

# DDT run-up distance for stoichiometric hydrogen-methane-oxygen

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## 1 Introduction

Metal tubes equipped with repeating obstacles are typically used to study flame acceleration and DDT in fuel-air mixtures initially at 1 atmosphere. Peraldi et al. identified the steady choked-flame (or fast-flame) and quasi-detonation propagation regimes and proposed the DDT limit criterion  $d \geq \lambda$ , where  $d$  is the orifice diameter and  $\lambda$  is the detonation cell size [1]. Detonation propagation was inferred from a measured average velocity greater than the product speed of sound, roughly one-half the CJ detonation velocity ( $1/2 V_{CJ}$ ). Rainsford and Ciccarelli [2] performed experiments in a polycarbonate tube equipped with orifice plates using high-speed photography to study steady combustion front propagation. The flame propagation distance required for transition to detonation, i.e., DDT run-up distance represents an important fundamental parameter that is also relevant to explosion safety. Hashemi and Ciccarelli [3] used high-speed visualization in a polycarbonate tube to obtain the DDT run-up distance for ethylene-oxygen-nitrogen mixtures, as well as for argon-diluted hydrogen-oxygen mixtures. They found that for the most reactive conditions (highest initial pressure) tested, the measured DDT run-up distance,  $X_{DDT}$ , was successfully predicted by the Silvestrini et al. correlation [4]:

$$\left[ \frac{X_{DDT}}{D} \right]_{BR} = \frac{1}{0.006(\sigma-1)} \left( \frac{0.15}{D} \right)^{0.4} \ln \left( 0.077 \frac{V_{CJ}}{\sigma S_L} \right) \left( \frac{1}{1+15BR} \right) \quad (1)$$

where  $\sigma$  is the density ratio across the flame,  $S_L$  is the laminar burning velocity, and  $BR$  is the obstacle area blockage ratio. However, the measured  $X_{DDT}$  was consistently larger than the prediction for the lower initial pressure tests corresponding to less reactive conditions. It was proposed that Eqn. (1) could be used for the flame acceleration distance to  $1/2 V_{CJ}$ , an additional "DDT induction" distance, governed by the detonation cell size and effective activation energy, is required to predict the DDT run-up distance [3]. Specifically, the DDT induction distance decreases with increasing mixture reactivity to zero for the most reactive condition, i.e., highest initial pressure. The objective of this study is to extend the study reported in [3] by capturing more detailed flame velocity measurements in order to investigate the DDT induction distance. Stoichiometric hydrogen-methane (0% to 100% methane) in oxygen was studied because of its importance to power generation applications and wide range in detonation cell structure regularity; argon-diluted hydrogen-oxygen was also tested to further increase the range.

## 2 Experimental

The 283.5 cm long combustion chamber consisted of two-mated polycarbonate cylindrical tubes with an inner-diameter of 7.6 cm was equipped with repeating orifice plates. For most tests ignition was from a standard automotive glow plug, but for the least reactive mixture conditions it was combined with a coil-over-plug spark ignition system. The 1.27 cm thickness orifice plates had an inner-diameter of 5.3 cm (50% blockage area), and were equally spaced at one tube diameter. The last 1 m of the tube was free of orifice plates. A Photron SA5 captured the combustion wave luminescence in the field-of-view from the ignition endplate to the 19<sup>th</sup> orifice plate. The frame rate and shutter speed for the Photron SA5 was varied from 75,000 fps to 175,000 fps and 0.37  $\mu$ s to 7.82  $\mu$ s, respectively. The shutter speed was selected based on the intensity of the combustion luminosity. For very low combustion luminosity intensity, it was difficult to measure the flame propagation speed, hence the more light-sensitive Photron SAZ camera was placed closer to the tube covering a smaller field-of-view that included the first nine orifice plates. Tests were performed with stoichiometric hydrogen/methane/oxygen, i.e.,  $(1-x) \text{H}_2 + x \text{CH}_4 + 1/2(1+3x) \text{O}_2$ , where the methane fuel content tested was  $x = 0, 0.25, 0.5, 0.75$  and 1. In addition, tests with stoichiometric hydrogen-oxygen with 40% argon dilution were performed because of its very regular detonation cell structure. The initial pressure was varied between 5-40 kPa absolute to control the mixture reactivity. A soot foil inserted into the end of the tube, well after the last orifice plate, was used to measure the average detonation cell size. In some limited tests, a flat soot foil was placed across the tube diameter between orifice plates located around the DDT location observed in the video.

