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A VERIFICATION AND VALIDATION EFFORT FOR HIGH EXPLOSIVES AT LOS ALAMOS NATIONAL LAB

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Abstract. We have started a project to verify and validate ASC codes used to simulate detonation waves in high explosives. Since there are no non-trivial analytic solutions, we are going to compare simulated results with experimental data that cover a wide range of explosive phenomena. The intent is to compare both different codes and different high explosives (HE) models. The first step is to test the products equation of state used for the HE models. For this purpose, the cylinder test, flyer plate and plate-push experiments are being used. These experiments sample different regimes in thermodynamic phase space: the CJ isentrope for the cylinder tests, the isentrope behind an overdriven detonation wave for the flyer plate experiment, and expansion following a reflected CJ detonation for the pate-push experiment, which is sensitive to the Gruneisen coefficient. The results of our findings for PBX 9501 are presented here.

Keywords: High explosive modeling, ASC, verification and validation, detonation waves
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INTRO

Simulations of detonation phenomena have not yet advanced to the stage of plug and play. Verification and validation (V&V) are critical to knowing what high explosive (HE) models apply to which applications and to estimate the accuracy of simulated results. Since there are no non-trivial analytic solutions, verification cannot be separated from validation, and it is essential to compare model predictions with experimental data.

HE models are empirically calibrated. Since the effects of model parameters are highly non-linear, fitting procedures are heuristic and non-unique. This raises two issues; first, what is the uncertainty in model parameters that are compatible with calibration experiments. Second, how much of an effect does a reasonable variation of model parameters have on simulation results for engineering applications?

We have started on a systematic approach to address these issues. As a first step, we focus on the equation of state (EOS) of the HE products. Several experiments are used to cover the domain of thermodynamic phase space of interest for propagation detonation waves. Here, we report exclusively on PBX 9501; a high performance HMX based plastic-bonded explosive.

APPROACH

We compare experimental data with simulated results from two ASC codes: the Lagrangian 'Flag' code and the Eulerian 'xNobel' code. To assess the current state of implemented models, we performed "out-of-the-box" simulations. That is, the setup matched the initial conditions of the experiment but standard model parameters are used. With fine-tuning, the simulations could be made to match experimental data much more closely. Here, our intent is a conservative estimate of predictive capability.

Initially, we simulate three types of experiments that access different regimes of thermodynamic phase space of the detonation products. Several different EOS models for PBX 9501 are used [1,2]. For each experiment, several comparisons are made: between experimental data and simulated results, between simulated results with Lagrangian and Eulerian codes, and between simulated results with different EOS models on the same code.

We also compared different HE burn models (Ignition and Growth, Forest Fire and Programmed Burn). However, the experiments we study were designed to obtain EOS data. They are dominated by the propagation of a steady detonation wave. As expected, they are insensitive to the burn model.

TEST SUITE

We have chosen to study three experiments. The first is two-dimensional and the other two are one-dimensional.

Cylinder Test

In this experiment there is a copper tube filled with 9501. The HE is ignited at the bottom with a booster and burns up the copper tube, see figure 1. A streak camera is used to measure the copper walls location at a given axial position as it expands outwards [3,4]. The data is used to obtain the radial wall velocity as a function of time. This test provides data on the products EOS for the release isentrope from the CJ state of an under driven detonation wave. Comparisons with experiment and simulations are shown in figures 2-4.

We find that out of the box for the cylinder is very different from the other experiments. Most of the models have been calibrated to cylinder test data. We do find that the results are very sensitive to the products EOS.

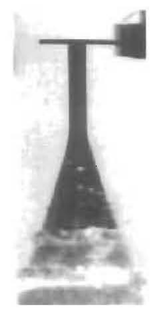

Figure 1. Experiments by Larry Hill, data is corrected and smoothed to get velocity [3].

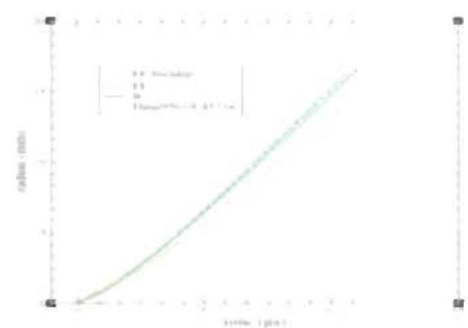

Figure 2. Radial wall motion for cylinder experiment shot C4521 comparing models in xNobel.

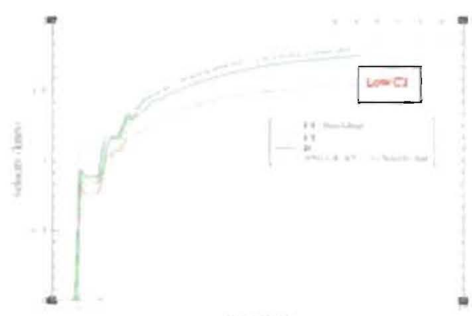

Figure 3. xNobel simulations of cylinder experiment, comparing different models and associated EOS for products.

