

# Comparison of critical conditions for DDT in regular and irregular cellular detonation systems

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**Abstract.** The results of an experimental study of DDT in mixtures with regular and irregular detonation cellular structures are presented. Experiments were carried out in a tube 174 mm i. d. with obstacles (blockage ratios were 0.1, 0.3, and 0.6). Mixtures used were hydrogen–air and stoichiometric hydrogen–oxygen diluted with N<sub>2</sub>, Ar, and He. The critical conditions for DDT are shown to depend on the regularity of the cellular structure of test mixtures. The critical values of the cell sizes in Ar- and He-diluted mixtures are shown to be significantly smaller than those in N<sub>2</sub>-diluted mixtures. This means that systems with a highly regular detonation cellular structure have far less capacity for undergoing DDT compared to irregular ones with the same values of detonation cell sizes.

**Key words:** Deflagration-to-detonation transition, Detonation cellular structure, Critical conditions

## 1 Introduction

Critical conditions for deflagration-to-detonation transition (DDT) in obstructed tubes have been studied extensively in different mixtures. Most of the studies have been carried out on mixtures of hydrogen and hydrocarbon fuels with air, oxygen, and nitrogen. It was shown that the minimum tube diameter (or other characteristic sizes) for the onset of detonations may be correlated with the detonation cell widths  $\lambda$  of these mixtures (Lee et al. 1984; Peraldi et al. 1988; Teodorczyk et al. 1988; Dorofeev et al. 1996 and other studies). In mixtures of this type, the detonation cell sizes were also shown to give good correlations in the classical relationships for dynamic detonation parameters (minimum initiation energy, limiting tube diameter  $d_l$ , critical exit diameter  $d_c$ , critical radius under direct initiation  $R_c$ , etc.). However, these relationships have been shown to be invalid in mixtures with highly regular cellular structure (Shepherd et al. 1986; Dupre et al. 1991; Desbordes et al., 1993). The effect of regularity of the cellular structure of test mixtures on the critical conditions for DDT is studied in the present paper.

## 2 Experimental

Experiments were carried out in a detonation tube measuring 174 mm in internal diameter and 11.5 m length.

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Circular obstacles were installed inside the tube with blockage ratios ( $BR = 1 - d^2/D^2$ , where  $D$  is tube diameter and  $d$  is orifice diameter in obstacle plates) equal to 0.1, 0.3, and 0.6. The distances between obstacles were equal to one diameter. The mixtures tested were hydrogen–air and stoichiometric hydrogen–oxygen diluted with N<sub>2</sub>, Ar, and He. The concentrations of hydrogen and diluent were variables in the tests.

Test mixtures were prepared by a precise partial pressure method in a special mixing tank. A preliminary evacuated tube was filled with test mixtures before tests. The mixtures were ignited with a weak electric spark at one end of the tube. All tests were at a normal initial temperature (about 293 K) and pressure (1 atm).

Pressure transducers PCB H113A, collimated photodiodes FD-10, and ion probes were installed along the tube to record details of propagation of deflagrations and detonations. A schematic of the experimental apparatus is shown in Fig. 1.

## 3 Results

### 3.1 DDT processes

Typical  $X-t$ -diagrams of explosion processes are presented in Figs. 2–9. Figures 2–7 show the development of explosion processes and transition to detonations in hydrogen–air mixtures with different blockage ratios  $BR = 0.1, 0.3,$  and  $0.6$ . Figures 8 and 9 show  $X-t$ -diagrams of DDT processes in hydrogen–oxygen mixtures diluted with Ar and He for  $BR = 0.3$ .

