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Evaluation of XHVRB for Capturing Shock Desensitization

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Abstract. Explosive shock desensitization phenomena have been recognized for some time. It has been demonstrated that pressure-based reactive flow models do not adequately capture the basic nature of the explosive behavior. Historically, replacing the local pressure with a shock captured pressure has dramatically improved the numerical modeling approaches. A pseudo-entropy based formulation using the History Variable Reactive Burn model, as proposed by Starkenberg, was implemented into the Eulerian shock physics code CTH. Improvements in the shock capturing algorithm in the model were made that allow reproduction of single shock behavior consistent with published Pop-plot data. It is also demonstrated to capture a desensitization effect based on available literature data, and to qualitatively capture multi-dimensional desensitization behavior. This model shows promise for use in modeling and simulation problems that are relevant to the desensitization phenomena. Issues are identified with the current implementation and future work is proposed for improving and expanding model capabilities.

INTRODUCTION

Desensitization is a characteristic of explosive behavior that has been recognized for some time [1]. Recently reactive flow models have been developed with this characteristic of explosive behavior in mind [1-3]. XHVRB is a new reactive flow model, based on the History Variable Reactive Burn (HVRB) model, developed by Starkenberg [4]. The purpose of XHVRB is to capture desensitization behavior of explosive materials due to pre-shock.

HVRB [5] is a pressure-based reactive flow model in the shock physics code CTH [6] developed at Sandia National Laboratories. The model integrates the current pressure to calculate the history variable, as given in Equation (1). The history variable is used to determine the extent of reaction. Compared to other reactive flow models [1-3] HVRB has relatively few parameters and is easy to fit to Pop-plot data. The history variable is defined in Equation 1 as

$$\phi = \frac{1}{\tau}\int_0^t \left(\frac{P-P_i}{P_r}\right)^{Z_r} dt \tag{1}$$

where Pr and Zr are related to the Pop-plot and Pi is a threshold pressure below which no reaction will occur. XHVRB introduces a concept called pseudo-entropy, which is defined in equations 2a – 2c. The cumulative pseudo-entropy is the previous value of pseudo-entropy plus the change for a given shock input. The change in pseudo-entropy is defined in Equation 2c as a ratio of shock pressures taken to the power, n_d, which is the desensitization exponent. This parameter can be used to fit the model to quantitative desensitization data. The equation to be integrated to give the new history variable for XHVRB is given in Equation 2a. For a single shock, the pseudo-entropy is equal to the magnitude of the shock pressure, and the HVRB model results are approximately reproduced.

$$h(q_s) = \left(\frac{q_s}{c_{vo}} - \frac{p_i}{p_r}\right)^{n_s} \text{ (a)} \qquad \frac{q_s}{c_{vo}} = \frac{q_{su}}{c_{vo}} + \frac{\Delta q_s}{c_{vo}} \text{ (b)} \qquad \frac{\Delta q_s}{c_{vo}} = \frac{\Delta P_s / P_r}{\left(P_{su}/P_0\right)^{n_d}} \text{ (c)} \tag{2}$$

MODEL IMPLEMENTATION

One distinguishing feature of XHVRB from HVRB is the capturing of the shock pressure. Whereas HVRB uses the current pressure at every time step to calculate the history variable, XHVRB uses the captured shock pressure. To capture the shock pressure, the shock must be detected. The current implementation of the model uses the magnitude of the artificial viscosity to detect the shock. The artificial viscosity is responsible for the formation of the shock wave which makes it an ideal choice for shock detection. Figure 1 shows a 1D calculation of a double shock scenario at a given time. The left image in this figure shows the artificial viscosity in red, demonstrating its localization at the shock front. The solid black line in this figure is the current pressure.

One the right in Fig. 1 the shock counter (dashed blue) and incrementer (solid black) are plotted for the same time step in the double shock scenario calculation. The incrementer ensures that the shock pressure is accurately captured given the numerical smearing that is necessary to resolve shocks. The counter shows the arrival of the first shock and has a value of 1, and then registers the arrival of the 2nd shock and the count is increased to 2. The logic for XHVRB calculates the new value of pseudo-entropy, shown on the left in dashed-purple, and for the second shock this value is less than the magnitude of the second shock pressure. The history variable is calculated based on this value, effectively desensitizing the material's response to the second shock pressure.

