Investigation of the Hugh James Criteria Using Estimated Parameters

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ABSTRACT:

The ability to predict the response of an energetic device to IM stimulus is one of the major focus areas within the IM community. Several methodologies have been proposed and used for this purpose, including direct calculation via reactive burn models, analytic criteria such as Held's V^2D criteria, and semi-empirical techniques such as the Hugh James criteria. A method was recently presented that leverages the James criteria with estimated parameters combined with the ALE3D hydrocode and statistical models to predict reaction threshold. In this paper, this methodology is examined in detail by applying it to a well-characterized explosive.

The basis for the methodology is in threshold statistics, as detailed by Hrousis, et al. Energetic materials are often characterized in terms of '50% go/no-go' thresholds, underscoring the inherent variability in material response. These concepts were initially applied to an explosive for which James parameters were not readily available (LX-14), but a large body of Fragment Impact (FI) test data was. Values for the missing parameters were 'guessed' by substituting parameters from a similar explosive. The initiation threshold was developed by applying the 'guess' parameters to the existing data, and extrapolated forward through a Binary Logistic Regression (BLR) model.

To test this methodology, the UF-TATB parameters from Hrousis, et al, were used in place of test data. The mean and variance of the ignition threshold were calculated using the QMU method and applied to a BLR model. Model variations were then simulated to test the predictive capability of the method.

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Introduction

Computational prediction of munition response to impact stimulus is routinely performed via hydrocode analysis. The material models used to simulate energetic materials are usually either a reactive flow model, such as Tarver-Cochran Ignition & Growth Reactive Burn (IGRB) or History Variable Reactive Burn (HVRB) or an inert material. Reactive models are capable of directly predicting the material response, but carry some disadvantages, such as increased computational load and binary response. Simulations using this type of model are capable of predicting detonation or non-detonation, but do not provide an estimate of distance from initiation threshold.

When instead an inert material model is used, prediction of initiation behavior relies on an external analysis. Multiple initiation criteria are used for this purpose, such as the Held's[1–3] V^2D for shaped charge jets, Walker & Wasley's[4] $P^2\tau$, or the James criteria[5] combined specific kinetic energy and energy fluence. These approaches are capable of producing excellent agreement with experiment, provided a suitable threshold value has been provided for the explosive under investigation. Previously, a method for predicting energetic response to impact stimulus has been presented[6] that relies on the James method, but uses the outcome of previous tests[7] instead of compiled critical values.

In the previous study, the critical values of James' parameters were not located for LX-14, but several Fragment Impact (FI) tests had already been conducted. These values were substituted arbitrarily for those of another explosive, and a BLR model was used for threshold to reaction. The justification for doing so was that within the geometry and impact conditions investigated, the calculated result should at least trend in a physically meaningful way. At that time, no further justification was offered for the approach. This paper investigates the idea further, and provides a validation study for the previous effort.

James Criteria and QMU Threshold

The James criteria has roots[8] in the critical energy criteria of Walker & Wasley[4]. James extended[5] the critical energy concept to include both the energy fluence across a unit area, E_c, and a specific kinetic energy, Σ_c. The resulting initiation threshold is hyperbolic in E-Σ space, in accordance with the relationship

$$1 = \frac{E_c}{E} + \frac{\Sigma_c}{\Sigma} \qquad (1)$$

The concept was further extended by Hrousis, et al[9] to develop a single parameter, J, as a combination of the two critical parameters. Additionally, a functional form of energy fluence was suggested that is well-suited to hydrocode calculation. Their relationships are

$$J = \frac{E_c}{E} + \frac{\Sigma_c}{\Sigma}, \qquad E = \int P\,u\,dt\,, \qquad \Sigma = \frac{u^2}{2} \qquad (2)$$

In the above equation, P represents pressure and u is particle velocity. In this form, the value of J_{max} = 1 corresponds to marginal initiation, while numbers less than 1 or greater than 1 imply non-initiation or initiation with margin, respectively. By carrying forward the measured uncertainty in experimental results and assuming that $J_{critical}$ is normally distributed with a mean of 1.0, they developed an engineering sense of margin from initiation.

