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Calibrating reaction rates for the CREST model

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Abstract. The CREST reactive-burn model uses entropy-dependent reaction rates that, until now, have been manually tuned to fit shock-initiation and detonation data in hydrocode simulations. This paper describes the initial development of an automatic method for calibrating CREST reaction-rate coefficients, using particle swarm optimisation. The automatic method is applied to EDC32, to help develop the first CREST model for this conventional high explosive.

Keywords: Reactive burn, CREST, EDC32, calibration, particle swarm optimisation.
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INTRODUCTION

In recent years, the hydrocode-based CREST reactive-burn model has had success in modelling a range of shock initiation and detonation propagation phenomena in polymer bonded explosives, see e.g. [1]. CREST uses empirical reaction rates that depend on a function of the entropy of the non-reacted explosive, allowing the effects of initial temperature, porosity and double-shock desensitisation to be simulated without any modifications to the model. In contrast, the majority of reactive-burn models use pressure-dependent reaction rates and are not able to do so [2].

Until now, the reaction-rate coefficients have been manually calibrated by trial and error, using hydrocode simulations of sustained-shock gas-gun experiments and the detonation size-effect curve for the explosive. This paper describes a new automatic method for calibrating CREST reaction-rate coefficients using the well-established particle swarm optimisation technique [3]. The method is demonstrated by applying it to EDC32 to develop, in conjunction with appropriate equations of state, the first CREST model for this conventional high explosive.

EDC32 comprises 85 wt.% HMX and 15% Viton A, with 1.5% porosity. Various experimental data are available, though unfortunately not a detonation size-effect curve. In this work, the reaction rate was calibrated only to data from four sustained-shock gas-gun shots on EDC32 and an estimated size-effect curve.

AUTOMATIC CALIBRATION METHOD

The form of reaction rate used in CREST has been described previously [1]. The reaction rate equations are (1) to (4), where λ is the mass fraction of explosive that has reacted, and the reaction rate $\dot{\lambda}$ is its derivative with time. The m and b parameters depend on a function of entropy of the non-reacted explosive, Z_s, which is obtained from the equation of state. The algebraic form of $m(Z_s)$ and $b(Z_s)$ has recently been changed and is given by equations (5) to (10).

$$\dot{\lambda} = (m_1\dot{\lambda}_1 + m_2\dot{\lambda}_2 + m_3\dot{\lambda}_3)(1-\lambda) \quad (1)$$

$$\dot{\lambda}_1 = (1-\lambda_1)\sqrt{-2b_1 ln(1-\lambda_1)} \quad (2) \qquad b_1 = c_0(Z_s - c_{12})^{c_1} \quad (5) \qquad m_1 = c_6(Z_s - c_{13})^{c_7} \quad (8)$$

$$\dot{\lambda}_2 = \lambda_1(1-\lambda_2)\sqrt{2b_2\left(\frac{b_2\lambda_1}{b_1} - ln(1-\lambda_2)\right)} \quad (3) \qquad b_2 = c_2(Z_s - c_{12})^{c_3} \quad (6) \qquad m_2 = c_8(Z_s - c_{13})^{c_9} \quad (9)$$

$$\dot{\lambda}_3 = \lambda_1(1-\lambda_3)\sqrt{2b_3\left(\frac{b_3\lambda_1}{b_1} - ln(1-\lambda_3)\right)} \quad (4) \qquad b_3 = c_4(Z_s - c_{12})^{c_5} \quad (7) \qquad m_3 = c_{10}(Z_s - c_{13})^{c_{11}} \quad (10)$$

For $Z_s \leq c_{12}$, the b parameters are set to a small but finite value. Coefficient c_{13} is an entropy threshold, below which no reaction will occur. The m parameters are, therefore, set to zero for $Z_s \leq c_{13}$. Limiters are applied to the b and m parameters to prevent the reaction rate from becoming unfeasibly fast for very high entropies.

