

# Flame Acceleration in Hydrogen-Air Mixtures with Concentration Gradients

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## 1 Introduction

The main goal of our research project is to characterize flame acceleration, transition to detonation and the detonation regime in hydrogen-air mixtures with concentration gradients. The orientation of these gradients is perpendicular to the main direction of flame propagation. This stratification of hydrogen and air constitutes a realistic setting of mixture composition as a consequence of accidental release of hydrogen into the ambient air [1]. The motivation is to find out if explosions in such mixtures can lead to higher flame speeds and related pressures compared to homogeneous mixtures and thus pose a higher risk for the containing structure. If this can be confirmed during the investigations, existing criteria for flame acceleration and transition to detonation for homogeneous mixtures cannot be considered conservative for such scenarios. An extension of these criteria could become necessary. In this paper flame acceleration leading to critical conditions for the onset of detonation is investigated experimentally.

## 2 Experimental Setup

Experiments are conducted in a closed rectangular channel with a height of 60 mm, a width of 300 mm and a length of 5.4 m. In this volume, hydrogen-air mixtures with vertical concentration gradients of defined steepness can be generated at ambient pressure and temperature. The channel is filled with air before hydrogen is injected through supply pipes at the top plate. The hydrogen flow is deflected so that a compact layer of hydrogen along the top of the channel is formed. Subsequent diffusion leads to defined concentration gradients over the channel height, depending on the diffusion time  $t_d$  elapsed since injection. The shorter the diffusion time the steeper the gradient. Diffusion times of 3 s, 5 s, 7.5 s, 10 s and 60 s are investigated. A diffusion time of 60 s leads to a homogeneous mixture. At one end of the channel the mixture is ignited using a central spark plug. At distances between 0.25 m and 2.05 m from the point of ignition, obstacles of different blockage ratio (BR) and spacing (S) can be placed. The subsequent part of the channel remains unobstructed in all configurations. Flame velocities are measured using UV-sensitive time-of-arrival photodiodes at about 40 positions at the channel axis. Piezoelectric pressure transducers are employed to capture combustion pressures and the dynamics of pressure waves. Further details about the facility can be found in [2]. Three different geometric configurations will be discussed. In configuration BR00, no obstacles are applied. However, a blockage ratio of 2 %

is generated by the hydrogen deflection mechanism. In the other configurations, horizontal flat plate obstacles at the top and bottom of the channel are used to promote flame acceleration by turbulence production, local increase of macroscopic flame surface and instabilities.

Table 1: Obstacle configurations investigated.

Configuration	Blockage Ratio BR [%]	Spacing S [mm]
BR00	2	-
BR60S300	60	300
BR30S300	30	300

### 3 Results and Discussion

In order to characterize flame acceleration as a function of average hydrogen concentration, concentration gradient and obstacle configuration, two parameters are evaluated. Firstly, the distance from the ignition plate to the point where the measured speed of the flame tip reaches the speed of sound of the unburned mixture calculated for the respective average hydrogen concentration. This parameter can be interpreted as the run-up distance to fast flames characterizing early flame acceleration. Secondly, the distance from the ignition plate where the flame speed reaches the speed of sound of the combustion products. This parameter is referred to as the run-up distance to choked flames. It can be observed that accelerating flames sometimes remain at velocities slightly below the speed of sound of the combustion products for a small distance prior to further acceleration. Therefore, a value of 95 % of this velocity is chosen as a criterion for the run-up distance to choked flames in order to reduce scatter, comparable to the approach in [3]. In case of the unobstructed channel, run-up distances generally decrease with the introduction of concentration gradients. This result is presented in Figure 1. Each point depicts the average of five experiments. It is noteworthy that run-up to choked flames in the unobstructed channel can only be reached very close to the end plate. Thus, it is expected that these results are strongly influenced by repeated reflection of compression waves off the end plate. However, the run-up distance to fast flames shows an equal trend which confirms the strong accelerating influence of concentration gradients at all average hydrogen concentrations investigated.

