Chemical kinetics of multi-component pyrotechnics and mechanistic deconvolution of variable activation energy

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Abstract

This study reports an experimental investigation into the chemical kinetics of several commercial pyrotechnic compositions. Differential Scanning Calorimetry (DSC) was utilized to elucidate the thermo-kinetic characteristics of four multicomponent pyrotechnic compositions. The combustion process of typical pyrotechnics is primarily driven by condensed phase reactions including processes such as phase change, decomposition, and oxidation. The multicomponent nature of practical pyrotechnics results in a particularly complex interaction between the components when heated. A thermo-kinetic study was performed to simulate the heating experienced by the pyrotechnics before the combustion zone. The physical processes occurring within these temperature limits provide important insight into the overall combustion rate. The non-isothermal DSC experimental technique combined with isoconversional methods, such as Friedman and Starink methods were utilized to evaluate the apparent chemical kinetics parameters for these propellants. The observations from the DSC study and isoconversional kinetic analysis provided an insight into the phenomenology of the combustion process of pyrotechnics. The problem of highly variable activation energy due to the presence of multiple reactions was addressed through a mechanistic deconvolution using nonlinear regression technique. The study confirmed the prominence of oxidizer decomposition on overall combustion reaction kinetics.

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Keywords: Pyrotechnics; Chemical kinetics; Non-linear regression; Variable activation energy

1. Introduction

Reaction kinetics of energetic materials is often investigated using one of the thermal analysis techniques simulating the temperature conditions of actual combustion process. The subsequent kinetic analysis of the experimental data aims to estimate the ‘kinetic triplet’ comprising the chemical activation energy \( E_a \), the pre-exponential factor \( A \), and the reaction model \( f(\alpha) \). Various isoconversional methods are commonly utilized for this purpose and the study by Starink [1] reveals the so-called Type B-1.92 method [1] and Friedman method [2] to be most accurate.

Typical isoconversional methods evaluate the activation energy \( E_a \) as a function of reaction progress \( \alpha \) and despite a varying value of \( E_a \), an
average activation energy ($\bar{E}_a$) may be used to indicate the nominal activation energy. However, the $\bar{E}_a$ value, evaluated using isoconversional methods, may not specify the correct minimum energy required for initiating the chemical reactions in certain cases. In practice, $\bar{E}_a$ may be considered meaningful and independent of $\alpha$, provided the maximum deviation relative to the $E_a$ for a given $E_a-\alpha$ relationship is less than 10% [3]. This condition essentially signifies a single-step reaction [4], while a large variation in the $E_a-\alpha$ relationship [5,6] as well as the dependence of $E_a$ values on the heating rates [7] is related to competing or overlapping reactions. In the latter case, the prediction of the isoconversional methods may be rendered inaccurate and additional mechanistic modeling may be necessary.

Thus, for a complex process, the kinetic analysis must extract the details of the constituent reactions from the overall process in a physically meaningful way. The overlapping reactions may be deconvoluted using standard statistical functions such as Fraser-Suzuki equation [8,9], followed by a kinetic analysis of the separated peaks. Alternatively, non-linear regression (NLR) techniques may be employed, which assume a certain reaction scheme. The corresponding kinetic parameters are optimized iteratively to minimize the difference between the experimental and simulated curves. Most recent attempts to elucidate the kinetics of the complex processes triplet include the novel NLR technique by Pomerantsev et al. [10] and the algebraic method presented in the review by Vyazovkin [11].

The Pomerantsev method utilizes generalized kinetic models with multiple adjustable parameters and subsequently requires substantial efforts to ensure convergence to reliable results. These computational challenges may be expected to increase significantly with large number of constituting reactions. Vyazovkin utilizes pre-determined theoretical algebraic equations between the experimentally determined isoconversional $E_a-\alpha$ relationship and the singular activation energies of the constituting reactions. The parameters of the algebraic equation are optimized to fit the experimental activation energy ($E_a$) for calculating the effective activation energy ($\bar{E}_a$) with multiple constituting reactions.

