DDT Limits in H_2-Air Mixture In a Tube Filled With Obstacles

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1 Introduction

Deflagration to detonation transition (DDT) limits are crucial values for every fuel defining the range of fuel in oxidizer for which the transition to detonation might occur. The knowledge about these limits is of great practical importance for process safety management and designing the in-line detonation extinguish devices like detonation arresters. The DDT limits are dependent on initial and boundary conditions of the experimental setup including fuel type, concentration, geometry, level of confinement and the scale of the setup. Example measurements of lower limits in a 30.5 cm [1], 43 cm [2] diameter tubes and 2.3 m high channel [3] gave values of 15%, 13.6% and 12.5% of hydrogen in air, respectively. This simple comparison shows that the scale of the experimental setup is of great importance. As the essential condition for the detonation front to propagate is the presence of developed cellular structure (fuel concentration dependent) it was possible to correlate the characteristic cell size width λ with the characteristic dimensions of the channel. For example Dorofeev et al. [4] provided the critical correlation of $L/\lambda \approx 7$, where L is the characteristic dimension of the experimental setup which might be interpreted as the minimum distance for detonation formation. This criterion was further confirmed by studying the blockage ratio influence on the DDT in a CH_4-air mixture [5]. In case of spinning detonation the criterion of sustained detonation in a tube of diameter d, is close to $d = \lambda/\pi$. However, this type of detonation is of specific nature and occurs in round tubes only while the mixture approaches the detonability limits [6]. In case of obstacle filled tubes the main origin of the hot spot leading to detonation onset is the surface of the obstacle or the corner between the obstacle and bottom wall [7–10] where formed Mach stem reflects. Depending on the obstacles spacing and arrangement additional sub-regimes for detonation formation might be also distinguished [7]. For obstacles filled channels Thomas [11] provided criterion for detonation to develop as $\eta >\sim 3$ where η is the ratio between the obstacle height h and product of a_r – sound speed and τ_r – ignition delay time in the undisturbed reflected shock region.

The research presented in this paper is mainly focused on the experimental measurements of the DDT limits in a 4 - m long obstacle filled channel (Blockage ratio BR = 0.5) filled with H_2-air mixture. Apart from the measurements of the DDT limits, the experimental setup allows simultaneous measurements of

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the shock wave and flame position along the channel. This arrangement allows to measure the time of existence of shocked flammable gas and compare it with the ignition delay time calculated with the 0-D Cantera software for reflected wave conditions. Additionally, the results are compared with the available criteria for successful detonation onset in obstacle filled obstacles.

2 Experimental setup

The experimental setup has been previously used for the investigation of scale effect of the obstacle filled 2 - m long channel and the results are reported in paper of Teodorczyk [8]. The current setup has been extended 4 – m length to observe further flame acceleration, transition to detonation and stable detonation. The tube consists of two 2-m long tubes of 0.08 x 0.11 m in cross-section (H x W). The tubes were filled with obstacles 10 mm thick and 40 mm high giving the blockage ratio of 0.5. The spacing S between obstacles varied in range of S = H, 2H, 3H. Initial conditions for the H_2-air mixture were T = 295 ±3K and P = 0.1 MPa, stoichiometric coefficient in range of 0.42-2.92 which corresponds to 15 - 55% of hydrogen in air. The mixtures were prepared with partial pressure method and stored horizontally for at least 24 hours to mix due to the diffusion process. Number of experiments for each mixture composition and geometrical configuration was 10-13 for the majority of tests, three configurations were tested with 4, 5 or 7 single experiments. The total number of experiments was nearly 300. The ignition source was automotive spark plug placed at one end of the channel at its half-height middle-width. The Data acquisition system (DAS) consisted of 16 channels sampling pressure sensors and ion probes with frequency up to 2 MHz. The Pressure sensors and ion probes arranged in pairs to simultaneous measure the flame and shock wave time-of-arrival (ToA). The scheme of the experimental setup is shown in Fig. 1.

