4 Applied Methods and Approach

The Micromix (MMX) research aims for the flexible combustion of high-hydrogen syngas up to pure hydrogen in a gas turbine. The chosen gas turbine for the research is the Honeywell/Garrett GTCP 36-300, Figure 18.

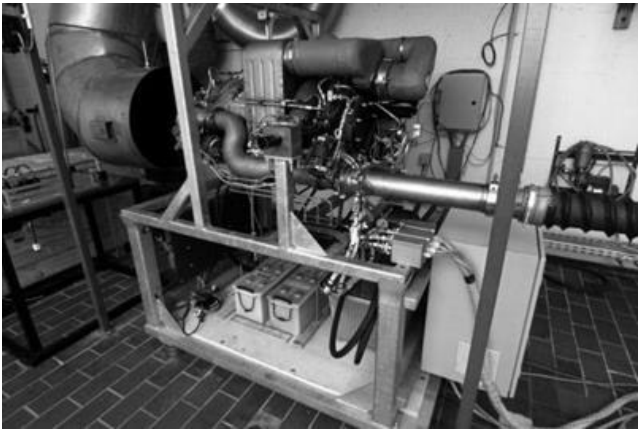

Figure 18: APU GTCP 36-300 gas turbine test rig at AcUAS

Prior to gas turbine integration, the identification of influencing phenomena on the MMX combustion and emission performance is necessary. The identification is done by an applied approach using experimental test burner investigations on an atmospheric combustion chamber test rig accompanied by numerical simulations. Based on the gained knowledge, a prototype-combustor is designed, manufactured and integrated into the GTCP 36-300 to prove the feasibility under real gas turbine conditions. This prototype MMX combustor is designed for dual-fuel combustion of pure gaseous hydrogen and a high-hydrogen syngas mixture that is defined to contain 90%-vol. H_2 and 10%-vol. CO (SG 90/10). This syngas-mixture is customized for the use under laboratory conditions and not derived from

IGCC-gasification. The properties of the SG 90/10 syngas-mixture is presented in the appendix.

4.1 APU GTCP 36-300 gas turbine

The GTCP 36-300 (Figure 18) is a single-shaft aviation gas turbine engine. It has a single-stage radial compressor and a single-stage radial turbine. The combustion module consists of an annular reverse flow combustion chamber section where the MMX combustor is integrated, Figure 19.

