Macroscopic Structure of Fast Deflagrations and Detonations in Hydrogen-Air Mixtures with Concentration Gradients

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1 Introduction

Research on explosion hazards in nuclear power plants has shown that hydrogen-air mixtures with concentration gradients constitute realistic accident scenarios [1]. Distribution of hydrogen released into large rooms is dominated by the buoyancy effect rather than by diffusion. Only comparably long times allow for formation of homogeneous mixtures via molecular diffusion. Little is known about the influence of concentration gradients on flame acceleration and the onset of detonation for gradients being oriented perpendicularly to the main direction of flame propagation. Previous studies mainly focused on flame front and shock tracking via photodiodes and pressure transducers [2–4], as well as on 2D numerical simulation of the entire process [5–8]. However, all this experimental and numerical data is rarely validated by means of optical measurement techniques. Ishii et al. [9] analyzed detonation propagation in hydrogen-air mixtures with vertical concentration gradients and gave an insight into detonation structure. Lieberman and Shepherd [10] optically examined detonation propagation through mixtures forming a spatial concentration gradient with a diluent. Both studies concluded influences on propagation velocity and detonation front curvature. The present work thus aims at giving further details on deflagration and detonation propagation in inhomogeneous hydrogen-air mixtures.

2 Experimental Setup

Deflagration and detonation phenomena are studied in a closed rectangular channel with a length of 5.4 m and a cross section of 300 mm x 60 mm as described in detail in [3]. The channel comprises two sections, one part for promoting flame acceleration via obstacles after spark ignition and an unobstructed second part. The first section is 2.05 m long and enables obstacle application. In this work, the configuration BR60S300 with a blockage ratio (BR) of 60 % and an intermediate spacing (S) of 300 mm is investigated. Optical access is achieved via two facing quartz glass windows. Individual positioning of the window section along the channel axis allows for observation of all relevant phenomena. A defined hydrogen concentration gradient in air is generated perpendicular to the main direction of flame propagation. For this purpose, a deflection mechanism at the channel's top is used to build up a hydrogen layer in the upper part of the channel which stratifies through buoyancy and diffusion as a function of time. Diffusion times t_d vary from 3 s up to 60 s and define the steepness of the gradient.

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The latter time represents an entirely homogeneous mixture. Further details on the injection mechanism including validation measurements and simulations can be found in [3]. All experiments are conducted at an initial pressure of 1 atm and ambient temperature. Optical investigations include color schlieren, shadowgraph and OH* chemiluminescence imaging. Schlieren and shadowgraph images are captured simultaneously to OH* chemiluminescence. Images are taken at a maximum frame rate of 72000 fps and a minimum shutter speed of 370 ns using Photron SA-X, SA5 and image intensified Photron APXI^2 high-speed cameras. For illumination, a constant 300 W Xe arc light source is used. It is noteworthy that self-absorption plays a role for OH* chemiluminescence imaging due to the considerable optical depth of the channel. Therefore, structures emerging from positions closer to the recording camera may appear with a higher weighting than structures at a larger distance.

3 Fast Flames in Inhomogeneous Mixtures

Figure 1 shows representative images of shock waves and flames in a homogeneous (left) and inhomogeneous mixture (right, t_d = 3 s) for 15 %vol hydrogen in air. Records are taken at the last obstacle passage at a distance of 2.05 m from the point of ignition. Although the channel width of 300 mm is distinctly larger than in comparable facilities, a low curvature of the observed structures in the spanwise-direction of the channel leads to an adequate image quality.

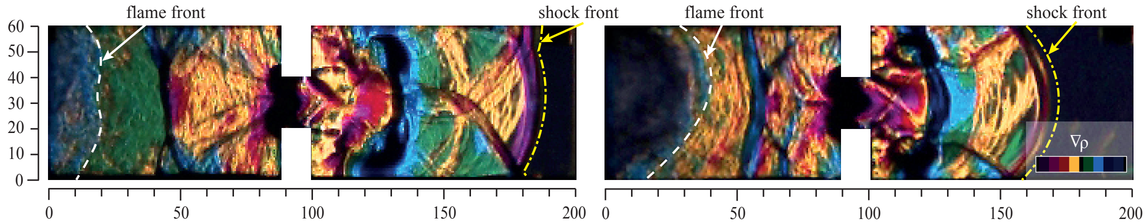

Figure 1: Color schlieren images showing shock waves and flame front in 15 %vol H_2-air mixture in the BR60S300 obstacle configuration; Left: homogeneous mixture; Right: inhomogeneous mixture with steep concentration gradient (t_d = 3 s).