### 3 Results and Discussion

Figure 1 shows an x-t diagram obtained by plotting a series of video frames from a test. Yellow dotted lines track the leading edge of the combustion wave, the slope of the line represents the average propagation velocity between orifice plates. The light emission from the flame near the ignition end is very faint and the flame is difficult to track. Once a strong shock develops ahead of the flame, e.g., after orifice plate #9 (OP6), shock reflection off the orifice plate face produces a reflected shock wave that converges at the centerline. This shock focusing increases the temperature of the combustion products, producing a more intense local light emission along the centerline (see red dotted line between OP9-10). A detonation initiates following shock reflection off the face of OP11, producing a strong nonreactive shock (retonation) that propagates through the products towards the ignition end (see solid red line between OP10-11). Before this point, the flame accelerates to a maximum velocity of 1218 m/s, after this point the combustion front velocity is steady at roughly 2300 m/s, indicative of detonation propagation. The DDT run-up distance is defined as the axial distance from the igniter to the location where detonation initiates for the first time, i.e.,  $X/D=11$  for this test. The detonation decouples as it diffracts after the orifice plate, evidenced by a sudden drop in light intensity after OP11, and then reinitiates following shock reflection at OP12. This cycle of detonation failure and initiation continues through the rest of the tube; for this test, detonation initiation alternates from the top to the bottom of the orifice plate.

In order to verify the DDT location determined by high-speed video, some limited tests were carried out with a flat soot foil placed across the tube diameter near the DDT location. There was no damage to the foil since the fast flame was axisymmetric, and DDT always occurred following uniform shock reflection across the orifice plate face. Photos of soot foils from different tests with stoichiometric hydrogen-oxygen at 10 kPa are provided in Fig. 2. Soot foils placed before OP8 showed no distinguishable features. The foil between OP10 and 11 shows cell structure in the triangular region bounded by the tube wall and the orifice plate face. The diagonal irregular-edge of the triangular region corresponds to the flame position when traversed by the detonation wave propagating away from the orifice plate upstream surface. The detonation cells in the region are extremely small because the detonation wave propagates into a pre-compressed gas region. Outside these two regions there are streaks indicating a strong flow. For the OP8-9 and OP9-10 foil, a similar smaller triangular region appears but there is no discernible cell structure within. These tests with foils confirm the DDT location of OP11 interpreted from the video frames in Fig. 1.