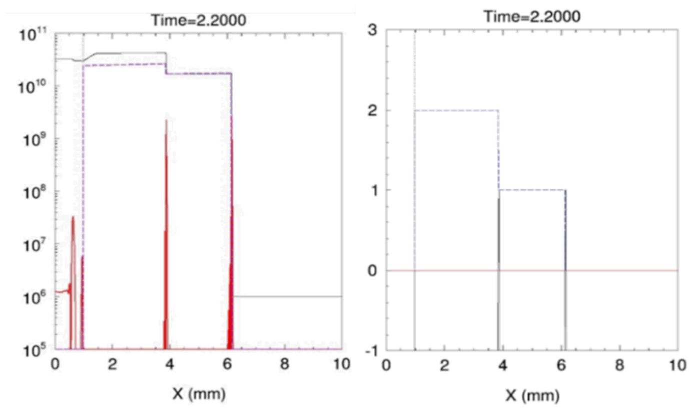

Figure 1: 1D double shock simulation showing (left) pressure in solid black, shock tracker in red, and pseudo-entropy in dashed purple and (right) shock counter in dashed blue.

SINGLE SHOCK RESPONSE

The first requirement of any reactive flow model is that it reproduce an explosive's Pop-plot behavior in shock-to-detonation scenarios. HVRB uses the parameters Pr and Zr in Equation 1 to calibrate an explosive's response to match the detonation distance for a given pressure. The Pop-plot for EDC-37, an HMX based explosive, is given in Fig. 2. Experimental data is shown as squares [7], the fit to the HVRB model is shown in solid green, and the XHVRB fit is shown in dashed purple.

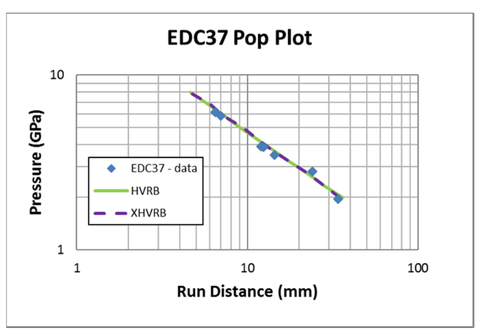

Figure 2: Pop-plot data for EDC-37 (blue diamonds) shown with the Pop-plot fit for HVRB (solid green) and XHVRB (dashed purple).

Figure 3 shows test data taken from Salisbury et al. [7] in which embedded gauges were used to measure particle velocity as a function of time for a single shock experiment with EDC-37 explosive (solid black). The test data are compared with the result from a 1D CTH calculation using HVRB (left) and XHVRB (right). The same Mie-Gruneisen equation of state (EOS) was used for both simulations, and a reacted products EOS for PBX9501, a similar HMX based explosive, was also used in both simulations. While both models demonstrate the same location of shock-to-detonation transition (which is not apparent in the data as transition happened after the last gauge), the characteristics of that transition are different between the two models. HVRB shows a sharper transition with little reaction or build up at the earlier gauges, whereas XHVRB shows a slower building of the pressure as reaction increases towards transition.

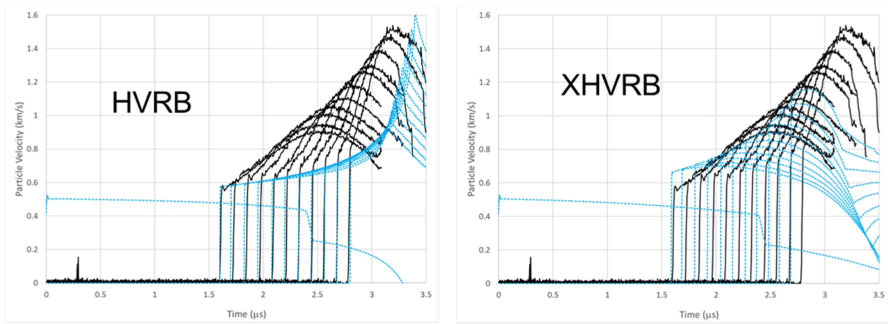

Figure 3: Single shock data from embedded gauges in EDC-37 explosive shown in solid black with comparison to simulation results in dashed blue for HVRB (left) and XHVRB (right).