The formation of shock waves ahead of the turbulent reaction zone is clearly visible. Shock waves reflected off the obstacle have not yet interacted with the flame front at the stage shown in Figure 1. The particular strength of the leading shock front and the reflected waves can be qualitatively assessed by interpreting the recorded colors (see $\nabla\rho$ plot, Figure 1). The maximum deflection of parallel light exceeds the colored region of the schlieren edge and indicates the highest appearing density gradients. Extensive studies of flame acceleration by means of conventional measurement techniques (photodiodes and pressure transducers) in this facility demonstrate the accelerating effect of concentration gradients for this obstacle configuration at average volumetric hydrogen concentrations lower than 22.5 %vol [11]. Concentration gradients lead to a reduction of the distance between leading shock and reaction zone at the examined position with a flame slightly oriented towards the top. Despite the mixture inhomogeneity, macroscopic flame surfaces remain in the same order of magnitude in the obstructed channel.
Figures 2 and 3 show fast deflagrations in the unobstructed part of the channel for two different average volumetric hydrogen concentrations. The white rectangles at the top mark the positions of the hydrogen deflection mechanism. The propagation behavior in the smooth channel is clearly different from the obstructed channel. Nearly symmetrical flame fronts and leading shock waves with respect to the channel axis can be observed in homogeneous mixtures. In contrast, steep concentration gradients cause streched flames with very large macroscopic flame surfaces and curved leading shock waves. The large flame surface leads to a high integral heat release rate, which is likely to cause the observed accelerating effect of concentration gradients in unobstructed channels [11]. As the mixture is most reactive at the channel top, providing the highest local laminar burning velocity and the highest local expansion ratio,

the flame tip is located in this region. An interaction of flame and turbulent boundary layer along the upper wall is believed to additionally support this enlargement of flame surface. Figure 3 shows the most pronounced difference in flame shapes observed in the reported series of measurements. While the flame in the homogeneous mixture is clearly separated from the leading shock, the flame in the inhomogeneous mixture is almost coupled with the leading shock in the upper region. Subsequent onset of detonation seems likely in this mixture. Shock and flame velocities extracted from the optical records are presented in Table 1. The inhomogeneous mixture clearly causes higher shock and flame velocities compared to the homogeneous mixture.

Table 1: Measured average velocities in the observed area corresponding to Figures 2 and 3.

15 %vol	t_d = 60 s	t_d = 3 s
shock velocity [m/s]	660	700
flame velocity [m/s]	350	390
20 %vol	t_d = 60 s	t_d = 3 s
shock velocity [m/s]	810	950
flame velocity [m/s]	570	$\approx v_{shock}$

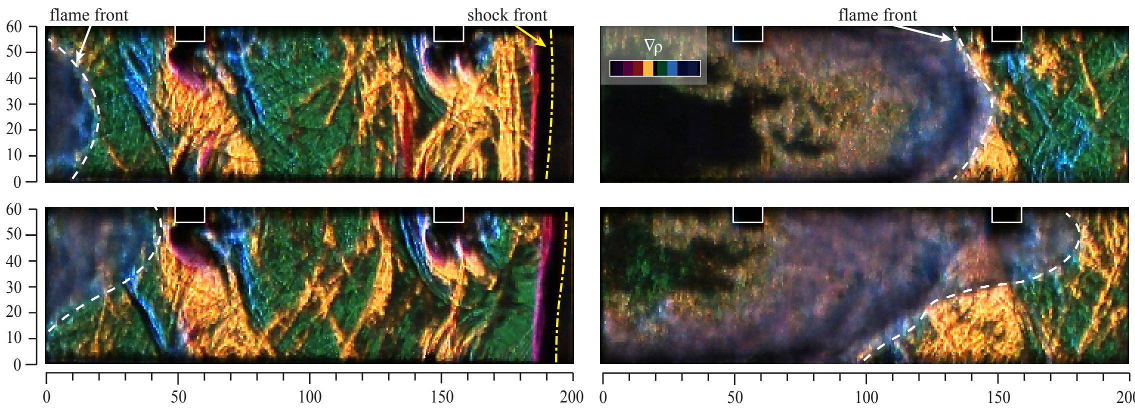

Figure 2: Color schlieren images showing shock waves and flame front in 15 %vol H_2-air mixture propagating in the unobstructed part of the channel; First row: homogeneous mixture at two different stages; Second row: inhomogeneous mixture with steep concentration gradient (t_d = 3 s) at two different stages.

