Optimization of low-NO_x partially premixed hydrogen burners using numerical simulation and flame diagnostics

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Abstract

This study presents fundamental numerical and experimental investigations on hydrogen combustion in model burners. The effects of the equivalence ratio, pressure and preheating temperature on the laminar flame speed and combustion temperature are numerically investigated using CANTERA (based on GRI-Mech 3.0 as reaction mechanism). Furthermore, the aspect of nitric oxides (NO_x) reduction by lowering the flame temperature was examined more closely. Based on these fundamental studies, a partially premixed single nozzle burner was developed using the 3D-CFD-code (CFD: Computational Fluid Dynamics) STAR-CCM+ (Siemens PLM) to optimize mixture formation and combustion. The overall burner design enables the variation of some important geometrical parameters of the nozzle for mixture preparation during the optimization process. The aim is homogeneous distribution of the fuel-air ratio (equivalence ratio) at the nozzle exit after a short mixing duct. The flame of the manufactured burner was investigated using an IR-camera and exhaust gas analysis. Stable operation of the micro-nozzle burner was found for a global equivalence ratio of 0.40 at 0.3 kW-1.0 kW at low NO_x-emissions (below 10 ppmv).

Introduction

Hydrogen is probably the most important energy carrier for a future global energy supply [1]. It has become a real alternative to conventional fuels and energy sources. This is due to the increasing share of renewable energies and the efficiency increase of electrolysers as well as their availability in various power classes nowadays [2]. On the one hand, hydrogen serves as a feedstock for synthetic fuels and gases, and on the other hand, it can be converted directly into thermal and electrical energy in fuel cells or in combustion applications. The major advantage of using hydrogen as an energy carrier is its theoretically unlimited availability and climate-neutral conversion into other forms of energy. However, there are particular challenges in using hydrogen as a thermal energy source, given its special combustion behavior. There are already a few burner concepts for hydrogen, such as porous media burners or swirl burners [3-5]. However, stability problems may occur when a wide range of thermal loads must be covered. Alternatives to these concepts could be multi-nozzle burners. For their development, basic investigations on stabilization and pollutant formation are necessary, which are presented in this study.

Numerical Investigations

The numerical 0D/1D-flame studies in the presented work were performed using the open source code CANTERA [10], based on the GRI-Mech 3.0 reaction mechanism. One common parameter to evaluate the combustion behavior of premixed fuel/air mixtures is the laminar flame speed. It is of fundamental importance for the modeling of technical combustion processes and especially, for the design of combustion chambers or free flame burners. Compared to other conventional gaseous fuels, hydrogen has a significantly higher laminar flame speed, as shown in *Figure 1*. While the highest laminar flame speed of methane and propane results at an equivalence ratio of around 1.1, hydrogen shows its maximum at approximately 1.6 for ambient conditions. At lean conditions, the laminar flame speed decreases significantly.

Another essential combustion property is the adiabatic combustion temperature and the associated formation of thermal nitric oxides [6]. Compared to the conventional gaseous fuels listed above, hydrogen has a slightly larger combustion temperature, which is about 150 K higher than for methane and 110 K higher than for propane at stoichiometric conditions. Increased combustion temperatures favor the formation of thermal nitric oxides: especially at temperatures above 1600 K to 1800 K, there is an exponential increase [7,8].

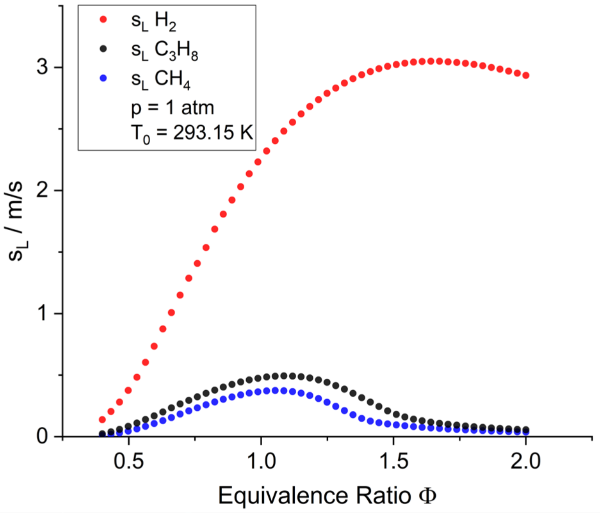

Figure 1: Calculated laminar flame speeds of H_2, CH_4 and C_3H_8 at various equivalence ratios.

