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## DDT in fuel–air mixtures at elevated temperatures and pressures

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**Abstract** An experimental study was carried out to investigate flame acceleration and deflagration-to-detonation transition (DDT) in fuel–air mixtures at initial temperatures up to 573 K and pressures up to 2 atm. The fuels investigated include hydrogen, ethylene, acetylene and JP-10 aviation fuel. The experiments were performed in a 3.1-m long, 10-cm inner-diameter heated detonation tube equipped with equally spaced orifice plates. Ionization probes were used to measure the flame time-of-arrival from which the average flame velocity versus propagation distance could be obtained. The DDT composition limits and the distance required for the flame to transition to detonation were obtained from this flame velocity data. The correlation developed by Vesper et al. (run-up distance to supersonic flames in obstacle-laden tubes. In the proceedings of the 4th International Symposium on Hazards, Prevention and Mitigation of Industrial Explosions, France (2002)) for the flame choking distance proved to work very well for correlating the detonation run-up distance measured in the present study. The only exception was for the hydrogen–air data at elevated initial temperatures which tended to fall outside the scatter of the hydrocarbon mixture data. The DDT limits obtained at room temperature were found to follow the classical  $d/\lambda = 1$  correlation, where  $d$  is the orifice plate diameter and  $\lambda$  is the detonation cell size. Deviations found for the high-temperature data could be attributed to the one-dimensional ZND detonation structure model used to predict the detonation cell size for the DDT limit mixtures. This simple model was used in place of actual experimental data not currently available.

**Keywords** Deflagration-to-detonation transition · Detonation · Flame

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### 1 Introduction

The phenomenon of flame acceleration leading to detonation initiation in obstacle-laden tubes, commonly referred to as deflagration-to-detonation transition (DDT), has been studied experimentally. The investigation was carried out in connection with industrial explosion safety and Pulse Detonation Engine (PDE) development. For both applications the detonation run-up distance, defined as the distance traveled by the flame from the point of ignition to the point of detonation onset, is a key parameter. For industrial safety the detonation run-up distance has been used to characterize the detonability of reactive mixtures. In PDEs the detonation run-up distance provides a rough estimate of the shortest possible combustor length for a PDE operating with the flame acceleration and DDT mode of initiation. Flame propagation in an obstacle-laden tube is characterized by an initial acceleration phase. In order for the flame to accelerate and transition to detonation the mixture must be of sufficient reactivity. The detonation limits represent the leanest and richest mixtures that can support a detonation wave in a given diameter tube. It has been shown by Peraldi et al. [1] that in order for transition to detonation to occur the detonation cell size of the mixture must be smaller than or equal to the orifice plate diameter.

There is an abundance of data in the literature on DDT in fuel–air mixtures at ambient temperature and pressure [2–4]. For both the industrial safety and PDE applications under normal operating conditions the combustible mixture is often at an elevated temperature. In this investigation emphasis has been placed on determining the affect of initial temperature on both the detonation run-up distance and DDT limits. A comprehensive study of DDT in high-temperature hydrogen–air–steam mixtures was reported by

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Ciccarelli et al. [5] in connection with nuclear reactor safety. In the context of PDEs, results from DDT experiments with propane-air at elevated temperature were reported by Ciccarelli and Dubocage [6]. In the present investigation DDT experiments were performed in fuel-air mixtures, the fuels tested include hydrogen, acetylene, ethylene. Experiments were also performed with JP-10 aviation fuel at prototypic PDE combustor pressures and temperatures.