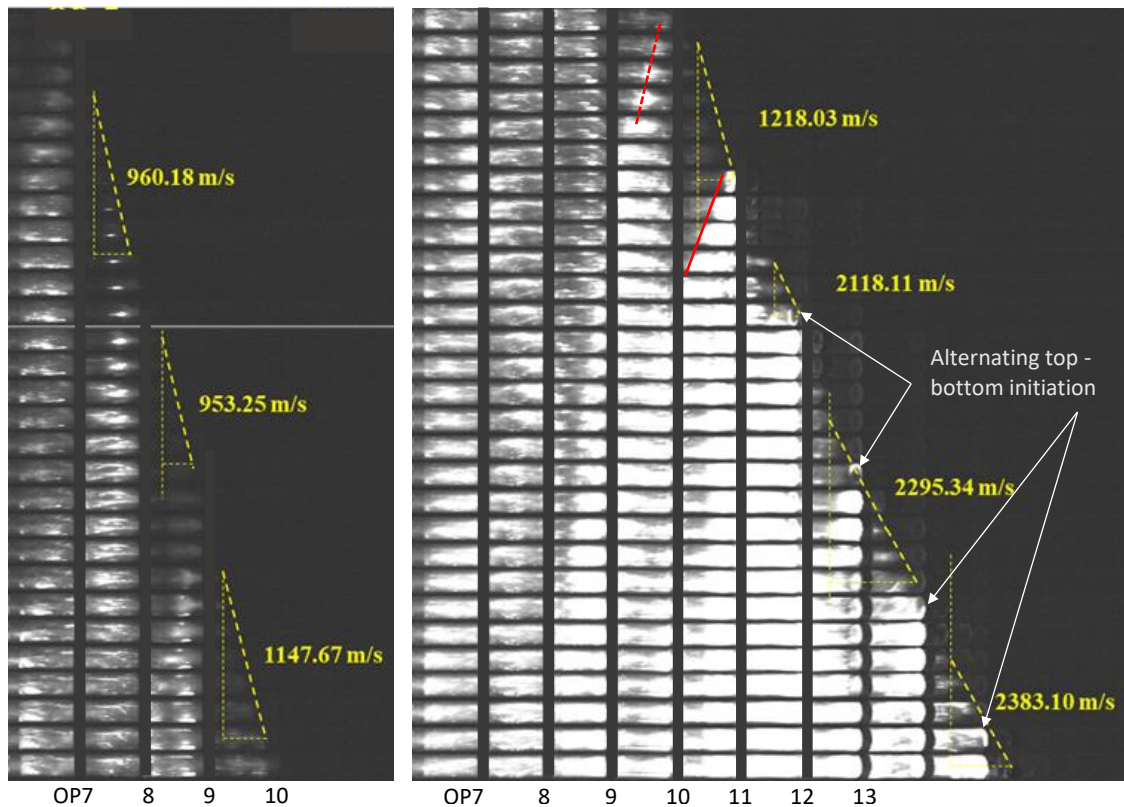


Figure 1: X-t diagram from video frames recorded at  $7.3 \mu\text{s}$ , showing DDT at OP11 for stoichiometric hydrogen-oxygen at initial pressure of 10 kPa.

The average flame velocity between orifice plates was deduced from the straight line that best fit the flame tip position versus time. Average velocity versus distance (normalized by the tube diameter) for stoichiometric hydrogen-oxygen and at different initial pressures is plotted in Fig. 3a; the velocity is assigned to the downstream orifice plate location. The data points correspond to the average from three different tests performed at the same condition, the error bars correspond to the minimum and maximum values. In all tests, onset of detonation occurred following shock reflection off an orifice plate similar to that observed in Fig. 1. The DDT location for each initial pressure test, deduced directly from analysis of the video, is denoted by a circle around the data point corresponding to the DDT axial position. For stoichiometric hydrogen-oxygen at pressures of 9 kPa and above, there is a clear jump in velocity to a quasi-steady velocity just below the CJ detonation velocity, see Fig. 3(a). This jump in velocity coincides with the DDT location observed directly from the video. For pressures between 6 and 8 kPa, there is only a mild increase in velocity above the products speed of sound following DDT. For 5 kPa the flame velocity stabilizes below the products speed of sound and there is no DDT observed in the video.

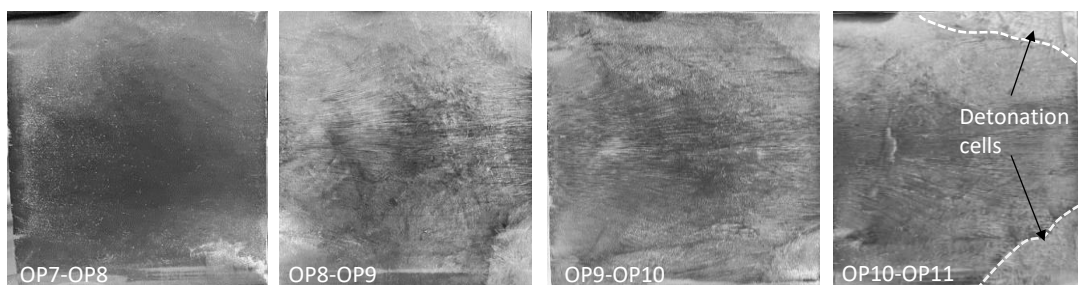


Figure 2: Flat soot foils placed across the diameter between orifice plates for  $2\text{H}+\text{O}_2$  at 10 kPa

