional heating scenario postulated by them, a sharp grit particle can easily act like a cutting edge producing hot chips if the adjacent material is softer than the particle. This would be the typical situation for a metal surface. We believe a separate type of model is needed to cover this situation. A challenge for this surface ignition model is to deal with the inherent variability of grit particles, their orientation with respect to the surfaces and the direction of motion between the surfaces. The behavior of a broken grit particle with a sharp edge will depend heavily on the cutting edge angle with respect to the embedding surface and the angle with respect to the sliding velocity vector. The interest here is not just in mean values, but also in the statistical distribution at the extremes.

CONCLUSIONS

Overall we believe that any of the constitutive models in the hands of a knowledgeable analyst can be used for a variety of important problems. Our comparison of SCRAM and ViscoSCRAM is influenced heavily by implementation details that are not inherent in the models. Our experience with SCRAM is limited to date, but we believe the model has capabilities that need exploration and usage. We hope to continue using the model as less restrictive implementations are released. We believe ViscoSCRAM is easier than SCRAM to calibrate for a new material, but appears to have some inherent problems with large-scale fracture behavior. The tension-compression shear failure mode is not in agreement with experiments, and is important in applications without an obvious work-around. The tensile stress cutoff option in the elastic-plastic model gives only a very rough approximation of gross fracturing but frequently this rough approximation is adequate. More accurate models of gross fracture behavior are badly needed.

The lack of localization behavior in both SCRAM and ViscoSCRAM may be the result of fitting the models primarily to low pressure data. Wiegand[15] reported some very interesting results on compressive strength as a function of pressure. At relatively modest pressures the behavior of PBX 9501 changed from viscoelastic roll off to something closely resembling traditional elastic-plastic behavior. We only noticed this paper recently and hope to investigate this behavior further.

We were surprised by the sensitivity of the calculated Steven test results to assumed friction values between the explosive, Sylgard, and metal layers. This one example emphasizes the influence that mechanical properties can have on non-shock ignition problems.

The actual experiments are very reproducible, implying that the frictional behavior is also reproducible. Our problem is finding the correct model. Experiments to study dynamic friction characteristics of these materials would be very helpful.

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