There are fourteen reaction-rate coefficients c_0 to c_{13}. For this work, the reaction rate has been simplified so that only seven calibration coefficients, defined below as convenient functions of c_0 to c_{13}, are needed. This simplified form

of reaction rate is sufficient for conventional high explosives (CHEs) like EDC32, for which there is relatively little calibration data available. It was developed from the following observations:

- $\dot{\lambda}_3$ is not required for CHEs, so m_3 is set to zero by defining $c_{10} = 0$. Its other coefficients are set to tractable values of $c_4 = 1$, $c_5 = 0$ and $c_{11} = 0$.
- The b-entropy threshold c_{12} is unlikely to be required for explosives with a sparse data set, so is set to zero.
- Unless there is a need for $b_1 \neq b_2$, for simplicity it is assumed that $b_1 = b_2 = b(Z_s)$ so $c_0 = c_2$ and $c_1 = c_3$. This constrains the shape of the reaction rate $\dot{\lambda}(t)$. Parameter $b(Z_s)$ is represented by two calibration coefficients, $BSHO = \log b(Z_1)$ and $BDET = \log b(Z_2)$, where Z_1 is an entropy of relevance to the shock-initiation regime and Z_2 is an entropy in the detonation regime.
- Parameter $m_2(Z_s)$ is represented by calibration coefficients $C9 = c_9$, m-threshold $MTHR = c_{13}$ and $M2HI = m_2(Z_2)$, which is a high-entropy constraint on m_2 to limit its magnitude in the detonation regime.
- The remaining two calibration coefficients controlling $m_1(Z_s)$ are $C7 = c_7$ and $SUMM = \Sigma_i m_i(Z_2)$, which needs to be large enough to guarantee that $\lambda \to 1$ in the detonation regime.

The reaction rate is calibrated by simultaneously varying the seven coefficients ($BSHO$, $BDET$, $C9$, $MTHR$, $M2HI$, $C7$ and $SUMM$) in order to improve the fit to the calibration data. Many different optimisation methods are available in the literature. We have used particle swarm optimisation (PSO) which is a mature and widely applicable technique.

PSO [3] works by moving a user-supplied number of "particles" ($\sim$32 are recommended) through coefficient space for a number ($\sim$40) of iterations, known as "generations". The coefficients to be optimised, as well as their allowed ranges (minimum and maximum values), are also supplied by the user. Each particle has a "position" which is its current set of coefficients, and a "velocity" which is the change in its coefficients from one generation to the next. At the start of the PSO run, a random position (within the allowed ranges for each coefficient) and velocity is chosen for each particle. Then the PSO submits hydrocode simulations for the first generation, waits until they finish, and analyses the results to generate a goodness-of-fit value known as the "misfit" for each particle. The "best" misfit (in our case, the minimum) for each particle and all the particles, from this and any previous generations, is identified.

Each particle's velocity is updated using an equation containing three terms, the first depending on the particle's previous velocity, the second based (with a degree of randomness) on the difference from the best set of coefficients that particle has seen, and the third based (with a degree of randomness) on the difference from the global best that all particles have seen. Then each particle's position is updated by adding the velocity to its previous position, before the hydrocode simulations are repeated for the next generation. Appropriate choice of the PSO control parameters helps the particles to explore the coefficient space effectively, before converging on the global best solution.

Our PSO code is written in Python with ancilliary Bash and Fortran 90 programs, and runs on AWE's BULL B510 Linux cluster. Although the code has multi-objective capability [4], only single-objective PSO has been used in this work. The code, as tailored to CREST model calibration, is known as *CalibrateHE*. For each particle, it runs 4 gas-gun simulations in a 1D Lagrangian hydrocode, using 100 zones/mm meshing, and 3 different-diameter rate-stick simulations in a 2D Eulerian hydrocode using either 50 or 100 zones/mm.
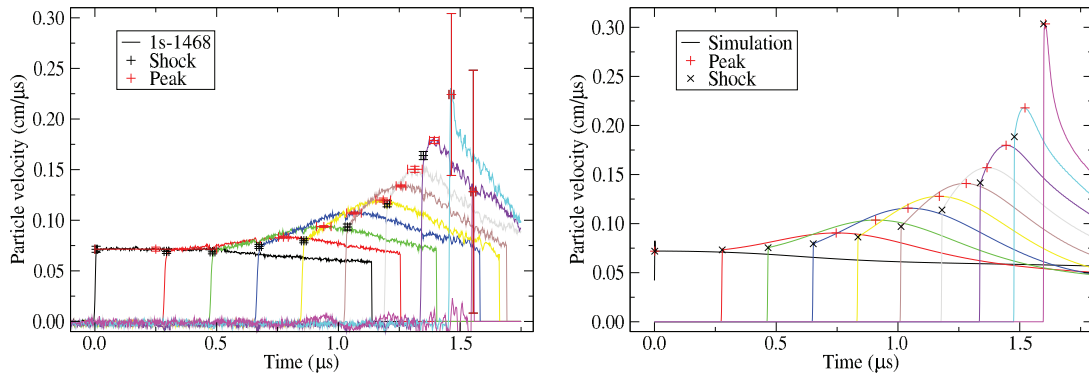

FIGURE 1. Embedded gauge data for EDC32 gas-gun shot 1s-1468 [5] (left), and a CREST simulation of the same shot (right).