## 2 Experimental details

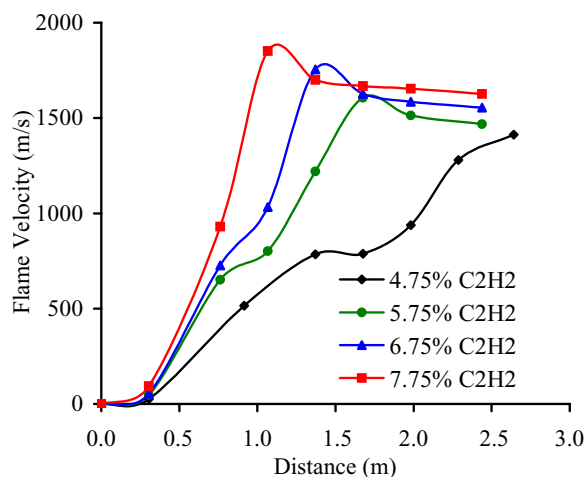
The experiments were performed in a 3.1-m long, 10-cm inner-diameter heated detonation tube. The tube is completely filled with 0.43 blockage ratio (BR) orifice plates equally spaced at one tube diameter. The blockage ratio for an orifice plate is  $BR = 1 - [d/D]^2$ , where  $d$  is the inner-diameter of the orifice plate and  $D$  is the inner-diameter of the tube. The test mixture is prepared by the method of partial pressures in a separate mixing chamber and then downloaded into the evacuated preheated detonation tube. The constituents are mixed using a pneumatic-motor driven propeller inside the mixing chamber. The mixing chamber is maintained at room temperature except for the JP-10 tests where it is heated to 410 K in order to vaporize the fuel. The fuel-air mixture is heated to the test temperature in transport through heat-traced tubing connecting the mixing chamber to the detonation tube. Since the gas is prepared at a low temperature there is no concern for pre-oxidation during mixing. In order to minimize pre-oxidation in the test vessel the mixture is present in the detonation tube at the test temperature for no more than 15 s before ignition. Combustion is initiated at one end of the tube via a standard automobile engine induction spark plug system. The average flame velocity is derived from time-of-arrival data obtained from ionization probes located along the complete length of the tube, typically spaced at 30.5 cm. Details on the experimental facility can be found in Ciccarelli et al. [7].

## 3 Results

### 3.1 Detonation run-up distance

The average flame velocity along the length of the tube was measured for different fuel-air mixtures. The fuels investigated include hydrogen, acetylene, ethylene, and JP-10. For each fuel-air mixture the flame acceleration history and detonation run-up distance was measured at temperatures between 300 and 573 K. A sample of the flame velocity versus distance data obtained for acetylene-air at 473 K and 1 atm for four different compositions is shown in Fig. 1. In all four tests with acetylene-air mixtures shown in Fig. 1, flame acceleration resulted in transition to detonation at different axial locations down the tube. As expected the highest flame acceleration and shortest DDT run-up distance is observed for the stoichiometric mixture, i.e., 7.75% acetylene.

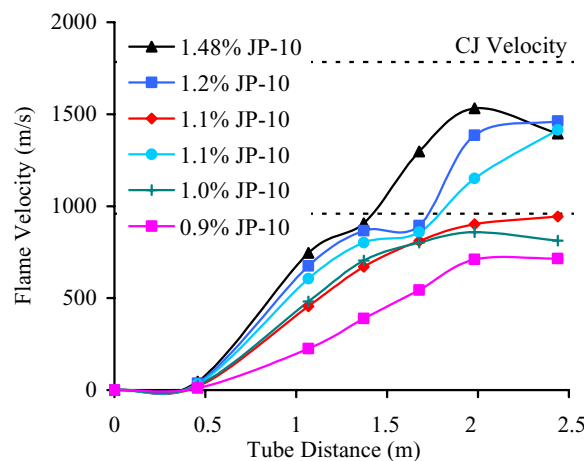
Because of the importance of JP-10 fuel in the PDE application a comprehensive study of flame acceleration and