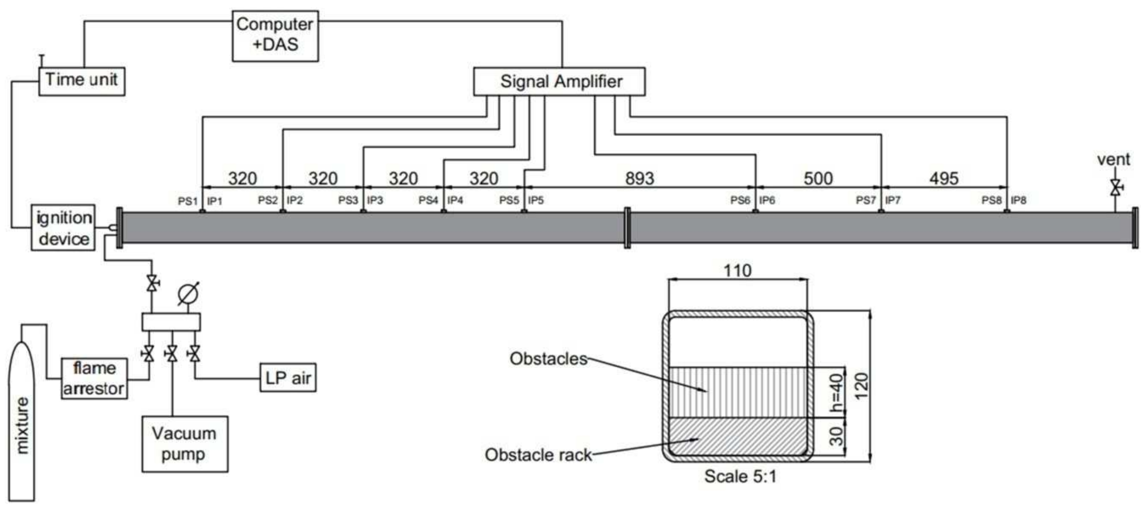

Figure 1. Experimental setup scheme.

3 Results

The total number of experiments performed was 304 including 77 for S = H, 121 for S = 2H and 106 for S = 3H. The reason for such amount of experiments was that for configuration S = H tested initially, transition to detonation was observed in some experiments and in some deflagrative regime was observed only. Figure 2 shows such feature for configuration S = H and stoichiometric H_2 - air mixture. The experiments present good experimental repeatability of the flame acceleration process till the velocity close to isobaric speed of sound in products, however the transition to detonation does not always occur. This points at the stochastic nature of DDT process, especially for low obstacles spacing. Therefore it was arbitrarily decided to define lower (upper) DDT limits as the concentration where at least one of experiments indicated detonation within particular experimental set while in lower (higher) concentration were experiments with deflagration only. Table 1 summarizes experiments performed together with the combustion regimes marked with colors: green - deflagration, red – detonation. Table also shows the number of deflagration and detonation only experiments over the total number of experiments for particular mixture. In case of S = H there is no 100% probability for the detonation to occur as for the ϕ = 1.2 in 8 experiment of 10 detonation was observed. With the criterion for DDT limit introduced earlier, for configuration S = H, lower and upper DDT limits are 27.4% and 38.6% of hydrogen in air, respectively. In case of higher spacing between obstacles S = 2H DDT limits are 25% and 50% of H_2 in air. For spacing S = 3H, the DDT limits are slightly wider as 22.7% - 50% of H_2 in air.

Table 1 Summary of experiments performed with the deflagration (DEFL) and detonation (DET) regimes observed. Values in bold are for concentrations at defined DDT limits.

Φ (%H_2)	**DEFL** / **DET** + mean velocity [m/s] at the end of channel											
	S = H				**S = 2H**				**S = 3H**			
0.42 (15%)									10/10	595		
0.6 (20.1%)					10/10	753			10/10	797		
0.7 (22.7%)					11/11	801					**10/10**	**1565**
0.8 (25%)	10/10	833					**11/11**	**1341**			10/10	1584
0.9 (27.4%)	**7/11**	**908**	**4/11**	**1497**								
1.0 (29.6%)	6/13	925	7/13	1653			11/11	1547			11/11	1719
1.2 (33.5%)	2/10	941	8/10	1679			11/11	1663			11/11	1789
1.4 (37%)	5/11	952	6/11	1474			11/11	1619			11/11	1788
1.5 (38.6%)	**8/11**	**935**	**3/11**	**1381**								
1.6 (40%)	11/11	916					11/11	1569				
1.7 (41.6%)											11/11	1740
1.8 (43%)							11/11	1516				
2.0 (45.6%)											10/11	1257
2.1 (46.9%)					7/11	943	5/11	1403				
2.4 (50%)					**7/11**	**939**	**4/11**	**1344**	**3/7**	**738**	**4/7**	**1235**
2.92 (55%)					11/11	921			4/4	646		

What can be also seen is that the DDT limits are wider and more distinct as the spacing increases. Additionally, the mean velocities at the channel end increase with the increase of spacing. The increase of the mean velocities is linked with less heat and momentum losses due to the less obstacle number along the tube. As the detonation velocities are below the ideal Chapman-Jouguet velocities (see fig. 2 and fig.

3) almost all experiments with successful transition to detonation could be classified as quasi-detonation regime, term initially introduced by Teodorczyk et al. [9] applying to the tube with high roughness and cyclic detonation initiation and attenuation due to the diffraction behind obstacles.