Figure 1 shows one of the sustained-shock EDC32 gas-gun shots used for calibration [5]. The coloured lines are experimental data from particle-velocity gauges embedded at known depths within the explosive. In order to construct the misfit, it was decided to compare two features of these data, the shock and peak states, because experience from manual calibration shows that it is difficult to match these states without fitting the whole particle-velocity history. The experimental data were analysed to determine the shock and peak states, and error bars were estimated. Results from the gas-gun simulations for each particle are analysed automatically, and the misfit calculated using the first term in:

$$misfit = \underbrace{\frac{1}{ngm}\sum_1^n\sum_1^g\sum_1^m\left[\frac{calc-data}{\sigma_{data}^{est}}\right]^2}_{shock\,initiation\,regime} + \underbrace{\frac{1}{r}\sum_1^r\left[\frac{calc-fitted\,data}{\sigma_{fitted\,data}^{est}}\right]^2}_{detonation\,regime} \qquad (11)$$

where n is the number of successful gas-gun simulations, g is the number of gauges in each gas-gun shot, m is the number of metrics for each gauge (currently 4: the peak time, peak magnitude, shock time and shock magnitude) and r is the number of rate-stick simulations. The σ^{est} values are estimated errors; providing that PSO is used only to optimise coefficients and not to estimate uncertainties on the coefficients, it is sufficient to estimate the errors.

The second term in equation (11) represents the fit to the detonation size-effect curve. This gives the variation in detonation velocity with diameter, as obtained from unconfined cylindrical rate-stick experiments. Since a size-effect curve is required to calibrate the detonation behaviour of CREST but no EDC32 data are available, it was necessary to estimate a size-effect curve. This was done by scaling the measured detonation velocities for two similar HMX-based explosives, LX-04 and EDC29, and using an established fitting form with an estimated failure diameter of 2mm. It is hoped that the resulting curve, shown by the black line and error bars in figure 4 (right), is plausible. Three points on this curve, at 3mm, 5mm and infinite diameter, are compared to detonation velocities automatically extracted from rate-stick simulations, using pressure traces from marker particles positioned along the axis of symmetry.

APPLICATION TO EDC32

CalibrateHE was first run for 40 generations of 20 particles, using 50 zones/mm rate-stick simulations, in order to demonstrate that it was working correctly. Figure 2 shows how the PSO has converged upon best-fit values for four of the calibration coefficients; results are similar for the other three coefficients. The particles explore the parameter space for $\sim$10 generations before beginning to converge. In this case, the particles move to a better minimum with a higher value of *M2HI* after $\sim$20 generations though, due to its stochastic nature, this behaviour might be different if the PSO run was repeated. Figure 3 shows that *BSHO* and *BDET* are tightly constrained by the calibration data because they control $b_1 = b_2$. It is known that the most important parameter in the CREST reaction rate is b_1, since it largely determines the time and magnitude of the peak overall reaction rate [1]. Coefficients *M2HI* and *SUMM* have wider minima because they are inter-related, so several combinations could give good fits to the calibration data.
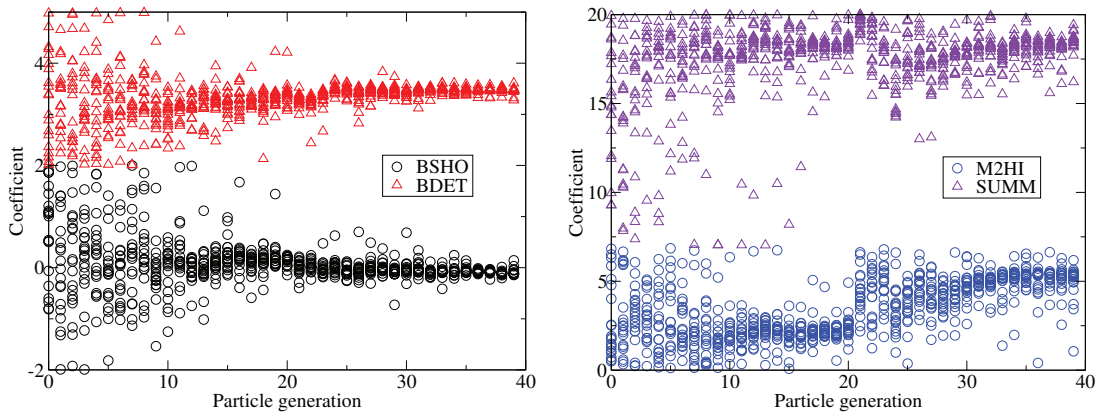

