2D and 3D Flame Surface Analysis of Flame Acceleration and Deflagration-to-Detonation Transition in Hydrogen-Air Mixtures with Concentration Gradients

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1 Introduction

Our project aims at improving the understanding of deflagrations and detonations in hydrogen-air mixtures. A special focus lies on the flame acceleration phase and the sudden transition to detonation which is a critical issue for nuclear reactor safety considerations. Whereas in the past homogeneous mixtures have intensely been investigated, concentration gradients perpendicular to the main direction of flame propagation are taken into account here. In case of a core meltdown, this represents a more realistic scenario of hydrogen distribution within a reactor containment dome [1]. Once a reliable prediction in terms of flame speeds and pressure loads is possible, the structural response of the containment can be evaluated.

Besides experimental research, numerical simulations are a promising way to study the combustion process. The latter approach is discussed in this paper to make a contribution in the analysis of an explosion channel experiment on laboratory scale. Responding to an idea raised in [2], two different obstacle configurations are examined. Thus, the orientation of obstacles (which are necessary to promote flame acceleration) relative to the concentration gradient is varied. Three-dimensional computations were performed to capture the full geometrical complexity of the problem. Moreover, two-dimensional and three-dimensional simulations are checked against each other. We want to demonstrate the potential of flame surface analysis to identify the relevant differences. To study the DDT (deflagration-to-detonation transition) process in detail is not the goal using the simplified but computationally very efficient approach described. Unlike simulation techniques requiring high spatial resolution, the analysis can therefore be applied to real-world scenarios.

2 Numerical approach

The unsteady compressible Navier-Stokes equations, together with a transport equation for the total internal energy and the ideal gas law, form the basis of the solver. An explicit and density-based formulation ensures accurate reproduction of gasdynamic effects, e.g. shocks, which is especially important when autoignition phenomena have to be considered. To take account of the wave characteristics of gasdynamic discontinuities, a Riemann solver is implemented for the calculation of convective fluxes. The equation system is discretised via the finite-volume method, provided by OpenFOAM technology.

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Weller's flame area combustion model [3], primarily suited for the flamelet regime, is applied. It is based on a transport equation for the reaction progress variable c, where $c = 0$ indicates the entirely unburned mixture and $c = 1$ the fully burned state. The commonly used gradient ansatz defines its source term. For that purpose, an additional transport equation, derived through conditional averaging, has to be solved for the flame wrinkling factor

$$\Xi = \frac{S_T}{S_L} = \frac{A_T}{A_\perp}. \tag{1}$$

Ξ represents the ratio of turbulent burning velocity S_T to laminar burning velocity S_L, but can also be interpreted as the ratio of average flame area A_T to average flame area projected onto the mean propagation direction $A_\perp$ in each control volume. Accordingly, Ξ measures the wrinkling of flame sheets by turbulent eddies and is equal to 1 for laminar combustion. It is therefore possible to distinguish between the macroscopic growth of flame surface that is reflected in $A_\perp$ and the microscopic growth of flame surface determined by the turbulence level that is reflected in Ξ. Both phenomena increase the consumption of premixed reactants and eventually enhance flame acceleration in a closed system through the expansion of products. Following the definition of the reaction progress variable, the isosurface for $c = 0.5$ can be considered as the flame front. During post-processing, a contour-based reconstruction algorithm calculates $A_\perp$ for all cells which are intersected by the front as this quantity is not directly available from the solver. Integrating the reconstructed values of $A_\perp$ finally yields the overall macroscopic flame surface in the computational domain. Since not only deflagrations have to be described, but also the transition to detonation, an extension of the combustion model for autoignition effects is essential. The approach by Colin et al. [4] uses a fictitious intermediate species specifying time and position where autoignition takes place. Required ignition delay times are stored in a database obtained from zero-dimensional isochoric explosion calculations [5] with a detailed reaction mechanism [6] during pre-processing. Besides, chemical kinetics is incorporated via the S_L-polynomial and a factor for quenching. Turbulence-chemistry interaction is therefore an inherent part of the combustion model itself. Menter's k-ω-SST turbulence model [7] provides the turbulent quantities needed. Buoyancy effects are included but play only a minor role in the process studied. Details on the numerical methodology, including further measures for sub-grid modelling, can be found in [8].

