VOID COLLAPSE-INITIATED DEFLAGRATION: PROGRESS TOWARDS PREDICTIVE MODELING FOR RISK EVALUATION PT. 2

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ABSTRACT

The unexpected deflagration of explosives and propellants due to the collapse of void-type defects is a matter of paramount concern, impacting both personnel safety and mission success. In munitions systems, high-acceleration events such as target impact or gun-launch are known to rapidly compress void defects such that their entrained gases reach explosive ignition temperatures almost instantaneously. Following ignition, two possible outcomes emerge: quench or sustain. A self-quenching reaction occurs when insufficient heat is generated to support further reaction growth. Such reactions often elude detection and pose no risk to munition functionality or personnel safety. Conversely, a sustained reaction generates ample heat, enabling growth, and depending on its rate, may result in a rapid deflagration that can hinder mission objectives and endanger gun-launch personnel. Emphasizing the refinement of modeling techniques to evaluate safety and survivability risks associated with void-type defects in various energetics is imperative.

Predictive models have been developed, specifically tailored to assess thermal ignition in polymer-bound explosives. The thermal ignition phase is critical as it marks the initial step in potentially weapon-damaging deflagration reactions. Drawing upon Arrhenius kinetic models, commonly used for cookoff predictions in the Insensitive Munitions (IM) field, ignition risk is effectively predicted. The models are validated using a limited dataset collected from innovative hardware designed specifically to gain visual insights into void collapse and thermal ignition. As these models continue to improve, they yield valuable insights into fundamental questions concerning void collapse, defect geometry, and explosive sensitivity. This knowledge, in turn, may inform void collapse deflagration risk assessments, offering potential insights relevant to the Insensitive Munitions (IM) community and enhancing our understanding of warfighter-relevant environments.

INTRODUCTION

Cast-cured polymer bonded explosives (PBX) are commonly employed as the main charge explosives in the bodies of penetrating warheads across various military services globally. The manufacturing process for cast-cured PBXs entails mixing the explosive components under high shear which is suspected to entrain gas in the mix. Sometimes pockets of entrained gas are not able to escape the system prior to cure and remain in the explosive. These are referred to in this paper as they are commonly described: void defects. The complete elimination of entrained gas is not practical under the current manufacturing processes. Instead, acceptance guidelines are used to limit the size and quantity of voids in fielded systems.

Main charge explosives in penetrating munitions are subjected to high pressure mechanical insults during impact events. Because these pulses usually take a half-sine shape, insults can be described in terms of peak pressure and pulse duration. For some penetrating munitions, peaks as high as 300 MPa (43 KSI) have been observed in test. Pressure durations can range from 2 milliseconds to 45 milliseconds. Previous work on the topic has indicated adiabatic compression [1] of void gases as a likely root cause of deflagration for several RDX-based PBXs [2]. The high pressure loads quickly compress the void defects. The gas inside of the defects undergoes rapid heating and can reach temperatures that thermally ignite the RDX in the surrounding explosive materials. Once thermally ignited, the reaction can follow two possible types of trajectories: Self-sustaining or Quenching. Figure 1 illustrates the post-ignition pathways that these reactions typically follow.

It is important to distinguish between what we term *thermal ignition* and *self-sustained* reactions. Thermal ignition refers to the localized ignition of the energetic. Self-sustaining reactions refer to reactions in which a deflagration front is established with the potential to consume the sample completely. These self-sustaining reactions are likely to generate enough pressure to damage the munition they are contained within. Previous work [2] has shown that reaching ignition is not sufficient to obtain a *self-sustaining* reaction. More energy is required past ignition to trigger a *sustained* reaction. *Quench* refers to a reaction where thermal ignition is likely achieved, but where the input energy is not sufficient to continue the burn. In quenching events, the reaction extinguishes and does not generate enough pressure to damage the system.