There are two ways to reduce nitric oxide emissions: One involves exhaust gas after treatment via SCR (selective catalytic reduction), in which nitrogen oxides are converted into nitrogen and water vapor usually by

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adding a NO_x reducing agent and a catalyst [9]. The other option is to optimize the combustion process itself to avoid the formation of nitrogen oxides, e.g. by lowering the combustion temperature. This can be realized, e.g. via lean operation, internal or external exhaust gas recirculation, or the introduction of liquid water or water vapor. In this study, the focus is on the potential of lean operation and the addition of water vapor to the fresh gas. The basis of these numerical investigations is a premixed 1D flat flame. In the first study, the equivalence ratio is varied from 0.67 to 0.4. *Figure 2* shows the NO concentration as a function of the spatial coordinate z, which indicates the path through the flame front. The boundary conditions are a reactant temperature of 293.15 K and an ambient pressure of 0.1 MPa. It can be clearly seen that NO formation is inhibited by a lower equivalence ratio and thus lower combustion temperatures. In this case, the most significant change is seen between $\Phi = 0.67$ and $\Phi = 0.5$, which can be explained by the exponential increase in formation of thermal nitric oxides above the threshold temperature range of approx. 1600 K to 1800 K [7,8] as mentioned above.

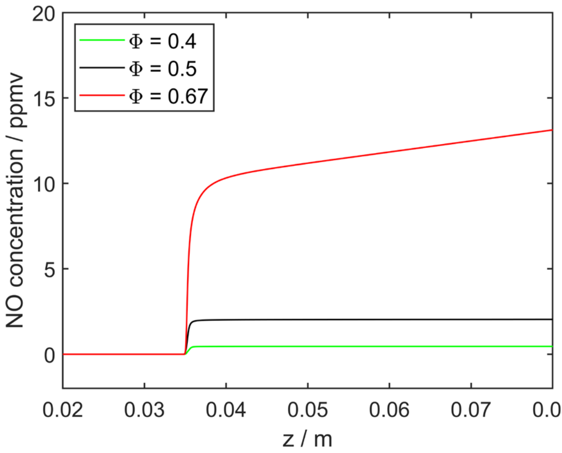

Figure 2: NO concentration as a function of the spatial variable z for different equivalence ratios Φ (T_0 = 293.15 K, p = 0.1 MPa).

A second way to lower the combustion temperature is the addition of water or steam to the unburned mixture. For a partly premixed free flame burner, the addition of water in a liquid form may cause problems. A very uniform droplet size would have to be introduced to avoid local flame instabilities caused by larger droplets. The addition of steam or even the use of water-saturated air could suffice here as a temperature reduction measure. In *Figure 3* results for the addition of water vapor at a temperature of 373.15 K for different water-fuel ratios Ω are presented. The equivalence ratio is set to 0.67. The results show a very similar NO minimization potential as a combustion at lean conditions.

Based on these preliminary investigations, a single-nozzle burner was designed, which was numerically optimized and then experimentally tested. The burner is based on a partially premixing of fuel and air (as well as mixing with additional components such as steam in some cases). Air and hydrogen are guided in separate concentric pipes, where the hydrogen pipe is mounted centrally. The gases are mixed shortly before the nozzle outlet. There, the hydrogen exits through radially symmetrically arranged holes in the air duct.

