LA-UR-12-20591
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Title:	Systematic approach to verification and validation: High explosive burn models
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Intended for:	New Models and Hydrocodes conference, 2012-04-23/2012-04-27 (London, ---, United Kingdom)

Systematic approach to verification and validation: High explosive burn models

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Abstract. Most material models used in numerical simulations are based on heuristics and empirically calibrated to experimental data. For a specific model, key questions are determining its domain of applicability and assessing its relative merits compared to other models. Answering these questions should be a part of model verification and validation (V & V). Here, we focus on V & V of high explosive models. Typically, model developers implemented their model in their own hydro code and use different sets of experiments to calibrate model parameters. Rarely can one find in the literature simulation results for different models of the same experiment. Consequently, it is difficult to assess objectively the relative merits of different models. This situation results in part from the fact that experimental data is scattered through the literature (articles in journals and conference proceedings) and that the printed literature does not allow the reader to obtain data from a figure in electronic form needed to make detailed comparisons among experiments and simulations. In addition, it is very time consuming to set up and run simulations to compare different models over sufficiently many experiments to cover the range of phenomena of interest. The first difficulty could be overcome if the research community were to support an online web based database. The second difficulty can be greatly reduced by automating procedures to set up and run simulations of similar types of experiments. Moreover, automated testing would be greatly facilitated if the data files obtained from a database were in a standard format that contained key experimental parameters as meta-data in a header to the data file. To illustrate our approach to V & V, we have developed a high explosive database (HED) at LANL. It now contains a large number of shock initiation experiments. Utilizing the header information in a data file from HED, we have written scripts to generate an input file for a hydro code, run a simulation, and generate a comparison plot showing simulated and experimental velocity gauge data. These scripts are then applied to several series of experiments and to several HE burn models. The same systematic approach is applicable to other types of material models; for example, equations of state models and material strength models.

1 Introduction

We discuss a methodology for objectively assessing the strength and weaknesses of different material models. To illustrate our approach, we use high explosive (HE) burn models for a plastic-bonded explosive (PBX). A PBX is a heterogeneous solid composed of explosive grains, a polymeric binder and a small amount of porosity.

HE burn models are heuristic in nature, motivated by the concept of hot spots; see for example, [1] and references therein. They are defined by a homogenized burn rate representing a coarse-grain volume average of the chemical rate over a temperature field with short wavelength variations.

A burn rate is specified as a fitting form, typically a function of pressure and reaction progress variable(s). Model parameters are calibrated to experiments. The calibration is an empirical fit based on comparing simulated and experimental data. Since the dependence on the parameters is very non-linear, a good fit to one experiment may not do so well on another.

There is a wide range of detonation wave phenomena. To simplify the discussion, we focus on shock initiation. At a minimum, a good initiation model should reproduce data for distance of run-to-detonation as a function of initial shock pressure. When plotted as $\log x$ vs $\log P$, this is known as a Pop plot. Many HE burn models can be calibrated to fit Pop plot data.

More detailed behavior of shock initiation is provided by shock-to-detonation transition (SDT) experiments with embedded velocity gauges; see for example, [2]. These experiments provide a sequence of Lagrangian time histories of the particle velocity for multiple gauges at different starting positions within the HE. The time histories describe the buildup of the lead shock and the reaction behind the shock front.

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1.1 Model issues

An HE burn model really consists of four parts: (i) equation of state (EOS) for the reactants, (ii) EOS for the products, (iii) mixture rule for the EOS of partially burned HE, (iv) burn rate.

Rate parameters, to some extent, depend on the EOS and the mixture rule. Moreover, the calibration of rate parameters is based on simulations. Unless the reaction zone is 'sufficiently' resolved, the parameters may depend on the cell size used for the simulations.

The porosity of a PBX varies with the manufacturing process. This can affect the density by as much as one percent. Though the density variation is small, experiments have shown that a lower density increases initiation sensitivity. Initiation is also sensitive to initial temperature; less sensitive at low temperature and more sensitive at high temperature. Many HE burn models require different parameter sets for different initial densities or initial temperatures. In effect, these models treat the same PBX at different initial states as distinct explosives.