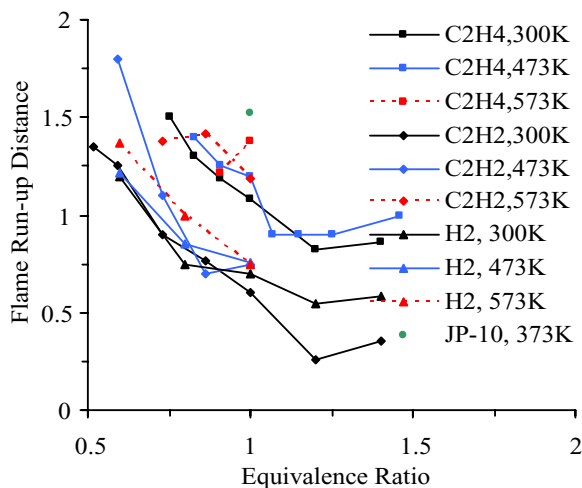
**Fig. 1** Flame acceleration data for acetylene-air mixtures at 473 K and 1 atm

DDT in JP-10/air mixtures was performed. Experiments carried out at an initial pressure of 1 atm did not result in detonation initiation. In general there was only a moderate enhancement observed in flame acceleration at 573 K compared to 373 K. This observation is consistent with the results from the other two hydrocarbon fuels tested. In experiments performed at 2 atm detonation initiation was observed over a range of mixture compositions at all temperatures. Shown in Fig. 2 is the measured flame velocity history along the tube in various JP-10/air mixtures at 473 K and 2 atm.

Transition to detonation occurs at an axial position in the tube where the flame velocity jumps abruptly from a value equal to the isobaric speed of sound in the combustion products to the Chapman-Jouget detonation velocity. For stoichiometric acetylene-air the CJ detonation velocity and the isobaric speed of sound in the products at 473 K and 1 atm are 1848 and 927 m/s, respectively. Experimentally this jump in velocity is not always well



**Fig. 2** Flame acceleration in JP-10/air mixtures at initial temperature and pressure of 473 K and 2 atm, the legend gives the mixture equivalence ratio and percent JP-10 in brackets. Also shown is the CJ detonation velocity for a 1.48% JP-10 mixture and the speed of sound in the combustion products for a 1.1% JP-10 mixture



**Fig. 3** Measured run-up distance for various fuel–air mixtures at 1 atm and different initial temperatures (JP-10 data is at 2 atm)

defined due to deviations from these two theoretical velocities caused by obstacle-induced momentum and heat losses, most notable in Fig. 1 is the results for the least reactive mixture containing 4.75% acetylene. For the purpose of this study the detonation run-up distance is determined based on the tube location where the average flame velocity equals the isobaric speed of sound in the combustion products. Typically this involves interpolating between two velocity measurement points. The location of detonation transition can only be measured to within the spatial resolution of the average flame velocity measurements, which for this study is 30.5 cm.

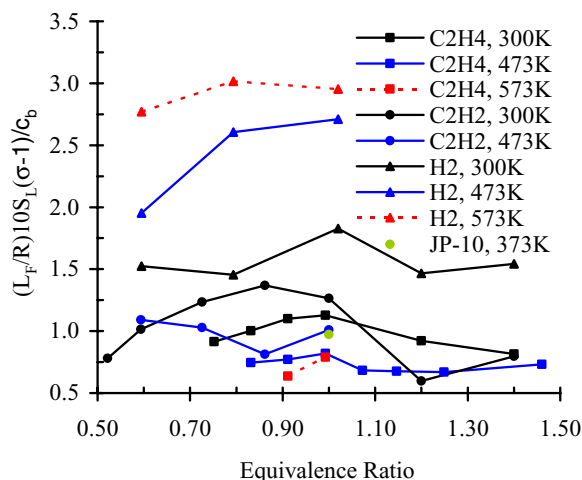
A summary of the detonation run-up distance measured for the four fuels at an initial pressure of 1 atm, (note the JP-10 data is for 2 atm) and initial temperatures of 300, 473 and 573 K is provided in Fig. 3 as a function of the equivalence ratio. Most of the data obtained corresponds to lean mixtures. This data clearly indicates that the run-up distance decreases as the mixture composition approaches the stoichiometric composition. The detonation run-up distance is mainly governed by the flame acceleration process. Therefore, the finding that the run-up distance decreases as the stoichiometric condition is approached from the lean side is expected since the laminar burning velocity and the density ratio across the flame both increase monotonically. For initial temperatures where data was also obtained on the rich side, the detonation run-up distance is minimum for mixtures with an equivalence ratio between 1.05 and 1.2. This corresponds to the composition for which the laminar burning velocity is maximum [8]. There is no strong dependency of detonation run-up distance on the initial temperature for the ethylene–air mixtures or the hydrogen–air mixtures. The hydrogen data does show a small increase in the run-up distance with initial temperature. The run-up distance for the acetylene–air mixture at 573 K is significantly larger than the run-up distance measured at 300 and 473 K. This could be due to some pre-ignition decomposition of acetylene in the tube at 573 K.