3 Computational setup

The computational domain represents an experimental facility [2] which consists of a closed rectangular channel (5.4 m long, 300 mm wide and 60 mm high) and seven identical obstacles yielding a blockage ratio of 30 % with respect to the cross-section of the channel. The first obstacle is installed at a distance of 250 mm from the left end plate where the mixture is ignited by patching selected cells to the fully burned state. The remaining obstacles follow at a constant spacing of 300 mm. Consequently, the rest of the channel from 2.05 m to 5.4 m is unobstructed. These internals are necessary to promote flame acceleration, primarily by means of turbulence generation and flame surface growth in their wake, and ultimately to reach critical conditions for DDT on laboratory scale. Horizontally as well as vertically oriented obstacles are examined to check whether blocking the region of highest fuel concentration (which is the case for horizontal obstacles) has an influence on flame acceleration or not. The obstacles' shape is indicated in Figure 2. In contrast to single-gap horizontal obstacles, a multi-gap configuration has been chosen for vertical obstacles. This assures analogous length scales which are crucial for the jet behaviour when the flow passes the obstacle. The buoyancy and diffusion driven mechanism to generate typical non-linear vertical concentration gradients in experiments is described in [2]. For the simulations, a similar initial hydrogen concentration profile with a maximum value of 45.2 vol.-% (at the top of the channel) and a minimum value of 7.2 vol.-% (at the bottom of the channel) at an average value of 25 vol.-% is assumed. Initial temperature and pressure are set to 293 K and 1 atm, respectively.

In order to save computational resources for three-dimensional (3D) simulations, symmetry is assumed with respect to the width of the channel. This is not possible in the vertical direction due to the concentration gradient. In case of the two-dimensional (2D) simulation, only one slice in the middle of the channel is discretized. Span-wise variations are therefore not considered. Apart from the symmetry boundary, no-slip wall boundary conditions are imposed. The corresponding computational domain is partitioned with a cartesian mesh of 2 mm spacing in each direction which yields approximately 80 000 cells for 2D calculations and 6 million cells for 3D calculations. The uniformity of the grid assures resolving the same length scales in each spatial dimension. It has been demonstrated that this cell size is sufficient to predict the global behaviour (i.e. flame speeds and pressure loads) at a reasonable accuracy without resolving all mechanisms on small scales [8,9]. Since turbulent wall boundary layers cannot be resolved properly by 2 mm cells, wall functions are employed. All computations have been executed on SuperMUC, a Sandy Bridge architecture based system, operated by Leibniz Supercomputing Centre in Garching. For 3D simulations, massive parallelization (512 cores) has been applied.

4 Results and discussion

To get a first overview of the results, the flame-tip velocity is plotted over the axial distance from the ignition point. All simulations were stopped shortly after DDT to save computational resources. It becomes evident from Figure 1 that the flame accelerates faster in the case of 3D calculations. Subsequently, after DDT, the flame is expected to slow down in the range of the Chapman-Jouguet velocity of a steadily propagating detonation. The generally good agreement with experiments is shown in [8].