In this study, the authors have attempted a quantitative analysis of variable activation energies in the context of pyrotechnics. Pyrotechnics are granular heterogeneous porous composite energetic materials utilized in a wide range of applications. These multi-component energetic materials undergo a complex combustion process involving multiple parallel and competing reactions. An accurate estimation of the kinetic triplet is essential to obtain, in the context of pyrotechnics, reasonable predictions of burning rate, reaction progress, ignition temperature, and storage life under given conditions. The thermo-kinetic phenomena occurring in composite energetic materials can be expected to be more complex than the idealized binary mixtures. However, numerous investigations on simple binary pyrotechnic compositions [12-18] have been reported in the literature, while far fewer investigations [19,20] concerning the chemical kinetics of practical multicomponent pyrotechnic compositions can be found.

The current study aims to investigate a set of commercial multicomponent pyrotechnic compositions for elucidating their thermo-chemical behavior and extracting the thermo-kinetic parameters. The chemical kinetics of these composite energetic materials was explored using the Differential Scanning Calorimetry (DSC) technique. The observations gleaned from the DSC thermograms for each composition were correlated with the pyrotechnic composition to obtain an insight into the combustion phenomenology. The kinetic parameters obtained using established analysis techniques such as Friedman and Starink methods were compared to identify the optimal method. The variation in the $E_a-\alpha$ relationship for a given heating rate range was addressed for obtaining a meaningful split of the overall reaction into a series of single step reactions. We use the so-called Bayesian approach, where known data relevant to the kinetics under consideration are collected to form the a priori information. This approach defines a model for the effective activation energy based on a set of proposed reactions. The adjustable model parameters are obtained through numerical optimization. A comparison of the combustion parameters predicted using the isoconversional average kinetics and the newly calculated kinetics has been presented.

2. Experimental study

The current study follows the ICTAC Kinetics Committee recommendations for collecting experimental data [21] as well as thermal analysis and data processing [22]. The optimal sample mass was pre-determined to be between 1.2 and 1.5 mg for preventing self-heating of the sample, while providing sufficient sensitivity to resolve various peaks. The particle size of the samples was closely controlled using 200 mesh (75 μm) particle sieves. DSC experiments were conducted with a Mettler Toledo DSC 3 instrument under constant heating rates of 1, 2, 5, 10, 20, 40, and 50°C/min with a purge flow of nitrogen maintained at 80 mL/min. The Dutch Society for Thermal Analysis (TAWN) sensitivity and resolution for the instrument was 11.9 and 0.12 respectively. A wide range of heating rates was selected to increase the overall accuracy of the predictions. The samples were contained within the standard 40 μL aluminum pans sealed with an aluminum lid with a perforation of approximately 0.5 mm diameter. The sample mass was spread across the bottom of the pan in a thin layer to ensure a rapid and uniform heat distribu-
tion, and to minimize the temperature gradients inside the sample.

The mass-based pyrotechnic composition and the sample images showing the flames currently being studied have been reported previously [23,24] and reproduced in Table 1. These compositions, typically utilized in display pyrotechnics, have been designated according to the flame color they generate.

The components of the pyrotechnic compositions could be assumed to undergo a specific process based on their intended role. The magnesium (Mg) invariably acts as the fuel, while potassium perchlorate (KClO₄), copper (II) oxide (CuO), and barium nitrate (Ba(NO₃)₂) act as the oxidizers. Strontium carbonate (SrCO₃) as well as the polymers polyvinyl chloride ((C₂H₃Cl)ₙ) and chlorinated rubber (C₁₀H₁₁Cl₁₇) are additives which undergo decomposition to provide reactive species in the gas phase. Sulfur (S) is known to act as a catalyst while Cryolite (Na₃AlF₆) decomposition occurs only at extremely high temperatures. Further observation indicates that red, blue, and yellow pyrotechnics have excess oxidizer, while the green pyrotechnic may be assumed to be stoichiometric in composition. It should be noted that the pyrotechnic flame color originates from the spectral emissions of certain species and does not depend on the stoichiometry of the composition.

3. Results and discussion

Typical DSC analysis elucidates the heat flow associated with the chemical reaction occurring within a given sample. The data from the DSC thermograms were used for understanding the chemical kinetics of the pyrotechnics.