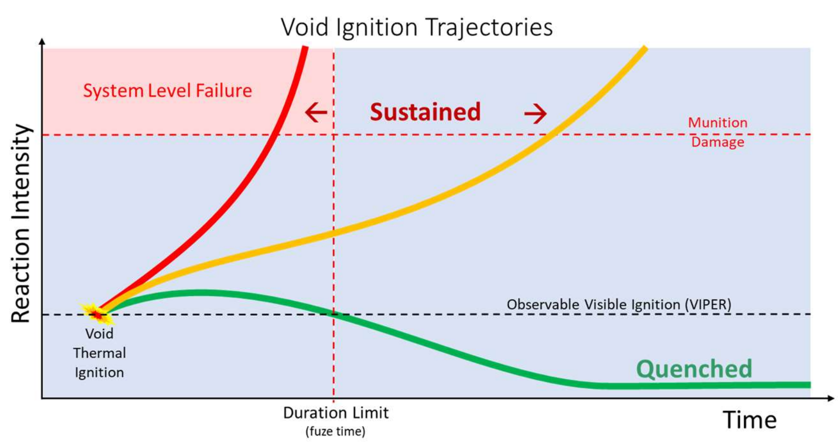

Figure 1. Possible post-ignition reaction trajectories

This paper leverages test data from two types of novel testing designed to expose explosive voids to relevant mechanical insults and perform deflagration root cause analysis. VIPER (Visible Insight for Penetrator Explosive Risk) and LIGER (Long-duration Ignition and Growth of Reactions). Both test types apply relevant pressures magnitudes, durations, and rates on the explosive by way of variable weight/height drop tower. A polycarbonate window in the VIPER test allows the void to be observed as it is compressed but it limits the maximum pressure achievable. The LIGER test can achieve higher pressures but does not allow the void to be observed during compression. In both tests, the explosive pressure is measured through transducers both above and below the explosive defects. The explosive defects for each test are cast in the desired defect shape into the two halves of the sample (LIGER) or into the single half of the sample (VIPER). As previously mentioned, the VIPER test allows for direct visual observation of the explosive response to a mechanical insult. Some still frames from high-speed video showing a typical void defect response to pressure loading are shown in Figure 2.

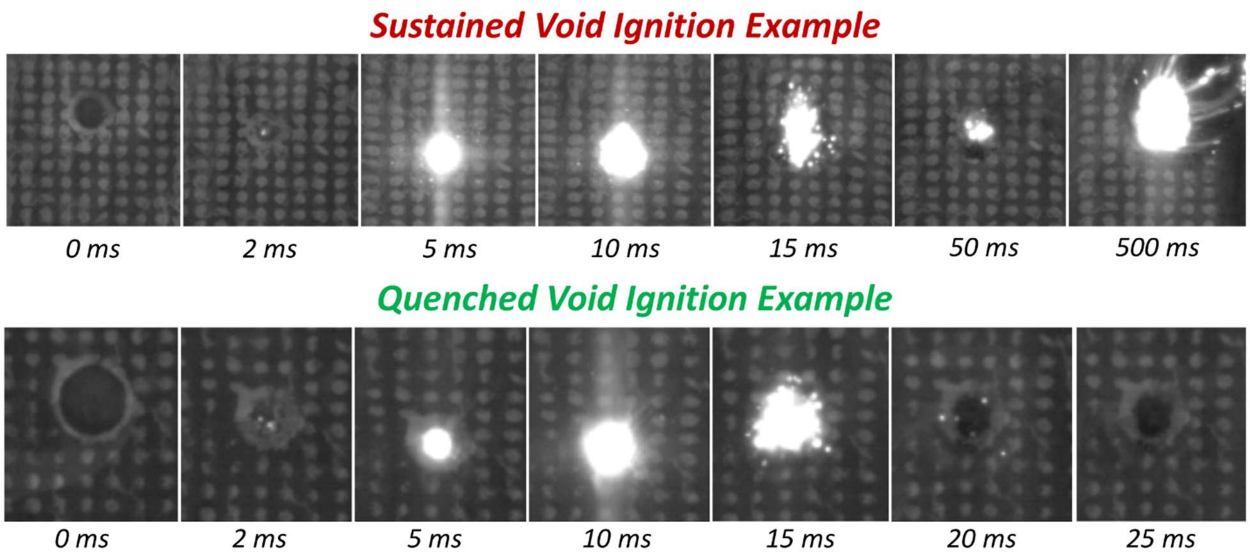

Figure 2.Examples void ignition reactions from Visible Insight for Penetrator Explosive Risk (VIPER) test

Of concern to this work is a single RDX based aluminized PBX containing ammonium perchlorate (AP). The relative composition of this explosive, termed Explosive 1 (E1) is shown in Figure 3. E1 will be referred to throughout this paper.