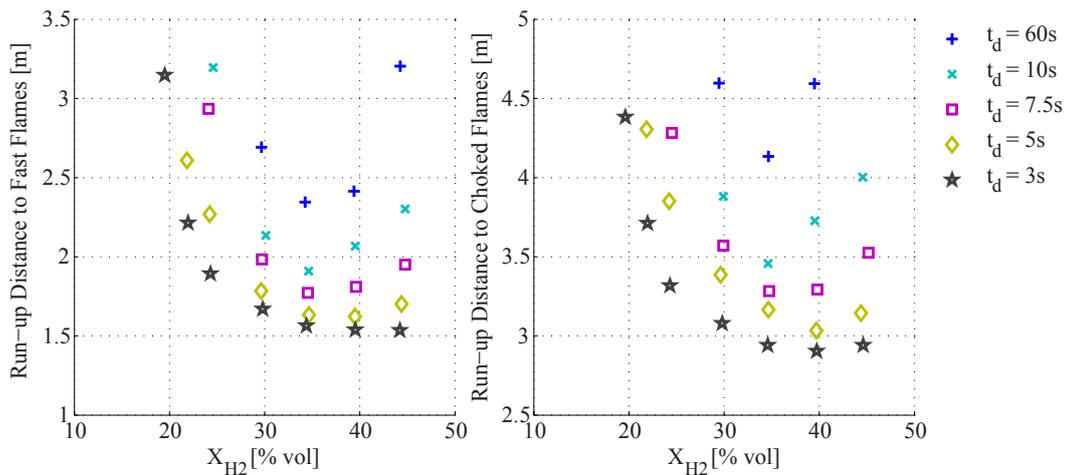


Figure 1: Run-up distances in the unobstructed channel for different average volumetric hydrogen concentrations and concentration gradients, BR00.

Run-up distances in the obstructed channel behave differently. Results for BR60S300 are shown in Figure 2. At average hydrogen concentrations lower than 22.5 %vol, concentration gradients cause faster flame acceleration. Run-up distances higher than 2.05 m mean that the criterion for choked flames is not reached within the obstacle path. Analysis of the run-up distance to fast flames is therefore more unambiguous showing equal trends. Above this concentration of 22,5 %vol, gradients lead to higher run-up distances. Flame acceleration is clearly retarded by the gradient in this region of high average hydrogen concentrations.

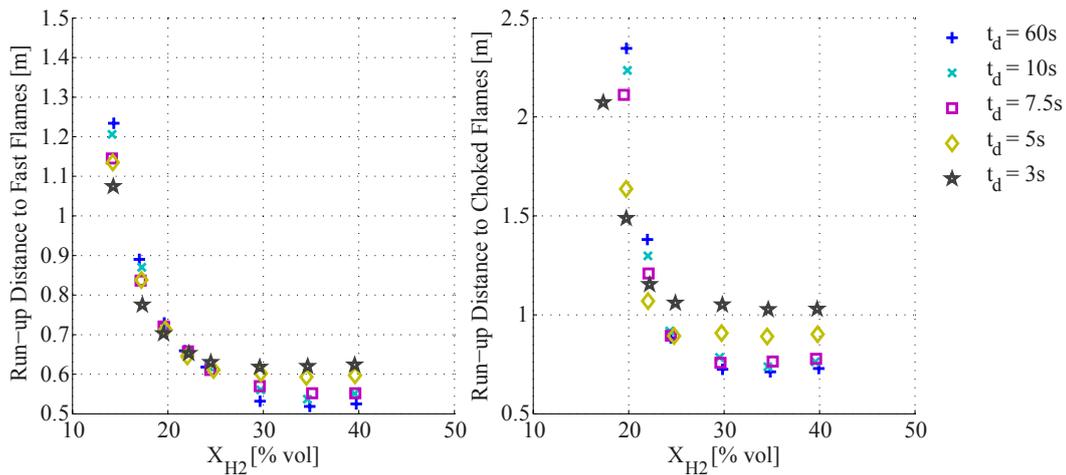


Figure 2: Run-up distances in the obstructed channel for different average volumetric hydrogen concentrations and concentration gradients, BR60S300.