Burn models for shock initiation can also be used for propagating detonation waves. Some models, however, require different parameter sets for initiating and propagating detonation waves. Thus, it is important to determine for a particular model and a choice of parameters that go with it for a specific HE, what is its domain of applicability.

Shock initiation depends on the driving pressure pulse. SDT experiments using a gas gun with a layered projectile to initiate the HE can vary the shape of the pressure pulse at the HE interface by the choice of projectile materials with appropriate shock impedance and thickness. The achievable pressure pulses include those from a sustained shock (constant pressure pulse assumed for a Pop plot), a short shock (pressure pulse of duration less than the time-to-detonation), a double shock, and a shock followed by a rarefaction.

Experiments have shown that a double shock leads to the phenomenon of shock desensitization. Many models require *ad hoc* modifications — limiting the rate based on detecting the pressure of the lead shock — in order to account for shock desensitization.

The gap test is one of many HE sensitivity tests. It uses a detonation wave in a donor explosive to drive a shock through a gap (inert of variable thickness) to initiate an acceptor explosive. Since a Taylor wave follows the detonation wave in the donor HE, the pressure pulse driving the acceptor HE is of the form of a shock followed by a rarefaction. Increasing the thickness of the gap clips the pressure peak. The maximum gap width that can still detonate the acceptor is a measure of its sensitivity to initiation.

For an initiation model to be predictive over a wide range of applications, such as the gap test, it needs to be able to handle different drive conditions. Because rate models are empirical and do not have a firm physical foundation, many tests are needed to assess the capabilities and limitations of a model.

1.2 Model comparisons

Many HE models have been developed over the past 35 years and are described in the literature. These include the following: Forest Fire model [3, 4], Ignition & Growth model [5], History Variable Reactive Burn model [see 6], Johnson-Tang-Forest (JTF) model [7], Wescott-Stewart-Davis (WSD) model [8], CREST model [9], and SURF model [10]. There is a need to compare these models on a suite of test problems in order to determine their relative strengths and weaknesses.

There are several difficulties with using published results to compare models: (i) Model developers use different experiments to calibrate their models. (ii) Models are calibrated using different EOS models for the same HE and sometimes different mixture rules. (iii) The reported simulations are done with different codes and utilize different mesh resolutions. (iv) There is no standard set of experiments that all models use as test problems.

Moreover, results of simulations are not available in electronic form. Thus, in order to compare models by plotting simulated data for the same experiment on the same graph, a researcher has to implement the models in the same code and then perform the simulations on his/her code.

A model developer faces similar issues with calibrating and testing a model for a specific HE. The data is scattered in the literature. Due to page constraints, especially for conference proceedings, some experimental details, which later turn out to be important for modeling, are often overly concise or omitted. The most detailed data are in the form of velocity time histories, from either VISAR, PDV or embedded magnetic gauges. Typically, these are presented as figures in a published paper and are not readily available in electronic form. Beyond five or ten years, the experimentalist may have retired or the original data file misplaced, leaving the printed paper as the only record of the experiment.

2 Approach to V & V

A systematic testing approach is needed to address the modeling issues raised in the previous section. To cover the range of phenomenon of interest, simulations of many experiments are needed. Two elements would greatly facilitate model testing: a database of experimental data and procedures for automating simulations.

A web based database would enable data from experiments to be readily accessible in electronic form. Having all available data in one place would allow a researcher to find quickly the relevant information for an explosive of interest.

Many experiments used for model calibration and testing are designed to be simple to analyze and require only one-dimensional simulations. These take a small amount of CPU time on a PC. The time consuming part of model testing is setting up the simulations and the mechanics of picking out and comparing simulated and experimental data. Procedures to automate model simulations would avoid the tedium of setting up a simulation by hand and greatly reduce the time to carry out a simulation. Automation would be less error prone and could ensure that the simulation corresponds precisely to the intended experiment.

In addition, automation allows simulations to be easily repeated. This is important when a model is extended or the rate parameters are modified to better fit new experiments. Redoing simulations is necessary to check whether any changes have an adverse effect on experiments that were previously well fit.