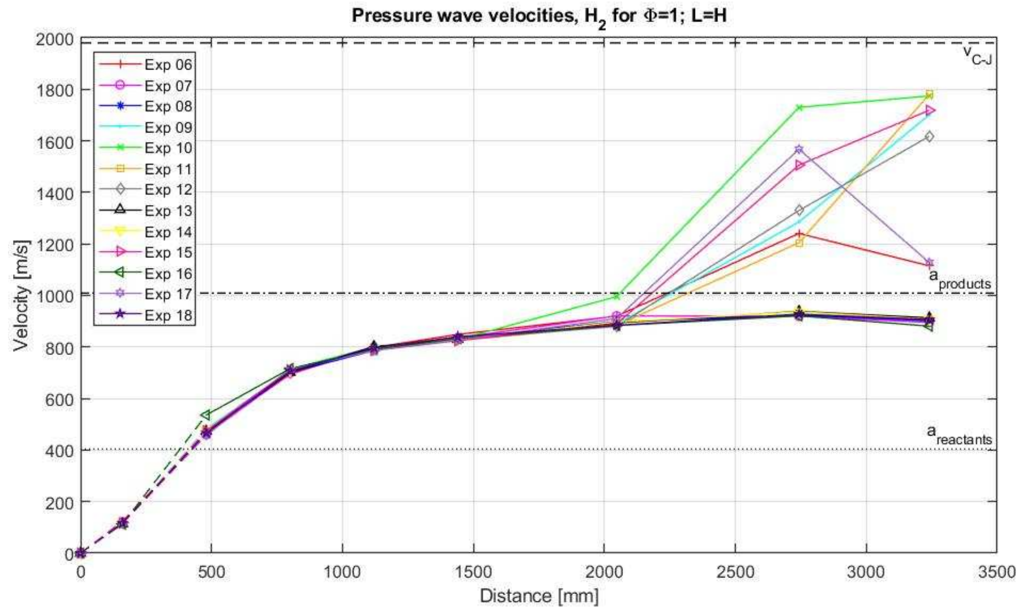

Figure 2. Example results of the 13 experiments performed for stoichiometric H_2-air mixture and S = H configuration.

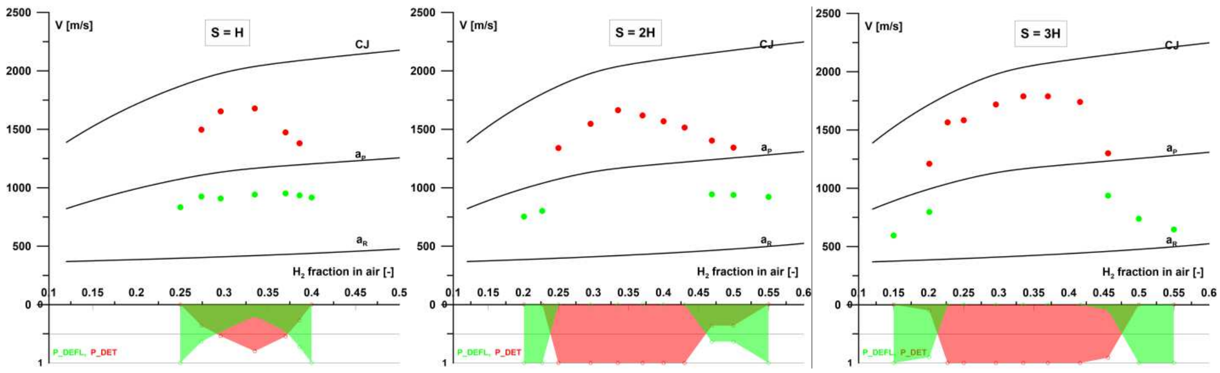

Figure 3. Velocities observed for three spacing configurations: L = H, L = 2H, L = 3H. Lower graph shows the probability for the detonation (red area) and deflagration (green area) to occur. Three black solid lines are

Next step of the experimental data analysis was to calculate the time between the leading shock wave and following flame front and compare it within the experimental sets and to the ignition delay time for post-reflected shock conditions. The code utilised was Cantera code [12] with SDToolbox module [13] and constant volume reactor model. The detailed reaction mechanism was of O Conaire et al. [14]. The data calculated were compared with the Thomas [11] criterion for successful transition to detonation.

