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A CREST Model for the RDX/TNT Explosive Composition B

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Abstract. The high explosive Composition B (Comp B), which comprises approximately 60% RDX and 40% TNT by weight, is still widely used for a range of applications, and reactive burn models able to simulate its shock initiation and detonation response are required for modelling assessments. CREST is unique among such models in using an entropy-dependent reaction rate to convert the solid unreacted explosive to gaseous detonation products. This paper describes the calibration of a CREST reactive burn model for Comp B. The equations of state are fitted to available shock Hugoniot, sound speed and overdriven detonation wave data, and are demonstrated to be suitably robust and compatible. The reaction rate has been tuned to fit recent sustained-shock-gas-gun data and, owing to a lack of modern data, a detonation size-effect curve dating from the 1950's on a slightly different Comp B variant. This made it necessary to accept a compromise fit to the calibration data, and which is explored further in the paper. The model is then tested against other Comp B data from the literature to assess its ability to predict a wide range of behaviour. CREST now adds to those reactive burn models available for simulating this well-studied explosive.

INTRODUCTION

Composition B (Comp B) is a widely-used military ordanance whose composition consists of approximately 60% RDX and 40% TNT by weight, usually with a small amount of wax desensitiser. Owing to its widespread use around the world, there are many different variants of Comp B having slightly different proportions of RDX, TNT, and wax, different manufacturing routes, a range of initial densities, and some have a known amount of HMX contamination in the RDX. Several Comp B formulations are listed below to illustrate some of the differences.

1. UK Comp B [1]
    - Nominal composition 59.5% (by weight) RDX, 39.5% TNT, 1% Wax
    - Hot isostatically pressed, initial density ~1.702 g/cm^3
    - ~3% HMX contamination in the RDX [2]
2. LANL Comp B [3, 4]
    - Nominally 59.5% (by weight) RDX, 39.5% TNT, 1% Wax
    - Melt cast (vacuum or open), initial density ~1.713 g/cm^3
    - ~6% HMX contamination in the RDX
3. Comp B Grade A [5]
    - 63% (by weight) RDX, 36% TNT, 1% Wax
    - "Enriched" melt castings, initial density ~1.715 g/cm^3
4. Comp B-3 [6, 7]
    - Nominally 60% (by weight) RDX, 40% TNT, with no wax
    - Melt cast or hot pressed, initial density ~1.68-1.73 g/cm^3
    - ~6.5% HMX contamination in the RDX in LANL Comp B-3 [7]

The variability of the explosive formulation can result in a significant spread in the experimental data for Comp B. For example, Burns et al. [1] performed gas-gun tests on UK Comp B and, when comparing Pop-plot data (run distance to detonation vs input pressure), found that this variant was significantly more shock sensitive than LANL Comp B and Comp B Grade A material. Similarly, in explosively-driven wedge tests, Jacobs et al. [6] observed that Comp B-3, which contains no wax, was more shock sensitive than Comp B with ~1% wax.

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From the modelling perspective, the variability of the material and its response presents significant difficulties when attempting to define a model for a "typical" Comp B, or a global model for Comp B. The hydrocode-based CREST reactive burn model has previously been shown to accurately predict a wide range of shock initiation and detonation behaviour in HMX- and TATB-based explosives [8]. CREST requires reaction information from embedded gauge gas-gun shots to help calibrate the model, and such data on Comp B has recently become available [1, 3, 4] which has enabled an initial model for this RDX/TNT based explosive to be developed.

MODEL CALIBRATION

The CREST model comprises equations of state (EoS) for the solid unreacted explosive and the gaseous detonation products, and a reaction rate dependent on shock strength using a function of entropy of the non-reacted explosive. To allow for porosity in the model, the component EoS are constructed at theoretical maximum density (TMD) and the Snowplough model is used. The model coefficients for the solid and gaseous EoS and the reaction rate are fitted to available experimental data, and the extrapolation of porous EoS data to TMD is performed as part of the calibration process. The calibration of the CREST model for Comp B is described in the sub-sections below.