It is useful to present the detonation run-up data from Fig. 3 using a non-dimensional group such that the dependency on the fuel type and mixture equivalence ratio could be eliminated. Vesper et al. [9] used the following non-dimensional parameter grouping to normalize the distance,  $L_{choke}$ , required for a flame to accelerate to 95% of the isobaric speed of sound in the combustion products, also referred to as flame choking, i.e.,

$$\frac{L_{choke}}{R} \left( \frac{10S_{lam}}{c_b} \right) (\sigma - 1) \approx \frac{a(1 - BR)}{1 + b \times BR} \quad (1)$$

where  $a$  and  $b$  are empirical constants,  $S_{lam}$  is the laminar burning velocity,  $\sigma$  is the ratio of the unburned to burned gas density,  $c_b$  is the isobaric speed of sound in the combustion products, and  $R$  is the tube radius. This relationship is obtained by assuming that the flame takes on a conical shape that is perturbed by the orifice plates. It is also assumed that the local burning velocity is constant and is taken to be 10 times the laminar burning velocity. The authors point out that this is typically the maximum turbulent burning velocity attained during flame acceleration in an orifice plate laden tube. In this study only a single blockage ratio was investigated so the right-hand side of Eq. (1) is taken to be a constant. In most cases the flame accelerates to the choking velocity at which point a detonation is initiated. As a result, the flame acceleration run-up distance defined by Vesper et al. is typically the same as the detonation run-up distance.

Plotted in Fig. 4 is the measured normalized run-up distance versus equivalence ratio for the various fuel–air mixtures and initial temperatures tested. The density ratio and the speed of sound in the combustion products are calculated using the chemical equilibrium code STANJAN. The laminar burning velocity is also required to calculate the normalized detonation run-up distance. The laminar burning velocity data for ethylene and acetylene at room temperature is taken from Law [10] and for hydrogen at 300 K, 473 K from Gavrikov et al. [11] and at 573 K from Lui et al. [12].



**Fig. 4** Measured normalized run-up distance for various fuel–air mixtures at 1 atm and different initial temperatures

The laminar burning velocity for the ethylene and acetylene mixtures at elevated initial temperature was obtained by using the following relationship [8]

$$S_{\text{lam}} = \left[ \exp\left(\frac{-E_a}{RT_f}\right) \right]^{\frac{1}{2}} \quad (2)$$

where  $E_a$  is the activation energy,  $R$  is the universal gas constant and  $T_f$  is the adiabatic flame temperature. The activation energy in Eq. (2) is obtained by the following equation given by Egolfopoulos and Law [13]

$$E_a = -2R \left\{ \frac{\partial[\ln(\rho_u S_{\text{lam}})]}{\partial[1/T_f]} \right\} \quad (3)$$