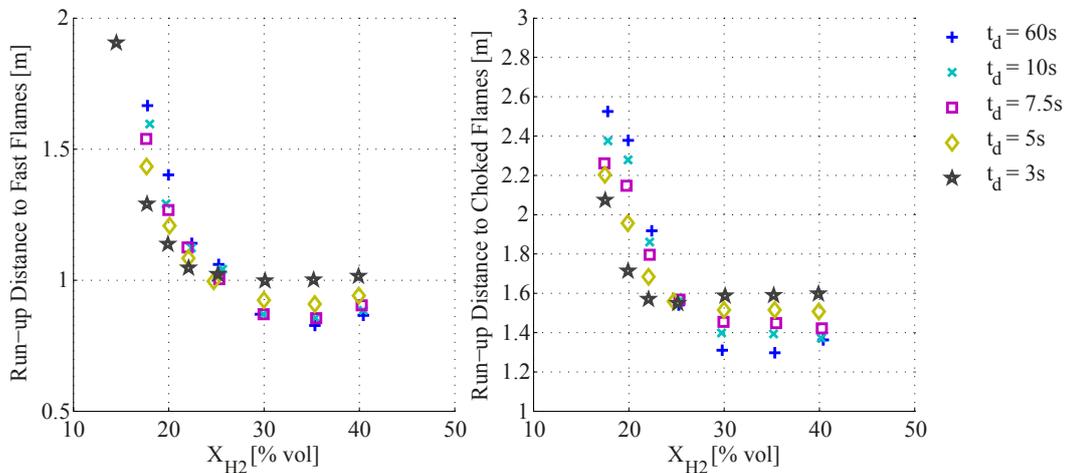


Figure 3: Run-up distances in the obstructed channel for different average volumetric hydrogen concentrations and concentration gradients, BR30S300.

Another obstacle configuration with a blockage ratio of 30 % and spacing of 300 mm was investigated in order to check the universality of the findings for obstructed channels. The results are shown in Figure 3. The same general effect of global concentration combined with concentration gradients on run-up distances can be seen. The average concentration where the change takes place is slightly shifted to 25 %vol. At the same time, the difference in run-up distances to fast flames between homogeneous and inhomogeneous mixtures at low average hydrogen concentrations is much more pronounced in this configuration than in BR60S300. These differences are comprehensible as this configuration has a blockage

ratio which lies in between the configurations BR60S300 and BR00. One could assume that the lower the blockage ratio, the higher the average concentration where the change in the concentration gradients' impact takes place. Thus, a substantial difference in the effect of concentration gradients on flame acceleration between the unobstructed and the obstructed channel can be observed. In order to obtain possible explanations for this fundamental difference, flame shapes and mixture properties need to be studied. High-speed OH\* chemiluminescence images were taken that give further insight. Figure 4 shows flames in the unobstructed channel (BR00) moving from left to right at a distance of 2 m from the point of ignition.

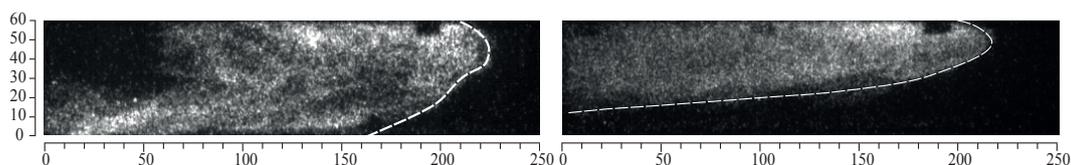


Figure 4: OH\* chemiluminescence images of flames in homogeneous (left) and inhomogeneous (right, 3 s diffusion time) mixtures, 20 %vol average hydrogen concentration, BR00.