3 High Explosive Database

Over the past $2\frac{1}{2}$ years we have undertaken to develop an online web based high explosive database (HED) at LANL. Currently it contains data for about 100 experiments. Many of these are SDT experiments performed on the two-stage gas gun at LANL with embedded velocity gauges of the type described by Gustavsen et al. [2]. We will use this data in the next section to illustrate our approach to model testing.

Much of the data in HED is stored as simple ASCII text files. In addition to the experimental data (such as velocity profiles), meta-data is included to make the data files self-contained. The meta-data identifies the experiment, describes the format of the data for multiple gauges, and specifies the units. It also contains key information needed to simulate the experiment (such as gauge positions). An html-like format is used in order to enable automated scripts easily to parse the data file and pick out blocks with the desired information.

3.1 Example of meta-data

Meta-data will vary with the type of experiment. To illustrate the kind of information that meta-data is meant to provide, we use a gas gun experiment as an example.

Conceptually, a gas gun experiment consists of three parts: projectile, target and diagnostics. A simulation is specified by the following information:

1. Projectile materials and their thicknesses, and the measured projectile velocity. These parameters determine the pressure pulse driving the target.
2. Target materials and their thicknesses. For an HE, density and temperature are key parameters.
3. The type of diagnostic (such as magnetic velocity gauge, VISAR or PDV probe) and the positions of all gauges or probes are needed to be able to interpret the experimental data.

For multiple gauges the data format needs to be specified. For example, each data line may consist of tab separated fields for the time and velocities of each gauge. Finally, the units for the measured quantities (such as time or velocity) needs to be specified.

4 Automated model testing

To illustrate how model testing can be automated we have written a script for SDT gas gun experiments with embedded velocity gauges. The purpose of the script is three fold: (i) To generate an input file for a reactive-hydro code corresponding to a specified experiment. (ii) To run the simulation. (iii) To compare simulated and experimental gauge data.

The script utilizes three inputs: (i) The name of a data file with both meta-data and experimental data. (ii) The name of a parameter file with information needed for the selected hydro code. (iii) A library of EOS and HE model parameters. The script starts by parsing the data file to determine from the meta-data the key experimental parameters needed to setup the mesh (geometry + materials) for the code input file. The gauge positions from the meta-data are used to setup the needed output to generate the simulated data, such as Lagrangian tracer particle output for each gauge.

The parameter file contains the desired cell size and other code specific inputs. It also contains maps for meta-data material names onto EOS models and the HE name onto a specific HE burn model. The model parameters are then fetched from the EOS/HE library and included in the code input file.

Next the code is run with the generated input file. After the simulation is completed, the script picks out the experimental data from the data file and the simulated data from the code output files. This is used to generate a comparison plot.

Having both the experimental data and meta-data in one file enforces consistency; *i.e.*, the simulation corresponds to the experiment. By changing the input to the script, names of the data and parameter files, any SDT experiment can be run with any HE model contained in the EOS/HE library. The part of the script that generates the input file is code specific. It can be thought of as analogous to a device driver for a printer, and can easily be modified for any code.

The next level of automation is to have another script that loops over the single experiment script for a series of experiments. Series are used for testing shock initiation models with different initial shock pressures. For gas gun experiments this is achieved by varying the projectile velocity.

As previously noted, a gas gun experiment can be simulated in 1-dimension. Since the simulation is so small, nothing is to be gained from running it on parallel processors. However, on a multiprocessor workstation or cluster, each simulation in a series can be run on a separate processor. This is a form of 'parallel' processing that is often overlooked.

5 Examples of automated testing

The script to run a SDT simulation has been written to use the Rage code [11]. This is an Eulerian hydro code with adaptive mesh refinement. As test cases we used several initiation experiments with PBX 9502 at room temperature.

Automated simulations were run with two burn models using PBX 9502 model parameters taken from the literature: the Forest Fire (FF) model using HOM EOS, Mader [3, table 4.5, pp. 233–237] and the Ignition & Growth (IG) model using JWL EOS, Tarver and McGuire [12, table 1, p. 644]. All simulations used a 0.5 mm cell size with two levels of refinement by a factor of 2; *i.e.*, finest cell size of 0.125 mm.