where  $\rho_u$  is the unburned gas density. By plotting the natural log of the laminar burning velocity versus the inverse of the flame temperature the activation energy can be obtained from the slope of the curve. This was done using the laminar burning velocity data from Law [10] and the flame temperature computed using STANJAN. Equation (2) is then used to scale the room temperature laminar burning velocity data to the elevated initial temperatures of 473 and 573 K using the calculated adiabatic flame temperature at room temperature and at the elevated temperature. Due to a lack of published laminar burning velocity data in the literature at this time only a single JP-10 data point corresponding to a stoichiometric mixture with air at 373 K and 2 atm is included in Fig. 4. This data point is based on a laminar burning velocity of 0.6 m/s at 373 K and 1 atm obtained via private communication with Joseph Shepherd from the California Institute of Technology. As can be seen from Fig. 4 the hydrocarbon data correlates very well over a wide range of equivalence ratios and initial temperatures. The average value of the normalized run-up distance is roughly unity and the spread in the data is roughly  $\pm 25\%$ . The hydrogen-air data at 300 K falls just outside the scatter of the hydrocarbon-air mixture data but the higher temperature hydrogen-air data falls well outside the scatter.

### 3.2 DDT limits and cell size prediction

Detonation run-up distance data presented in Fig. 3 corresponds to tests with mixtures that resulted in detonation propagation. Under certain conditions the flame acceleration results in a choked flame and no DDT is observed. Based on the final steady-state flame velocity, one can determine whether a mixture undergoes detonation, typically the velocity is just under the theoretical Chapman–Jouget velocity. A comprehensive series of experiments were performed at different initial temperatures and pressures with ethylene to determine the lean and rich composition limits for which DDT was observed within the length of the tube. These so-called “DDT limits” are not fundamental properties of the fuel–air mixture, they are highly apparatus dependent. The detonation limits reported represent the range of mixture compositions that result in detonation propagation for the particular

geometry and initiation method used in these tests. Knowing orifice plate inner diameter,  $d$ , and the detonation cell size,  $\lambda$ , for the limit mixture composition we can check the applicability of the classical  $d/\lambda = 1$  DDT limit correlation at the various initial temperatures and pressures tested. This criterion represents a necessary condition for detonation propagation in an obstacle-laden tube but compliance with this criterion does not necessarily ensure that DDT will occur. For example, the tube geometry (e.g., tube diameter, tube length, orifice plate blockage ratio and orifice plate spacing) must promote flame acceleration to a velocity on the order of the mixture isobaric speed of sound of the combustion products. Therefore, the detonation limit criterion represents a necessary but not sufficient condition for DDT.

The experiments were performed at initial temperatures of 300, 373, 473, and 573 K and initial pressures of 1 and 2 atm. The DDT limit results for ethylene-air are shown in Figs. 5 and 6 for 1 and 2 atm, respectively. The results are

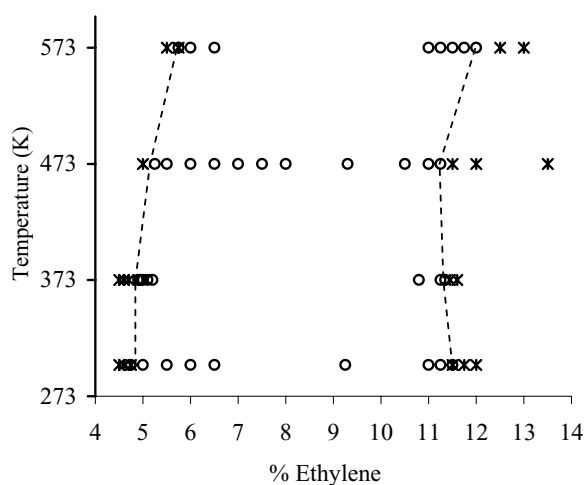


Fig. 5 Detonation limits of ethylene–air at 1 atm as a function of initial temperature (circles denote DDT and crosses denote no DDT)