In the homogeneous mixture (left) an almost symmetric flame front can be seen. It is slightly oriented towards the top of the channel, possibly due to a region of elevated turbulence around the hydrogen deflection mechanism at the top. Looking at the flame in the mixture with a steep concentration gradient (right), a stretched flame with a very large macroscopic flame surface is observed. This large surface leads to a higher overall heat release rate which might be a first explanation why flames in mixtures with concentration gradients in the unobstructed channel, where an undisturbed flame shape can develop, show faster acceleration. In case of the obstructed channel, the flame shape is influenced by the geometry. In the vicinity of each obstacle the flame shape is dominated by the flow generated by thermal expansion of the reaction products. It takes a certain distance behind each obstacle until the undisturbed flame shape is regenerated. Additionally, shock-flame interaction between the obstacles has a major influence on flame acceleration in the obstructed channel. Flames passing an obstacle at 1.15 m from the point of ignition are shown in Figure 5.

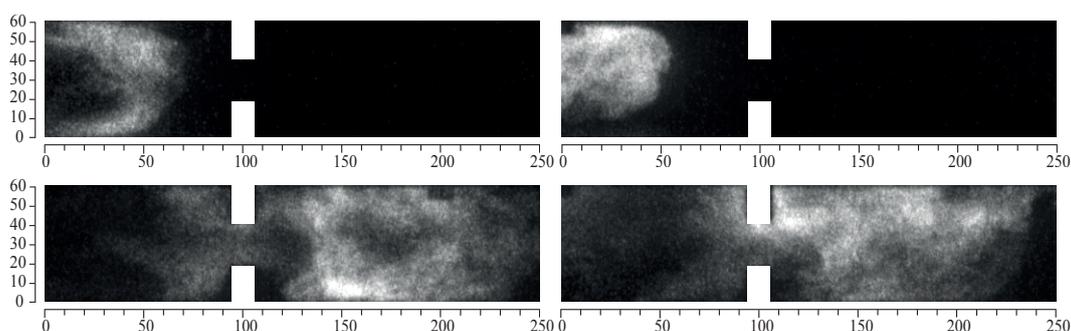


Figure 5: OH\* chemiluminescence images of flames in homogeneous (left) and inhomogeneous (right, 3 s diffusion time) mixtures, 20 %vol average hydrogen concentration, BR60S300.

Flame shapes in the homogeneous and inhomogeneous mixture look similar behind the obstacle due to the influence of geometry and induced flow. With increasing average hydrogen concentration and thus increasing flame and flow velocities as well as increasing strength of pressure waves, macroscopic flame shapes and surfaces assimilate in the obstacle path. Large blockage ratios (BR60) support this effect compared to lower blockage ratios (BR30). This could explain why flame acceleration becomes independent of the concentration gradient at a certain average concentration. Similar trends in macroscopic flame shapes were observed using the color schlieren technique at the facility [4].

The remaining question is why concentration gradients in mixtures with high average hydrogen concentrations lead to even slower flame acceleration than measured in homogeneous mixtures. A first idea was that horizontal obstacles may retard flame acceleration in mixtures with gradients because they particularly obstruct the parts of the mixture with the highest local reactivity. This could not be confirmed. Vertical obstacles with equivalent blockage ratio and spacing show the same general behavior as horizontal obstacles. Another promising approach is to study characteristic properties of homogeneous and inhomogeneous mixtures. One of the central mixture properties for flame acceleration, the expansion ratio  $\sigma$ , is examined. Further basic parameters like the laminar burning velocity could be studied in a similar manner. The expansion ratio is commonly used to describe flame acceleration and is especially useful to predict if slow or fast flames will develop in a mixture [5]. It can be calculated for the homogeneous mixture of hydrogen and air as shown in Figure 6, left part, red solid line. Cantera [6] is employed for these calculations. A first idea to capture the properties of a mixture with concentration gradients is to calculate an effective expansion ratio:

$$\sigma_{eff} = \frac{1}{H} \int_0^H \sigma(h) dh, \quad (1)$$

where  $H$  is the channel height and  $\sigma(h)$  the local expansion ratio calculated for the corresponding local mixture composition at each height  $h$ . In Figure 6, the effective expansion ratio as a function of average volumetric hydrogen concentration is shown for different concentration gradients, blue dashed lines. It remains below the values for a homogeneous mixture at all average concentrations due to the non-linear dependency between expansion ratio and hydrogen concentration.

