

Deflagration-to-Detonation Transition in Hydrogen-Air Mixtures with Concentration Gradients

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1 Introduction

The hazardous potential of hydrogen-air mixtures has intensively been studied assuming a perfect mixture of fuel and oxidant. However, comprehensive risk assessment studies [1] have shown that an inhomogeneous mixture with a vertical concentration gradient is much more likely to be generated in a real accident scenario. The influence of such a concentration gradient on flame acceleration has been studied previously [2]. From a safety point of view, the open question remaining is if the established criteria to determine whether deflagration-to-detonation transition (DDT) can occur or not, like the 7λ criterion [3], can be applied to inhomogeneous mixtures as well. Thus, the present study aims at quantifying the DDT potential of mixtures with a vertical concentration gradient in comparison to homogeneous mixtures.

2 Experimental setup

The experiments are conducted in a 5.4 m long, closed channel. It has a rectangular cross-section with a height of 60 mm and a width of 300 mm. Different obstacles can be arranged inside the channel in order to promote flame acceleration and observe DDT. The results presented in this study were obtained with flat plate obstacles mounted on top and bottom of the channel, leading to an effective blockage ratio (BR) of either 30% or 60%. The obstacles are installed in the first part of the channel, up to a distance of 2.05 m from the end plate where the gas is ignited. The remaining part of the channel is unobstructed. The obstacle spacings (S) investigated are either 100 mm or 300 mm.

In order to detect the arrival time of pressure waves and flames, the channel is equipped with seven pressure transducers (Kistler 601A) and 30 UV sensitive photodiodes (Hamamatsu S1336) operating at a sampling rate of 250 kSamples/s.

As concentration gradients on such a small scale are quickly being destroyed by molecular diffusion, different ways of hydrogen injection have been studied. The mechanism finally chosen for the experiments uses injection holes ending in small serrations on the top obstacles. From there, the injected hydrogen can flow to both sides of each obstacle (Fig. 1). Numerical simulations show that due to buoyancy and diffusion, the hydrogen plumes are quickly stratified so that no *horizontal* concentration gradients remain

and the vertical concentration gradient forms the typical S-shaped diffusion curves. With this injection mechanism, a concentration gradient of the desired strength can be produced by varying the waiting time between injection and ignition of the gas. The hydrogen distribution simulations have been confirmed qualitatively by color schlieren photography and quantitatively by gas chromatography. The measurements show good agreement with the simulations, except for very short waiting times ($t_W < 5$ s), see Fig. 2. For long waiting times ($t_W > 30$ s), the mixture can be considered as homogeneous.

The procedure for the DDT experiments is as follows: before hydrogen injection, the channel is flushed with fresh air. Next, the channel is partially evacuated to achieve the desired partial pressure. The amount of hydrogen injected is chosen to result in a pressure of 1 atm and a temperature of 20 °C. After the desired waiting time the gas is ignited with a spark plug.

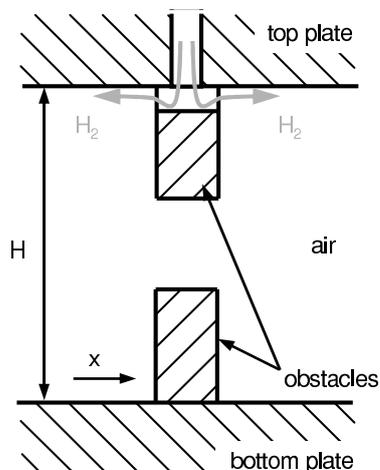


Figure 1: Sketch of the injection mechanism.

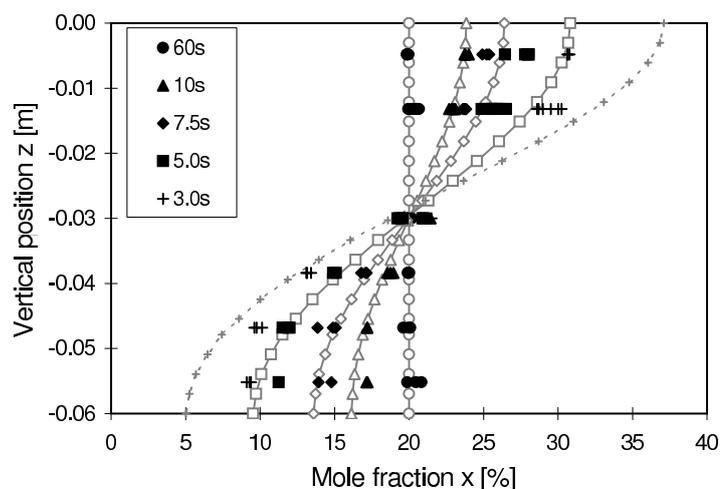


Figure 2: Hydrogen mole fraction over channel height, depending on the waiting time after injection. (Exemplary results for a hydrogen content of 20%; black symbols: experiment; grey symbols: simulation.)