FIGURE 2. Variation of four of the seven reaction-rate calibration coefficients during 40-generation 20-particle PSO run.
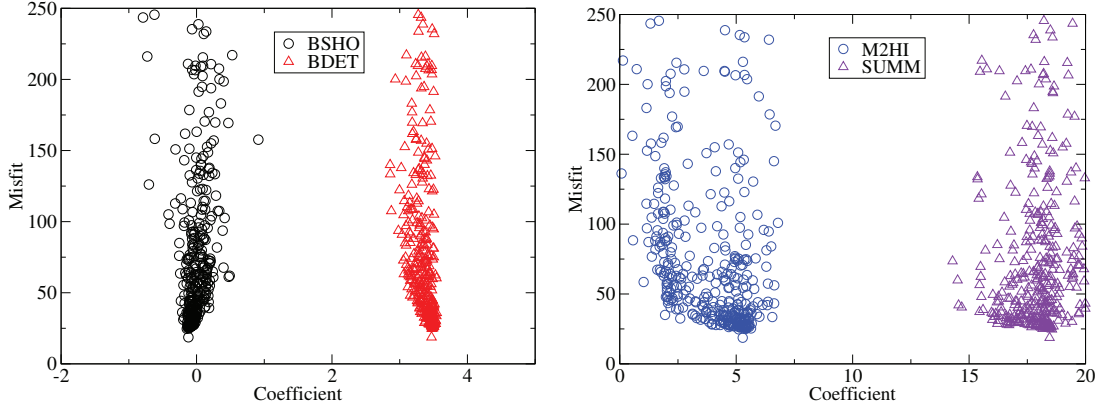
FIGURE 3. Misfit plots for four of the seven calibration coefficients, from the 40-generation 20-particle PSO run. The misfit scale is truncated in order to focus on the best reaction rates.
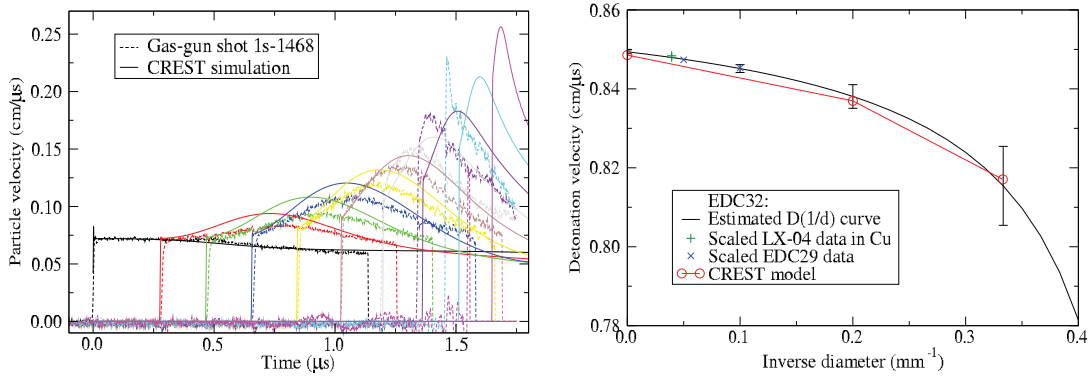

FIGURE 4. Fit to calibration data for the global best particle from the 26-generation 8-particle PSO run that was used to calibrate the CREST model for EDC32. Left: one of the four sustained-shock gas-gun shots. Right: detonation size-effect curve.