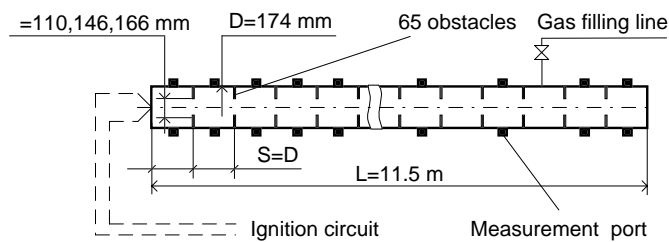


Fig. 1. Schematic of experimental apparatus

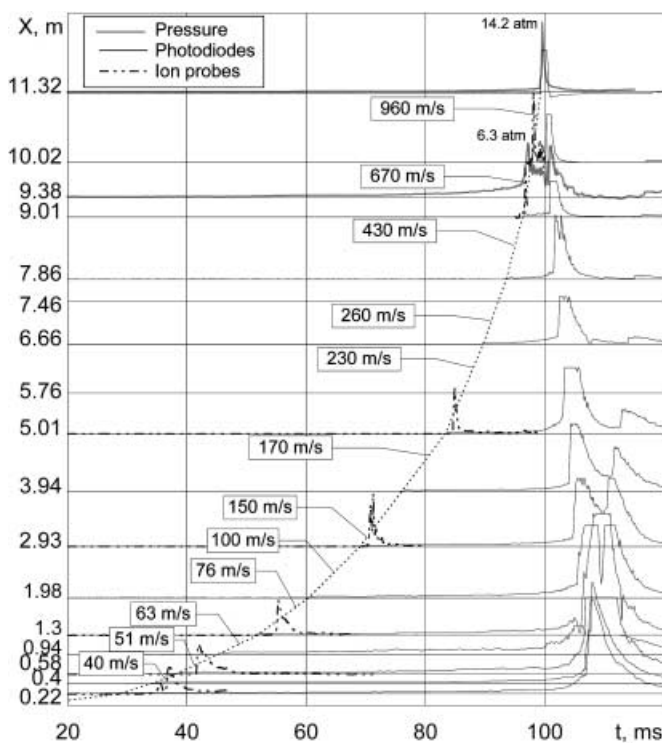


Fig. 2.  $X-t$ -diagram of explosion process in 17%  $H_2$ /air mixture ( $BR = 0.1$ ). Dotted line – flame trajectory

In the present study, cases of DDT were distinguished on the basis of the following requirements. A detonation wave should be formed and should propagate for some distance along the tube, such that the speed of the wave can be determined from the arrival times. The speed and characteristic overpressure of this wave should be close to characteristic Chapman–Jouguet (CJ) values (a velocity deficit was assumed to be possible for high  $BR$ ). Typical cases of DDT are presented in Figs. 3 and 6–9. The cases of strong local explosions of the compressed gases at the end of the tube, as shown in Fig. 2, were not considered as DDT cases.

The configuration of obstacles was found to noticeably influence general pictures of the explosion processes and DDT. With the smallest blockage ratio,  $BR = 0.1$  (see Figs. 2, 3), the flames accelerated continuously and either the flame reached the end of the tube or transition to detonation was observed. This means that in some tests, where DDT was not observed, it might occur if the tube were longer.

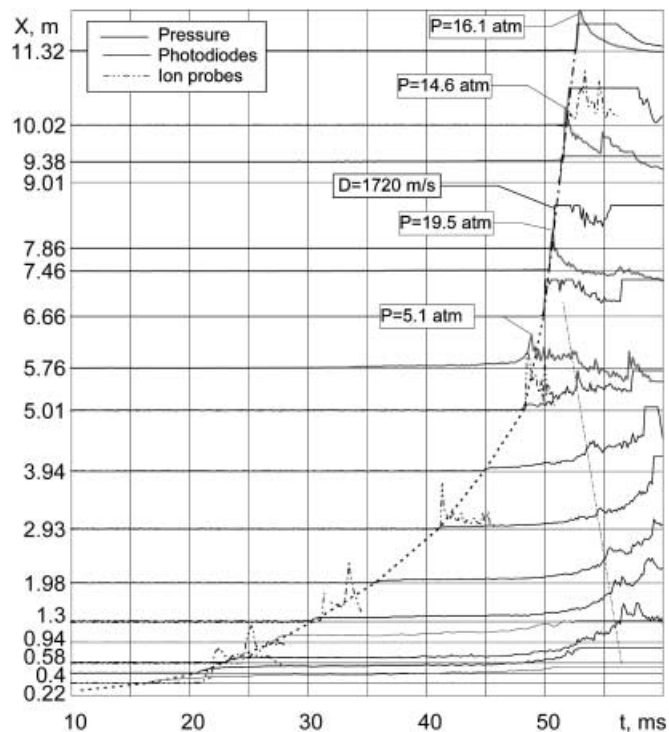


Fig. 3.  $X-t$ -diagram of explosion process in 20%  $H_2$ /air mixture ( $BR = 0.1$ ). Dotted line – flame trajectory, dash-dot line – detonation trajectory, dash-dot-dot line – retonation wave trajectory

Examples of  $X-t$ -diagrams of explosion processes with  $BR = 0.3$  are shown in Figs. 4 and 7. With this blockage ratio, either development of so-called choked flames or flame acceleration and DDT were observed. In the first case the flames propagated with a quasi-stationary speed, which was close to the isobaric sound speed in combustion products. In the second case (DDT), transition to detonation was observed very soon after the flame speed reached the value close to the sound speed in combustion products.

With  $BR = 0.6$  (see Figs. 5, 6), flame acceleration and development of choked flame were observed. After flame propagation at a quasi-stationary speed for some distance along the tube, DDT occurred in some tests. This was different from the case with  $BR = 0.3$ , where DDT, if it occurred, followed the flame acceleration almost immediately.