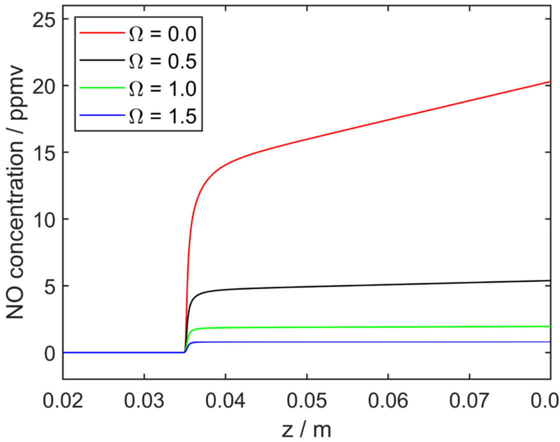

Figure. 3: NO concentration as a function of the spatial variable z for different water fuel ratios Ω (T_0 = 373.15 K, p = 0.1 MPa).

Mixing takes place in a small volume between the fuel outlet and the nozzle exit, improved by an additional flow body in between.

The described nozzle principle was studied in a series of 3D simulations using the 3D-CFD-code (CFD: Computational Fluid Dynamics) STAR-CCM+ (Siemens PLM), which was utilized for optimization of the mixture formation and combustion. Mixing fields at the nozzle exit were evaluated using the surface average of the equivalence ratio. Furthermore, the minimum and maximum values of the equivalence ratio served as an indicator for the homogeneity of the mixture. Geometric parameters, such as diameter of the flow body, length of the premixing section or diameter of the nozzle exit were varied during 3D-simulation and in the experiment.

Figure 4 shows the mixing fields at the nozzle exit for two different configurations.

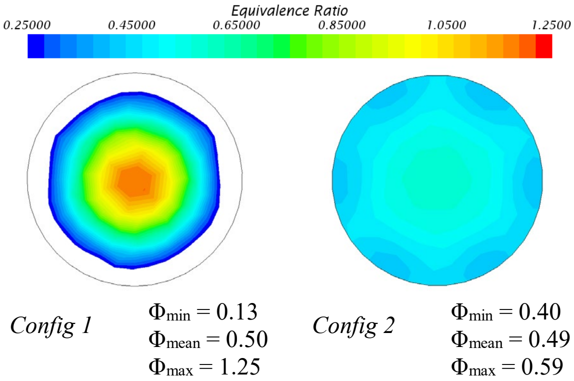

Figure 4: Mixture formation in terms of the equivalence ratio at the nozzle exit for two mixing configurations.

Both configurations have a mixing duct length of 15 mm and a nozzle diameter of 2 mm. The equivalence ratio was set to 0.5 and the thermal power to 0.1 kW. *Configuration 1* contains no geometric optimization based on a flow body. The hydrogen flow enters the air stream through six radially symmetric holes. The fuel distribution shows a large gradient from the nozzle center to the nozzle edge. While there is a high proportion of hydrogen in the center, the mixture in the peripheral areas is very lean. This is illustrated by the two extreme values (Φ_{min}, Φ_{max}), whose deviations from the mean value are significant. In *Configuration 2* the flow guiding is optimized by a flow body in the premixing section. There, the end of the hydrogen line is covered with a larger flat disk, which actively guides the hydrogen into the air flow. This results in a significantly improved homogenization hydrogen and air since the extreme values of the equivalence ratio in this area are quite close to the surface average (Φ_{mean}).

Experimental Results and Discussion

Parts of the numerical single nozzle optimization process were also tested in experimental studies. The test rig set up for this purpose includes the single nozzle, mass flow controllers (El-FLOW®, Bronkhorst) for air and hydrogen, an infrared camera (Velox 327k SM, IRCAM) for flame diagnostics and an exhaust gas analyzer (Testo 350 XL). The exhaust gas temperature was tested at one point using an S-type thermocouple. In order to avoid dilution of the exhaust gas, the burner was mounted into a small measuring cell. The optical access was realized by sapphire windows. An optionally connectable humidifier made it possible to increase the relative humidity of the combustion air up to 90 %.