DOUBLE SHOCK DATA COMPARISON

A double-flyer can be used to produce two shocks sequentially in the same material such that the effect of a pre-shock can be studied. In the same paper referenced above for the single shock data, Salisbury et al [7] performed this kind of experiment using a relatively low impedance material at the front of the flyer to produce a low level shock, backed by a higher impedance material to produce a stronger shock. These two shocks enter the material, and in the absence of significant reaction they can be seen clearly by the embedded gauges in the EDC-37 sample. If no reaction occurs, the second shock, travelling faster than the first, will catch up to the first shock and the shocks will coalesce and then behave as a single shock going into pristine or un-shocked material. Two such experiments were performed, and the results of the first of these experiments is shown in the left image in Fig. 4 (solid black) along with the results the simulation done in CTH with XHVRB (dashed blue). The model shows the distinct arrival of both shocks, and it approximately captures build-up to transition well. Changing the value of the desensitization exponent can produce faster build up in the model. This comparison demonstrates that the model can be used to represent the change in behavior of the explosive in response to shock re-shock scenarios.

Figure 4 (right) shows the results from another experiment from that same study [7] (solid black) compared to the results from the simulation (dashed blue) using the same set of parameters from the simulation shown in Fig. 4 (left). The model under-predicts the magnitude of the second shock or the amount of reaction contributing that that shock value, but shows a build-up to reaction similar to that shown in the data. These experiments yielded two results for transition distance, varying from 8.4 to 9.4 mm, and the model showed transition at 9 mm.

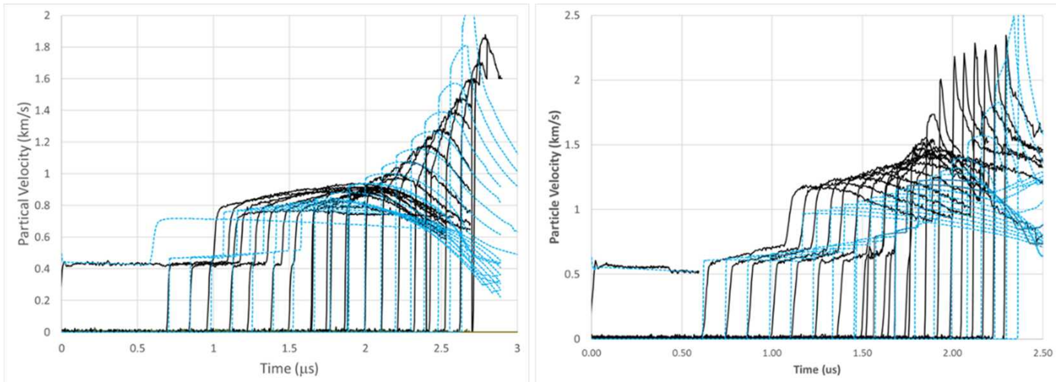

Figure 4: Double shock data for EDC37 for shots 1175 and 1176 (left) and shot 1194 and 1195 (right) [7] shown in solid black and compared with simulation results for XHVRB with Nd=1.0 and Ns=0.75.

MULTI-DIMENSIONAL SCENARIO

All simulation results and experimental data shown to this point have been 1D, but a complete reactive flow model should be useable in multidimensional simulations as well. Figure 5 shows a scenario in which a metal penetrator is moving towards a sandwich configuration consisting of two metal plates surrounding explosive material. The initial shock from the penetrator is not enough to cause the material to transition to detonation in the distance available. The HVRB result, shown on the top in Fig. 5, shows that the material responds to the increased pressure upon reflection at the interface with the back plate by rapidly transitioning to detonation. In reality, this material has likely been desensitized by the initial shock. The XHVRB model shows no transition upon reflection, demonstrating a qualitative ability to capture desensitization in multi-dimensional scenarios.