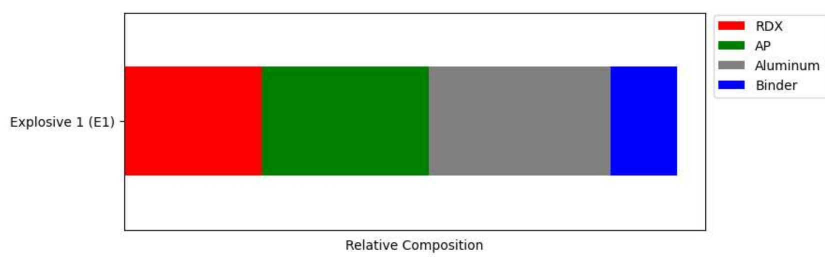

Figure 3. Explosive Composition

Previous work [3] leveraged high-speed video data, like shown in Figure 2, to estimate the void thermo-physical conditions leading up to the first visible sign of ignition. The result of this work has uncovered an empirical relationship between the applied pressure load and the apparent gas temperature inside the void defect over range of test shots. These relationships were derived by assuming that these voids are composed of ideal gas air at standard atmospheric conditions (5,200 ft altitude), and that the void compression can be modeled as an adiabatic compression event. The empirical relationships observed between applied pressure and estimated temperature are shown in Figure 4. The data shown in Figure 4 was collected in VIPER tests between the years 2020 and 2023, using void defects between diameters 0.25" and 1.0", and utilizing peak pressures up to 6 KSI (kilo pounds per square inch) and loading durations up to 12ms. The general relationship between applied load and estimated temperature is appears to be linear and may have a void size dependence. Using the apparent linear relationship, a pressure time-history can be converted into an estimated temperature time history and the temperature at visible ignition can be estimated as shown in Figure 5.

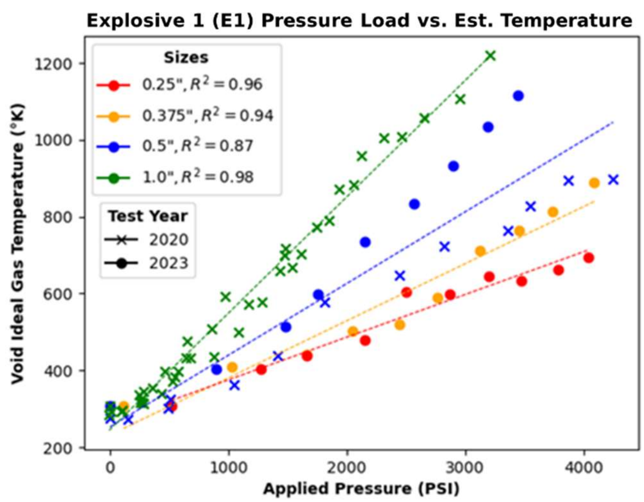

Figure 4: Empirically Derived Mechanical-Thermal Relationship During Void Collapse Prior to Ignition [3]

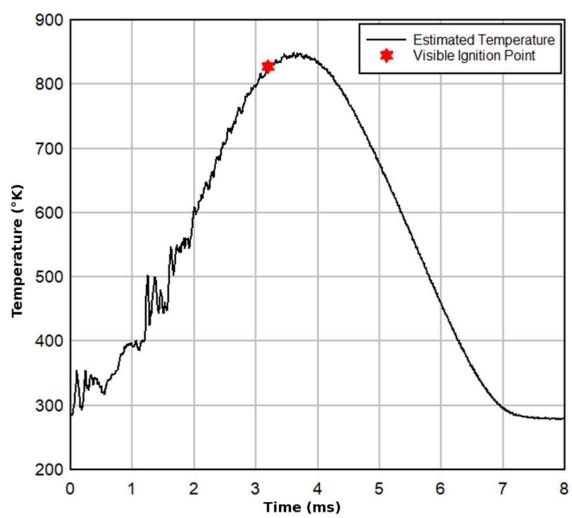

Figure 5: Example estimated temperature time-history

While the VIPER data provides insight for ignition, the LIGER tests help distinguish between the two reaction growth trajectories. A sample of higher-pressure LIGER data collected on E1 is shown in Figure 5. are expected to have ignited but extinguished without developing significant pressure. The red sustain points represent applied loads that generated self-sustained reactions that generated enough pressure to burst the pressure relief feature. A notional sustain/quench threshold is depicted which separates the responses.