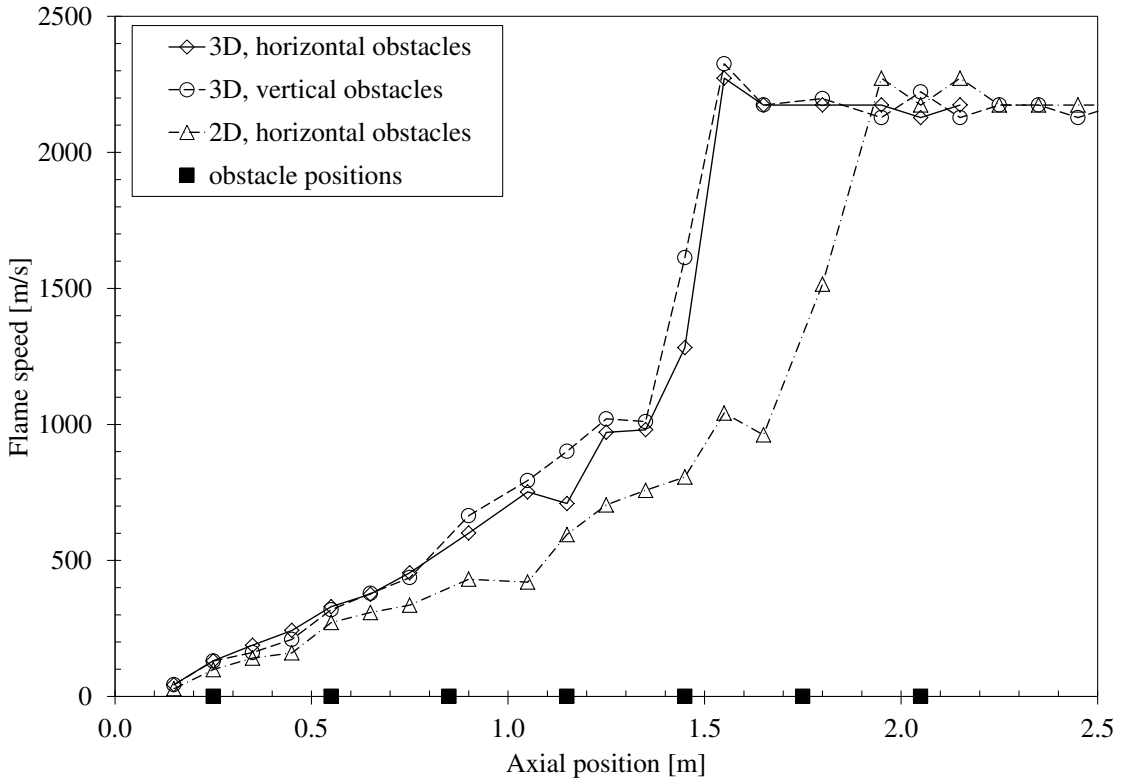
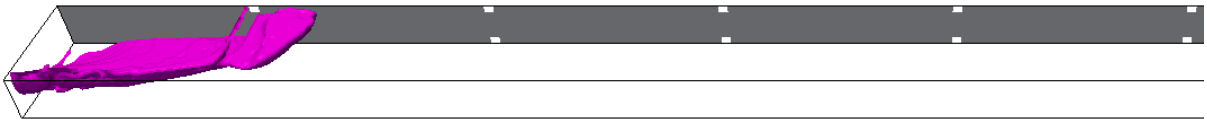


Figure 1: Flame-tip velocity versus axial distance from ignition point

The reason for this 2D/3D discrepancy is probably related to the complex shape of the macroscopic flame front (coloured purple in Figure 2) that determines the overall consumption rate. Thus, there is a direct feedback on flame acceleration through the expansion of products that pushes the flame front forward. Two noticeable observations can be made: First, there are strong variations in vertical direction due to the concentration gradient. Despite the induced flow ahead of the flame, the initial concentration gradient is not completely homogenized. Reaction in the richer zone towards the top of the channel is clearly faster than in the leaner zone towards the bottom of the channel. Second, compared to the middle of the channel, delayed reaction towards the side walls is recognized. Unlike the first, this influence cannot be captured by 2D calculations. In 3D however, span-wise variations can contribute to the growth of the macroscopic flame surface. Another interesting fact appears from Figure 2(d). Contrary to the highly three-dimensional deflagration front, the detonation front is almost perfectly two-dimensional. Note that a pseudo-stable detonation front has evolved as the intrinsically unstable structure of a real detonation cannot be reproduced by the coarse 2 mm mesh.



(a) Slow deflagration passing the first horizontal obstacle after 0.0074 s

(b) Fast deflagration passing the fourth horizontal obstacle after 0.0096 s

(c) Fast deflagration passing the fourth vertical obstacle after 0.0098 s

(d) Detonation passing the sixth horizontal obstacle after 0.01 s

Figure 2: Macroscopic flame front in 3D simulations

Only a qualitative explanation has been given so far. Figure 3 facilitates a quantitative evaluation since the development of the macroscopic flame surface seems to be the key point in understanding the different flame acceleration behaviour. Conclusions in [10] support this conjecture. A similar flame surface analysis has been conducted in [11] for slow deflagrations with flame speeds below 100 m/s in homogeneous methane-air mixtures. To allow for a direct comparison, the 2D surface is multiplied by 300 mm, the width of the channel, and the 3D surface is multiplied by 2 because of the symmetry assumed. It has to be mentioned that the circular ignition zone in 2D corresponds to a cylinder in 3D, whereas for 3D computations, a spherical zone has been ignited since this is closer to spark ignition in experiments. Accordingly, the initial value of the 2D flame surface is higher than the 3D flame surface. The diagram shows an exponential rise of flame surface in both cases. The process starts as a slow laminar deflagration and quickly turns into a fast turbulent deflagration after approximately 0.007 s when passing the first obstacle. But apparently the 3D computation predicts a clearly faster increase in flame surface. It is