Non-reacted EoS

The EoS for the non-reacted explosive is assumed to be of Mie-Gruneisen form with the principal isentrope, written in finite strain form, as its reference curve [9]. A large amount of experimental Hugoniot [1, 3, 4, 5, 10, 11, 12, 13, 14] and bulk sound speed [13, 14, 15, 16] data on Comp B is available to aid calibration of the non-reacted EoS. This collection of data, in shock velocity (U_s)-particle velocity (u_p) space, is shown in Fig. 1(a). Despite the data covering a number of Comp B variants, there is reasonable consistency between the different measured datasets. The one dataset that is somewhat different is on Grade A material (green diamonds), and was ignored in the fitting procedure.

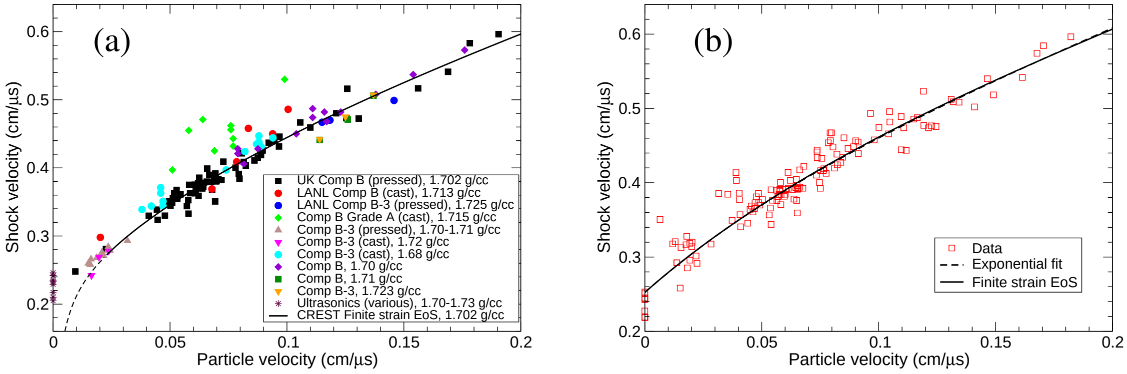

FIGURE 1. Finite strain EoS fit to shock Hugoniot and bulk sound speed data for Comp B.

The extrapolation of porous Hugoniot data to TMD, under the assumption of using the Snowplough model, has been described previously [17]. For CREST, the corrected data is firstly fit using an exponential $U_s - u_p$ relation, which is then converted to a finite strain relation for the principal isentrope [9]. In both these steps, the relevant parameters are determined via constrained least squares processes. Figure 1(b) shows the final EoS fit to both the exponential $U_s - u_p$ relation and Hugoniot data corrected to TMD. Using the TMD EoS in conjunction with the Snowplough model at a typical porous density for Comp B gives the black line shown in Fig. 1(a). Overall, this fits the original (porous) Hugoniot data reasonably well over the range of interest. The EoS is shown as a dashed line below u_p ~0.02 cm/μs, which corresponds to a reaction threshold of 1 GPa in the reaction model based on experimental evidence [14].

Detonation products EoS

The detonation products are modelled using a modified JWL EoS in which additional terms are added at high densities in order to match overdriven detonation data. Similar to the non-reacted EoS, porous JWL parameters *e.g.* fit to cylinder test data, need to be extrapolated to a set of parameters at TMD for use with CREST. Due to a lack of modern published cylinder test data on Comp B, a JWL EoS on UK Comp B from the 1960's fit to cylinder and sphere test data was chosen as the starting point for formulating the detonation products EoS at TMD. The extrapolation procedure to the fully dense state involves ensuring that the TMD EoS, when used at porous density, matches the detonation velocity and power of the original EoS from which the TMD EoS was deduced.

In addition to the expansion isentrope, the detonation products EoS must also be able to reproduce overdriven detonation data, and such data, where available, is included as part of the calibration procedure. Overdriven detonation states in Comp B have been measured by Skidmore & Hart [18], and Kineke & West [19]. Figure 2(a) shows the final fit of the detonation products EoS to the Comp B overdriven detonation data at TMD, where the calculated $U_s - u_p$ relation gives a good match to the corrected data.