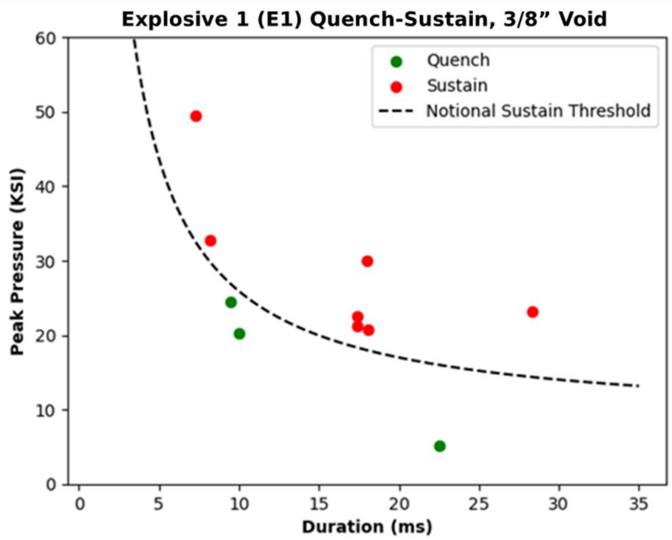

Figure 6: Quench-Sustain Example

BACKGROUND

Previously [3], the focus of void collapse ignition modeling was on the study of the relationship between applied load and estimated temperature, as shown in Figure 4. In this work, the focus is turned on the analytical estimation of an ignition threshold and efforts directed at understanding the barrier between visible ignition and reactions that eventually grow into weapon-damaging events. Although understanding of the sustain threshold is a long-term goal for this program, the primary focus of this work is on the study and development of models that predict the thermal ignition.

VOID COMPRESSION

Through the adiabatic assumption, the void compression ratio can be directly related to void gas pressure, temperature, and available thermal energy. Figure 7 shows that for moderately low compression levels, the thermal energy available in the void exceeds the mass specific activation energies for RDX [4], found by dividing the activation energy by the molar mass of the energetic.

Although the energy density of the void gas can exceed the activation energies at these low levels, heat transfer lag will play a significant role in determining the actual ignition energy level.

$$E_m\left(\frac{kJ}{kg}\right) = \frac{E_a\left(\frac{kJ}{mol}\right)}{MW\left(\frac{kg}{mol}\right)} \tag{1}$$

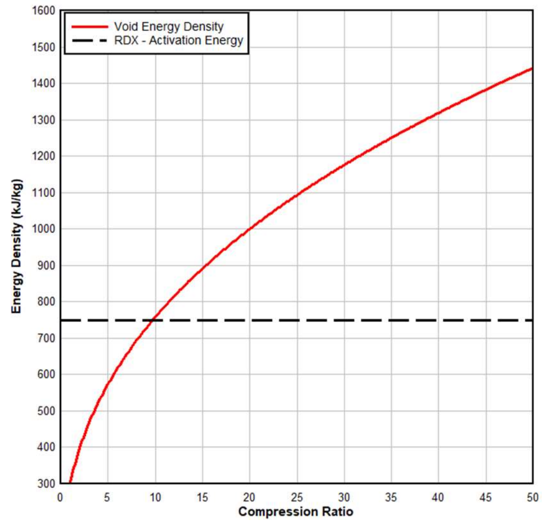

Figure 7: Void Collapse Thermal Energy

THERMAL IGNITION

The thermal ignition of energetic materials is typically modeled using an Arrhenius kinetic model that relates the energetics' temperature to the characteristic reaction time. Two such models for RDX, one based on experiment [4] and one based on high fidelity molecular dynamics simulations [5], are shown in Figure 8. The temperatures expected during void collapse ignition are outside the fitted range for both models. Reaction kinetics models for explosives with ammonium perchlorate (E1) are generally unavailable in the literature.

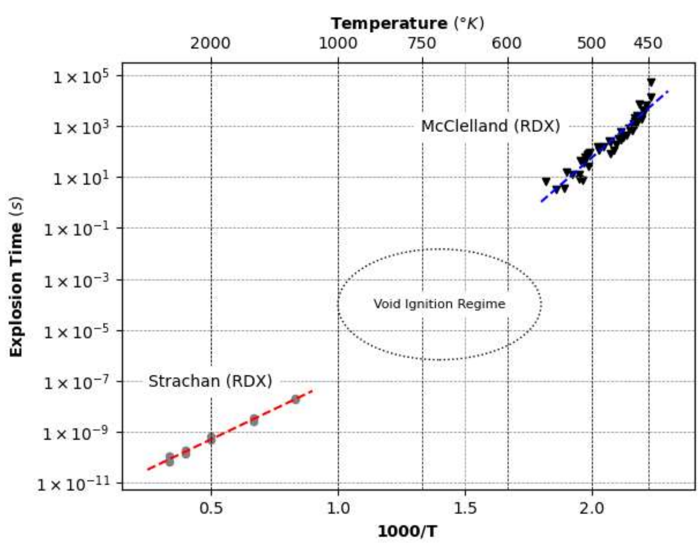

Figure 8: RDX Reaction Kinetics Models [4] [5]