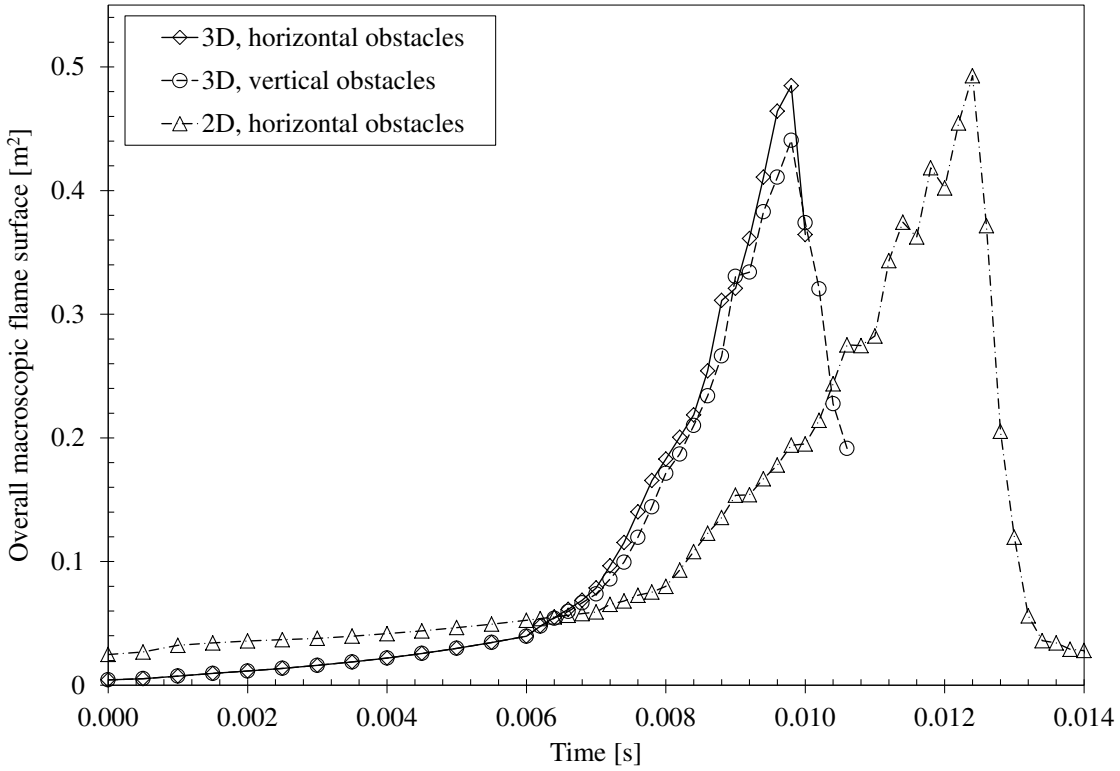


Figure 3: Temporal evolution of the overall macroscopic flame surface

surprising that the maximum values for all simulations are more or less identical. In other words, DDT happens at the same critical macroscopic flame surface. The obstacles' orientation does obviously not have a decisive influence on flame acceleration. The 2D computation enables further insights. After DDT, instead of a sudden drop, the flame surface asymptotically approaches the level of a steadily propagating detonation because of after-burning in some regions behind the front. Such unburned regions can be seen in Figure 2(d).

5 Conclusion and outlook

The comparably simple combustion model is not suited to analyze the chemical reaction part in detail but it facilitates the investigation of the whole flame acceleration process, from ignition to DDT, in real-world scenarios.

For the laboratory scale experiment investigated, we can observe clear differences between 2D and 3D computations. This is primarily traced back to the complex shape of the flame front which cannot be reproduced by 2D calculations. Variations in span-wise direction are playing an important role in the growth of the overall flame surface and are consequently affecting flame acceleration. Our advice would be to do 3D deflagration simulations provided that adequate computational resources are available. Otherwise, one has to be aware of making a systematic error. In the detonation regime however, it appears to be sufficient to do 2D simulations if only the global propagation behaviour is of interest.

The obstacles' orientation relative to the concentration gradient seems to be an inferior parameter regarding flame acceleration. This conclusion is in accordance with experimental findings [12].

The study furthermore demonstrates the benefit of numerical simulations by providing data on flame surfaces which is difficult to obtain in an experimental way.

In the future, we want to compare the evolution of $A_\perp$ and $A_T = A_\perp \Xi$ to quantify the influence of both phenomena – macroscopic growth of the flame surface and turbulent wrinkling of the flame front on microscopic level.

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