General pictures of DDT in hydrogen–air mixtures and in  $H_2/O_2$  mixtures diluted with Ar or He were similar. Explosion waves differ by their speed and by characteristic values of overpressures. This is connected with different thermodynamic properties of the mixtures. A comparison of the CJ detonation velocities for the mixtures tested with the measured average detonation velocities is presented in Table 1. The measured values are close to CJ velocities for  $BR = 0.1$ . Lower propagation velocities are observed with higher  $BR$ , because of the momentum losses during propagation of detonation wave through the obstacle array. The velocity deficit is about 10% for  $BR = 0.3$  and about 30% for  $BR = 0.6$ .

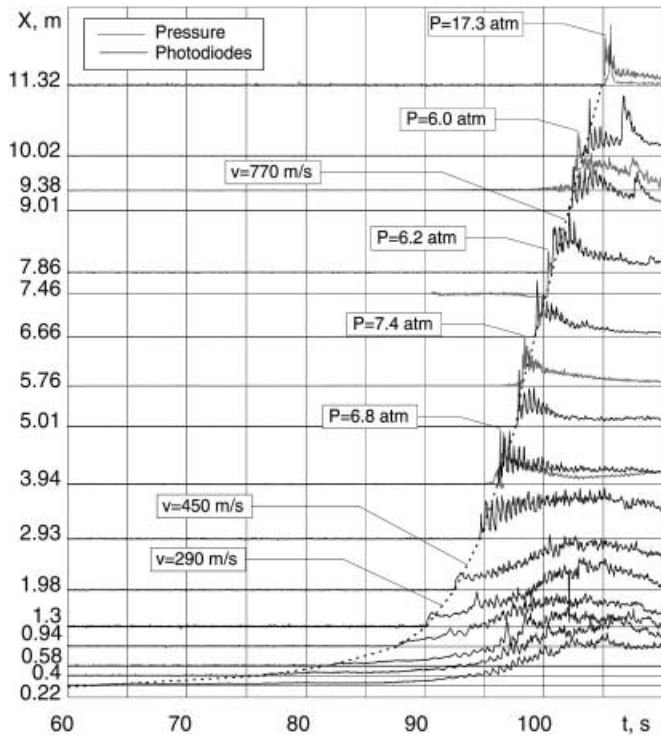


Fig. 4.  $X-t$ -diagram of explosion process in 13%  $H_2$ /air mixture (BR = 0.3). Dotted line – flame trajectory

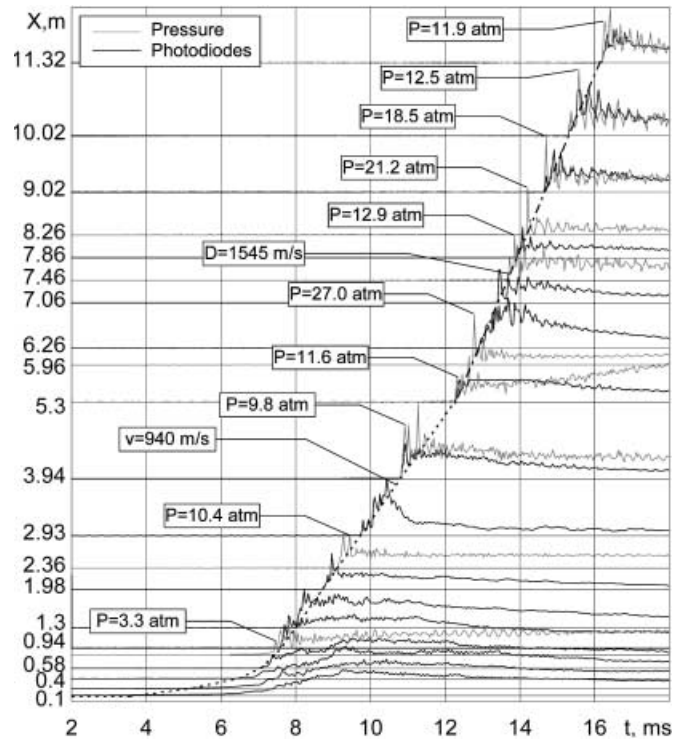


Fig. 6.  $X-t$ -diagram of explosion process in 51%  $H_2$ /air mixture (BR = 0.6). Dotted line – flame trajectory, dash-dot line – detonation trajectory