IGNITION RISK MODEL DEVELOPMENT

By establishing a link between the input loading and the void thermal response for each explosive, a model for the ignition threshold can be developed. We start with the linear relationship between the applied loading and the observed ideal gas temperature, as depicted in Figure 4.

$$T(P) = \alpha + \beta P \tag{2}$$

The applied pressure time history can be expressed as a half sine pulse of given pressure magnitude (P_m) and duration (ω).

$$P(t) = P_m \sin(\omega t) \tag{3}$$

These functional forms can be combined with the Arrhenius kinetic model to yield and estimation of the time until ignition as a function of time where E_n is the normalized activation energy E_a/R and Z' is the natural logarithm of the pre-exponential factor.

$$\tau(t) = e^{\frac{E_n}{\alpha+\beta P_m sin(\omega t)} - Z'} \tag{4}$$

Due to the challenges of estimating the heat transfer at the void-explosive boundary, a simplification is to define an *available* time for ignition that this estimate must be within. Equation 5 expresses the available ignition time as the time up until the peak of the pressure pulse.

$$r_t(t) = \frac{\pi}{2\omega} - t \tag{5}$$

Equations 5 and 6 are visualized in Figure 9, where the overlap of the two curves indicates high ignition probability.

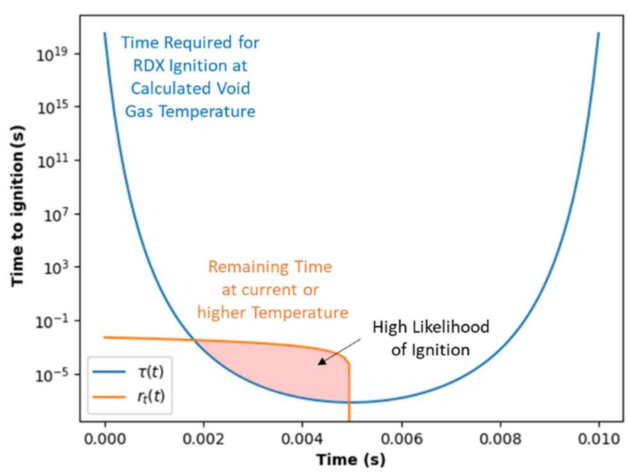

Figure 9: Ignition time availability

An ignition threshold may be described as a function $P_m(\omega)$ that ensures equality and tangency of Equations 4 and 5 at only one point. Through numerical experimentation, it has been found that the function given by Equation 6 satisfies these conditions.

$$P_m(\omega) = \frac{1}{\beta sin\left(\frac{\pi^2}{8}\right)}\left[\frac{E_n}{ln\left(\frac{\pi}{\omega}\right) + ln\left(\frac{4-\pi}{8}\right) + Z'} - \alpha\right] \quad (6)$$

That is, the ignition threshold is a function of the pressure pulse duration, reaction kinetics parameters, and the slope of the observed mechanical-thermal response curve. It should be noted that this is an *ignition risk model* that, given a certain pressure load duration, predicts a peak pressure that will likely result in visible ignition of the explosive. It does not predict the pressure *at ignition*.

RESULTS

EXPLOSIVE 1 (E1): IGNITION THRESHOLD

A body of VIPER data for E1 has been collected over the last three years, which can be used to assess the quality of the developed ignition model. This includes voids of different shapes which are exposed to different pressure environments. This data can be thought of as an out of sample test of the developed model. Due to the apparent *void-size-effect* seen in E1 shown in Figure 4, a different ignition threshold is determined for each void size. These ignition thresholds have been developed based on the single step kinetic model specified by AFRL [6].

