

Influence of concentration gradients on flame acceleration in tubes

Klaus Gerhard Vollmer^{*†}, Florian Ettner^{*}, and Thomas Sattelmayer^{*}

^{*}Lehrstuhl für Thermodynamik, Technische Universität München,
Boltzmannstr. 15, 85747 Garching, GERMANY
TEL : +49-89-289-16240

[†]Corresponding address : vollmer@td.mw.tum.de

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Abstract

Experimental results are presented for accelerated flames in gas mixtures with vertical concentration gradients in a smooth and an obstructed tube. Hydrogen-air mixtures with a global hydrogen content between 13 and 30 vol.% are investigated at an initial pressure of 1 atm. An injection mechanism is described that is capable of creating homogeneous mixtures as well as mixtures with vertical concentration gradients inside the tube. It is shown that the vertical concentration gradient has a major influence on flame acceleration (FA), indicated by the change of maximum flame velocity and pressure. Mixtures of the same hydrogen content can produce three different flame regimes, viz. slow flames, fast flames, and detonations, depending on the concentration gradients present. The peak over-pressure at the end of the tube can increase up to two orders of magnitude compared to homogeneous mixtures. It is shown that the maximum (local) concentration is a good criterion to compare different mixtures. The transition from slow flames to fast flames and even the deflagration-to-detonation transition (DDT) in different mixtures can be correlated well using the maximum fuel concentration near the upper wall.

Keywords : flame acceleration, inhomogeneous mixture, vertical concentration gradient, hydrogen

1. Introduction

Severe accidents in a nuclear power plant can result in the production and release of a large amount of hydrogen. If the released gas reacts with the ambient air, the combustion induced pressure results in a major risk for the integrity of the containment. Several studies were conducted in explosion tubes to get a better understanding of the flame acceleration (FA) process resulting from such hazardous events. The goal was to derive criteria when fast flames occur. Breitung *et al.*¹⁾ investigated the behaviour of turbulent flames in hydrogen-air mixtures in a series of experimental studies. It was found that in tubes containing different obstacle configurations a well-defined difference in flame behaviour can be observed between slow, subsonic flames, and fast flames. Dorofeev *et al.*²⁾ analyzed the data of Breitung *et al.*'s FA experiments in depth. The data cover a wide range of tube scale and obstacle configurations and mixture compositions. Temperatures and pressures were

at normal and elevated levels. Critical conditions for the effective FA are suggested in the form of correlations of critical expansion ratio σ^* versus dimensionless effective activation energy. Ciccarelli and Dorofeev³⁾ gave an overview of the FA process and discussed the flame propagating mechanism in obstructed and unobstructed tubes. However, all these experiments were conducted with homogeneous hydrogen-air mixtures.

In the case of a hydrogen release into an air-filled vessel, the hydrogen rises to the top of the vessel, producing an inhomogeneous mixture. Due to the interaction of buoyancy and diffusion the mixture initially forms a vertical concentration gradient with hydrogen concentration increasing towards the top of the vessel. This gradient levels out with time and the mixture becomes more and more homogeneous on the global scale. In the case of a large volume (such as a reactor containment) this process can take several hours before the homogeneous state is reached.

Even though this scenario is very realistic, studies on the combustion of mixtures with an inhomogeneous concentration are scarce. Bleyer et al.⁴⁾ investigated flame propagation with a vertical hydrogen gradient in a vertical tube. The flame propagates in the upward direction, away from the igniter, into a gradually richer or leaner mixture depending on the concentration gradient. It was shown that the concentration at the ignition source has a significant influence on the flame development. Ishii and Kojima⁵⁾ put a focus on detonation propagation in mixtures with vertical concentration gradients in a horizontal tube. However, to the knowledge of the authors, flame acceleration in horizontal tubes has only been investigated for perfectly homogeneous mixtures so far.

As an inhomogeneous fuel distribution represents a more realistic assumption for the initial state of the hydrogen-air mixture in an accident scenario⁶⁾, it needs to be taken into account in safety-related combustion studies.

2. Experimental setup

The experimental investigation of flame acceleration with inhomogeneous mixtures is conducted in a closed, 5.4 m long tube with a rectangular cross section of height $H = 60$ mm and width $W = 300$ mm. The tube is either completely smooth (blockage ratio $BR = 0\%$) or partially equipped with turbulence-producing obstacles. In the latter configuration the blockage ratio is chosen to be 60% and the distance between the obstacles is $S = 100$ mm. The final of the 19 obstacles is at a distance of 2.05 m from the ignition source which is mounted on one of the end plates. The remaining part of the tube is smooth. Seven pressure transducers and 30 flame sensors (photodiodes) are installed along the length of the tube to record the pressure wave velocity and the flame velocity, respectively, at a sampling rate of 250 k samples s^{-1} .