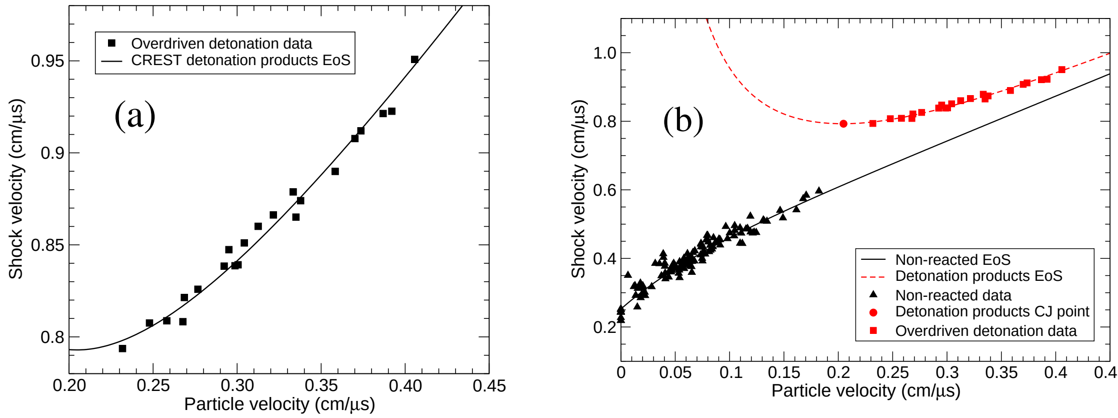

FIGURE 2. Comparison of (a) detonation product Hugoniot for Comp B with overdriven detonation data corrected to TMD, and (b) non-reacted and detonation products Hugoniots for Comp B at TMD.

Compatibility of the Non-Reacted and Detonation Products EoS

The non-reacted and detonation products EoS are not independent. In addition to robustness tests of the individual EoS [20], it needs to be demonstrated that the two EoS are well suited so that their combined use (when calculating the EoS of the reacting mixture) does not cause hydrocode calculations to break down or produce non-physical results. Part of the compatibility criterion, as suggested by Lambourn [21], is to ensure that the non-reacted and detonation product Hugoniots do not cross at high pressures, since this can cause robustness issues when simulating overdriven detonation states in excess of any crossing point.

Figure 2(b) shows that the detonation product Hugoniot for Comp B lies above the corresponding Hugoniot for the non-reacted explosive. This is also the case out to much higher values of particle velocity than shown in the figure, with the two curves running roughly parallel for $u_p > 0.45$ cm/μs. Therefore, the developed EoS for Comp B should be sufficiently robust in the hydrocode modelling of Comp B problems of interest.

Reaction rate

CREST uses empirical reaction rates that depend on a function of entropy of the non-reacted explosive, and the form of the rate equations used was as described in [22]. As per other CREST models [20], the reaction rate for Comp B was tuned to experimental data for sustained shock initiation and the detonation size-effect curve only, using 1D and 2D hydrocode simulations of a suite of embedded-gauge gas-gun shots and rate-sticks, respectively. The calibration data in the shock initiation regime was from Burns et al. [1] on UK Comp B. Unfortunately, there is no rate-stick data on this Comp B variant, so it was decided to use the size-effect curve from Campbell & Engelke's definitive paper [23], which is for Grade A material, to calibrate the Comp B reaction rate at high entropies.

Automatic calibration of the reaction rate was undertaken using the Particle Swarm Optimisation (PSO) method [24]. The utilisation of PSO for CREST has been described previously [22], and the same procedure was applied to Comp B to determine the reaction rate coefficients that give the best fit to the calibration data. Unfortunately, achieving a good fit to both the shock initiation and detonation size-effect data simultaneously proved impossible, for reasons that will be discussed below. This made it necessary to accept a compromise fit to the calibration data. Figures 3 and 4(a) show the final fits to the gas-gun and rate-stick data respectively. Only two of the gas-gun comparisons are shown in Figure 3 but the level of agreement obtained with experiment is similar over all 7 sustained-shock shots performed [1], where the jagged lines are the measured data and the smooth lines show the simulated results.