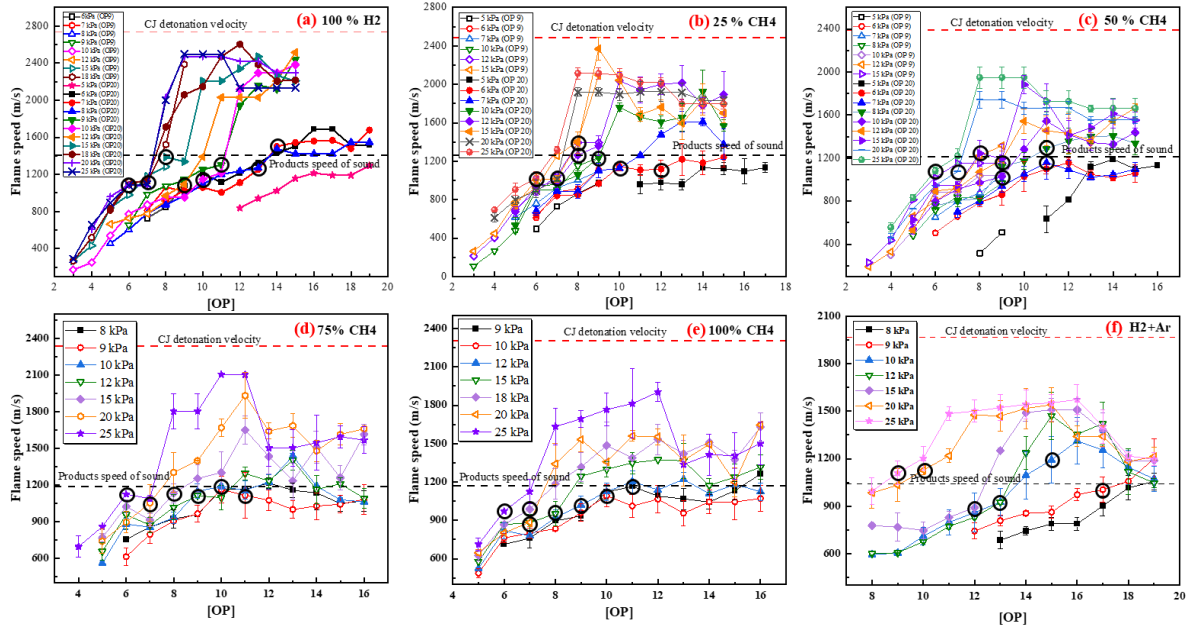


Figure 3: Combustion front velocity for different initial pressures, a) 100% H<sub>2</sub>, b) H<sub>2</sub> diluted with argon, c) 25% CH<sub>4</sub>, d) 50% CH<sub>4</sub>, e) 75% CH<sub>4</sub>, f) 100% CH<sub>4</sub>. Circles denote detonation onset. Error bars represent range in velocity measured for three different tests. Dotted lines represent the CJ detonation velocity and the speed of sound in the products for a constant pressure/enthalpy process.

The same flame acceleration and DDT behaviour is observed for the four mixtures with methane in Fig. 3 (b)-(e). For the lowest pressure where DDT was observed in the video, the average velocity does not increase above the products speed of sound. This is because the detonation generated at the orifice plate face immediately decouples during diffraction through the orifice plate, so the DDT does not contribute to increasing the average velocity between the orifice plates [3], i.e., the fast-flame leading shock wave controls the average velocity. Since methane is less reactive than hydrogen, for 75% and 100 % CH<sub>4</sub>, the DDT limit is larger, i.e., 8 kPa.

The normalized DDT run-up distance ( $X_{DDT}/D$ ) is plotted in Fig. 4 (a). DDT occurred sufficiently fast that flame interaction with the end wall reflected shock wave does not play a role in DDT. In general,  $X_{DDT}/D$  decreases monotonically with increased initial pressure. The DDT run-up distance for argon-diluted stoichiometric hydrogen-oxygen is significantly larger because of the smaller density ratio across the flame (lower energy content) that governs flame acceleration. For the other mixtures, the data essentially merges above 15 kPa; for pressures below 15 kPa the shortest DDT run-up distance corresponds to the 25% CH<sub>4</sub> mixture and longest is for 100% H<sub>2</sub>. Although hydrogen has a significantly higher laminar burning velocity than methane, the addition of methane to hydrogen makes the flame density ratio larger, compensating for the reduction in laminar burning velocity.

Also shown in Fig. 4a is the  $X_{DDT}/D$  predicted by the Silvestrini et al. [4] correlation (solid lines). The correlation is based on DDT data obtained in smooth tubes that was extended to rough tubes by including a blockage ratio term. The correlation, given in Eqn. (1), includes the flame density ratio and laminar burning velocity that were calculated using Chemkin and the GRI-Mech 3.0 [5]. The correlation consistently under predicts the experimental data, see Fig. 4 (b), with good agreement at the highest initial pressure. For the methane containing mixtures, the correlation predicts very little influence of initial pressure on  $X_{DDT}$ , and for the hydrogen-only mixtures, the effect at lower pressure is much less than that observed in the experiment. A head-to-head comparison of the experimental DDT run-up distance with that predicted by the Silvestrini et al. correlation is provided in Fig. 5 (a), where the straight line corresponds to a perfect match. The data points approach the line with increasing initial pressure (for each mixture the upper data point corresponds to the limit), similar to that observed in Fig. 4 (b).