The infrared camera was used to detect the flame (via water molecules), flame instabilities and to define the load range of safe operation. *Figure 5* shows three single shots and the averaged images of two operating points of the single nozzle burner. The averaged image was obtained from 600 individual shots, taken at a frame rate of 100 Hz. The equivalence ratio was set to 0.5, the diameter of the nozzle exit was 5 mm and a flowbody with a diameter of 10 mm was used. With this setup, a stable operation was possible from 0.2 to 0.7 kW, i.e. the flame showed no lift off, quenching or flashback. Using a larger nozzle diameter of 7.5 mm and an equivalence ratio of 0.4 the stable load range was between 0.3 and 1.0 kW (not shown in *Figure 5*). For all measurements, the equivalence ratio was adjusted by changing the air mass flow rate to maintain a constant load. It should be noted that the flames are slightly bent to the “left” for these two operating points as the flowbody is not perfectly centered.

The flame brush is broader for the increased load, and the zone of the highest signal intensity is shifted more downstream due to the increased flow velocity and turbulence.

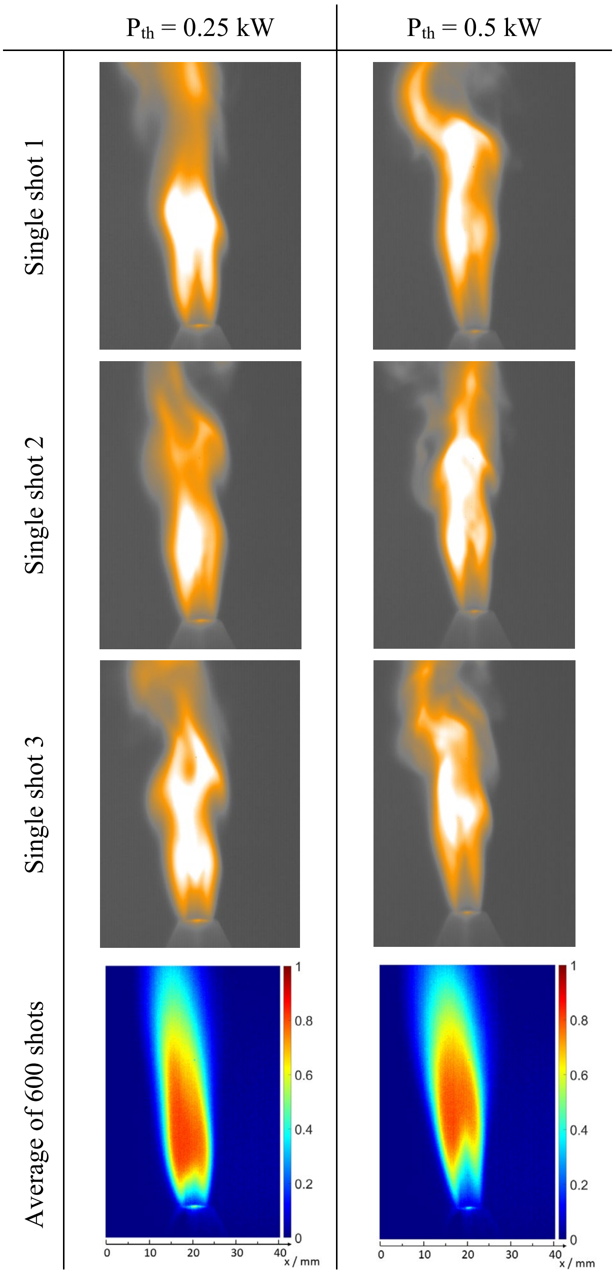

Figure 5: Single shots and averaged images of the hydrogen flame for two thermal loads at Φ=0.5.

In addition to the optical investigation of the flame stability, the combustion was evaluated by measuring the exhaust gas composition with an exhaust gas analyzer (with a measurement accuracy of ± 5 ppmv for NO_x). The measurement position is about 160 mm above the burner. Several measurements with different nozzle configurations were tested. The diagram in *Figure 6* shows the concentration of nitric oxides in the exhaust gas for three equivalence ratios with and without geometrical optimization. In this case the thermal load was set to 0.3 kW. As calculated in the 1D-simulations, nitric oxide emissions decrease with lower equivalence ratios. The experimental results also show that the adjustment of the short premixing section by using flow bodies leads to lower NO_x concentration in the exhaust gas, although the improvement is relatively small. For an equivalence ratio of 0.4, the time average value of the optimized configuration is around 8 ppmv. The error bars represent standard deviations that occurred during the measurement period of 5 minutes.