3.1. DSC thermograms

Figure 1(a)–(d) show the characteristic DSC thermograms obtained at various heating rates for the different pyrotechnics under study. Despite utilizing potassium perchlorate as the primary oxidizer and magnesium as the primary fuel, a definite variation in the appearance of the thermograms of each composition was observed. However, certain features of pure component thermochemistry are evident in the DSC thermograms shown in Fig. 1.

The typical thermograms for pyrotechnics comprised of the first endothermic peak occurring before the onset of exothermic reactions, the primary exothermic peak that was a composite of multiple peaks, and the second endothermic peak overlapping the primary exotherm. The first endothermic peak manifested between 301 and 307°C for all pyrotechnics indicating the phase transition of KClO₄ as previously reported [12,25]. In case of green pyrotechnic, the phase transition was superimposed with a minor exothermic peak. The onset of the primary exothermic peak, associated with the combustion reactions, changed from approximately 350–390°C and the exothermic peaks moved towards higher temperatures along the x-axis with increasing heating rates due to the kinetically driven nature of the processes involved. The second endothermic peak, shown in the detailed views within Fig. 1, was highly muted for the least heating rate, was conspicuously absent for the blue pyrotechnic, and occurred approximately at 460°C for other compositions without significant movement with heating rates. The second endotherm...
Fig. 1. DSC thermograms at various heating rates for (a) red (b) green (c) blue and (d) yellow pyrotechnic compositions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

was attributed to the simultaneous melting and decomposition of KClO₄ which was corroborated by the sharp increase in the slope of primary exotherm immediately after the second endothermic peak. The pyrotechnic oxidizer-fuel reactions are typically triggered by melting or decomposition of the oxidizer [13,14]. Here, the onset of exothermic peaks occurred prior to the second endothermic peak indicating the melting of KClO₄ which itself occurred at significantly lower temperatures than the reported values [12,25]. This reduction in the melting temperature and the early onset of oxidation reactions has been attributed [15–17] to the solid-state reactions, increased inter-diffusion of reactive components beyond the Tammann temperature, and inadvertent formation of local hotspots in the sample, as well as crystal defects such as distortions, dislocations, and cracks. The absence of the second endotherm for blue pyrotechnic was attributed to catalytic effect of promoting solid-state reactions. Similarly, the minor exotherm observed in case of green pyrotechnic was attributed to the partial decomposition of the Ba(NO₃)₂ and subsequent minor oxidation reactions.

3.2. Isoconversional reaction kinetics

Chemical kinetic parameters for each pyrotechnic composition were evaluated from the DSC thermograms using the Friedman method and the nonlinear method by Starink using a custom MATLAB code. The review by Starink [1] provides a detailed description of these isoconversional methods. Both methods rely on conducting a number of non-isothermal calorimetric experiments at different heating rates (β) to yield several temporal coordinates at which a certain reaction progress is achieved for each heating rate. The differential Friedman method plots ln [dα/dt] against 1/T for a given reaction progress yielding $E_a$ from the slope of the linear fit. Similarly, for the integral Starink method, the plot of ln [β/Tα] against 1/T for a given reaction progress yields the value of $E_a$.

Thus calculated, the kinetic parameters were verified against the AKTS thermo-kinetics software [26] which allows implementation of the isoconversional method by Friedman. The analysis was restricted to the alpha range of 0.02 to 0.98 for excluding the extreme values of conversion with higher measurement uncertainty. Figure 2 shows the $E_a$-$α$ distribution for each pyrotechnic composition evaluated using the Friedman and Starink methods, as well as the variation of the logarithmic term ln(A × f(α)) calculated by the Friedman method. The $E_a$ profiles show a significant variation with α while the results obtained by the isoconversional methods were comparable. This is in contrast with the earlier results obtained for RDX-based energetic material with fewer components [27]. The gradual heating of the sample in a DSC

Table 2
Variation in activation energy according to Friedman and Starink methods.