An injection mechanism has been designed that generates different vertical concentration gradients inside the tube. The concentration gradient is created in two steps. First, the tube is filled with air and hydrogen is injected through several holes in the upper plate of the tube. Modified obstacles deflect the injected hydrogen into the horizontal direction. The amount of hydrogen is controlled by the injection time and the pressure of the fuel supply. Second, diffusion takes place until the desired concentration gradient is achieved. The vertical concentration gradient finally achieved depends on the waiting time t_w , which itself is defined as the time between the end of hydrogen injection and ignition.

All combustion experiments are conducted with a hydrogen-air mixture at an initial pressure of 1 atm and an initial temperature of 293 K.

3. Generation and measurement of the concentration gradient

The experimental determination of the concentration gradient is done by collecting gas samples at different positions inside the tube. The samples are analyzed with a gas chromatograph. Due to safety aspects most of the concentration measurements have been conducted with

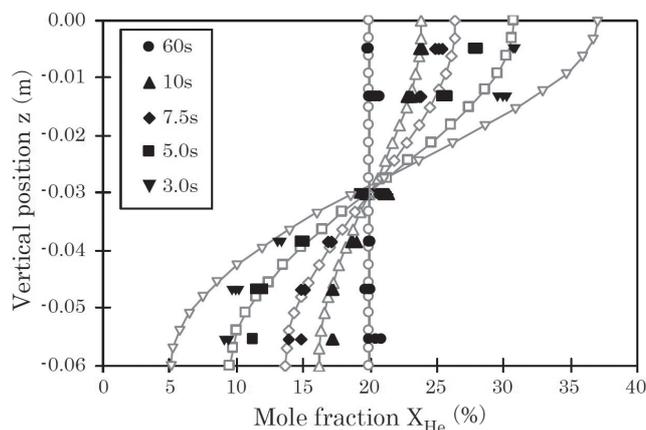


Fig. 1 Fuel concentration over channel height for different waiting times. The mixture is globally lean with an overall mole fraction of 20 vol.% fuel. Solid symbols indicate experimental results, transparent symbols numerical results.

helium. A comparison with hydrogen injection shows only minor differences in the mole fractions measured (relative deviation $< 6\%$).

Figure 1 shows the degradation of the vertical concentration gradient with time in a mixture with a fuel content of 20 vol.% in air. For short waiting times a globally lean mixture can be stoichiometric (i.e. 29.6 vol.% H_2) or even rich in the upper part of the tube ($z = -0.02 \dots 0$ m). In the configuration shown this is the case for a waiting time of $t_w = 3$ s. The influence of this local hydrogen excess on the flame propagation progress is shown in the following section. In the bottom part ($z = -0.06 \dots -0.04$ m) the local concentration is much lower. This yields a mixture with a strong vertical concentration gradient. With increasing waiting time the mixture becomes more homogeneous. The mechanism of this degradation of the concentration gradient is mainly based on diffusion - convection quickly becomes negligible. For $t_w = 60$ s the mixture is practically homogeneous.

A large number of injection experiments have been conducted in order to ensure the reliability of the injection mechanism. In order to further support these experimental results, 3D simulations of the injection mechanism have been conducted. Apart from the initial gradients ($t_w < 5$ s), the simulations show good agreement with the experiments. Consequently, this injection system has proven to be capable of producing both homogeneous mixtures as well as mixtures with a vertical concentration gradient in a reproducible manner.

4. Results of flame acceleration experiments

4.1 FA in smooth tube ($BR = 0\%$)

Figure 2 shows the development of the flame velocity over the channel length in mixtures with different vertical concentration gradients. The global hydrogen content of all these mixtures is constant at 20 vol.%. A transition of the flame regimes (i.e. slow flames - fast flames - detonation) can be observed for the investigated mixture gradients. In the homogeneous mixture ($t_w = 60$ s) and in mixtures with weak vertical concentration gradients ($t_w =$

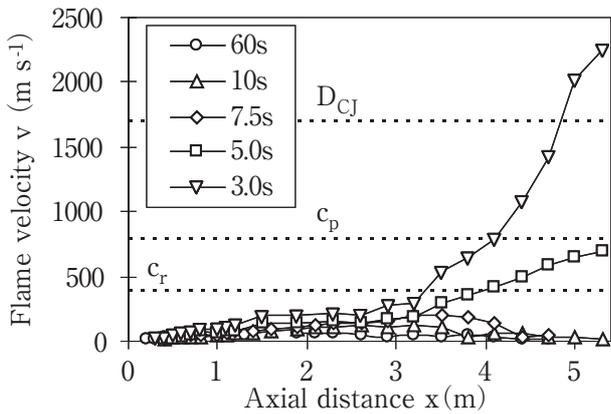


Fig. 2 Flame velocity vs. axial tube distance for different vertical concentration gradients (waiting time). All mixtures have a global hydrogen content of 20 vol.-%.