5.1 Model Pop plot

First we check the Pop plot. Numerically calculating the Pop plot for an HE model involves a series of simulations for 1-D gas gun experiments with different projectile velocities to vary the initial shock pressure. This can be done with a script analogous to the one described in the previous section to automate running an SDT experiment.

For each simulation the initial shock pressure and distance of run at which the transition to detonation occurs is picked off the output files. The criterion for the transition is based on the pressure time histories of tracer particles 0.5 mm apart; first particle with peak pressure within 5 or 10 cycles of the arrival of the lead shock using the initial shock pressure (which is much lower than the detonation pressure) as the threshold for detecting the shock rise. The result is shown in fig. 1.

With the original IG parameters, the run distance is much too small. Parameters for the 'growth term' in the rate [see 12, Eq. 2], $G_1(P/[\mathrm{Mb}])^y\,\mu\mathrm{s}^{-1}$, have been adjusted to get the model Pop plot to agree better with the experimental data; G_1 from 1100 to 7700 and y from 2 to 3.75 .

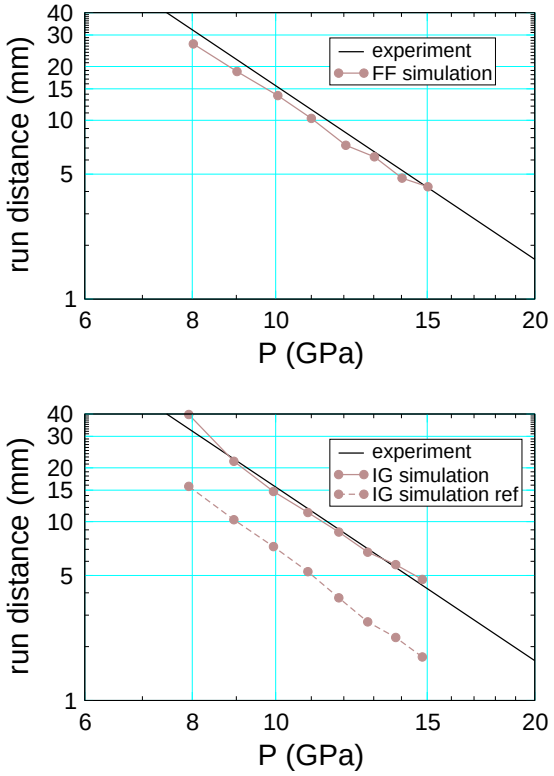

Fig. 1. Pop plot for PBX 9502. Black and brown lines are fit to experimental data and simulated data, respectively. Top and bottom plots are with FF model and IG model, respectively. For IG model, dashed and solid lines are the original and adjusted parameters, respectively.

There is insufficient information about the calibration in [12] to determine why an adjustment is needed. Possibly it is due to mesh resolution or the mix rule for partially burned HE. (The Rage code uses P-T equilibrium for the mix rule.) The need to adjust published parameters to fit the Pop plot has occured before [see 13, fig. 7 and § Simple Shock].

5.2 SDT experiments

The automation scripts were applied to two series. The first for experiments with a sustained shock driving the shock-to-detonation transition. The second for a short shock or pressure pulse of limited duration.

5.2.1 Sustained shock

The first series simulated shots # 2s40, 2s42, 2s58. Comparison plots of all gauges are shown in fig. 2. An expanded view of the gauges near the transition to detonation are shown in fig. 3 for shot # 2s40.

Several points are worth noting. The glitch in the first simulated gauge at $t = 0$ is due to a startup error