<table>
<thead>
<tr>
<th>Method</th>
<th>$E_a$ Range (kJ/mol)</th>
<th>$\bar{E}_a$ (kJ/mol)</th>
<th>Deviation (%)</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Friedman</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Red</td>
<td>158–380</td>
<td>267.82</td>
<td>83</td>
<td>0.95±0.03</td>
</tr>
<tr>
<td>Green</td>
<td>163–270</td>
<td>197.25</td>
<td>55</td>
<td>0.99±0.01</td>
</tr>
<tr>
<td>Blue</td>
<td>115–234</td>
<td>155.85</td>
<td>76</td>
<td>0.95±0.04</td>
</tr>
<tr>
<td>Yellow</td>
<td>159–225</td>
<td>183.50</td>
<td>36</td>
<td>0.97±0.02</td>
</tr>
<tr>
<td>Starink</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Red</td>
<td>131–346</td>
<td>215.68</td>
<td>100</td>
<td>0.98±0.02</td>
</tr>
<tr>
<td>Green</td>
<td>152–244</td>
<td>180.87</td>
<td>51</td>
<td>0.99±0.01</td>
</tr>
<tr>
<td>Blue</td>
<td>125–181</td>
<td>133.14</td>
<td>42</td>
<td>0.98±0.02</td>
</tr>
<tr>
<td>Yellow</td>
<td>167–204</td>
<td>176.51</td>
<td>21</td>
<td>0.98±0.01</td>
</tr>
</tbody>
</table>

...continues...
Table 3
A priori kinetic data for the proposed reactions.

<table>
<thead>
<tr>
<th>Sr. No.</th>
<th>Reactions</th>
<th>$E_a$ (kJ/mol)</th>
<th>$\ln A$ (1/s)</th>
<th>Reaction model</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1a [12]</td>
<td>$4\text{Mg} + \text{KClO}_4 \rightarrow 4\text{MgO} + \text{KCl}$</td>
<td>153.6</td>
<td>21.5</td>
<td>$f(\alpha) = (1-\alpha)^{3.9}$</td>
</tr>
<tr>
<td>R1b [29]</td>
<td>$3\text{Mg} + \text{Ba(NO}_3)_2 \rightarrow 3\text{MgO} + \text{BaO} + 2\text{NO}$</td>
<td>110.82</td>
<td>7.71</td>
<td>$f(\alpha) = [\ln(1-\alpha)]^{2/3}$</td>
</tr>
<tr>
<td>R1c [13]</td>
<td>$\text{Mg} + \text{CuO} \rightarrow \text{MgO} + \text{Cu}$</td>
<td>120</td>
<td>8.64</td>
<td>$f(\alpha) = (1-\alpha)^{3.9}$</td>
</tr>
<tr>
<td>R2 [30]</td>
<td>$\text{KClO}_4 \rightarrow \text{KCl} + 2\text{O}_2$</td>
<td>309.22</td>
<td>16.03</td>
<td>$f(\alpha) = 3(1-\alpha)[\ln(1-\alpha)]^{2/3}$</td>
</tr>
<tr>
<td>R3 [31]</td>
<td>$\text{SrCO}_3 \rightarrow \text{SrO} + \text{CO}_2$</td>
<td>241</td>
<td>12.1</td>
<td>$f(\alpha) = 3(1-\alpha)^{2/3}$</td>
</tr>
<tr>
<td>R4 [8]</td>
<td>$(\text{C}_2\text{H}_2\text{Cl})_n \rightarrow (\text{C}_2\text{H}_2\text{Cl})_n - (\text{C}_2\text{H}<em>2)</em>{n-m} + m\text{HCl}$</td>
<td>160.5</td>
<td>19.28</td>
<td>$f(\alpha) = (1-\alpha)[\ln(1-\alpha)]^{1/2}$</td>
</tr>
</tbody>
</table>