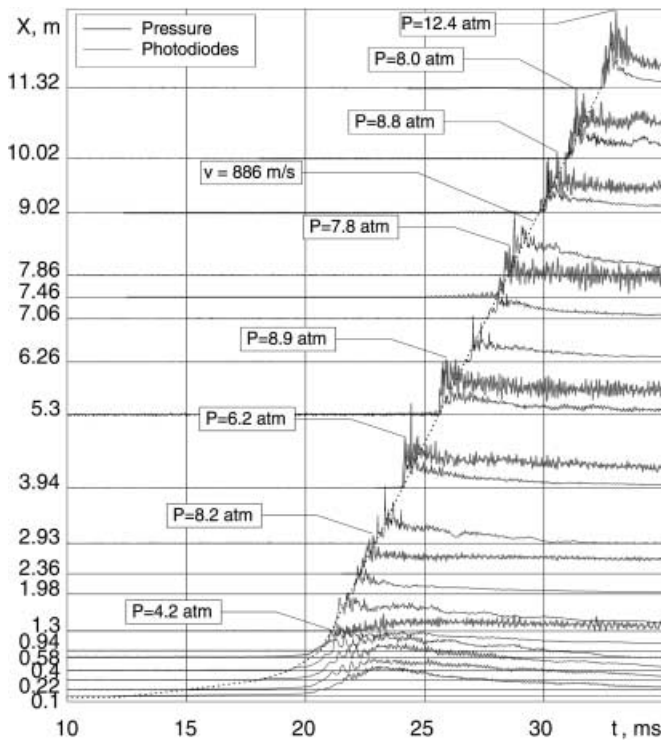


Fig. 5.  $X-t$ -diagram of explosion process in 65%  $H_2$ /air mixture (BR = 0.6). Dotted line – flame trajectory

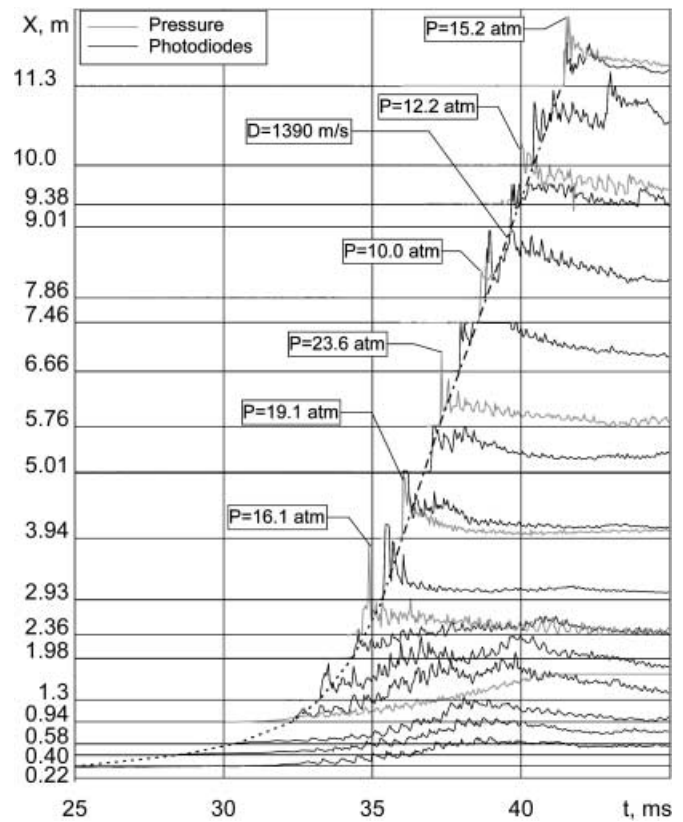


Fig. 7.  $X-t$ -diagram of explosion process in 17.5%  $H_2$ /air mixture (BR = 0.3). Dotted line – flame trajectory, dash-dot line – detonation trajectory

**Table 1.** Characteristic detonation velocities in obstructed channel

BR	H <sub>2</sub> % vol.	Diluent	<i>D</i> m/s	<i>D</i> <sub>CJ</sub> m/s	<i>D</i> / <i>D</i> <sub>CJ</sub>
0.1	17	air	1560	1600	0.98
0.1	20	air	1720	1710	1.01
0.1	21	N <sub>2</sub>	1970	1750	1.12
0.1	17	He	3840	3810	1.01
0.1	15	Ar	1560	1590	0.98
0.3	17.5	air	1390	1620	0.86
0.3	20	air	1500	1710	0.88
0.3	60	air	1960	2250	0.87
0.3	62.3	air	1900	2270	0.84
0.3	10	He	3330	3740	0.89
0.3	8	Ar	1250	1320	0.94
0.3	10	Ar	1400	1430	0.98
0.3	12	Ar	1470	1500	0.98
0.6	23	air	1170	1800	0.65
0.6	25	air	1350	1860	0.72
0.6	29.6	air	1510	1970	0.77
0.6	35	air	1610	2050	0.78
0.6	40	air	1600	2100	0.76
0.6	45	air	1550	2140	0.73
0.6	48	air	1550	2170	0.72
0.6	51.5	air	1540	2190	0.71
0.6	24	N <sub>2</sub>	1140	1840	0.62
0.6	26	N <sub>2</sub>	1340	1890	0.71
0.6	28	N <sub>2</sub>	1430	1940	0.74
0.6	15	He	2720	3830	0.71
0.6	12	Ar	1110	1500	0.74
0.6	13	Ar	1180	1540	0.76