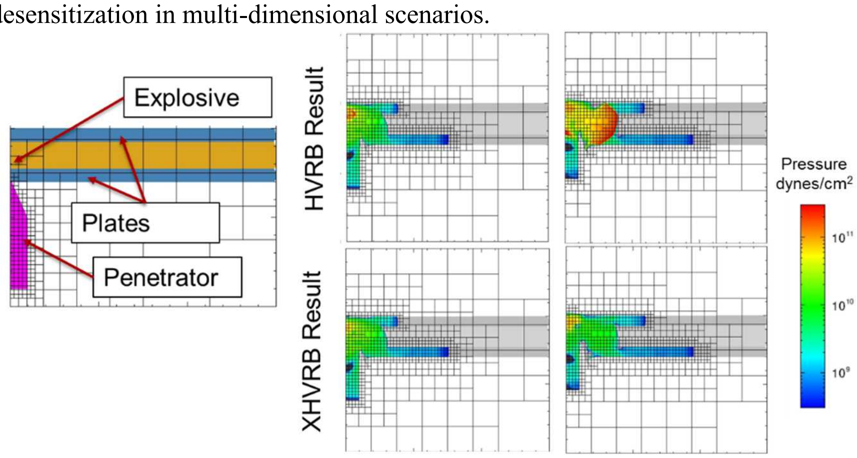

Figure 5: Multi-dimensional simulation result for a penetrator going into a sandwiched explosive, demonstrating XHVRB's capability to qualitatively represent desensitization due to a reflected shock wave.

THEORETICAL DISCUSSION

Desensitization has been observed for some time, but quantitative data that would allow for a deeper understanding of explosive sensitivity is difficult to obtain. Quantitative data is not available for many explosives. The simplest theory to describe the nature of desensitization which appears in the literature supposes that a desensitizing shock renders the material upon which it acts completely inert [7]. The explosive that has been pre-shocked cannot be detonated, and it is not until the two shocks coalesce and then act on pristine material that a transition to detonation can occur. For a given set of flyers of fixed thickness, the Pop-plots can be inferred for varying levels of pre-shock. The point of coalescence of the two shocks can be determined for a given flyer speed, and the transition to detonation from this point taken from the Pop-plot for the pristine material. This results in a new run distance to detonation, as demonstrated in Fig. 7. For a higher pre-shock magnitude, the new Pop-plot is further offset from the original due to the longer coalescence distance. Whether or not this behavior is a reasonable description of reality is difficult to say with the data available today. The data shown above from Salisbury, et al. suggests that some reaction is occurring before shock coalescence, but the measured run distance is within a millimeter of the result from the "rendered inert" theory described above. Systematic quantitative data is needed to populate the space in which desensitization to pre-shock occurs, and this data may lead to a better understanding of the nature of explosive desensitization.

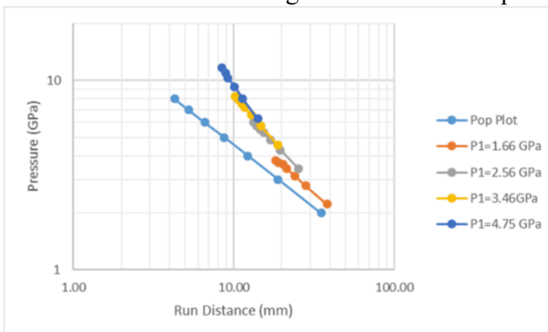

Figure 4: Pop-plot for EDC-37 with theoretical Pop-plots give for varying levels of pre-shock. Plotted values are secondary shock magnitude and total run to detonation distance.

CONCLUSIONS

XHVRB has been shown to reproduce the single shock Pop-plot, with improvement over HVRB in the representation of build-up to detonation compared to embedded gauge data. It is capable of representing desensitization behavior in double shock scenarios. The model may require more flexibility in order to fit a range of explosive behaviors. XHVRB has also been shown to qualitatively capture desensitization in multi-dimensional scenarios. Systematic quantitative data may reveal the nature of explosive desensitization, which would guide the evolution of this model to more accurately capture this phenomenon.

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