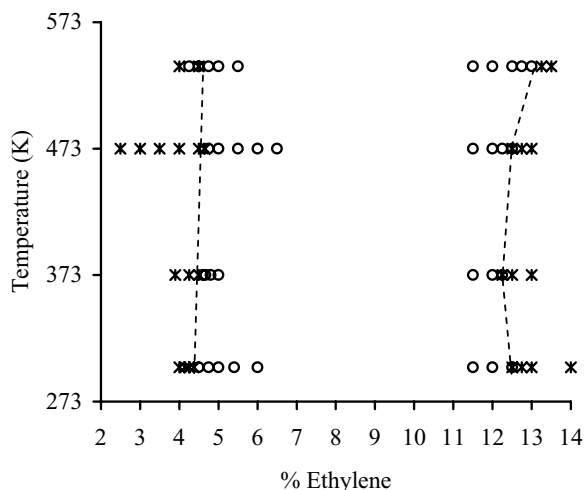
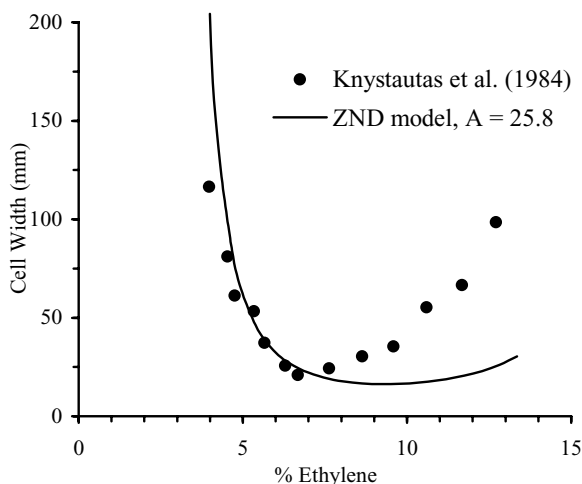


Fig. 6 Detonation limits of ethylene–air at 2 atm as a function of initial temperature (circles denote DDT and crosses denote no DDT)

presented in the form of “go” and “no go” data, where the open circles correspond to tests that resulted in DDT and the crosses represent no DDT. The two dotted lines indicate the trend in the lean and rich DDT limits as a function of initial temperature. A comparison of Figs. 5 and 6 indicates that the trend in the DDT limits with initial temperature is very similar for both initial pressures. The lean limit continuously increases approaching stoichiometric with increasing initial temperature, less so for the 2 atm results. The rich limit remains relatively unchanged between 300 and 373 K and then increases at higher temperatures. Overall the detonability limits do not vary that much with increased initial temperature, at most there is a variation of 1% ethylene.

Detonation cell size data for ethylene–air mixtures at 300 K and 1 atm is reported by is available from Knystautas et al. [14]. Detonation cell size data for ethylene–air at elevated initial temperatures and pressures are not available in the literature so the one-dimensional ZND detonation wave structure model is used to extrapolate available experimental detonation cell size data at 300 K to the elevated initial temperatures and pressures tested in this study. It is assumed that a linear relationship exists between the detonation cell size,  $\lambda$ , and the calculated ZND reaction zone length,  $\Delta$ , i.e.,  $\lambda = A\Delta$  where  $A$  is the proportionality constant. The Konnov [15] mechanism is used to calculate the reaction zone structure and the reaction zone length is defined based on the distance between the shock and the point in the reaction zone where the temperature gradient is a maximum. The proportionality constant  $A$  is evaluated using the experimental detonation cell size data obtained by Knystautas et al. [14] at 300 K and 1 atm, i.e.,  $A = \lambda/\Delta$ . The Knystautas et al. data is reproduced in Fig. 7 along with the ZND model prediction using a proportionality constant of 25.8 which anchors the model prediction to the cell size measured for the stoichiometric mixture. A comparison of the measured and predicted cell size data in Fig. 7 indicates that a single proportionality constant is not appropriate for all mixture compositions.