**Table 2.** Critical conditions for DDT in H<sub>2</sub>-air mixtures

BR	H <sub>2</sub> , % vol.	$\lambda$ , mm	<i>d</i> / $\lambda$	DDT	Label
0.6	23	34	3.2	Yes	d3
0.6	22	36	3.1	No	d3
0.6	51.5	37	3.0	Yes	d3
0.6	51.5	37	3.0	No	d3
0.3	17.5	140	1.0	Yes	d2
0.3	15	360	0.4	No	d2
0.3	60	150	1.0	Yes	d2
0.3	70	930	0.2	No	d2
0.1	17	170	1.0	Yes	d1
0.1	16	250	0.7	No	d1

The retonation waves can be distinguished in *X-t*-diagrams for BR = 0.1 and, in some cases, for BR = 0.3. The retonation waves in mixtures with Ar or He dilution are generally more pronounced compared to those in H<sub>2</sub>/air and H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixtures (compare Fig. 7 with Figs. 8 and 9).

With BR = 0.6, the retonation waves cannot be observed in *X-t*-diagrams. At the same time, numerous reflections of pressure waves from obstacles are very pro-

**Table 3.** Critical conditions for DDT in 2H<sub>2</sub>+O<sub>2</sub>+ $\beta$ N<sub>2</sub> mixtures

BR	H <sub>2</sub> , % vol.	$\lambda$ , mm	<i>d</i> / $\lambda$	DDT	Label
0.6	24	35	3.1	Yes	d7
0.6	23	43	2.6	No	d7
0.3	13	1200	0.1	No	d6
0.1	21	70	2.4	Yes	d5
0.1	19	120	1.4	No	d5

**Table 4.** Critical conditions for DDT in 2H<sub>2</sub>+O<sub>2</sub>+ $\beta$ He mixtures

BR	H <sub>2</sub> , % vol.	$\lambda$ , mm	<i>d</i> / $\lambda$	DDT	Label
0.6	15	10	11	Yes	e3
0.6	13	15	7.3	No	e3
0.3	10	30	4.8	Yes	e2
0.3	9	39	3.7	No	e2
0.1	17	7	24	Yes	e1
0.1	15	10	17	No	e1

**Table 5.** Critical conditions for DDT in 2H<sub>2</sub>+O<sub>2</sub>+ $\beta$ Ar mixtures

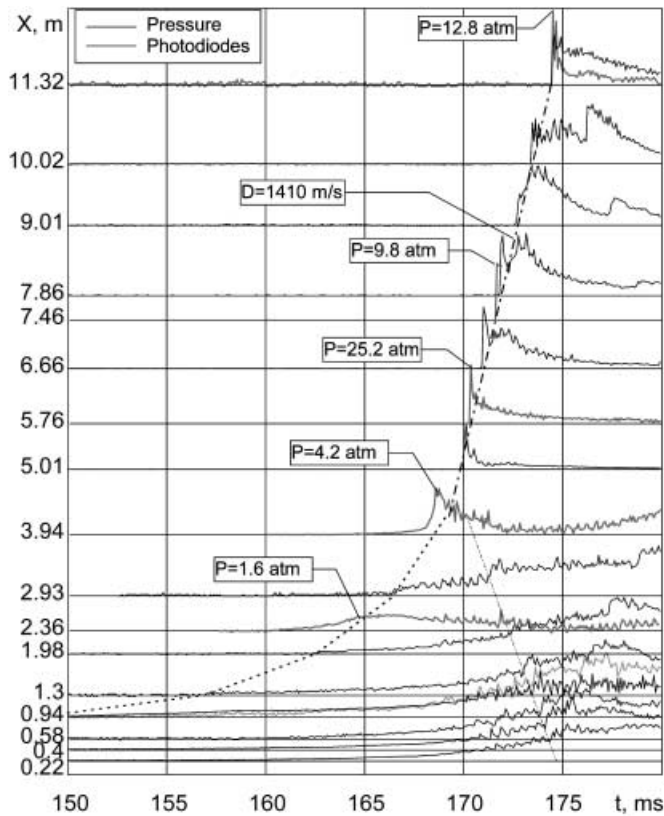
BR	H <sub>2</sub> , % vol.	$\lambda$ , mm	<i>d</i> / $\lambda$	DDT	Label
0.6	12	8.2	13	Yes	e7
0.6	11	9.8	11	No	e7
0.3	8	18	8.0	Yes	e6
0.3	7	22	6.6	No	e6
0.1	15	5.0	33	Yes	e5
0.1	13	7.0	24	No	e5

nounced in the readings of the pressure transducers and photodiodes. Figures 5 and 6 show that corresponding oscillations of the signals are typical for both fast deflagrations and detonations.