3 Results and discussion

For each of the obstacle configurations described above, a series of equivalence ratios has been studied, and for each of the equivalence ratios different gradients (indicated by different waiting times) have been investigated. Local flame velocities over the whole channel length were gained by recording the flame arrival time at the position of the photodiodes and differentiating this relation by time. A compilation of the maximum flame velocities measured in all experiments of the configuration “BR30-S100” (30% blockage ratio, 100 mm obstacle spacing) is shown in Fig. 3. It shows that almost independently of the concentration gradient, the maximum flame velocities jump from approximately 800 m/s to more than 1600 m/s if the volumetric hydrogen content of the mixture exceeds a value of 19%. This corresponds to a jump from the Chapman-Jouguet (CJ) deflagration speed a_p (the speed of sound of the combustion products) to the CJ detonation speed D_{CJ} and is a clear indication for the occurrence of DDT. It goes along with a strong rise in the pressures measured. The result is in fairly good agreement with Dorofeev’s modification of the 7λ criterion [3] which predicts DDT for this geometrical configuration at a hydrogen content of 21%.

The configuration “BR30-S300” (Fig. 4) shows quite a different picture. In the homogeneous case (waiting time $t_W = 60$ s), DDT requires a volumetric hydrogen content of 20%. However, with stronger

concentration gradients, DDT occurs much earlier. At a waiting time $t_W = 3$ s, the point of DDT can be located at approximately 17% hydrogen. Moreover, the transition from slow flames (velocity below the sound speed of the unburned reactants a_r) to fast flames (velocity at CJ deflagration speed a_p) can also be recognized quite distinctly in this configuration, but not in the configuration “BR30-S100”.

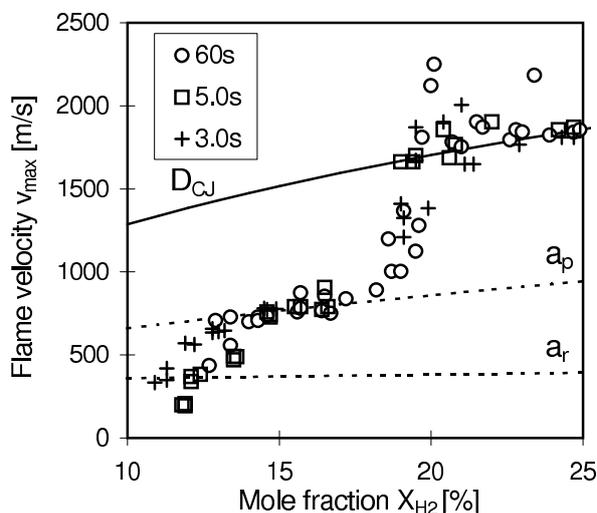


Figure 3: BR30-S100.

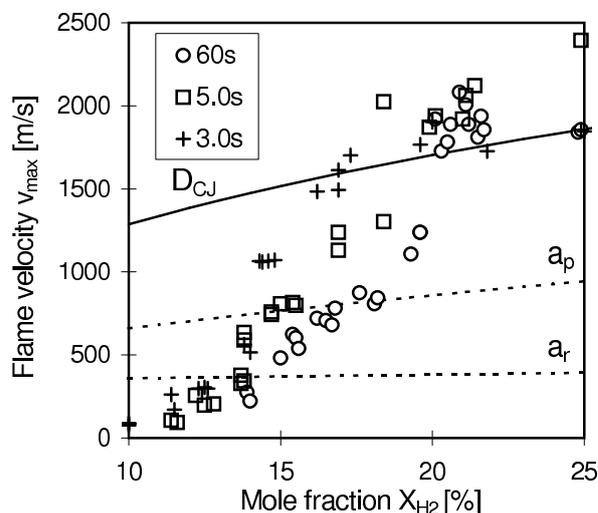


Figure 4: BR30-S300.

An explanation for the big difference in the two configurations can be found in the interaction of the flow with the obstacles. During the flame acceleration period, the deflagration acts like a piston on the unburned gas: the gas is displaced away from the reaction zone. This displacement flow is forced through the orifices between the obstacles mounted on top and bottom of the channel. Behind the obstacles, recirculation zones are generated that thoroughly mix the gas and destroy the concentration gradient locally. Numerical simulations revealed that the diameter of the recirculation zones approximately equals the obstacle height. In the case of narrow obstacle spacing (S100), most of the gas is mixed. When the flame arrives at the final obstacles, there is no big difference between a premixed gas and a mixture with an initial concentration gradient. On the other hand, in the case of wide obstacle spacing (S300), the mixing zones are limited to zones immediately behind the obstacles, while a large fraction of the volume between subsequent obstacles remains unmixed. In this case, the remarkable result is found that mixtures with strong concentration gradients are more prone to undergo DDT than homogeneous ones containing the same amount of fuel. In [1] a method is presented how the 7λ criterion can be applied to inhomogeneous mixtures. However, neither this method nor the averaged 7λ criterion are conservative when applied to the configurations studied here.