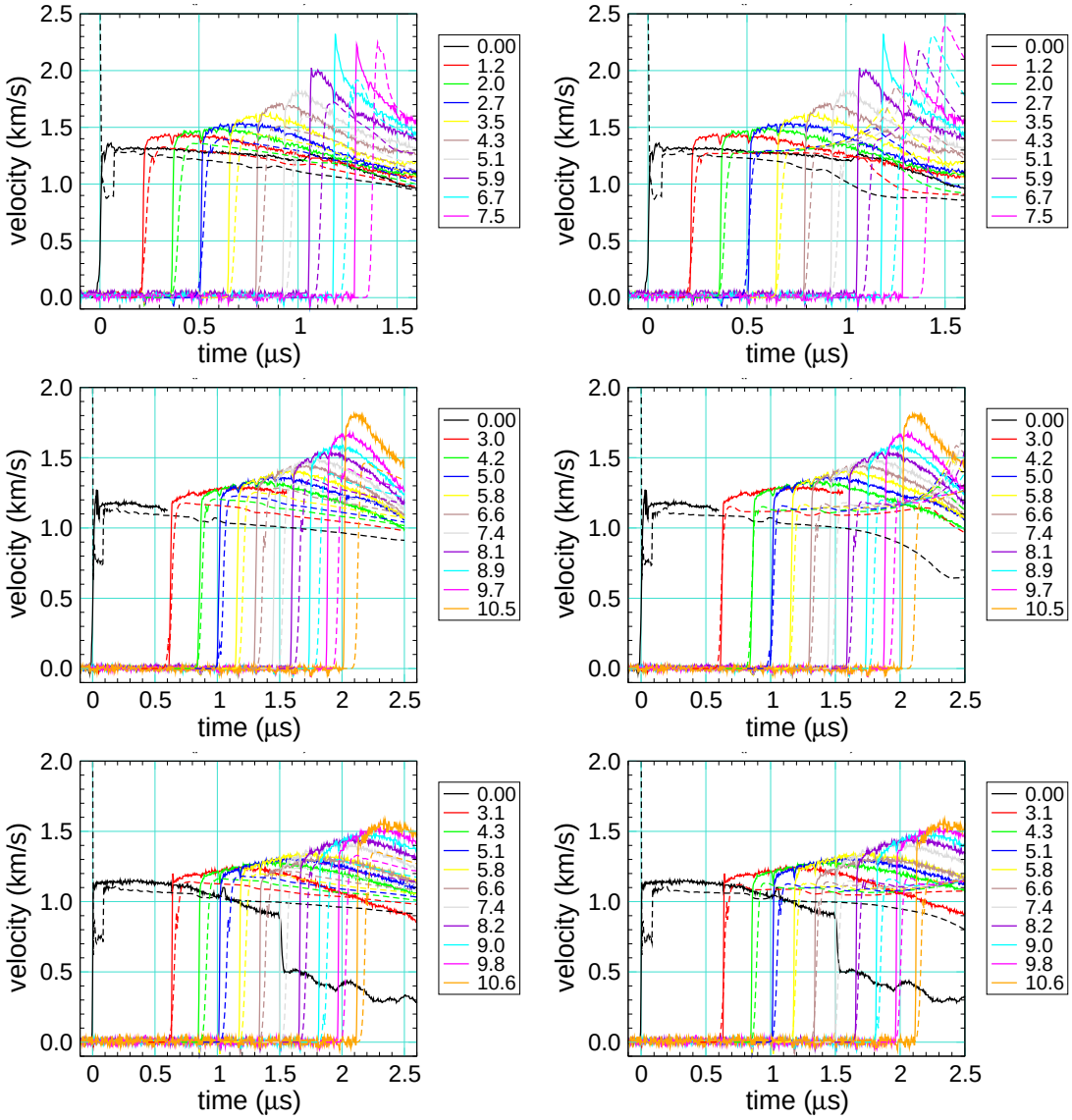

Fig. 2. SDT for sustained shock in PBX 9502. Solid and dashed lines are experimental and simulated embedded velocity gauge data, respectively. Top to bottom plots are for shots 2s40, 2s42, 2s58, respectively. Left to right plots are with FF model and IG model, respectively. Legend gives gauge positions in mm.