### 3.2 Critical conditions for DDT

Critical conditions for DDT in different types of mixtures are presented in Tables 2–5. Mixture compositions which are the closest to the borderline of DDT (both from deflagration and DDT sides) are the only ones given in the Tables. More detailed experimental data were reported by Dorofeev et al. 1999 and Kuznetsov et al. 1999. The results of Kumar 1990; Liu et al. 1984; Knystautas et al. 1982, and Gavrikov et al. 2000 were used to obtain values of the detonation cell sizes given in Tables 2–5.

The data presented in Tables 2–5 show that the critical mixture compositions for DDT depend on the blockage ratio. This is true for each type of mixture used in the tests. It is seen that the critical cell sizes increase with the decrease of BR. For each value of BR, the cell sizes of the critical compositions for DDT depend on the mixture type.

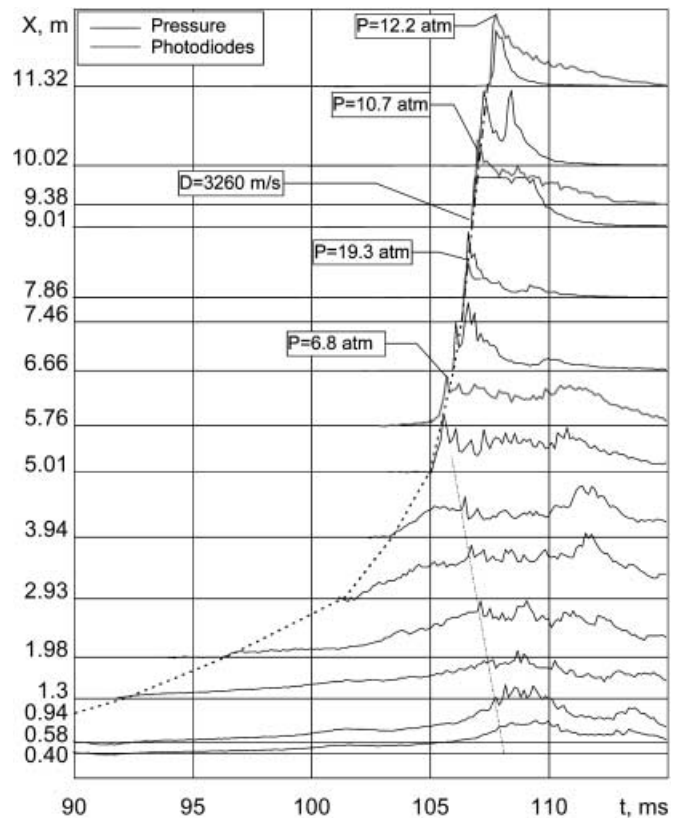


**Fig. 8.**  $X-t$ -diagram of explosion process in 10%  $H_2/O_2/Ar$  mixture ( $BR = 0.3$ ). Dotted line – flame trajectory, dash-dot line – detonation wave, dash-dot-dot line – retonation wave trajectory

According to the results of Peraldi et al. 1988, the critical compositions for DDT in obstructed tubes are expected to have a cell size smaller than or equal to the size of the unobstructed passage  $d$ . It may be assumed that the variations in the critical cell sizes for DDT with changes of  $BR$  (in the same tube and mixture type) can be explained by the different values of  $d$ . The values of  $d/\lambda$  are given in Tables 2–5. A comparison of the critical values of  $d/\lambda$  shows that this ratio is still a function of the blockage ratio. For each value of  $BR$ , the ratio  $d/\lambda$  of the critical compositions for DDT depends on the mixture type.

As mentioned in the previous section, the explosion processes in the tests with  $BR = 0.1$  were in some sense different to those with larger blockage ratios. Flame acceleration was not efficient in the case of  $BR = 0.1$ . This resulted in a situation in which the possibility of DDT was limited, in some cases, by the development of flame acceleration. It may be that the onset of detonations was possible for a particular mixture in the given tube, but fast flames were not formed and DDT did not occur. Despite this, the influence of the obstacle configuration on the critical conditions was still an important factor for  $BR = 0.3$  and 0.6, although the effectiveness of flame acceleration was clearly not a limiting factor for DDT in these cases.