The p-values associated with the computed value of J_{max} can then be viewed as a probability of initiation occurring. They demonstrated the developments with parameters for µF TATB as the explosive, providing a set of critical parameters and standard deviation of J as

$$E_c = 0.26 \frac{MJ}{m^2}, \quad \Sigma_c = 0.67 \frac{MJ}{kg}, \quad \sigma_J = 0.15 \tag{3}$$

These parameters were used in this study as the basis for computational predictions.

Binary Logistic Regression Model

Binary Logistic Regression[10] is a regression technique by which categorical data can be used as a response variable. The model approach allows overlap in predictor variables versus observed category to build a probabilistic function describing the likelihood of a predictor to fit into a given category. In the previous study[6] the predictor variable was J_{max} and the categorical response variable was detonation or non-detonation. Some attempt was made to delineate IM reaction type (I,II,III, etc) as the response variable, but the experimental uncertainty caused this analysis to be ineffective.

Mathematically, the approach takes the exponential of a linear function to represent the probability of category fit, as shown in Eq. 4 below, where *x* represents a predictor variable and *p* is the probability that the response will fit in a base (null) category.

$$p(x) = \frac{1}{1 + e^{-ax-b}} \tag{4}$$

In a least-squares regression model the parameters are fit by minimizing the squared error, which is analytically tractable in the case of continuous predictor and response variables. In the logistic regression models, a likelihood function optimization is used to fit the slope and intercept of the linear function to experimental data. The likelihood function is a measure of model error, and is defined

$$LL = \sum_{i=1}^{n} y_i \, ln(p_i) + (1 - y_i) \, ln(1 - p_i) \tag{5}$$

The *y* in Eq. 5 is the observed fraction of observations fitting into the null category, and the subscript *i* refers to the predictor variable level. This equation is maximized numerically to fit the slope and intercept (*a* and *b* from Eq. 4).

Simulation Approach

In order to validate the described approach, a simulation strategy was devised to represent the process. Using the parameters in Eq. (3) 2D, axisymmetric hydrocode simulations were performed in ALE3D[11] with a null-constitutive model and Mie-Gruneisen Equation of State for µF TATB. The explosive was modeled as a 100 mm diameter by 50 mm length cylinder, with a 3mm case and the impact occurring on one of the two flats. The standard IM fragment geometry (STANAG 4496) was used, and impact velocity varied from 300 – 3,000 m/s. The simulation geometry is shown in Fig. 1.

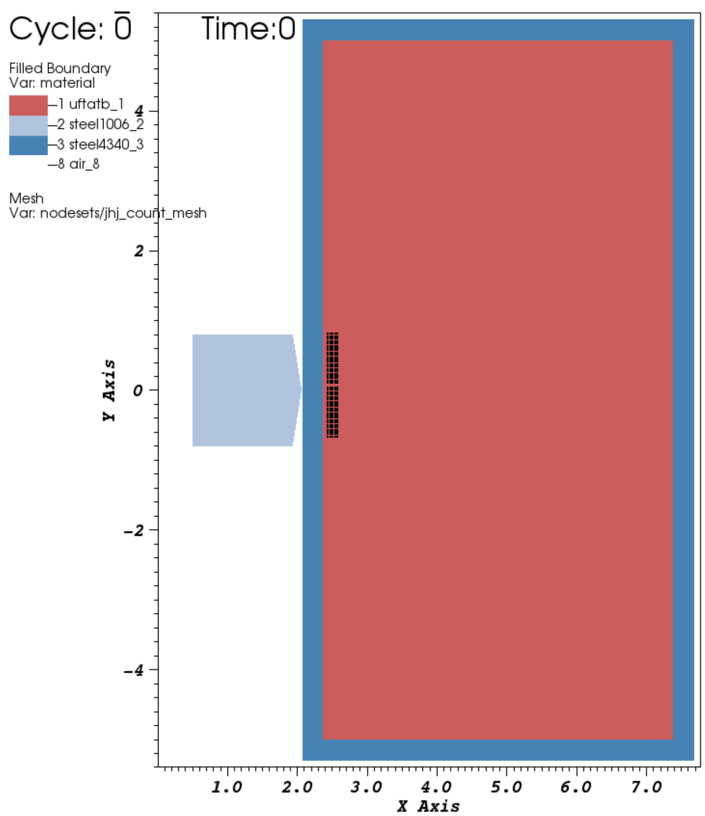

Figure 1. Hydrocode model geometry. This geometry was used throughout the simulation series.