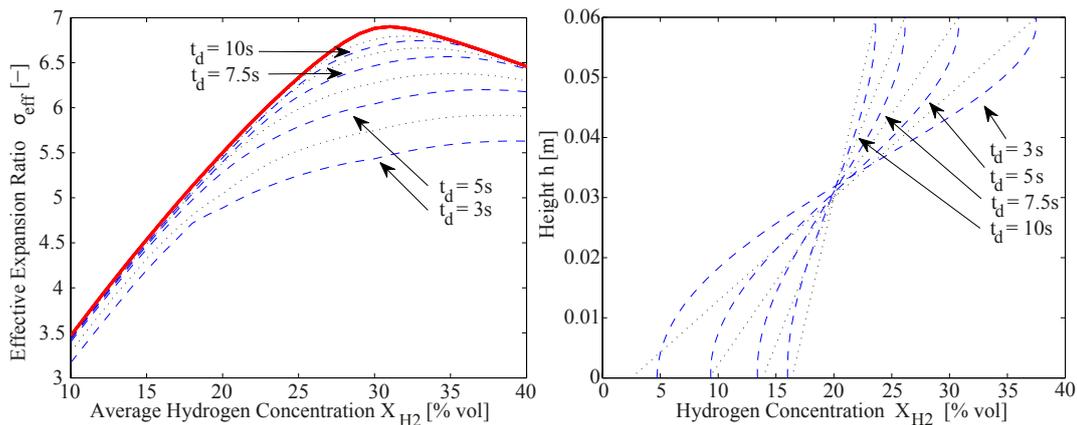


Figure 6: Calculated effective expansion ratio for homogeneous and inhomogeneous mixtures (left). Examples of concentration profiles used for the calculations (right, average hydrogen concentration 20 %vol) .

The shape of the gradients used for these calculations is obtained from numerical simulations of hydrogen injection and diffusion in the test facility [7]. Exemplary concentration profiles are plotted in Figure 6, right part, for an average hydrogen concentration of 20 %vol. For ease of comparison, linear generic concentration gradients with equal maximum and average concentrations are used to calculate the profiles shown with black dotted lines. It is noticeable that the maximum effective expansion ratio, which lies slightly above stoichiometry for homogeneous mixtures, is shifted towards higher average concentrations with gradients getting steeper. This trend can indeed be seen in Figure 1 for flame acceleration in the unobstructed channel. Summarizing these findings, there might be a decelerating effect of concentration gradients due to mixture properties if a global view by defining effective integral parameters is really justified. In the unobstructed channel, the effect of amplified flame surface might predominate. In the obstructed channel, the decelerating effect of a lower effective expansion ratio might prevail at high average concentrations and large blockage ratios where high flow velocities in the obstacle path dominate the flame shape in both homogeneous and inhomogeneous mixtures.

## 4 Conclusions and Outlook

Flame acceleration in hydrogen-air mixtures was studied with particular focus on the effect of concentration gradients. These generally lead to faster acceleration in the unobstructed channel. In contrast, concentration gradients can either increase or decrease the run-up distances in the obstructed channel, depending on the corresponding average hydrogen concentration. An attempt was made to explain this difference by studying the macroscopic flame shape using OH\* chemiluminescence imaging and by analyzing the effective expansion ratio of mixtures with concentration gradients. A concept for the interpretation of mixture properties by integral balancing was proposed in this context. Undisturbed flame surfaces in mixtures with gradients are significantly larger than in homogeneous mixtures, whereas the effective expansion ratio is lower. Obstacles tend to equalize flame shapes. The hazardous potential of inhomogeneous mixtures compared to homogeneous mixtures in case of accidental ignition in real-world scenarios, especially in unobstructed tubes, is considerable regarding the presented results. Criteria for effective flame acceleration like the well-known sigma-criterion [5] do not cover these effects and accordingly do not provide conservative predictions for safety considerations. In future studies, an emphasis will be placed on the use of highly time-resolved optical measurement techniques such as OH-PLIF (Planar Laser-Induced Fluorescence), as well as on in-depth analysis of decisive mixture properties and modeling approaches for further characterization of flame propagation in mixtures with concentration gradients.

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