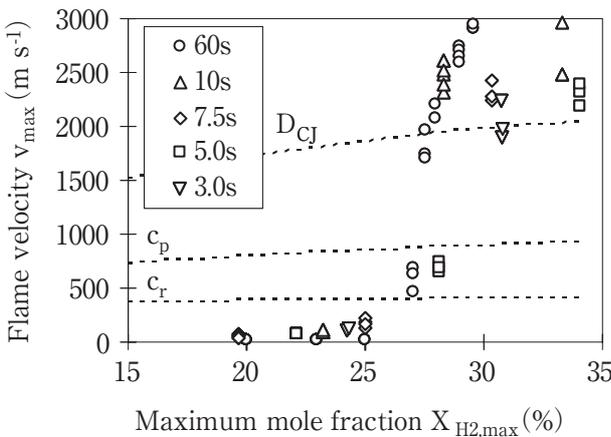


Fig. 3 Flame velocity vs. maximum hydrogen mole fraction for different vertical concentration gradients.

7.5 ~ 10 s) the flame velocity remains below the reactants' speed of sound (c_r). This combustion regime is generally classified as slow flames. For $t_w=5$ s a fast flame is observed which exceeds the reactants' speed of sound and reaches the speed of sound of the products (c_p). The mixture with the steepest concentration gradient ($t_w=3$ s) exceeds even this speed and undergoes DDT further downstream, reaching velocities above the Chapman-Jouguet detonation velocity (D_{CJ}). The peak over-pressure at the end of the tube increases up to two orders of magnitude compared to the homogeneous mixture.

This DDT mechanism is supported by the FA process, which itself is affected by the inhomogeneous mixing with locally enriched zones of hydrogen. Figure 3 summarizes the maximum flame velocities observed in a series of experiments with different global hydrogen concentrations and different concentration gradients. It has turned out to be advantageous to plot the maximum flame velocities not over the global, but over the maximum hydrogen content of the respective mixtures. The maximum hydrogen content in each mixture is the one that is present at the top of the tube (cf. Fig. 1). Displaying the results in this way leads to a clear velocity rise at 27 vol.-% hydrogen for all mixtures, no matter if homogeneous or with concentration gradient, while plotting the results over the global hydrogen content does

not lead to any coherent pattern.

4.2 FA in obstructed tube ($BR = 60\% / S = 100$ mm)

Mixtures with different concentration gradients have also been investigated in the tube with obstacles described in section 2. The flame propagation velocities for mixtures with a global hydrogen content of 20 vol.-% are shown in Fig. 4. In the obstructed part of the tube the flame velocity increases rapidly, but remains below the speed of sound of the combustion products. The maximum flame velocities of homogeneous and inhomogeneous mixtures are almost equal in this part of the tube. After a distance of 2.05 m the flame enters the smooth part of the tube and the leading shock decouples from the flame. The shock wave reflected at the end plate causes a deceleration of the flame. This phenomenon has also been observed by Eder⁷. However, a reacceleration can be observed for mixtures with a steep vertical concentration gradient ($t_w=3\sim 5$ s).

A comparison of mixtures with different global hydrogen contents and vertical concentration gradients shows that homogeneous mixtures reach an approximately 10% higher maximum flame velocity in the obstructed part than mixtures with strong concentration gradients ($t_w=3\sim 7.5$ s) of the same global hydrogen content. Thus, vertical concentration gradients have only a minor effect on the flame acceleration in this part of the tube. For a better understanding of this phenomenon, CFD simulations have been conducted⁸). The aim was to investigate if the initial concentration gradient in the unburned mixture remains or if it is destroyed during the flame acceleration process. For slow flames and narrow obstacle spacing ($S = 100$ mm as in the experiments), the simulations showed intensive mixing ahead of the flame front. This effect can explain the almost identical maximum flame velocities for homogeneous and inhomogeneous mixtures in the obstructed part of the tube. However, for faster flames and/or wide obstacle spacing, the simulations showed only minor mixing effects ahead of the flame front. Consequently, care should be taken not to generalize the results obtained in this experimental series before further investigation.