The value of J was calculated by defining a derived variable in the hydrocode analysis. The derived variable is calculated across the mesh domain. It is extracted as the mean value from a nodeset of the same radius as the tracer particle and 0.2 mm thick located 0.05 mm inside the explosive. Nodes on the case boundary and symmetry plane were excluded intentionally to avoid numeric noise. Calculated values of J_{max} are plotted versus velocity in Fig. 2.

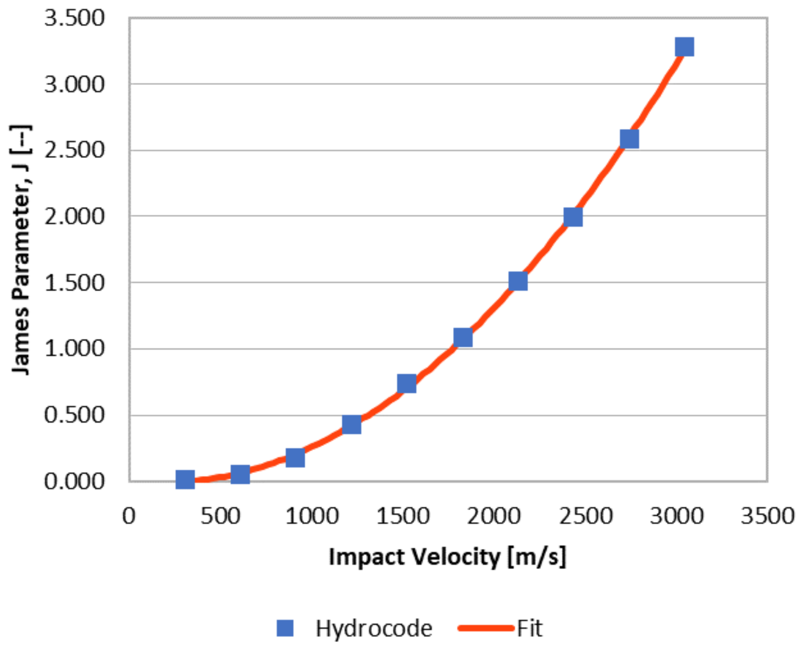

Figure 2. Calculated J_{max} at various impact velocities. Relationship is apprx. quadratic.

The mean (1.0) and standard deviation (0.15) of J were used to calculate the Z-statistic, leading to the probability of detonation represented in Fig. 3.