The PSO was run again to calibrate the reaction rate for EDC32, with 26 generations of 8 particles, using rate stick simulations with 100 zones/mm meshing which is converged for detonation propagation. This is fewer particles than is desirable from a computer-science perspective, but limited computational resource was available for this work. From a physics perspective, the results are sufficient to calibrate CREST providing that the fit to the calibration data is acceptable. The best particle, whose reaction rate has been adopted for the model, had the following coefficients: $c_0 = c_2 = 1.104 \times 10^8$ μs^{-2} (Mbar cm^3/g)$^{-c_1}$, $c_1 = c_3 = 2.300$, $c_4 = 1.0$ μs^{-2} (Mbar cm^3/g)$^{-c_5}$, $c_5 = 0.0$, $c_6 = 1.993 \times 10^5$ (Mbar cm^3/g)$^{-c_7}$, $c_7 = 2.48$, $c_8 = 11.12$ (Mbar cm^3/g)$^{-c_9}$, $c_9 = 0.325$, $c_{10} = 0.0$ (Mbar cm^3/g)$^{-c_{11}}$, $c_{11} = 0.0$, $c_{12} = 0.0$ Mbar cm^3/g and $c_{13} = 2.25 \times 10^{-4}$ Mbar cm^3/g. If these values are substituted into equations (5) to (10) and plotted, the entropy-dependence of the m and b reaction-rate parameters is similar to the previous manually-calibrated CREST model for the HMX-based explosive PBX 9501 [1], which is reassuring.

Figure 4 shows how well the model fits the calibration data. A reasonably-good fit to gas-gun shot 1s-1468 has been obtained, comparable in quality to the PBX 9501 model. Space does not permit the other three gas-gun comparisons to be illustrated here, but they are similar. The resulting misfit for the shock initiation regime, the first term in equation (11), is 31.35. The fit to the estimated size-effect curve for EDC32 is excellent, giving a misfit for the detonation regime of 0.99. The misfit for the gas-gun data is much higher than for the size-effect curve because the shock and peak states from the gas-gun simulations (figure 4) are often outside the estimated error bars on the experimental data (figure 1). While this suggests that the CREST model could be improved, it is also likely that the estimated errors are too small because they do not account for shot-to-shot variability. In future, a hierarchical model [6] could be used to estimate better errors for the gas-gun data.

CONCLUSIONS

An automatic calibration method, *CalibrateHE*, has been developed for CREST reaction-rate coefficients. A particle swarm optimisation code submits multiple hydrocode simulations, whose results are analysed to determine the "misfit" to calibration data. Over ~40 generations, the code finds a best set of reaction-rate coefficients that minimise the misfit. *CalibrateHE* has been applied to EDC32, to develop the first CREST model for this conventional high explosive. The reaction rate has been calibrated using four sustained-shock gas-gun shots and an estimated size-effect curve. The fit to the calibration data is comparable in quality to that for manually-calibrated CREST models for other explosives and, since multiple sets of reaction-rate coefficients have been tested, it is more likely that a best fit has been achieved.

It is much easier and quicker to run *CalibrateHE* than it is to manually calibrate a CREST reaction rate. However, there is a danger in reducing the level of human involvement because any automatic optimisation scheme can only work within the equation-set provided. Since the original development of CREST, both the reaction-rate equations and the entropy-dependence of their m and b parameters have been improved. The necessity to change the equations was identified during the manual calibration process, when attempting to tune the reaction rate to new data sets. It is important that, when automatic calibration methods are used, time is spent analysing the resulting reaction rates and, if necessary, changing the reaction-rate equations to improve the fit to experimental data.

CalibrateHE is computationally expensive because several rate-stick simulations are required for each particle, and each of these takes up to 8 hours to run on 32 Intel Sandy Bridge processors. In this work, the number of rate sticks was limited to three to reduce the computational expense, but defining the size-effect curve in this way is cumbersome. It is hoped that research currently underway at Leeds University using the straight and variational streamline approximations with CREST will, in future, enable the size-effect curve to be estimated in minutes. If successful, this has the potential to signficantly reduce the computational expense of reaction-rate calibration.

CalibrateHE currently uses a simplified reaction rate that is appropriate for conventional high explosives like EDC32 for which there is relatively little calibration data available. Well characterised and/or insensitive high explosives will require a more-complete reaction rate, possibly using all fourteen of the available coefficients. In due course, the code will be made compatible with these reaction rates, and with other types of calibration data e.g. Pop plots.

CREST equations of state (EoS) are calibrated to appropriate data using a separate automated code. It has been shown [7] that adjusting the EoS coefficients within the uncertainties in the underlying data can improve the fit to detonation corner turning behaviour. By combining the EoS and reaction-rate codes in future, to allow both sets of coefficients to be optimised simultaneously, it will become possible to account for uncertainties in the EoS data when CREST models are calibrated.

ACKNOWLEDGMENTS

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