Compared to  $H_2/air$  and  $H_2/O_2/N_2$  mixtures, the critical values of the cell sizes for DDT are smaller in mixtures with  $Ar$  and  $He$  dilution, which are characterised by regu-



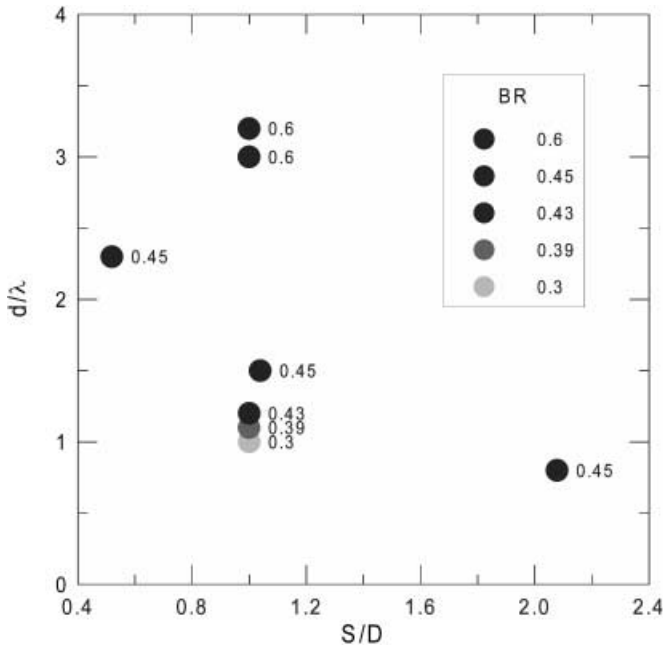
**Fig. 9.**  $X-t$ -diagram of explosion process in 10%  $H_2/O_2/He$  mixture ( $BR = 0.3$ ). Dotted line – flame trajectory, dash-dot line – detonation wave, dash-dot-dot line – retonation wave trajectory

lar cellular structure of detonation waves. This is true for all blockage ratios used in the tests.

## 4 Discussion

To isolate the effect of mixture composition on the critical conditions for DDT, the influence of the obstacle configuration should be addressed first. For tubes with repeated obstacles there are two main parameters characterising this configuration: the blockage ratio and obstacle spacing. The effect of these parameters on the critical ratio of  $d/\lambda$  for DDT in hydrogen–air mixtures is summarised in Fig. 10 (data from Teodorczyk et al. 1988 and present work), which shows that the critical values of  $d/\lambda$  decrease with  $S/D$  and increase with  $BR$ .

A correlation for the critical DDT conditions, which accounts for the configuration of obstacles, was suggested recently by Dorofeev et al. 2000. The critical conditions for DDT in tubes with different obstacle configurations were analysed in this work for mixtures of hydrogen and hydrocarbon fuels with air and  $O_2$  (diluted with  $N_2$ ,  $H_2O$ , and  $CO_2$ ). It was shown that a characteristic size  $L$  of an obstructed tube may be defined, which correlates with the detonation cell size  $\lambda$  of the critical mixture composition for DDT. The size  $L$  is defined by the tube diameter  $D$ , blockage ratio, and obstacle spacing  $S$ :



**Fig. 10.** The minimum ratio  $d/\lambda$  for DDT in obstructed channel versus dimensionless obstacle spacing  $S/D$ . Critical values  $d/\lambda$  for different BR are shown

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

where  $d$  is the diameter of the orifice of an obstacle. Applications of (1) are limited to sufficiently large  $D/d$  or blockage ratios, e.g., for  $BR \geq 0.1$ . For  $S = D$ , which was the case in our tests:

$$L = D/(1 - d/D). \quad (2)$$

For mixtures of hydrogen and hydrocarbon fuels with air, which are characterised by irregular cellular structures, the critical conditions for DDT was shown to agree with (Dorofeev et al. 2000):

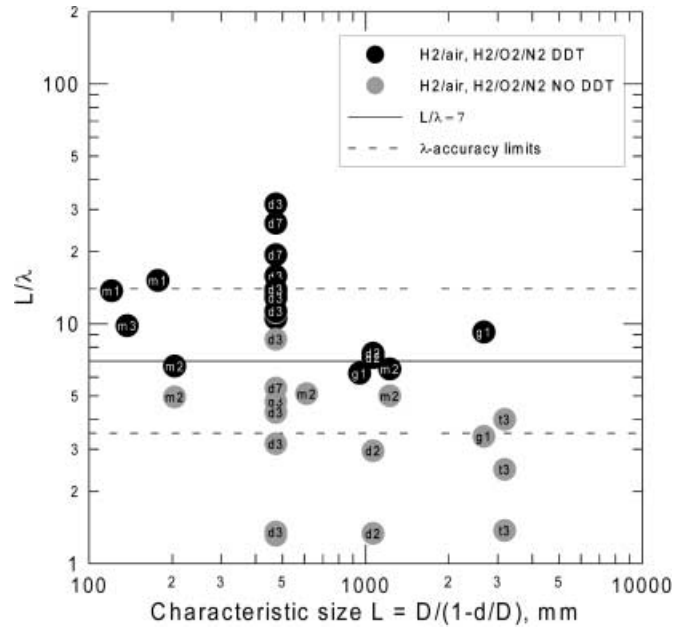
$$L/\lambda > 7, \quad (3)$$

within the limits of accuracy of the cell size data. A comparison of the experimental results for hydrogen mixtures with air and  $O_2$  (diluted with  $N_2$ ) with correlation  $L/\lambda > 7$  is presented in Fig. 11. Data point labels are given in Tables 2–5. The points labelled ‘m1’, ‘m2’, and ‘m3’ were reported by Teodorczyk et al. 1990, Lee et al. 1984, and Teodorczyk et al. 1988; those labelled with ‘c6’, ‘g1’, ‘g4’, ‘t2’, and ‘t3’ were obtained by Kuznetsov et al. 1999.