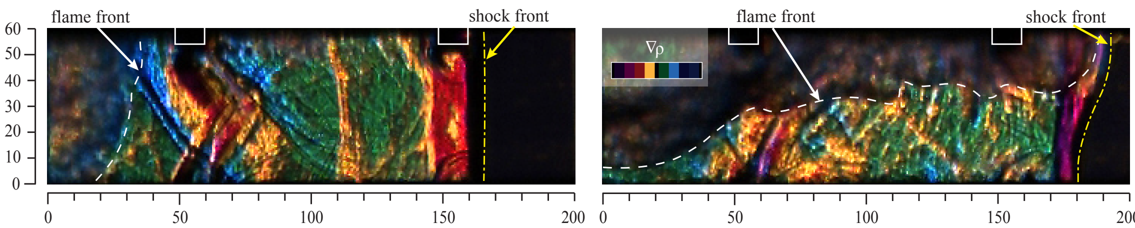

Figure 3: Color schlieren images showing shock waves and flame front in 20 %vol H_2-air mixture propagating in the unobstructed part of the channel; Left: homogeneous mixture; Right: inhomogeneous mixture with steep concentration gradient (t_d = 3 s).

4 Detonations in Inhomogeneous Mixtures

At average hydrogen concentrations higher than 20 %vol, detonations can be observed in the unobstructed section of the channel. Shadowgraph and OH* chemiluminescence images are presented in Figure 4, where 8bit greyscale OH* chemiluminescence records are transferred into color maps for better visualization of local intensities.

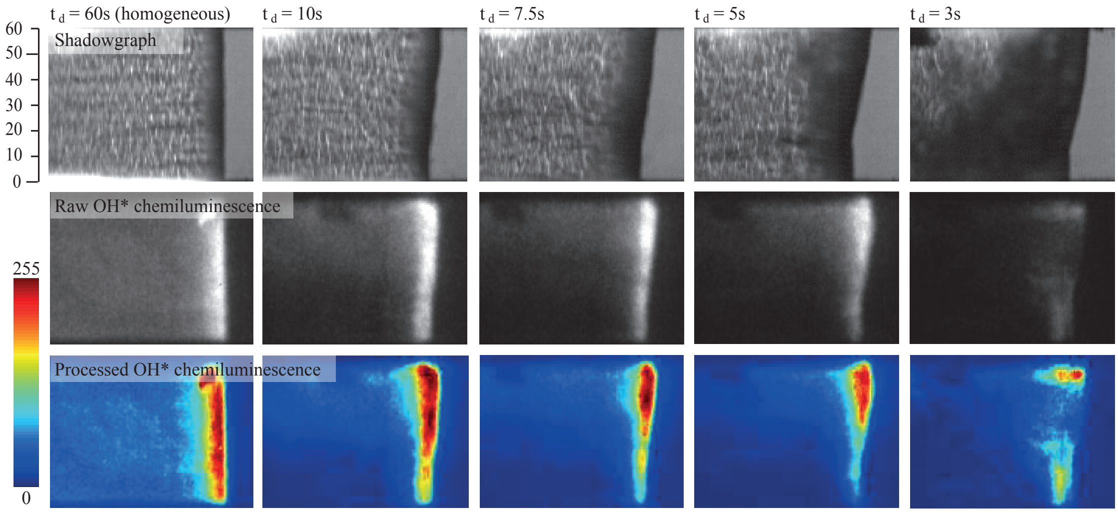

Figure 4: Shadowgraph and OH* chemiluminescence images of detonations in 30 %vol H_2-air mixture with different concentration gradients.