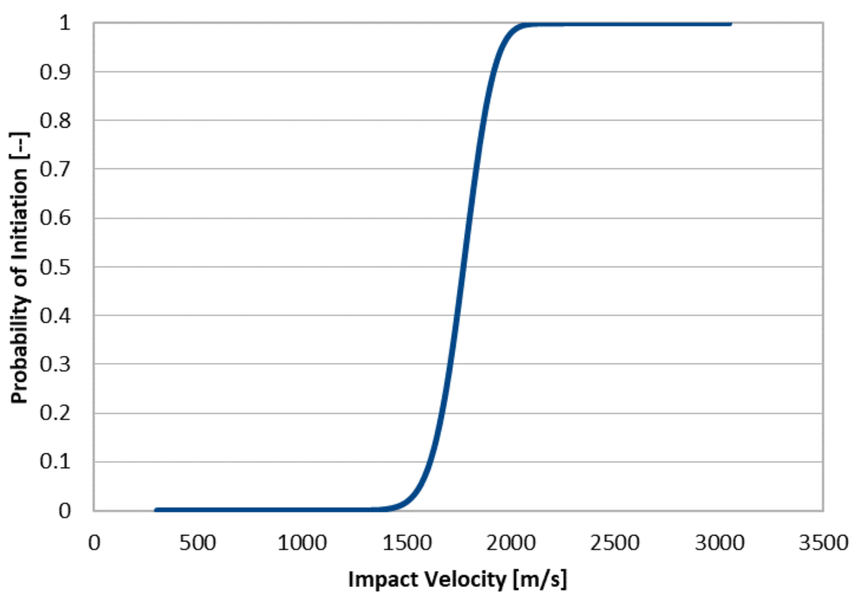

Figure 3. Probability curve plotted with impact velocity for known James parameters.

This probability function was used to generate a set of 25 'observations'. Using random numbers, impact velocities between 1675 and 1980 m/s were generated to represent test data. Another random number was compared against the p-value at the given velocity. If the random number exceeded the p-value, non-detonation (0) versus detonation (1) was recorded. This process represents experimental uncertainty such as impact location variations while providing the actual p-value (devoid of external influence) to compare with the predictions made with arbitrary critical values. The generated data appears in Table 1.

Table 1. Randomly generated observations from known parameter probability curve.

Impact Velocity m/s	J (KNOWN) --	Z --	P --	Random Number --	Result
1798	1.167	1.111	0.867	0.629	1
1719	1.075	0.501	0.692	0.836	0
1924	1.137	0.912	0.819	0.023	1
1873	1.019	0.128	0.551	0.313	1
1870	1.108	0.717	0.763	0.939	0
1768	1.095	0.632	0.736	0.584	1
1867	1.001	0.007	0.503	0.637	0
1798	0.947	-0.356	0.361	0.679	0
1693	0.996	-0.027	0.489	0.022	1
1829	1.035	0.233	0.592	0.184	1
1725	1.025	0.164	0.565	0.840	0
1837	1.200	1.332	0.909	0.119	1
1737	1.096	0.641	0.739	0.475	1
1816	0.966	-0.226	0.410	0.753	0
1683	1.057	0.381	0.648	0.251	1
1772	1.031	0.204	0.581	0.889	0
1901	1.144	0.961	0.832	0.442	1
1829	1.166	1.107	0.866	0.110	1
1848	1.124	0.828	0.796	0.122	1
1854	1.094	0.625	0.734	0.455	1
1803	1.030	0.201	0.580	0.964	0
1790	1.025	0.168	0.567	0.502	1
1843	1.153	1.018	0.846	0.923	0
1811	0.978	-0.144	0.443	0.296	1
1770	1.096	0.643	0.740	0.267	1

Further simulations were performed using arbitrary values of the critical parameters, which appear in Table 2.

Table 2. Simulation matrix showing the 'guess' values of E_c and Σ_c.

	E_c	Σ_c
	MJ/m2	MJ/kg
Known	0.26	0.67
Variation 1	0.1	0.1
Variation 2	0.1	0.9
Variation 3	0.9	0.9
Variation 4	0.9	0.1

Results & Discussion

When the arbitrary values of E_c and Σ_c are substituted for the known values, the response curve changes shape significantly, though a quadratic regression still fits extremely well. The J_{max} versus velocity plots for several iterations appear in Fig. 4.