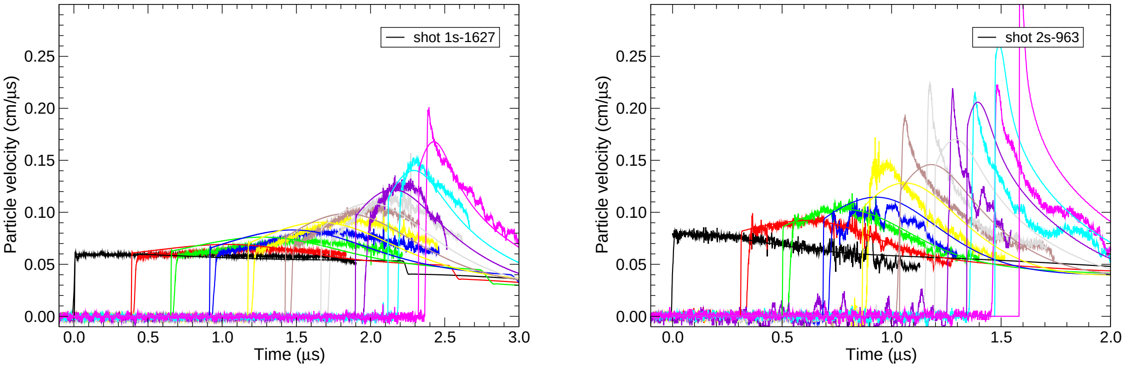

FIGURE 3. Fit of CREST model for Comp B to gas-gun shots 1s-1627 (left) and 2s-963 (right) of Burns et al. [1].

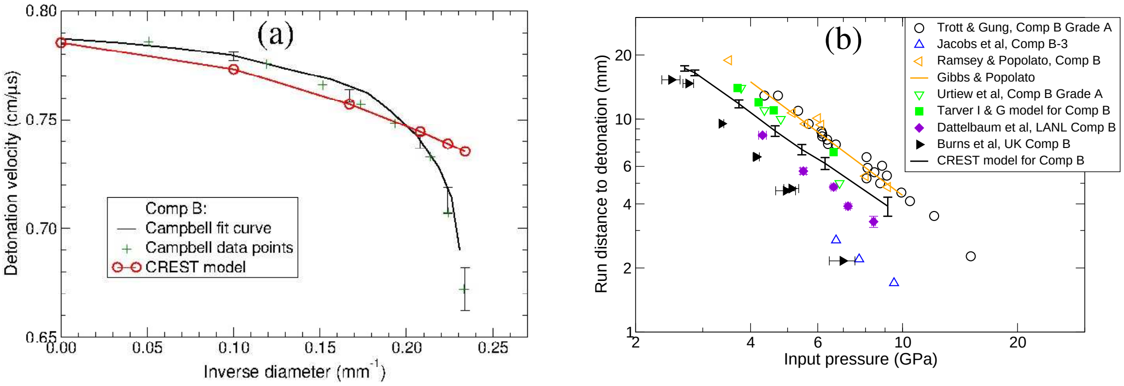

FIGURE 4. (a) Fit of CREST model for Comp B to detonation size-effect curve (Grade A material), and (b) comparison of CREST model with Pop plot data from experiments and models for various types of Comp B.

Qualitatively, the fit to the calibration data is fair. For the shock initiation regime, the fit to the early gauges is reasonable, but then the subsequent shock front and reaction growth is too slow in the model. This results in run to detonation distances that are longer than in Burns' experiments, as shown by the Pop plot in Fig. 4(b). Whilst it is far from ideal that the model does not fit the Pop plot data from the gas-gun shots to which it was calibrated, at least the predicted run distances are well within the spread of the data on Comp B.

The simulated detonation size-effect curve has a similar gradient to the experimental data, but is less curved. This was found to be typical of reaction rates that give a reasonable fit to the gas-gun data. Reaction rates that give a better fit to the size-effect curve give poorer fits to the gas-gun data, and vice versa. Thus, there appears to be an incompatibility between the shock initiation behaviour on UK Comp B and the detonation size-effect curve on Comp B Grade A, in that it was not possible to find a CREST reaction rate that fitted both data sets simultaneously.

The original source for the rate-stick data was Malin et al. [25] who investigated several different types of Comp B. They observed differences in the size-effect curves, depending on the RDX particle size distribution and the cooling rate during casting (which affects the TNT crystal size). This suggests that UK Comp B, by virtue of its manufacture by hot isostatic pressing rather than casting and our lack of knowledge of its particle size distribution, may have a different size-effect curve than that quoted by Campbell & Engelke for Comp B Grade A material.