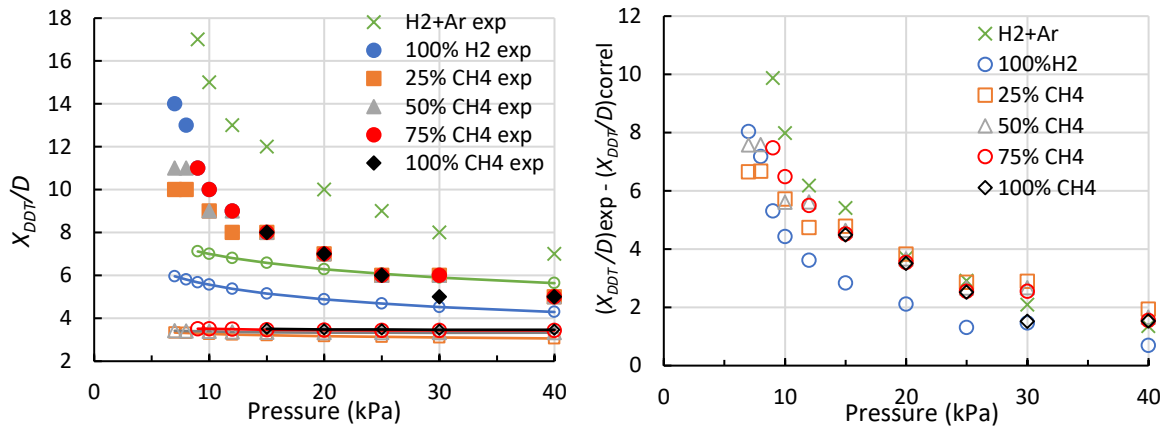


Figure 4: a) Normalized  $X_{DDT}$  versus initial pressure - experimental (symbols), Silivstrini correlation [4] -symbol line, b) the difference between the experimental and calculated DDT run-up distance.

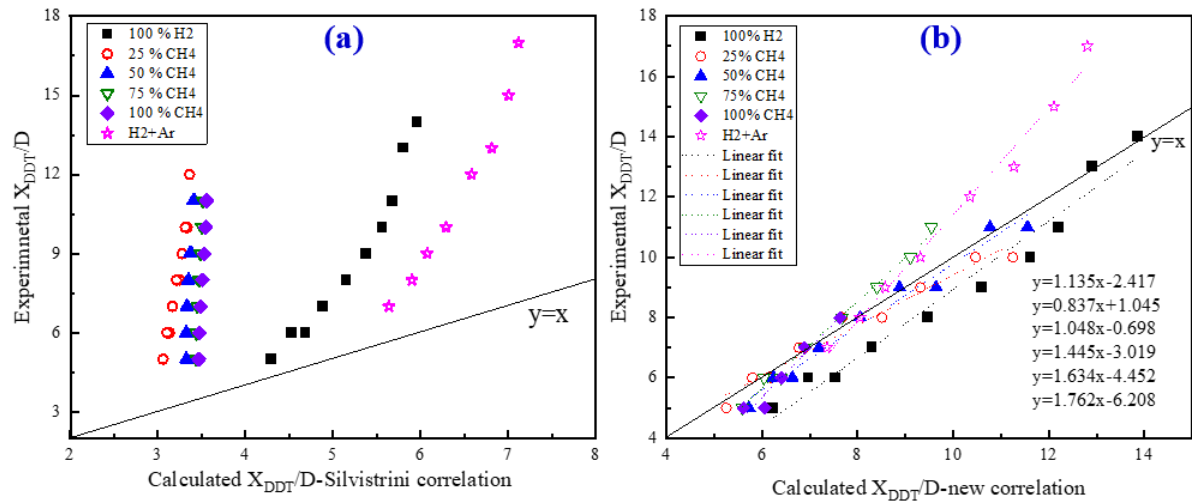


Figure 5: Comparison between the experimental and predicted  $X_{DDT}/D$  using correlation in a) Eqn. (1) [4], b) Eqn. (2) proposed in this study.