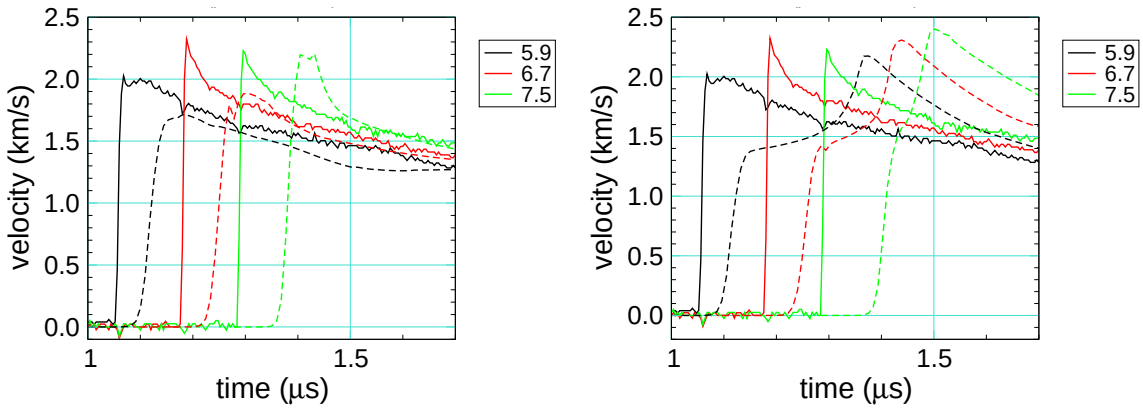

Fig. 3. Velocity gauges for shot 2s40 around transition to detonation. Left and right plots are with FF model and IG model, respectively.

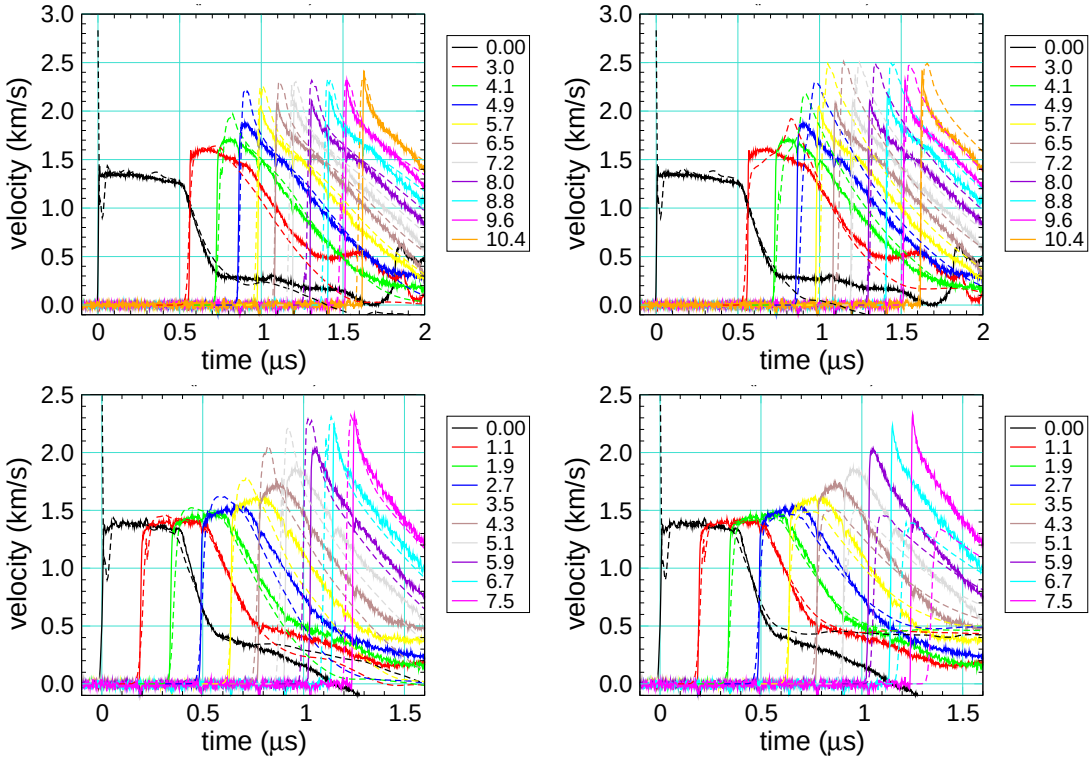

Fig. 4. SDT for short shock in PBX 9502. Solid and dashed lines are experimental and simulated embedded velocity gauge data, respectively. Top and bottom plots are for shots 2s97, 2s100, respectively. Left to right plots are with FF model and IG model, respectively. Legend gives gauge positions in mm.