VALIDATION AND APPLICATIONS

The developed CREST model was subsequently tested against a variety of published data on Comp B. Two examples, testing the models' 2D initiation capabilities, are given below where the inert materials were modelled using parameters from Steinberg's Compendium [26]. The mesh resolution used in the hydrocode simulations was 50 zones/mm.

Gustavsen et al. [7] fired flat-nosed 6.35mm or 12.7mm-diameter stainless steel rods at bare Comp B-3 charges of various thicknesses. These were diagnosed using PDV probes to record the velocity of the explosives' rear-surface through a PMMA window at several different positions from the axis of symmetry. The input pressure into the explosive in each shot was ~7 GPa. Figure 5(a) shows the comparison between the measured velocities and simulated results for a 12.7mm-diameter rod impacting a 3mm-thick Comp B-3 target. It is observed that reaction in the model (dashed lines) is too slow; these results were expected based on the Pop plot comparison in Fig. 4(b) which shows that the run distance to detonation in Comp B-3 at 7 GPa is shorter than that predicted by the CREST model.

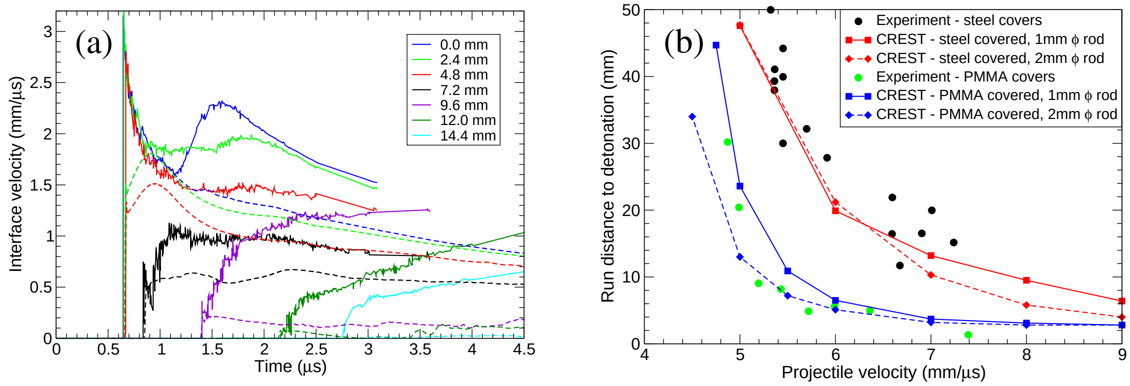

FIGURE 5. Comparison of CREST results with (a) velocimetry data from rod impact experiments [7], and (b) experimental shaped charge bow shock run distances to detonation [27].

Chick et al. [27] studied the shape charge jet initiation of Comp B charges (55% by weight RDX, 44 % TNT, 1% Wax) having steel or PMMA cover plates, where run to detonation was attained through a bow shock mechanism. The simulations of Chick's experiments described in [28] were repeated but using the Comp B CREST model in place of the previous surrogate model for the explosive, and a copper flat-nosed rod to represent the jet. Figure 5(b) shows that CREST accurately reproduces the experimental run distances to detonation, including the effect on run distance of changing the cover plate material from steel (subsonic jet penetration and long run distances) to PMMA (supersonic jet penetration and short run distances). The good agreement obtained with Chick's data is likely because the Comp B used has a lower weight % of RDX, and hence will be less sensitive than some of the other Comp B variants.

CONCLUSIONS

A CREST model has been developed for the RDX/TNT explosive Comp B. The non-reacted EoS is a good fit to the majority of the Hugoniot data, the detonation products EoS accurately represents the available overdriven data, and the overall EoS satisfies the compatibility criterion. Reaction rate calibration was hampered by an apparent inconsistency between the gas-gun shock initiation data for isostatically pressed UK Comp B and the detonation size-effect curve for melt-cast Comp B Grade A, which made it necessary to accept a compromise fit to the calibration data. The subsequent validation exercise demonstrated that the model is able give sensible predictions of both shock initiation and detonation behaviour, however the goodness-of-fit to available data is very much dependent on the type of Comp B used in the experiments.

To ensure consistency of the calibration data, new cylinder tests and rate-sticks are planned on UK Comp B so that an improved CREST model can be developed in the future. Consideration will then be given as to how to modify CREST to take account of Comp B compositional and manufacturing differences.

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