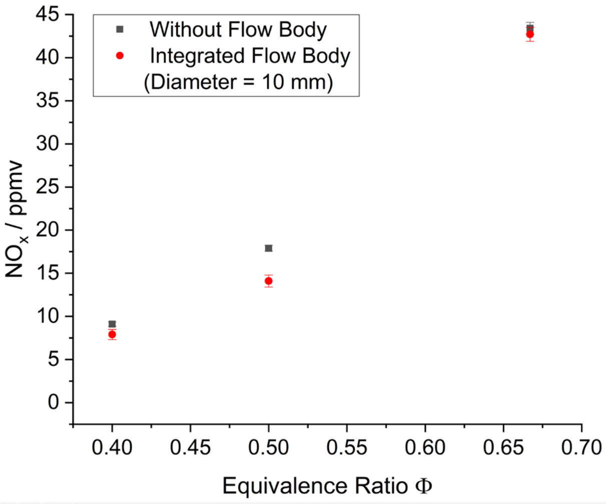

Figure 6: Experimental results of NO_x emission as a function of the equivalence ratio with geometric optimization. The thermal load was 0.3 kW.

To investigate the effect of water vapor on emissions, the combustion inlet air was humidified to a relative humidity φ of 90 % (measurement accuracy for φ: ± 3 %). The burner load was set to 0.3 kW, which corresponds to a water/fuel ratio of approx. 1. As can be seen in *Figure 7*, humidification has a positive effect on minimization of NO_x emissions, especially at higher equivalence ratios. At low equivalence ratios, no significant improvement is seen compared to dry air operation. In order to be able to make clearer statements at lean operation, exhaust gas measurements with a higher accuracy at low pollutant emission levels are necessary.

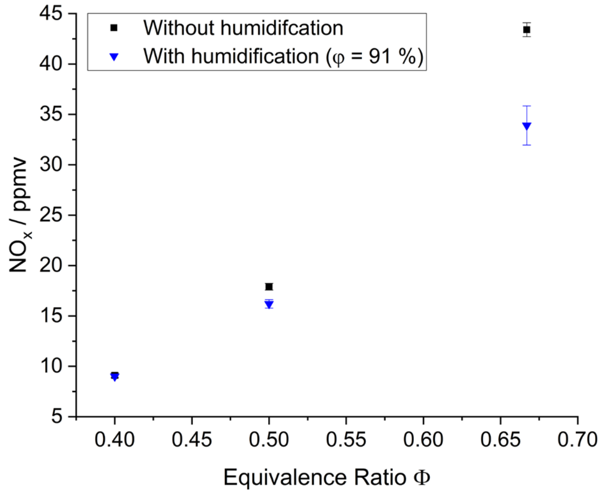

Figure 7: Experimental results of NO_x emission as a function of the equivalence ratio with humidification. The thermal load was 0.3 kW.

Conclusions

The combustion behavior of hydrogen-air flames was investigated in this paper. First, premixed flames were studied numerically using the GRI-Mech 3.0 reaction mechanism. The laminar flame speed and nitrogen oxide emissions indicate that operation at lean mixtures is preferable to lower NOx emissions. For flame stability and safety reasons, a partially premixed burner was designed afterwards in a numerical study. The single nozzle partially premixed burner was optimized regarding mixture formation by running 3D-CFD simulations. Despite a very short premixing section, a relatively homogeneous mixture was achieved at the nozzle exit. The designed burner was built and the influence of the equivalence ratio and the water-fuel ratio on the nitric oxide emissions was investigated. The experimental results show a similar trend as the numerical investigations.

Acknowledgements

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