The detonation front for the homogeneous 30 %vol hydrogen-air mixture is captured as a reference. A nearly planar front with a very narrow reaction zone is observed for this case, as can be expected. The measured propagation velocity is nearly constant with a deficit of about 2 % compared to the theoretical Chapman-Jouguet velocity. Reaction is evenly distributed along the whole channel height, as can be seen in the OH* chemiluminescence image. With increasing concentration gradients, the detonation front becomes curved. This has already been observed in general by Ishii et al. [9]. Ettner [7] analyzes possible solutions at the channel walls to achieve wall-parallel flow behind the leading shock in a curved detonation front. He distinguishes three possible mechanisms:

1. Bending of the leading shock
2. Regular shock reflection
3. Development of a Mach stem

In the presented work, a Mach stem can be observed at the bottom of the channel for steep concentration gradients corresponding to t_d = 3 s and 5 s. This observation confirms numerical simulations shown in [7]. At less pronounced concentration gradients (t_d = 7.5 s and 10 s), it can be seen that local deflection angles remain comparably small. The Mach stem height is either decreased, direct reflection of the shock front from the bottom wall occurs, or bending of the leading shock leads to wall-parallel flow. OH* chemiluminescence images show a shift of the reaction zone towards the top wall for moderate concentration gradients. The steepest concentration gradient (t_d = 3 s) with Mach stem formation leads to high local luminescence right at the top plate interaction, as well as behind the Mach stem. Detonation propagation is maintained even though measured propagation velocities decrease with concentration gradients, as reported in [2]. It cannot be concluded directly from the images whether the reaction zone is coupled to the leading shock along the whole channel height and width. Nevertheless, an important finding is that reaction in the lean region at the channel bottom is maintained due to the high temperature ratio produced by the Mach stem. This effect can be reproduced by calculating the thermodynamic conditions behind the Mach stem and the vertical part of the leading shock at the channel top. As argued in [7], the shape of the observed curved detonation structure remains unchanged during propagation if instability effects are neglected. Following this simplified approach and taking into account the local mixture properties along the channel height at a diffusion time of t_d = 3 s and 30 %vol average hydrogen concentration (Table 2), it is obvious that the local shock Mach number is higher at the channel bottom than at the top. This in turn results in a higher temperature ratio at the Mach stem. Induction times are calculated for the particular local mixture compositions with an exemplary detonation velocity of 2000 m/s. It can be shown that self-ignition is promoted behind the Mach stem in the leanest region of the channel. This is due to the more pronounced sensitivity of induction time on temperature than on hydrogen concentration. Additional calculations of corresponding induction lengths reveal a noticeable fact. At the channel bottom, the calculated length predicts close coupling of shock wave and reaction zone. At the top however, pronounced and easily visible decoupling should be expected. As this is not the case in the presented shadowgraph images, additional underlying mechanisms, which cannot be captured by simplified one-dimensional approaches, may be responsible for self-sustaining detonation propagation in mixtures with concentration gradients. This aspect requires further investigations.

Table 2: Parameters of detonation in the inhomogeneous mixture. Calculations are based on Cantera [12], combined with the Shock and Detonation Toolbox [13] employing a detailed reaction mechanism by O'Conaire et al. [14].

Location	H_2 conc. [%vol]	Shock Ma [-]	Post-shock temp. [K]	Induction time [s $\cdot 10^{-6}$]	Induction length [m $\cdot 10^{-3}$]
Channel top	52.4	4.1	1225	17	34
Channel bottom	9.5	5.5	1853	0.19	0.38

Another striking aspect, which is shown in the shadowgraph images, is the stretched indistinct grey area right behind the leading shock front for steep concentration gradients. The area width increases with decreasing diffusion time. This effect might either originate from viewing a curved detonation front in the channel with an optical depth of 300 mm, or from local decoupling of reaction zone and shock wave due to instability of the detonation front induced by concentration gradients. Turbulent burning of initially unburnt fractions of the mixture at a certain distance from the leading shock would consequently lead to an appearance of the detonation front as it is observed.

5 Conclusions and Outlook

Influences of concentration gradients on the macroscopic shape of fast deflagrations and detonations are optically investigated in this study. For deflagrations in the unobstructed channel, significantly larger macroscopic flame surfaces can be observed. Higher propagation velocities of flame and leading shock front are measured, which is most likely due to the growth of flame surface and the related increase of the integral heat release rate. The detonation study unveils curved detonation fronts resulting from concentration gradients. Steep gradients lead to the formation of a Mach stem at the bottom wall. Reaction in the leanest part of the mixture is maintained by the high temperature ratio produced by the Mach stem.

Future optical investigations should reveal further information on flame structure and details of the detonation front, especially on the dynamics and mechanisms of detonation propagation in mixtures with concentration gradients. Additionally, detonation characteristics will be studied with soot foil records.

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