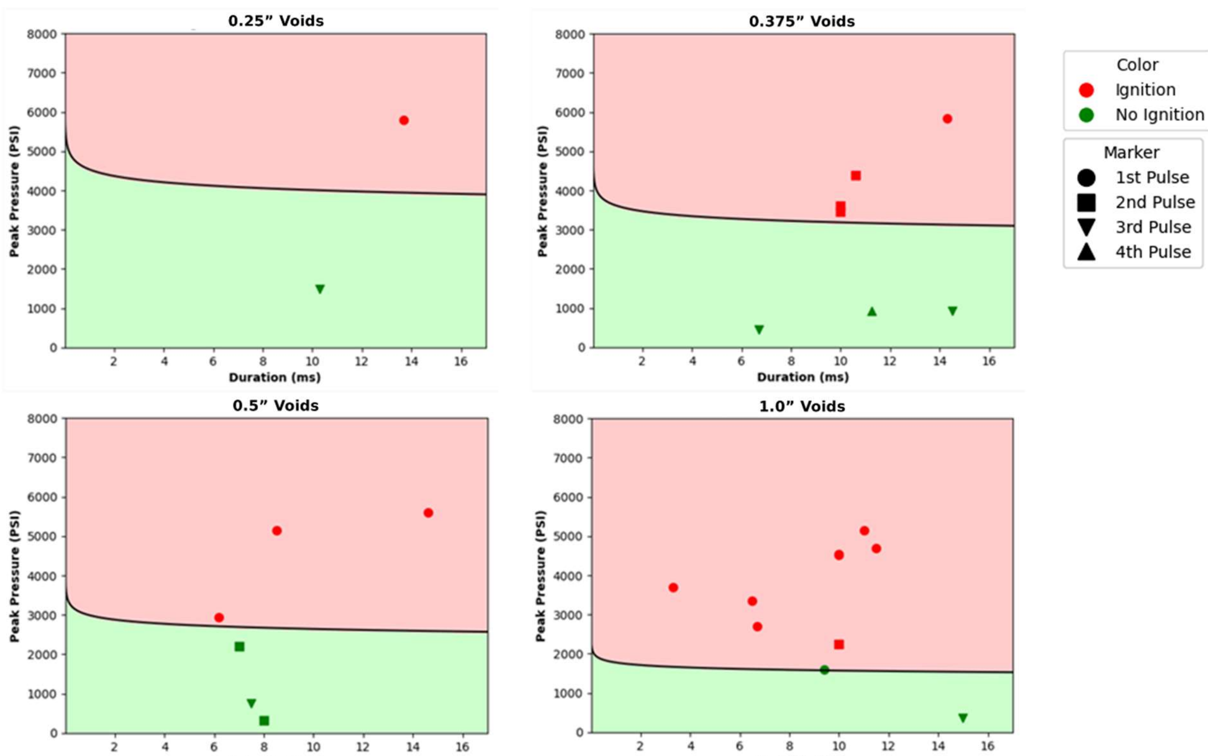

Figure 10: E1 Ignition Thresholds (a) Top left - ¼" Voids, (b) Top right - 3/8" Voids, (c) Bottom Left - ½" Voids, (d) Bottom Right – 1" Voids

Figure 10 depicts the predicted ignition threshold for all tested void sizes for E1. Alongside the ignition threshold model, we have plotted go/no-go ignition data across a variety of VIPER tests. These individual datapoints represent the *pulse shape* that resulted in an ignition; they do not represent the ignition pressure. Additionally, secondary pulses (secondary impacts of the drop weight [2]) have been included. Validation of the ignition thresholds can be done in part through the analysis of points near the boundary. More test data exists for both 0.5” and 1” voids, where the predicted ignition thresholds are generally observed.

DISCUSSION

THRESHOLD PROXIMITY

As mentioned previously, the ignition threshold is not a point in time prediction of the ignition pressure. Rather, it is a risk threshold for a given *pulse shape.* Figure 11 shows pressure measured during the compression of three pill-type voids, whose data was not used to inform model development.