After the final obstacle the flame propagates into the

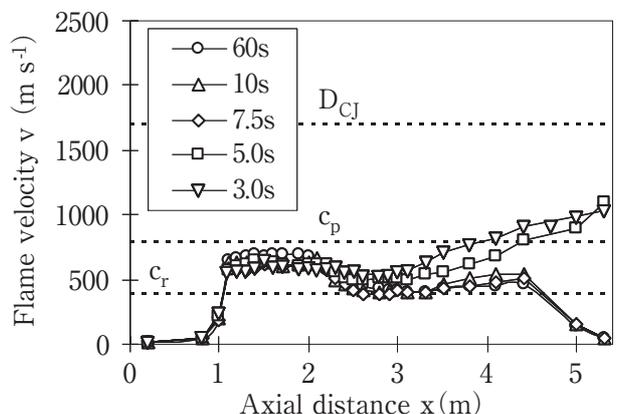


Fig. 4 Flame velocity vs. axial tube distance with 20 vol.-% hydrogen (global). The obstacle configuration in the tube is: $BR = 60\%$ and $S = 100$ mm. The final obstacle is located at 2.05 m.

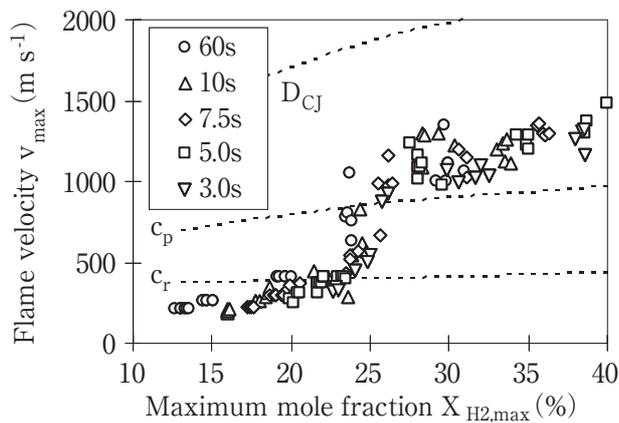


Fig. 5 Maximum flame velocity in the unobstructed part of the tube vs. maximum hydrogen mole fraction.

smooth part of the tube. As seen in Fig. 4, the vertical concentration gradient has a strong influence on the flame velocities achieved. Figure 5 shows the maximum flame velocity in the smooth part of the tube. Once again, the results are plotted over the maximum, not the global hydrogen content present in each mixture.

As for the smooth tube, good agreement of the maximum flame velocities can be observed for homogeneous and inhomogeneous mixtures by plotting the data in this way. With increasing hydrogen concentration the maximum flame velocity increases, too. For mixtures with concentrations of 20 ~ 25 vol.-% hydrogen the maximum flame velocity reaches the reactants' speed of sound. A transition to fast flames and quasi-detonations is observed for mixtures with a maximum hydrogen content of 24 and 26.5 vol.-%, respectively. However, DDT was not observed in the tube with close obstacle spacing. Mixtures with maximum concentrations near the stoichiometric value (26 ... 30 vol.-%) exhibit an increased scatter of the maximum velocities.

5. Conclusions

In order to extend the existing correlations for assessment of critical FA conditions, mixtures with vertical concentration gradients have been investigated. A series of systematic measurements unveils a major influence of the vertical concentration gradient on flame acceleration. In a smooth tube three distinct combustion regimes can be observed by keeping the global hydrogen concentration constant and varying the concentration gradient: slow flames, fast flames, and detonation. In a partially obstructed tube ($BR = 60\%$, $S = 100$ mm)

homogeneous mixtures accelerate faster than inhomogeneous mixtures as long as the flame travels through the obstructed part of the tube. The flame velocities show a deviation of only 10%. However, after the final obstacle the vertical concentration gradient has much stronger influence on FA. DDT has not been observed in this configuration for any of the mixtures investigated. Consequently, it cannot be recommended to use the existing safety criteria which have been derived for homogeneous mixtures in applications where inhomogeneous mixtures may occur. In general, it can be concluded that mixtures with vertical concentration gradients have a higher hazardous potential than homogeneous mixtures of the same hydrogen content. Comparing different mixtures not in terms of their global hydrogen content, but in terms of their maximum hydrogen content shows a first promising attempt for extending the relevant safety criteria to inhomogeneous mixtures.

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