DDT in Methane-Air Mixtures

M. Kuznetsov¹, G. Ciccarelli², S. Dorofeev¹, V. Alekseev¹, Yu. Yankin¹, and T. H. Kim³

¹Russian Research Center - Kurchatov Institute,

Moscow, 123182, Russia

²Queen's University,

Kingston, Ontario, Canada K7L 3N6

³E.I. Du Pont de Nemours & Company,

P.O. Box 1089, Orange, Texas 77630 U.S.A.

E-mail: dorofeev@iacph.kiae.ru

Introduction

Considering the common use of methane gas in the chemical process industry there is a lack of detonation phenomena data in the literature for methane-air mixtures. This lack of data is due to the relatively low detonation sensitivity of methane-air, and thus the need for large-scale apparatus. Experimental studies performed in tubes have shown that it is very difficult to achieve deflagration-to-detonation transition (DDT) in methane-air mixtures. The only reported observation of DDT in a methane-air mixture was by Lindstedt and Michels (1989) in a very long tube equipped with a Schelkin spiral. Experimental results from a study on the critical condition for DDT in methane-air mixtures are presented in this paper.

Experimental

A series of experiments were carried out at atmospheric initial conditions (i.e., 293K and 1 atm) using methane-air mixtures with methane concentrations, on a volume basis, ranging from 5.5 to 17%. These tests were performed in two different detonation tubes, one 12-m long with an innerdiameter of 174-mm and the other 520-mm inner-diameter and 34.5-m long. The tubes were equipped with orifice plate obstacles spaced at one tube diameter, with blockage ratios of 0.3 and 0.6. A weak electrical spark was used to ignite the mixtures at one end of the tube. Fast-response piezoelectric pressure transducers, photo-diodes and ionization probes were used to measure pressure and flame time-of-arrival.

Results

Typical data on visible flame propagation velocity as a function of propagation distance is presented in Fig. 1. Based on the test data presented in Fig. 1, two flame propagation regimes can be clearly distinguished. In the first regime the flame achieves a steady-state speed just below the theoretical CJ detonation velocity. This propagation regime is commonly referred to as "quasi-detonation." The velocity deficit relative to the CJ detonation velocity is attributed to energy losses due to shock and flow interaction with the obstacles. In the second regime the flame achieves a steady-state velocity which is roughly equal to half the CJ detonation velocity. This is known as the "choking" regime and is characterized by a flame speed close to the speed of sound in the combustion products (Lee et al., 1984).

In experiments with obstacles with a blockage ratio (BR) of 0.3, propagation in the quasi-detonation regime was observed for mixtures with 8, 9.5, 10.5, and 12 % CH₄ in the 520-mm tube and 9.5 and 11% CH₄ in the 174-mm tube. In tests with a BR= 0.6, propagation in the quasi-detonation regime was not achieved in either tube for any methane-air mixture.



Figure 1. Effect of initial mixture conditions on flame propagation in tube with BR = 0.3

Various investigators have demonstrated that the detonation cell size can be used to describe the critical condition for DDT in gaseous mixtures. The cell size represents a chemical length scale for the detonation wave. For DDT to be possible, the mixture detonation cell size must be small enough relative to the characteristic size of the tube. Thus, detonation cell size data is necessary to analyze the critical condition for DDT. This cell size data was obtained in tests performed in a smooth tube using both the smoked foil and the pressure oscillation technique. A photograph of a typical foil showing the cellular structure for a methane-air mixture at atmospheric conditions is presented in Figure 2. The detonation cell size measured for three different methane-air mixtures is shown in Table 1. They are in agreement with the measurement made by Moen et al. (1984) for a stoichiometric methane-air mixture.



Figure 2. Cellular structure of methane-air mixture with 11% CH4 at atmospheric initial conditions. (Scale: vertical length of foil is 1-m)

As a result of the limited available experimental cell size data, a model is used to estimate the detonation cell size for a wider range of mixture composition. In the present analysis a model developed by Gavrikov et al. (2000) is used to estimate the cell size for the mixture conditions corresponding to the DDT tests. The predicted detonation cell size for methane-air mixtures at atmospheric conditions is shown in Table 1 and Fig. 3.

CH ₄	Detonation	Pressure	Average	Calculation
content	cell width	oscillations	cell width	(Gavrikov et al.,
				2000)
%(vol.)	cm	cm	cm	cm
8	-	-		49
9.5	21±8	18±7	19	29
10.5	-	-		26
11	26±10	18±10	22	27
12	42±11	23±8	33	34
13.5	-	_		56

Table 1. Experimental data on detonation cell width and results of calculations.