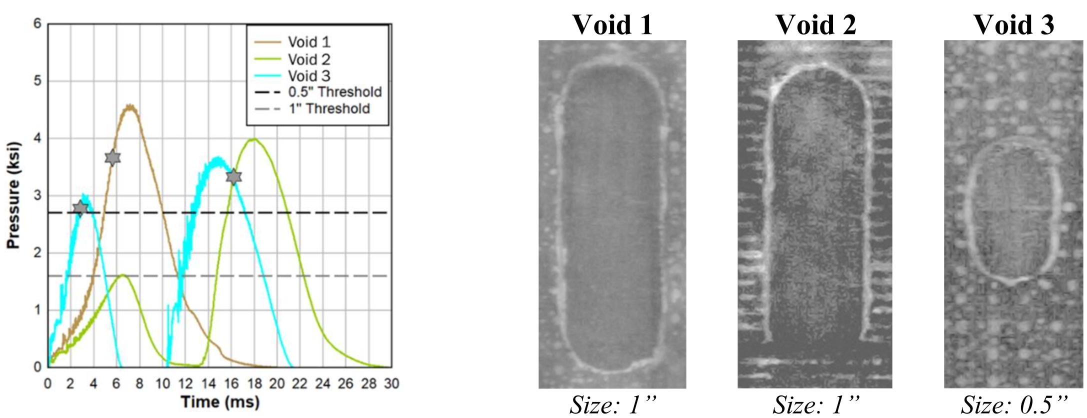

Figure 11: Pressure, Ignition Point, and Threshold Example

Although the shape of these voids does not favor the use of diameter as a measure of their size, the mechanical responses (see Figure 4) are in family with the sizes specified by their *width* (this is not shown for brevity). For example, Void 1 is 1” wide, and it’s mechanical response is in family with the 1” spherical void responses. It is for this reason that we will use the 1” threshold for these voids, because the threshold depends primarily on the mechanical response curve.

Figure 11 illustrates some nuances around the ignition threshold. Firstly, for Void 1 and Void 2, the actual ignition point occurs well above the threshold. Whereas for Void 3, the ignition point occurs very close to the threshold. This shows how the ignition threshold is not a prediction of the ignition pressure, but a risk threshold for a given pulse shape. Only when the pulse shape is very close to the threshold (Void 3, Void 2 first pulse), can we expect the ignition threshold to be a decent estimate of the ignition pressure.

We can also compare the second pulse from Void 1 (not pictured in Figure 11), which had an ignition, with the first pulse from Void 2, which did not have an ignition. These pulses were very similar in duration, but the second pulse from Void 1 was well above the ignition threshold, as shown in Figure 12.

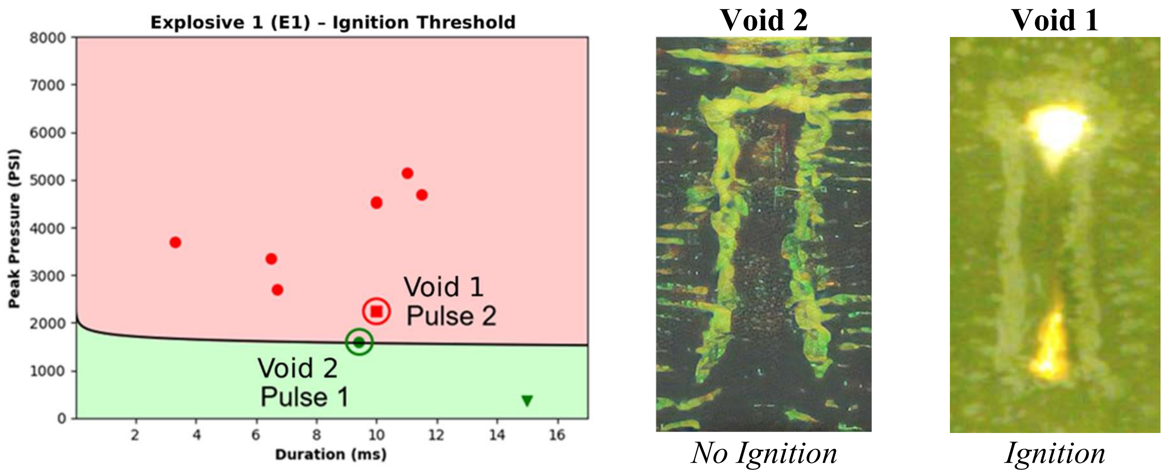

Figure 12: Void Shots above and below ignition, E1, 1" Class Voids

The difference in peak pressure between these two pulses was about 650 PSI, both with similar durations. Void shots just above and below the predicted ignition threshold, as depicted in Figure 12, are evidence for the local accuracy of the ignition threshold for a given void size. However, limited data in both the low and high duration pulse regimes makes it hard to validate the model across a wider range of pressure environments.

IMPLICATIONS ON QUENCH-SUSTAIN BEHAVIOR

Up to this point, the modeling effort has been concerned with predicting ignition risk for a given pulse shape. However, the apparent linear relationship between applied load and estimated temperature can be further leveraged to gain insight into the relationship between thermal energy and the quench-sustain behavior of void defects exposed to higher magnitudes of mechanical insult than available through VIPER testing. A simple, lumped analytical convection heat transfer model that only considers the specific heat of the energetic and the temperature of the void gas is considered. Similarly, we can compare this analytical model to a more complex FEM model under less strict assumptions. In the FEM model, a 1D simulation is considered with a convection boundary condition and the thermal properties of RDX. The results of these two models, across a range of pressure pulses, is shown in Figure 13.