According to the Dorofeev et al. [4] criterion for successful transition to detonation is $L/\lambda \geq 7$, where L is the characteristic dimension of the experimental setup which might be interpreted as the minimum distance for detonation formation. In case of the experimental stand described in this paper the characteristic distances L for S = H, S = 2H and S = 3H are equal to 0.160 0.32 and 0.48 m, respectively. The table 2 presents the L/λ ratio calculated for the cases considered. As one can see the Dorofeev's criterion is fulfilled for all of the cases with relatively large L/λ value in range of 10 - 28.8. Additionally, table 2 contains the ratio h/λ which seems to drop together with the increase of the spacing distance. This feature might be explained with the fact that for higher S the detonation is less disturbed by the obstacles therefore develops more stable velocity and cellular structure. As the volume between obstacles becomes longer, the importance of the distance between obstacle tip and top wall becomes limiting dimension. Table 3 presents the results of the calculations of η parameter based on the Thomas [11] criterion. The leading shock wave velocity V_{shock} has been taken from experiments for concentrations at DDT limits and recorded for experiments at the time shortly before successful transition to detonation. The post-reflected conditions has been calculated with Cantera and SDToolbox software and used as the initial conditions for the constant volume reactor model to calculate ignition delay time τ_r. The results of the calculations show that the calculated η according to Thomas criterion is well below limiting value of 3. This suggests that based on this criterion the mixture should not detonate. We should bear in mind that the ignition delay time is strongly related to temperature and τ_r is highly influenced by leading shock wave velocity and therefore due to the post-reflected temperature and pressure conditions.

Table 2 L/λ parameter calculated based on the DDT limits specified experimentally.

	S = H		S = 2H		S = 3H	
Det. Limits [% H2]	27.4	38.6	25	50.0	22.7	50
λ [mm] [15,16]	~9	~8	11.1	~20-30	~16	~20-30
L [m]	0.160	0.160	0.32	0.32	0.48	0.48
L/λ	17.8	20	28.8	10-16	30	16-24
h/λ	4.4	5	3.6	2-1.3	2.5	2-1.3

Table 3 Parameter η calculated for mixtures at DDT limits and leading shock wave travelling at velocities preceding transition to detonation. Δt is the measured time difference between pressure wave and ion probe at the time preceding transition to detonation.

	S = H		S = 2H		S = 3H	
DDT Limits [% H_2]	27.4	38.6	25	50.0	22.7	50
h [m]	0.04	0.04	0.04	0.04	0.04	0.04
Δt [μs]	20-25	28-36	30-80	80-110	60-90	90-150
V_{shock} [m/s]	~950	~900	~920	~960	~950	940
a_r [m/s]	697	690	678	745	690	734
τ_r [ms]	19.5	>1000	~40	>1000	8.6	>1000
η [-]	0.0029	<5.0E-5	0.0015	<5.0e-5	0.067	<5.0e-5

To compare the calculated ignition delay time with the experimentally measured time difference Δt between leading shock wave and following flame one can see that the available time is of the order of 20 - 150 μs, therefore the mixture at reflected conditions will not have sufficient time available to self-ignite because it will be consumed by the flame. This is quite simplified conclusion however, it points at the order of magnitude of ignition delay time that the mixture should achieve to successfully transit to detonation. The range of recorded Δt seems to increase with increase of the spacing S. This might also partially explain the increase of the DDT range with the increase of spacing S. As the leading shock wave does not only reflects from the obstacles surface but also from the bottom wall there exist areas near the corners where reflected shock waves meet and focus. This area has been very often pointed at as the main source of hot-spots leading to detonation [7–10]. To confirm that sooted foil technique has been used in case of stoichiometric mixture and S = 2H and such fine – cellular structures in the corners have been recorded.

4 Summary and Conclusions

The experimental research has been conducted in 4-m long, rectangular 0.08 x 0.11 m cross-section obstacle filled tube with constant blockage ratio BR = 0.5 to define DDT limits in H_2-air mixture. Three geometrical configurations of obstacles spacing were considered: S = H, 2H and 3H, where H is the unobstructed channel height. The results showed that the DDT limits highly depends on the obstacles spacing. The widest DDT limits and higher velocities were observed for largest spacing. This effect is due to lower heat and momentum losses behind the lower number of obstacles where detonation diffracts. It has been shown that criterion of Dorofeev et al. [4] for successful transition to detonation is valid with relatively large margin for the geometry and mixtures investigated. The criterion of Thomas [11] has not been confirmed however, the analysis is based on the velocity of the leading shock wave velocity. As the interaction of the reflecting and focusing shock waves in the corner is more complicated than simple reflection and pressure and temperature have not been measured for these conditions we are not able to calculate properly the ignition delay time and therefore the real η value. The measured experimentally time difference Δt between leading shock wave and following flame front points at the order of magnitude of ignition delay time that should be shorter to self-ignite the mixture before being consumed by the flame. The Δt increases with the increase of spacing and therefore might partially explain the increase of DDT range.

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