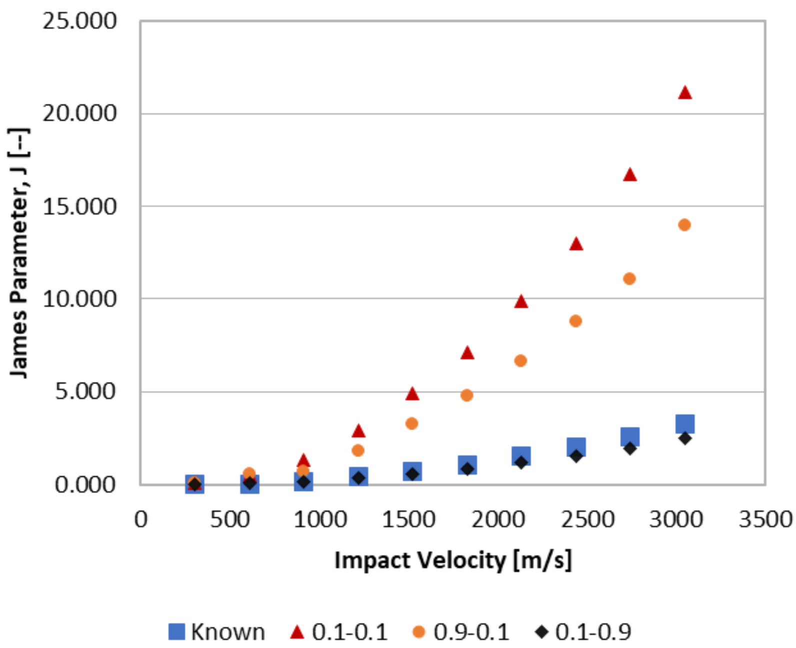

Figure 4. Predicted J_{max} values for arbitrary values at various velocities

For each set of parameters, the J_{max} parameter was computed from the regression fit for each velocity in the observation data. A BLR model was fit to the J_{max} predictor with the randomized result as response variable for the first 5, 10, 15, and 20 observations. The remainder of observations were then used to test predictive capability of the resulting model fit. Probability of detonation versus impact velocity is shown in Fig. 5 for the known case compared to the two most different sets of E_c and Σ_c in terms of J (0.1-0.1 and 0.1-0.9). The prediction is only marginally improved by increasing the size of the sampled dataset from 10 to 20. In each case, it was found that the BLR model detonation probability remained unchanged for any value of E_c and Σ_c, which does tend to validate the previous approach. No attempt has been made to verify this finding mathematically at this point. The function optimization aspect of the BLR method is handled numerically, making it difficult to analytically prove the finding.

In terms of model accuracy, 76% of observations were correctly categorized according to recorded reaction (1 or 0) and approximately the same proportion according to known probability. The number of observations correctly categorized remains consistent across the range of sample size. This is a similar accuracy to the previous study, though in that case the true underlying distribution parameters were unknown.

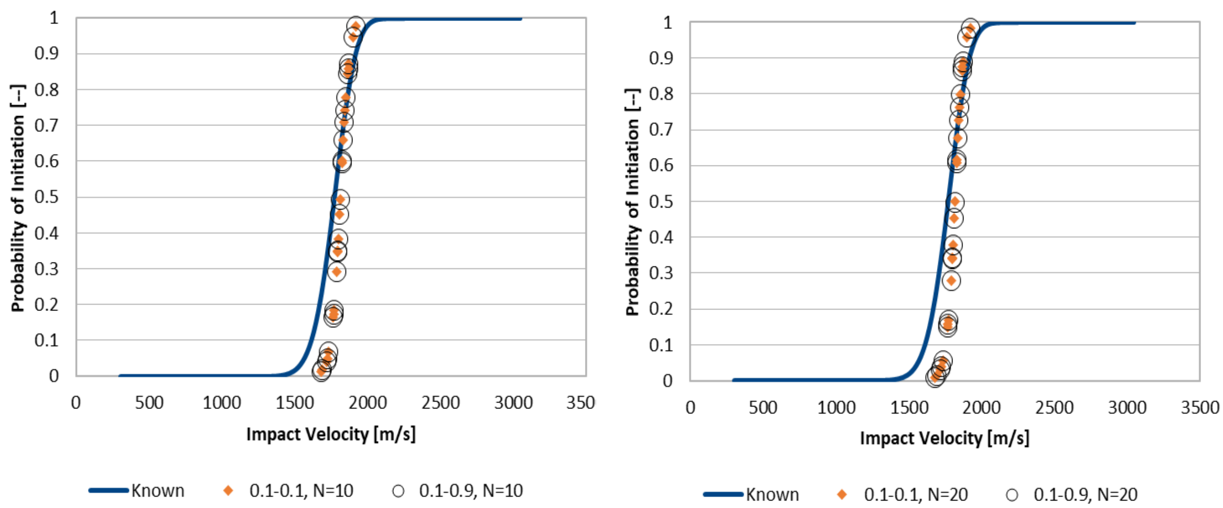

Figure 5. Estimated probability curves from BLR compared to known probability curve.