$E_a$-$\alpha$ relationship obtained in previous section, the physical meaning of such parameters is typically unknown. Furthermore, from an engineering point of view, knowledge of the reaction mechanism in terms of the concentration of propellant constituents or extent of certain reaction is far more important. Thus, a mechanistic deconvolution process was proposed in the current study. A set of reactions was postulated for the current analysis based on the known components of the pyrotechnic composition. These reactions include combustion reaction between Mg and KClO$_4$ (R1a), combustion reaction between Mg and Ba(NO$_3$)$_2$ (R1b), combustion reaction between Mg and CuO (R1c), decomposition reaction of pure KClO$_4$ (R2), decomposition reaction of pure SrCO$_3$ (R3), and the polymer decomposition reactions (R4) which may be nominally represented by the dehydrochlorination reaction. The kinetic triplets representing these reactions have been reported in the literature and listed in Table 3 along with the detailed reactions. The $f(\alpha)$ for R1a and R1c was assumed to be the same as reported by Umbrakar et al. [28]. Although, both R3 and R4 are known to contain two sub-reactions, in this study, the activation energy and pre-exponential factor for these sub-reactions was represented by a single pair of parameters, while the reaction model was represented by summation of the two $f(\alpha)$ functions.

Based on the composition of each pyrotechnic and the proposed set of reactions, the overall process followed by red and yellow compositions was postulated to comprise the reactions R1a, R2, R3, and R4. The green composition was assumed to follow the reactions R1a, R2, R1b, and R4, while the blue composition was proposed to undergo the reactions R1a, R1c, R2, and R4. A typical NLR technique would define a minimization function based on the constituent reaction kinetics modified by adjustable parameters. Subsequent minimization of this function would present with certain values of fitting variables. However, such techniques are hampered by the kinetic compensation effect. This signifies that a given set of experimental data may be fitted accurately by multiple pairs of kinetic parameters, which may render the fitted values of activation energy meaningless and non-unique.

In order to address this issue, the activation energy values in this study were assumed to remain unchanged and the deviation from ideal kinetics in the complex pyrotechnic mixture was represented through a change in the pre-exponential factor values. Furthermore, the reaction model represented by the $f(\alpha)$ function was proposed to use a fraction of $\alpha$ related to the total value through an adjustable parameter. The effective activation energy resulting from the superposition of the constituent reactions in this manner with the proposed modified kinetic parameters follows the relationship in Eq. (1).

$$E_a = \sum E_{ai}A_i'\exp\left(\frac{-E_{ai}}{RT}\right)f(\alpha_i)$$

(1)

Where, the subscript $i$ represents various reactions in the reaction scheme. The modified pre-exponential factor, and reaction progress are defined as shown in Eqs. (2), (3).

$$A_i' = A_i \times y_i$$

(2)

$$\alpha_i = \alpha \times z_i \text{ where, } \sum z_i = 1$$

(3)

Where, $y_i$ and $z_i$ indicate the adjustable parameters. Appropriate adjustable parameters were evaluated through numerically minimizing the error function given by $\text{error} = E_a - E_{ai}$. This technique was implemented using a custom MATLAB code and utilizes the known data regarding the kinetics and reactive behavior of the components instead of representing the constituent reactions through arbitrary parameters. The optimization was carried out using the pattern search technique with the ideal values of the activation energy as the initial guess. The pattern search technique was constrained between zero and infinity for $y_i$ and between zero and a maximum concentration determined by the pyrotechnic composition for $z_i$. The widest possible search domain along with physical
Table 4
Numerically optimized adjustable parameters.

<table>
<thead>
<tr>
<th></th>
<th>Red</th>
<th></th>
<th>Blue</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ln (A′) (1/s)</td>
<td>y_i</td>
<td>z_i</td>
<td>ln (A′) (1/s)</td>
</tr>
<tr>
<td>R1a</td>
<td>29.93</td>
<td>1.39</td>
<td>0.45</td>
<td>R1a</td>
</tr>
<tr>
<td>R2</td>
<td>52.32</td>
<td>3.27</td>
<td>0.20</td>
<td>R2</td>
</tr>
<tr>
<td>R3</td>
<td>3.02</td>
<td>0.25</td>
<td>0.20</td>
<td>R1c</td>
</tr>
<tr>
<td>R4</td>
<td>1.62E-04</td>
<td>1.50E-01</td>
<td>0.15</td>
<td>R4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Green</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ln (A′) (1/s)</td>
<td>y_i</td>
<td>z_i</td>
<td></td>
</tr>
<tr>
<td>R1a</td>
<td>8.76</td>
<td>0.41</td>
<td>0.16</td>
<td></td>
</tr>
<tr>
<td>R2</td>
<td>42.62</td>
<td>2.66</td>
<td>0.16</td>
<td></td>
</tr>
<tr>
<td>R1b</td>
<td>1.00</td>
<td>0.13</td>
<td>0.50</td>
<td></td>
</tr>
<tr>
<td>R4</td>
<td>17.66</td>
<td>0.92</td>
<td>0.16</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 3. Experimental and numerical $E_a$-$\alpha$ relationship for pyrotechnics.