The Silivstrini et al. correlation, Eqn. (1), does not include the detonation length scale, i.e., the cell size, as a parameter. However,  $X_{DDT}/D$  plotted versus the inverse of the detonation cell size (normalized by the orifice diameter) in Fig. 6 shows a clear dependency. Similar to that found for ethylene-oxygen-nitrogen mixtures [3], the data from this study fits very well with a power law. The cell size was obtained assuming a linear relationship with the ZND reaction zone length, calculated using the SDToolbox [6] and the GRI-Mech 3.0 [5]. The linear proportionality constant  $A$  for each mixture was obtained based on cell size measured at two initial pressures. For all the non-diluted mixtures,  $d/\lambda$  evaluated at the lowest initial pressure resulting in detonation, was close to unity, in agreement with [1]. For the argon-diluted hydrogen-oxygen,  $d/\lambda$  was 3.4 at the DDT limit. This is in agreement with previous work that showed that for mixtures with regular cell structure the critical  $d/\lambda$  is larger than one, but the effect was not as significant as reported in [7], most likely because they did not make direct observations of DDT.

As proposed in [3], the DDT run up distance is the sum of the distance required to establish a fast-flame propagating at roughly the speed of sound of the products (or  $1/2V_{Cf}$ ) and the DDT induction distance that takes into account the time required for the critical condition for DDT to be established. Unlike the flame acceleration, the induction distance is governed by the detonation cell size and regularity; the latter is quantified by the effective activation energy  $\theta = E_a/RT_{vN}$ , where  $T_{vN}$  is von Neumann post-shock temperature. The effective activation energy was obtained for all the test conditions using the sensitivity of the constant volume reaction time to a  $\pm 2\%$  variation of the initial temperature taken as  $T_{vN}$ . Based

on the cell size and effective activation energy evaluated for each test condition (mixture composition and initial pressure) the following correlation was obtained from Matlab fitting:

$$\frac{X_{DDT}}{D} = \left[ \frac{X_{DDT}}{D} \right]_{1/2 V_{CJ}} + 0.054 \left( \frac{2316}{d/\lambda} \right)^{\theta^{-0.21}} \quad (2)$$

where  $\left[ \frac{X_{DDT}}{D} \right]_{1/2 V_{CJ}}$  is the Silvestrini et al. correlation. This is the same correlation as in [3] but different empirical constants. A comparison of the DDT run-up distance predicted by Eqn. (2) with the measured values is provided in Fig. 5(b). The correlation does an excellent job of collapsing the experimental data to a spread of about 20%.

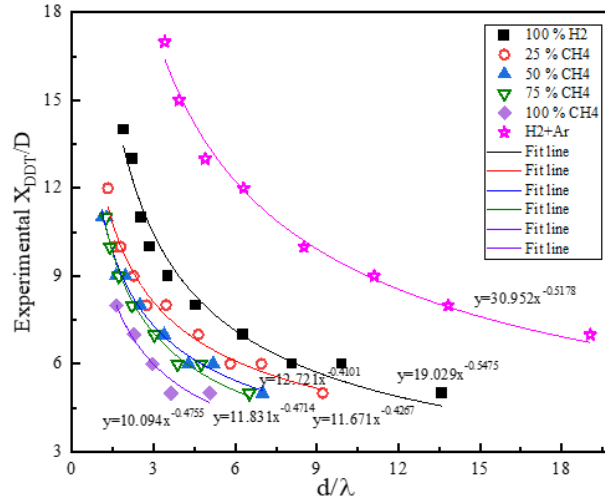


Figure 6: Experimental DDT run-up distance versus  $d/\lambda$  with curve fits.

## 4 Conclusions

Experiments were performed in an obstructed round tube to measure the DDT run-up distance using high-speed photography for stoichiometric hydrogen-methane-oxygen mixtures. For each mixture, the DDT run-up distance was found to monotonically decrease with the increase of initial pressure, or  $d/\lambda$ . A correlation was proposed based on the concept that the DDT run-up distance consists of a flame acceleration distance and a DDT induction distance that is governed by the detonation cell size and the effective activation energy, which represents the cell size sensitivity to temperature.

## References

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