In the configuration “BR60-S100” DDT was never observed, although the 7λ criterion allows it for hydrogen concentrations of 24% and higher. However, the maximum velocities observed in the inhomogeneous mixtures were considerably higher than in the homogeneous mixtures (see Fig. 5).

In the configuration “BR60-S300”, the 7λ criterion predicts DDT if the hydrogen content exceeds 21%. This is confirmed by the experiments with homogeneous mixtures (Fig. 6). However, the corresponding mixtures with strong concentration gradients require a higher hydrogen content to detonate in this configuration. The transition is a little less distinct than in the other configurations, but can be found in the range between 22% and 24% hydrogen for waiting times $t_W = 5$ s and $t_W = 3$ s. Contrary to the “BR30” configuration, a concentration gradient seems to lessen the tendency to undergo DDT. A possible explanation for this seeming paradox can be found in the arrangement of the obstacles. With a large fraction of the channel cross-section being blocked, the reaction front is forced to pass in the middle of the channel, where the hydrogen content approximately equals the content of the homoge-

neous mixture. The shock waves generated by explosions in the highly reactive gas in the upper part of the channel are mostly reflected by the obstacles and cannot contribute adequately to the propulsion of the reaction front. In this configuration the possible regime of repetitive explosion and subsequent failure of detonation fronts is likely to occur at hydrogen contents at which a homogeneous distribution might already produce DDT. However, further investigation will be required in order to enlighten the phenomenon.

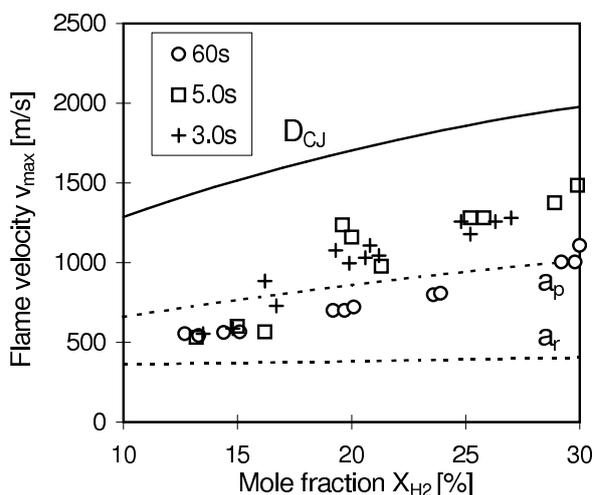


Figure 5: BR60-S100.

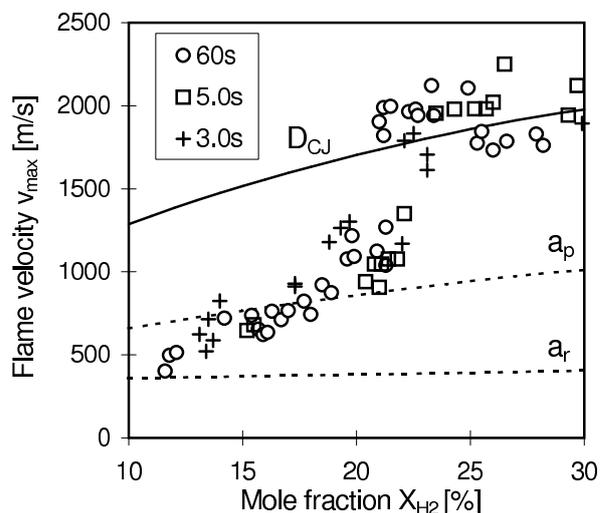


Figure 6: BR60-S300.

4 Conclusions and outlook

In the experiments conducted it was found that the 7λ criterion in its modification for obstacle-laden channels [3] predicts detonability relatively well in most cases, as long as the mixture is perfectly homogeneous. However, if the hydrogen content is distributed non-uniformly within the enclosing geometry (as it is likely to occur in accident scenarios), assessing the probability of DDT becomes challenging. Depending on the geometrical configuration, DDT can happen at considerably lower or higher fuel concentrations. The exact influence of the geometrical configuration is difficult to assess, but it is obvious that due to the concentration gradient the problem becomes a multi-dimensional one. One-dimensional parameters like blockage ratio and characteristic length scales [1, 3] are no longer sufficient to describe it, e.g. different results can be expected when the obstacles are arranged vertically instead of horizontally as in the present study. Further research is required and will be conducted by the authors in order to quantify the additional effects that have to be taken into consideration for DDT prediction in mixtures with concentration gradients.

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References

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