**Fig. 7** Comparison of the measured detonation cell size [14] and the ZND model prediction assuming  $\lambda = A\Delta$  for ethylene–air at 1 atm and 300 K

**Table 1** DDT limits for JP-10/air mixtures at 2 atm

$T$ (K)	Lean limit				Rich limit			
	% JP – 10	$\phi$	$\lambda$ (cm)	$d/\lambda$	% JP – 10	$\phi$	$\lambda$ (cm)	$d/\lambda$
373	1.15	0.77	7.0	1.1	2.10	1.42	5.7	1.3
473	1.20	0.80	5.7	1.3	1.75	1.19	2.2	3.4
538	1.25	0.84	3.8	2.0	1.75	1.19	2.2	3.4

**Table 2** Ethylene–air DDT limits at 1 atm

$T$ (K)	Lean limit				Rich limit			
	% C <sub>2</sub> H <sub>4</sub>	$\lambda/\Delta$	$\lambda$ (cm)	$d/\lambda$	% C <sub>2</sub> H <sub>4</sub>	$\lambda/\Delta$	$\lambda$ (cm)	$d/\lambda$
300	4.75	–	6.1 <sup>a</sup>	1.2	11.25	–	6.4 <sup>a</sup>	1.2
373	4.9	21.4	4.5	1.3	11.35	83.3	5.8	1.3
473	5.25	27.4	3.6	2.1	11.25	83.2	5.0	1.5
573	5.75	23.3	2.2	3.4	12.0	86.4	5.2	1.4

<sup>a</sup>Knystautas et al. [14]

There is a substantial difference for the rich mixtures where the predicted values are consistently below the measured cell size. As a result, for predicting the cell size at elevated initial temperature and pressure a different proportionality constant is evaluated for each mixture using the measured cell size at 300 K and 1 atm and multiplied by the calculated reaction zone length at the desired initial temperature and pressure. In doing this it is assumed that the proportionality constant for a mixture composition applies up to the maximum operating temperature of 573 K and a pressure of 2 atm.

The lean and rich ethylene–air DDT limits from Figs. 5 and 6 are tabulated in Tables 1 and 2 for an initial pressure of 1 and 2 atm, respectively. Also given in the table is the cell size corresponding to the limit mixture. The cell size data at atmospheric pressure and temperature is taken from Knystautas et al. [14], the remainder of the cell size data in the tables is calculated from the ZND model. The ratio of the orifice plate diameter and the detonation cell size is also given in the table. Examination of this data indicates that at room temperature the experimental data agrees very well with the classical DDT limit criterion  $d/\lambda = 1$ , within the experimental error associated with the detonation cell size data which can be as high as  $\pm 50\%$ . At the higher initial temperatures the  $d/\lambda$  ratio tends to increase with increasing initial temperature. This deviation is most likely the result of using a single value for the ZND proportionality constant  $A$  for a given composition over the temperature range tested. It has been shown that for hydrogen–air mixtures the ZND constant of proportionality decreases with increasing temperature [7]. Another possible cause for the increase in the value of  $d/\lambda$  for the limit mixtures with initial temperature could be the increase in cell regularity with increased initial temperature. Moen et al. [16] demonstrated that cell regularity has a dramatic effect on detonation phenomenon, in their tests the cell regularity was increased by adding argon to the fuel oxygen mixture. The possible influence of mixture initial temperature on cell regularity was raised by Ciccarelli [17] in connection with measured high values of  $d/\lambda$  in the range of 18–24 for limit mixtures obtained in critical tube

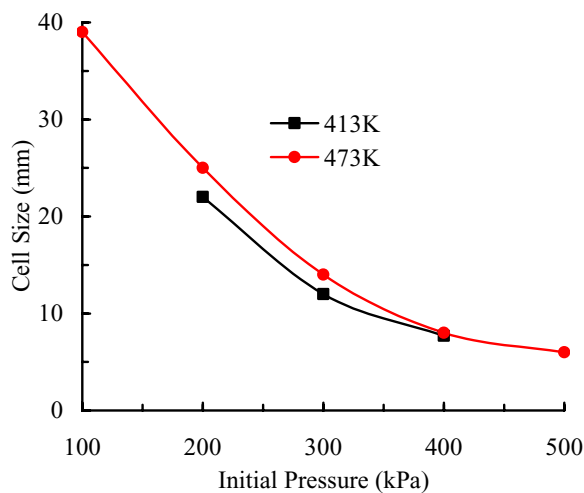
**Table 3** Ethylene–air DDT limits at 2 atm