Figure 3: Measured and predicted cell size for methane-air mixtures at 300K and 1 atm

Discussion

It has been shown by Peraldi et al. (1986), and other investigators, that for common hydrocarbon fuels in air the critical condition for DDT in obstacle laden tubes is given by $d/\lambda = 1$, where d is the orifice diameter and λ is the detonation cell size. In order to verify the applicability of this DDT criterion for methane-air mixtures, the value of λ for the critical mixture was estimated for each test. The detonation cell size was taken to be the average experimental value from Table 1, if available, or the calculated value using the Gavrikov model. For each test performed the value of d/λ is plotted as a function of the orifice diameter, d. Those tests resulting in DDT are shown as black symbols and the tests that did not result in DDT are shown as gray symbols. Also shown in the figure is a horizontal line corresponding to $d/\lambda = 1$.

In general, there is good agreement between the current DDT results and the DDT criterion within the range of uncertainty of the cell size determination. For the 0.6 BR tests DDT was not observed, even for a test with a corresponding d/λ value of 1.8. Since DDT was not observed, the critical value could be even larger than this value. A similar breakdown in the classic DDT criterion for high BR tubes was reported by Kuznetsov (1999) in hydrogen-air mixtures. The relatively high BR of 0.43 used in tests performed by Peraldi et al. (1986) in a 300-mm tube could explain why DDT was not observed in a stoichiometric methane-air mixture.



Figure 4: DDT results plotted as d/λ versus orifice diameter d.

Dorofeev et al. (2000) proposed an alternate DDT cell size correlation based on the analysis of a wide variety of experimental data. Instead of using just the orifice diameter in the correlation they introduced a characteristic length scale for the obstructed channel, L, defined as

$$L = (S + D)/2/(1 - d/D)$$

where S is the obstacle spacing, and D is the tube inner-diameter. This length scale includes the effect of area blockage and obstacle spacing. For the tests reported here the obstacle spacing is equal to the tube inner-diameter (S = D), so

$$L = D/(1-d/D)$$

Based on their analysis of previous experimental data, Dorofeev et al. proposed that the critical DDT condition could be expressed by $L/\lambda=7$. The data shown in Fig. 4 is re-plotted in Fig. 5 as L/λ versus L. The data shows good agreement with this correlation. For those tests performed using the 0.6 BR plates, where DDT was not observed, the maximum value of L/λ is close to the critical value of 7. This shows better agreement with the critical condition than the same data plotted as d/λ in Fig. 4.

Summary

The DDT process for methane-air mixtures in obstructed tubes at atmospheric initial temperature and pressure were studied. The relatively large size of the facilities make it possible to observe DDT in a range of conditions for an insensitive fuel such as methane. Critical conditions for detonation onset were determined in the tests.

The results indicate that for a tube cross-sectional area blockage ratio of 0.3 the critical condition for DDT can be characterized by the $d/\lambda = 1$ criterion proposed by Peraldi et al. (1986). However, for a tube area blockage ratio of 0.6 it was found that the critical value was significantly higher, up to a value of d/λ of at least 1.8. The data also shows that the critical condition for DDT can be better described by $L/\lambda = 7$, where L is a characteristic size for of the channel volume between orifice plates which depends on the orifice plate dimensions and spacing. This is in good agreement with previous data obtained for other hydrocarbon and hydrogen mixtures with irregular detonation cellular structure.



Figure 5: DDT results plotted as L/λ versus characteristic size L.

References

Dorofeev S.B., V.P. Sidorov, M.S. Kuznetsov, I.D. Matsukov, V.I. Alekseev, Effect of scale on the onset of detonations. *Shock Waves*, 10(2), pp 137-149, 2000

Gavrikov A.I., A.A. Efimenko, and S.B. Dorofeev, Detonation cell size predictions from detailed chemical kinetic calculations. *Combustion and Flame* 120, 19-33, 2000

Kuznetsov M.S., V.I. Alekseev, A.V. Bezmelnitsyn, W. Breitung, S.B. Dorofeev, I.D. Matsukov, A. Veser, and Yu.G. Yankin Effect of obstacle geometry on behavior of turbulent flames. Preprint IAE-6137/3, RRC "Kurchatov Institute", Moscow, 1999, Report FZKA-6328, Forschungszentrum Karlsruhe, Karlsruhe, 1999

Kuznetsov M.S., V.I. Alekseev, and S.B. Dorofeev, Comparison of critical conditions for DDT in regular and irregular cellular detonation systems. *Shock Waves*, 10(3), pp 217-223, 2000

Lee J.H., R. Knystautas, C.K. Chan, Turbulent flame propagation in obstacle-filled tubes, 20th Symposium (Int.) on Combustion, The Combustion Institute, Pittsburgh, PA, pp 1663-1672, 1984

Lindsted R. P. and H. J. Michels, Deflagration to Detonation Transitions and strong Deflagrations in Alkane and Alkene Air Mixtures, *Combustion and Flame* 76, 169-181, 1989

Peraldi O., R. Knystautas, J. Lee, 19th Symposium (International) on Combustion, The Combustion Institute, p. 1629, 1986.