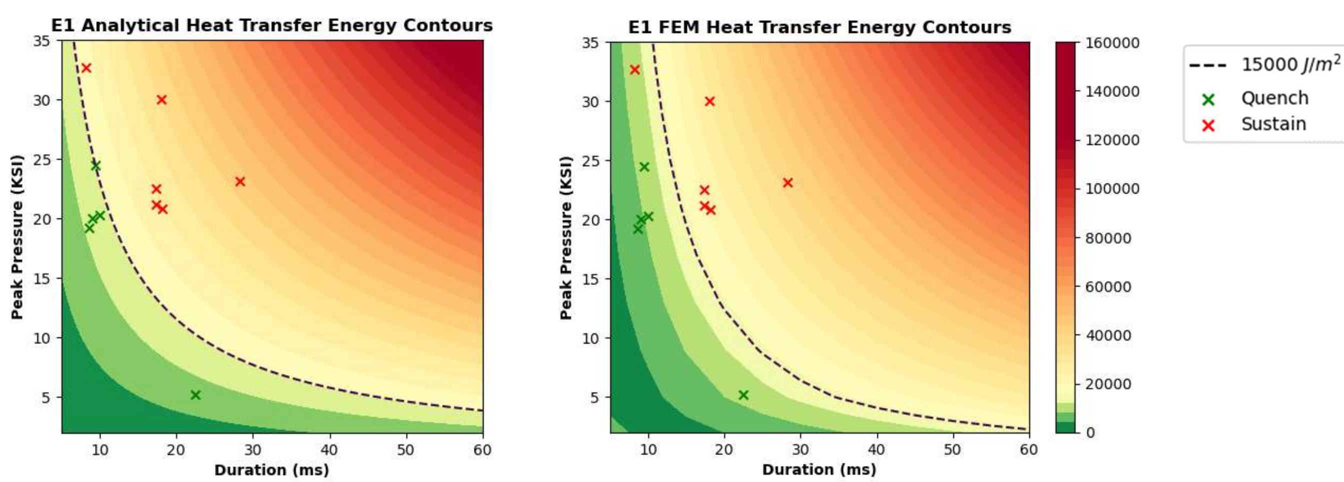

Figure 13: Heat transfer energy contours for (a) analytical model and (b) FEM models

Both models shown in Figure 13 seek to model the energy transferred between the void gas and the energetic. These heat transfer simulations were carried out using the 0.375” void size linear fit parameters from Figure 4, as well as a value of 500 W/m^2 for the convection coefficient. The quench-sustain test data that is plotted alongside the contours comes from single impact LIGER tests from 2020. The analytical model resolves the energy contours completely across the peak pressure and duration of pulses shown in Figure 13. Conversely, the FEM model has been evaluated at distinct grid points in pressure-duration domain, and the resulting contours are linear interpolations between those points. These simulations show that a line of constant energy may be capable of classifying between quenching and self-sustaining reactions. For both the analytical and computational (FEM) models, the 15 kJ/m^2 energy line is shown as a notional energy level needed to achieve self-sustaining reactions. For a void of 0.375”, this is equivalent to an energy of approximately 4.3 Joules. It is important to note that the selection of the convection coefficient is notional and the resulting energy lines are geared towards determination of a theoretical reason for the apparent ability of pressure impulse iso-contours to classify between reaction types; rather than an explicit prediction of required energy for RDX. With further LIGER testing at pulse durations above 20ms, it may be possible to fit a threshold line to the data, which could be used to back-calculate the implied linear coefficients of the mechanical-thermal response curve (Figure 4). This curve could then be directly compared with the curves observed in the VIPER data for a means of further model validation.

CONCLUSION

Models that predict the void-collapse-induced thermal ignition and deflagration of RDX based PBXs are being developed. A relationship between the applied load and the estimated ideal gas temperature was established with visible void collapse sub-scale test data. These relationships were leveraged to develop an analytical model for the prediction of ignition risk for the PBX of concern. Ignition risk model was validated using data that was not used in model fitting. Beyond ignition modeling, the observed mechanical-thermal relationship may be used in the assessment of the difference between insults that yield quenching vs. self-sustaining reactions. Two heat transfer model approaches were presented, which both show promise of being able to classify between these reaction types by a certain total heat transfer energy.

Upon establishing a theoretical or empirical understanding of the quench-sustain threshold, it may be possible to predict these phenomena for a wider variety of un-tested explosives, as well as begin to predict the timing of deflagration run up to a weapon damaging event.

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