$T$ (K)	Lean limit				Rich limit			
	% C <sub>2</sub> H <sub>4</sub>	$\lambda/\Delta$	$\lambda$ (cm)	$d/\lambda$	% C <sub>2</sub> H <sub>4</sub>	$\lambda/\Delta$	$\lambda$ (cm)	$d/\lambda$
300	4.5	19.1	6.5	1.2	12.5	96.7	7.6	1.0
373	4.6	20.2	3.8	1.9	12.25	97.8	5.7	1.3
473	4.75	19.7	2.2	3.4	12.5	96.7	4.0	1.6
573	4.5	19.1	2.2	3.4	13.0	95.0	3.8	1.9

experiments performed with hydrogen–air mixtures over an initial temperature range of 300–650 K. Based on smoked foil records it was shown that the high values could not be attributed to cell regularity. The effect of initial temperature on the detonation cell regularity for JP-10 air mixtures is not known. Neither explanation can be verified until detonation cell size data becomes available at these elevated initial temperatures.

DDT limits were also obtained from the JP-10/air mixture experiments. Based on the data shown in Fig. 2 the lean DDT limit for mixtures at 473 K and 2 atm is 1.1% JP-10 in air. In a similar fashion the lean and rich DDT limits in JP-10/air at 2 atm and 373, 473 and 538 K were measured, the data is summarized in Table 3. The data in Table 3 indicates that the lean DDT limit is only slightly influenced by initial temperature but a much more pronounced effect is observed for the rich limit. The rich limit decreases significantly with an increase in temperature from 373 to 473 K but then remains constant to 538 K.

There is limited detonation cell size data in the literature for JP-10 in air to use with the DDT composition limit data from this study to validate the  $d/\lambda$  criterion. Austin and Shepherd [18] measured cell size as a function of equivalence ratio at 373 K and 1 atm and Zhang et al. [19] measured cell size in a stoichiometric mixture at 413 and 473 K over a pressure range of 1–5 atm. The cell size measurements by Zhang et al. [19], reproduced in Fig. 8, indicates that there is very little effect of initial temperature on detona-

**Fig. 8** Cell size data for stoichiometric JP-10/air from Zhang et al. [19]

tion cell size over the limited temperature range tested (e.g., 12% increase in  $\lambda$  at 200 kPa) but a much larger influence of initial pressure. In the present study the experiments were performed over a temperature range close to that tested by Zhang et al. [19]. The cell sizes for the DDT limit mixtures from this study shown in Table 3 are obtained by interpolating the Austin and Shepherd [18] data at 1 atm and 373 K and then using the Zhang et al. [19] results from Fig. 8 to scale the data for the initial pressure and temperature. It is assumed that the temperature and pressure scaling observed for the stoichiometric mixture from Fig. 8 applies for off-stoichiometric mixtures.

The values of  $d/\lambda$  for the lean and rich limit mixtures at 373 K given in Table 3 show good agreement with the classical DDT criterion. The 473 and 538 K data show less agreement with the classical DDT criterion, especially for the rich limits. The apparent disagreement in the high temperature data could be the result of the inaccuracy in the temperature and pressure scaling of the Austin and Shepherd detonation cell size data.

## 4 Conclusions

Experimental results are presented for hydrocarbon fuels which were successfully correlated with Veser et al. [9] fast flame run-up distance correlation. Satisfactory agreement was not found for the hydrogen–air mixtures at the higher initial temperatures. The classical DDT limit criterion of  $d/\lambda = 1$  is validated for room temperature ethylene–air and JP-10–air mixtures at 373 K. Deviations from the correlation were observed for the high temperature ethylene–air mixtures. It is not possible to determine if these deviations are the result of the detonation phenomenon or the ZND detonation model cell size prediction method.

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