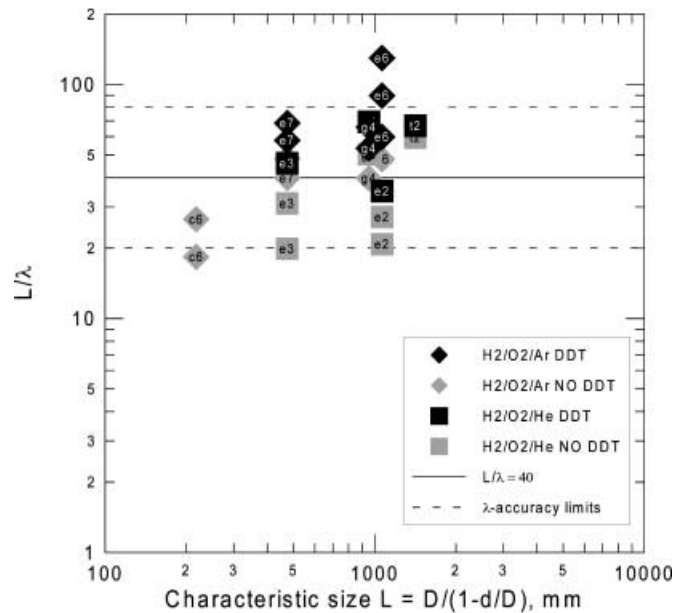
The results for mixtures diluted with Ar and He, which are characterised by regular detonation cellular structures, show that the critical conditions for DDT expressed by (3) are not valid for these mixtures. Figure 12 shows that the critical conditions for DDT in stoichiometric  $H_2/O_2$  mixtures diluted with Ar or He can be approximately described by:

$$L/\lambda > 40. \quad (4)$$

Deviations from this condition, which can be found in Fig. 12, are within the limits of accuracy of the cell size data.



**Fig. 11.** Critical conditions for onset of detonation in ‘irregular’ mixtures



**Fig. 12.** Critical conditions for onset of detonation in ‘regular’ mixtures

The difference in the critical conditions for DDT between ‘regular’ and ‘irregular’ systems show the same trend as that in the problem of detonation propagation from a tube to an unconfined space. The critical exit diameter  $d_c$ , expressed in terms of  $\lambda$ , has been found to be several times larger in regular systems compared to irregular ones (Shepherd et al. 1986; Desbordes et al., 1993). Similar behaviour was also observed in the problem of the minimum (limiting) tube diameter for self-sustained propagation of detonations. The limiting tube diameter  $d_l$ , expressed in terms of  $\lambda$ , has also been found to be at

least several times larger in regular systems compared to irregular ones (Dupre et al. 1991).

In all these cases, the cell size is used for the description of limiting conditions for detonation propagation and initiation as a characteristic chemical length scale. In regular systems the value of  $\lambda$  is generally well defined. Irregular systems are characterised by a rather wide range of characteristic chemical length scales. The values of  $\lambda$  reported are usually a sort of average of the cell sizes, or a size of dominant cells. It may be suggested that, if the smallest chemical length scale from the existing range are used for both types of mixtures, then the difference in correlations for the critical conditions between regular and irregular systems would be reduced. Further development of this assumption would suggest that the smallest available length scales might be those that define the mixture sensitivity and critical conditions for detonation propagation and initiation. Although such an explanation seems reasonable to describe the differences in critical conditions for regular and irregular systems, additional analyses are required for its evaluation.

## 5 Conclusion

The critical conditions for DDT (expressed both in terms of hydrogen concentrations and detonation cell widths  $\lambda$ ) have been shown to be strongly influenced by the regularity of the detonation cellular structure of the test mixtures. The critical values of the cell sizes in Ar- and He-diluted mixtures have been found to be significantly smaller than those in air mixtures and oxygen mixtures with N<sub>2</sub> dilution for the same tube and obstacle geometry. This means that systems with highly regular detonation cellular structures are much less capable of undergoing DDT compared to irregular ones with the same values of the detonation cell sizes. The difference in critical conditions between regular and irregular systems was shown to have the same trend in the case of DDT and in the problems of self-sustained detonation propagation.

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