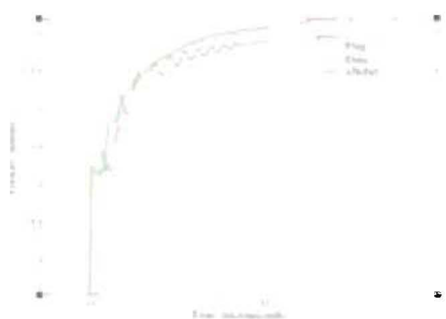

Figure 4. Experimental data for cylinder tests compared with Flag and xNobel. Both codes running Programmed Burn and using JWL equation of state.

Flyer Plate

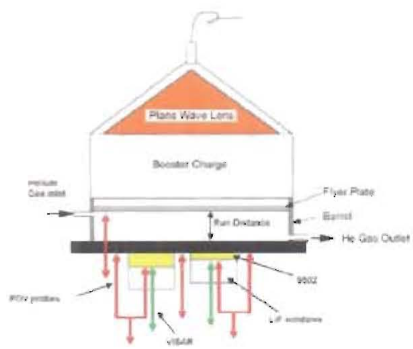

Figure 5. Experimental data from Hixson et al [5,6]. Improved setup and image from Jensen et al [7].

In this experiment a flyer plate impacts an HE target and provides the support for an overdriven detonation wave, see figure 5. The sound speed behind the detonation and release isentrope are measured. This experiment provides EOS data for a higher isentrope than obtained from the cylinder test. The experiment is essentially one-dimensional. Thus, it avoids the complication associated with radial flow in the cylinder test. Simulations were run with Flag and xNobel, both using Programmed Burn and JWL equation of state. The results are compared in figure 6.

The results demonstrate the use of non-compatible models for the type of experiment we are looking at. This is an overdriven problem and Programmed Burn models are not adequate for modeling this state.

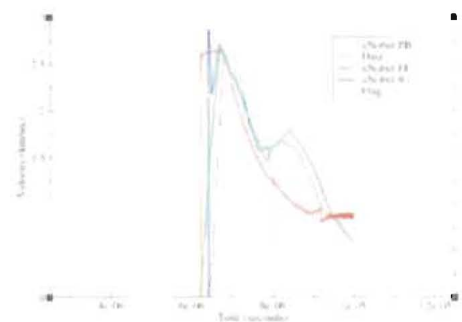

Figure 6. xNobel simulations of flyer plate experiment using different models with EOS that each model is calibrated to. Again the products EOS have a large effect on results.

Plate Push Test

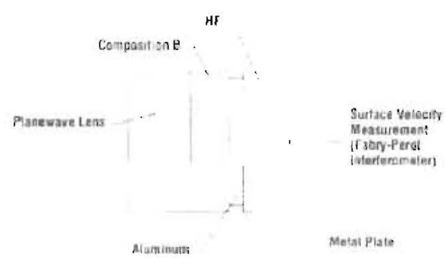

Figure 7. Example experimental setup by Tang et al[8]. Data is a figure in a detonation symposium paper and is not available as an electronic file.

This experiment is similar to the flyer plate experiment. Rather than using an impedance-matched window for a VISAR measurement, the HE pushes a metal plate and the velocity is measured on the free surface of the plate, see figure 7.

The detonation wave reflects off the metal and the subsequent shock in the HE propagates through the Taylor wave behind the detonation; data provides a good check on the products of EOS off the CJ isentrope. It is sensitive to the Gruneisen coefficient. This problem is in a very different phase space from the cylinder test problem. One will get a higher pressure from the reflected shock and this will kick above the isentrope. A comparison of results is shown in figures 8 and 9.

The plate-push problem demonstrates a dependence on the products EOS again.

Figure 8. xNobel simulations of plate push experiment, velocity time history at the air copper interface.

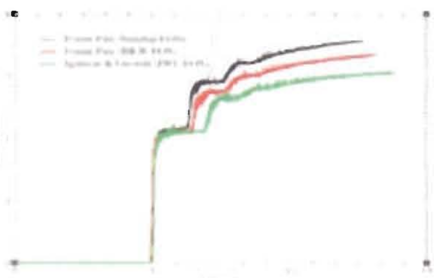

Figure 9. xNobel simulations of plate push experiment, time history at the air copper interface for different EOS.

SUMMARY & CONCLUSIONS

We have started on a systematic approach to verification and validation of high explosive modeling. Here we have reported preliminary results for HE products EOS, on what we hope will be an ongoing V&V project.

Long term there is a need for additional est problems to cover a wide range of detonation phenomena: such as, gas gun experiments on shock-to-detonation transition; rate stick experiments on the curvature effect and failure diameter; onion skin and corner turning experiments which combine aspects of both initiation and propagation. Also, other HE burn models, such as DSD and Crest, should be added to the list of models to be tested and evaluated.

To thoroughly assess the strengths and weaknesses of different HE models, there is a need for a standard suite of test problems. The goal should be to provide code users with guidance on the domain of applicability along with an estimate of the uncertainties associated with each model.

One of the largest impediments to a V&V program for HE is obtaining data along with a complete specification of an experiment. For a detailed comparison with simulations, it is especially important to have data for time histories or profiles in electronic form. We have proposed a common database for this purpose. It would include experimental data, EOS parameters for HE, and burn model parameters. Hopefully, such a database will be funded in the near future and would be accessible by other laboratories.

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