KClO$_4$ decomposition reaction on overall combustion process of pyrotechnics was also revealed previously [32]. The dominance of R2 in green pyrotechnic despite low concentration of KClO$_4$ in the pyrotechnic was attributed to the exothermic nature of KClO$_4$ decomposition, dependence of the subsequent exothermic magnesium combustion reaction on the R2 reaction, and the Mg-KClO$_4$ equivalence ratio being similar for all pyrotechnic leading to a similar reaction driving mechanism.

In certain cases, the optimization process was observed to result in very small value of the adjustable parameters. Although this value may be quantitatively inaccurate, qualitatively it indicates a low significance of the reaction to the overall process. Similar observation regarding the qualitative nature of the reaction mechanism can be made with higher confidence. The combustion reaction of Mg with KClO$_4$ was found to be the second most dominant reaction in case of red pyrotechnic, while the reaction between Mg and CuO was more prominent for the blue pyrotechnic. In case of green and yellow pyrotechnics, the polymer decomposition was found to be significant.

Contrary to purely numerical regression, this mechanistic deconvolution process assumes a set of reactions based on the composition, stoichiometry, and known thermal response of the individual components of the pyrotechnics. This scheme represents the exothermic reactions responsible for the propagation of combustion through the pyrotechnic bulk and decomposition of additives. Owing to the mechanistic approach, the reported values of optimized parameters are directly dependent on the chosen reaction pathways. Although, a more detailed mechanism consisting of additional reaction pathways may be envisaged, the current reaction mechanism was deemed sufficient for describing the overall combustion of pyrotechnics. Consequently, the proposed dominance of R2 reaction is unlikely to change despite additional modeling. Furthermore, a chemical equilibrium analysis of the pyrotechnics using NASA CEA
4. Uncertainty analysis

The authors have attempted to minimize the experimental error and uncertainty for improving the reliability of the results. Duplicate experiments were conducted for the extreme heating rates to ensure the repeatability of the thermograms and accuracy of the calculated parameters. The experiment was repeated twice for any thermogram showing peculiar variations. The minor variation in the appearance of peaks in the thermograms was attributed to the slight inhomogeneity in the sample and small variations in the particle size distribution. Furthermore, equivalency of the DSC results was established by ensuring the variation in the heat of reaction evaluated by integrating the thermograms to be less than 10%. The kinetic analysis by Starink method was considered accurate as the results satisfied the criteria of $R^2 \geq 0.98$. The results obtained through the numerical optimization were compared against the experimental value and the maximum deviation was found to be approximately 3%.

5. Conclusions

A calorimetric study of four multicomponent pyrotechnic compositions with colored flame used for display pyrotechnics has been reported followed by kinetic and numerical analysis. The Differential Scanning Calorimetry data was utilized to gain an insight into combustion-related chemical kinetics of the pyrotechnics. The calorimetric thermograms for each pyrotechnic indicated a superimposition of the thermo-chemical response of the pure component. This study provides an insight into how the pure component thermal behavior is reflected in the behavior of the mixture. The unsurprising occurrence of multiple simultaneous reactions in complex pyrotechnics was conspicuously quantified from the results of isoconversional analysis. The variable activation energy reported by these methods was found to indicate a complex reaction mechanism and extraction of the constituent reaction kinetics was carried out. A mechanistic deconvolution technique was implemented for elucidating the fundamental steps constituting the overall reactions. The most prominent reaction from the set of proposed reactions was discerned to be the $\text{KClO}_4$ decomposition reaction. The chemical kinetic parameter values evaluated through such a technique would be instrumental in theoretical estimation of the burning rate of the pyrotechnics.

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