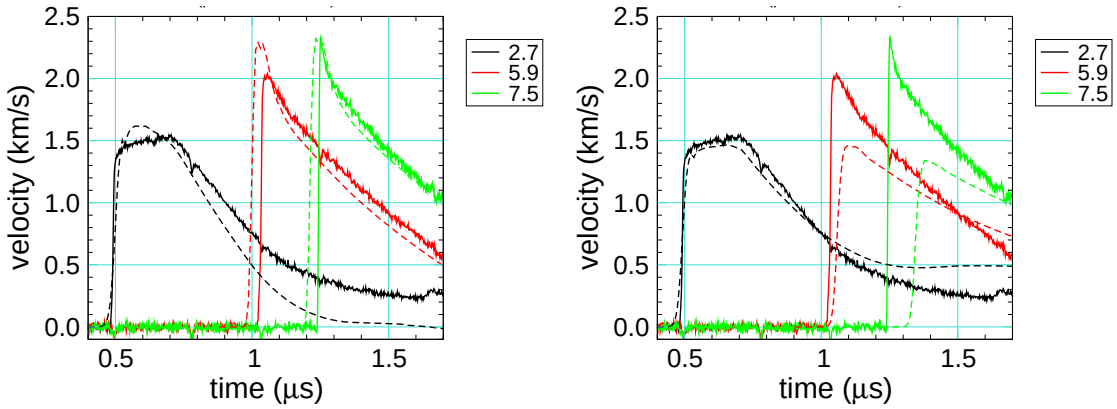

Fig. 5. Velocity gauges for shot 2s100 around transition. Left and right plots are with FF model and IG model, respectively.

from the velocity discontinuity when the projectile impacts the target HE. Its spatial and temporal extent is proportional to the cell size.

The expanded view of the embedded gauges shows that the transition is slightly earlier with the FF model parameters than with the IG model parameters. This is consistent with the model Pop plots. The transit time for the models differ from the experiment by a couple of tenths of μs. Since the detonation speed is 7.7 mm/μs, this correspond to a difference in run distance of only 1 or 2 mm. Thus the gauge data is a more sensitive measure of a shock-to-detonation transition than the Pop plot data.

On the first gauge the initial velocity jump is slightly lower than that of the experiment. The reactants EOS affects the initial shock pressure from the impedance match of the projectile impacting the target. The transition distance is sensitive to the initial pressure. This may explain some of the differences.

The rate parameters could be adjusted to give a better fit for this series. We have not done that as the point of V & V is to check how well a HE model does with a given set of parameters.

5.2.2 Short shock

The second series simulated shots # 2s97, 2s100. Comparison plots of all gauges are shown in fig. 4. An expanded view of select gauges are shown in fig. 5 for shot # 2s100.

Several points are worth noting. For a sufficiently short pulse, the transition to a detonation will fail. The threshold or minimum pulse width for a transition to occur is sensitive to the burn rate. On the wrong side of the threshold, simulated data will differ substantially from experimental data.

This is seen in the simulations with the IG model. The transition occurs for shot 2s97 with a pulse width of 0.5 μs, but not for shot 2s100 with a pulse width of 0.4 μs. The experiment and the simulations with the FF model show that a transition occurs for both shots. Again the difference in the simulations is consistent with the model Pop plots; FF model being more sensitive (shorter run distance for a given pressure) than the IG model.

6 Recommendations

Based on the approach presented for testing HE initiation models, we think progress in developing improved HE models that are predictive over a wide range of applications would be greatly facilitated by the following:

1. *A database supported by the research community.*
The database should make experimental HE data in electronic form accessible to all model developers. It should aim to be as complete as possible and updated when new experimental data becomes available.

2. *Encourage model comparisons.*
There is a need to objectively assess the strength and weakness of all models by comparing simulated and experimental data over a wide range of HE phenomena.

3. *Consensus for a standard suite of test problems.*
Using the same test problems for all models would enable a fair assessment of the relative merits of different models. It would also allow the research community to minimize the duplication of effort and work together to a greater extent than is currently done.

The same general approach can be adapted to other types of material models, such as equations of state and material strength.

Acknowledgments

This work was carried out under the auspices of the U. S. Dept. of Energy at LANL under contract DE-AC52-06NA25396.

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