In light of the findings that show BLR results remaining across different values of E_c and Σ_c another question is raised. How can the predictive capability of this approach be improved? From Fig. 5, it can be seen that the slope of the BLR probability is steeper than the known probability curve. It was speculated that this stems from all of the observation data being close to the threshold, without bounding values on the extremes. The first two observations were altered to 2,430 m/s (1.0 Reaction = Detonation) and 610 m/s (0.0 Reaction = Non-detonation) and the analysis was repeated for the E_c ,Σ_c = 0.1,0.1 case.

The BLR predictive capability improved to 96% using 20 observations, and dropped to 72% using 5 observations. This is likely due to the first two observations being changed, leaving only 3 threshold observations in the 5 sample dataset versus 18 in the 20 sample dataset. The effect is to skew the probability estimate, as there are fewer anchor points toward the center of the curve. When 20 observations, including the bounding samples, are included the curve is well enough characterized to nearly replicate the known probability curve. The improved probability estimates appear in Fig. 6.

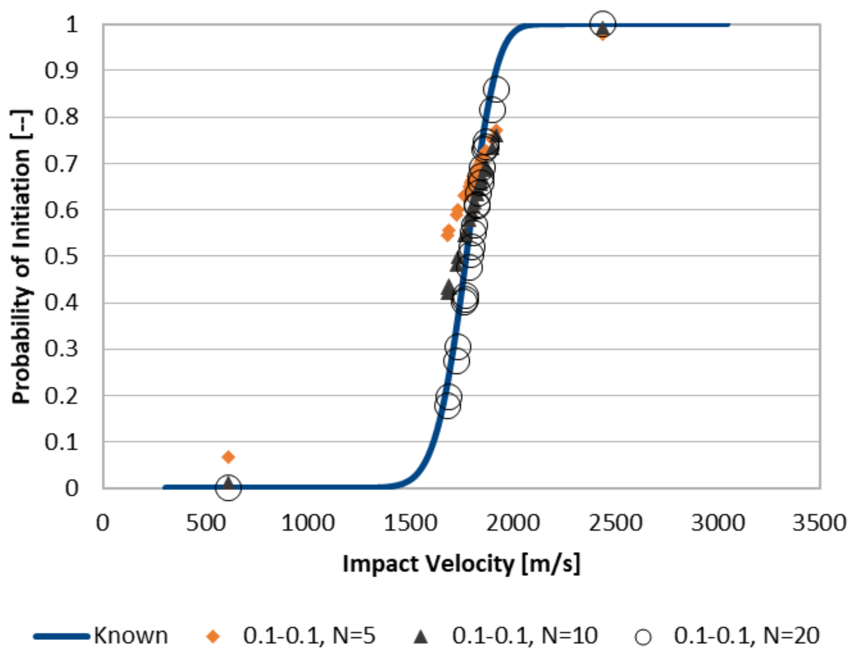

Figure 6. Improved estimate probability curves from BLR compared to known probability curve.

Conclusion

The simulation approach utilized in a previous study[6] has been validated through a series of hydrocode simulations designed to investigate the variance of predictions made with a combined James model / binary logistic regression model. Through these simulations, it was shown that the BLR predictions remain unchanged when parameters are selected arbitrarily. It was further shown that the addition of bounding cases to the data set drastically improves the predictive capability of the model.

The importance of this study lies in the ability to pivot from a relatively small number of impact tests into a predictive capability for further tests. As in the prior work, the intent is to provide a means to iteratively improve a munition's response to impact stimulus. As more design variations are tested within a geometry envelope, the model prediction will become increasingly accurate.

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