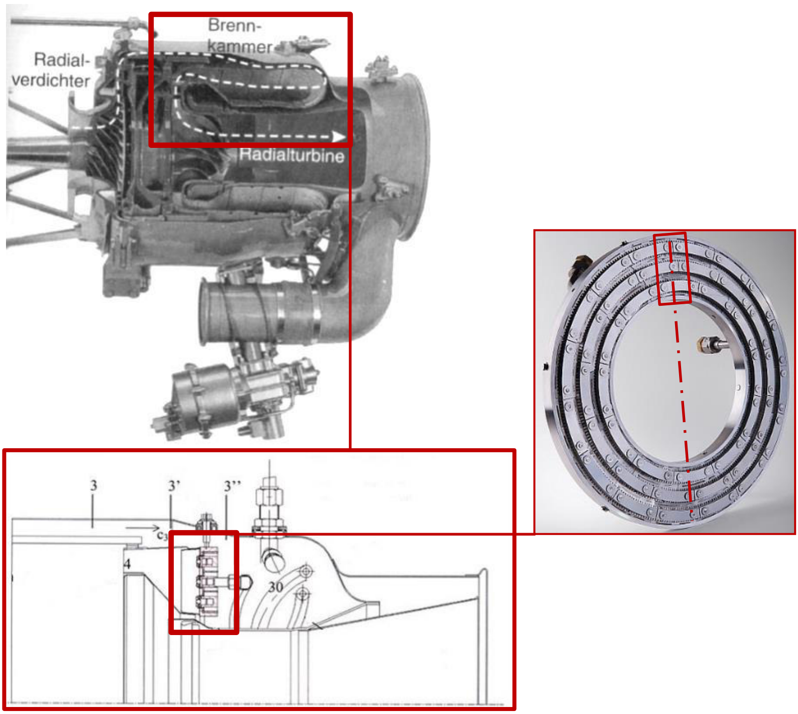

Figure 19: APU GTCP 36-300 combustion section crosscut

The GTCP 36-300 fuel supply system is already modified for the operation with gaseous hydrogen [11]. The combustion chamber creates around 1.6 MW thermal power, which are converted to shaft power in the turbine to drive an electrical generator and an additional single-stage radial load compressor. These accessories produce electrical and pneumatic power up to 370 kW in total.

The GTCP 36-300 is controlled by the Versatile Engine Control Box (VECB) built by Diehl Aerospace GmbH, Germany. Since it is a rotational speed controlled gas turbine engine, the flexible use of hydrogen and syngas is based on the concept of feeding the same requested amount of thermal power into the combustion chamber, regardless of the used fuel. Therefore, similar gas turbine operation characteristics for all modes of operation are achieved, and the designated rotational speed for each load condition can be maintained.

Several load modes are possible, depending on the required demand of the connected consumers. The GTCP 36-300 provides pneumatic power via a load compressor and electric power via a generator, hydraulic power is not provided. The load modes can be separated into two main modes. First, there is the Environmental Control Supply (ECS) mode where the APU delivers compressed air for the aircraft air conditioning system. It can be adjusted in stages to several load conditions from idle to maximum ECS load. All ECS stages operate at constant rotational speed of 99%, while the power output is controlled by movable Inlet Guide Vanes (IGV). These IGV open or close depending on the particular power demand. Second, there is the Main Engine Start (MES) mode delivering the maximum electric and pneumatic power output of the APU. This mode is required for the start procedure of the aircraft main engines. It runs at a constant rotational speed of 101%.

Table 2 summarizes the operational parameters in the gas turbine combustion chamber for the two modes ECS (Environmental Control Supply) and MES (Main Engine Start).

Table 2: Technical data of APU GTCP 36-300

compressor discharge temperature at MES	T_3	560 K
compressor outlet pressure at MES	p_3	6.69 bar
estimated fuel temperature at MES	T_{fuel}	300 K
primary air mass flow at MES	$\dot{m}_{air,MES}$	$1.37\ \frac{kg}{s}$
total kerosene mass flow at MES	$\dot{m}_{Kerosene,MES}$	$0.041\ \frac{kg}{s}$
primary air mass flow at ECS	$\dot{m}_{air,ECS}$	$1.35\ \frac{kg}{s}$
total kerosene mass flow at ECS	$\dot{m}_{Kerosene,ECS}$	$0.038\ \frac{kg}{s}$
turbine inlet temperature at ECS	$T_{4,ECS}$	1292 K
turbine inlet temperature at MES	$T_{4,MES}$	1356 K

4.2 Experimental Test Burner Applications

To develop a fuel-flexible Micromix combustor prototype, a multitude of parameter investigations is necessary to find out important phenomena, and to identify key design drivers for a stable combustion with low-NO_x characteristics. For this purpose, test burners are investigated on an atmospheric combustion chamber test rig, Figure 20. This method allows flexible, easy and cost efficient changes of different influencing geometry parameters. Atmospheric test rig means, that the combustion always takes place against atmospheric pressure. In the test set-up, two speed-controlled radial blowers supply up to 1 kg/s of air to the installed test burner. An electric heater with an electric power of 15.5 kW is used to heat the inlet air to about 560 K, the nominal APU combustor inlet temperature. The fuels (syngas and hydrogen) are supplied from 200 bar pressurized bottles. The test burner fuel inlet pressure is reduced to around 4 bar with a fuel inlet temperature of around 300 K.

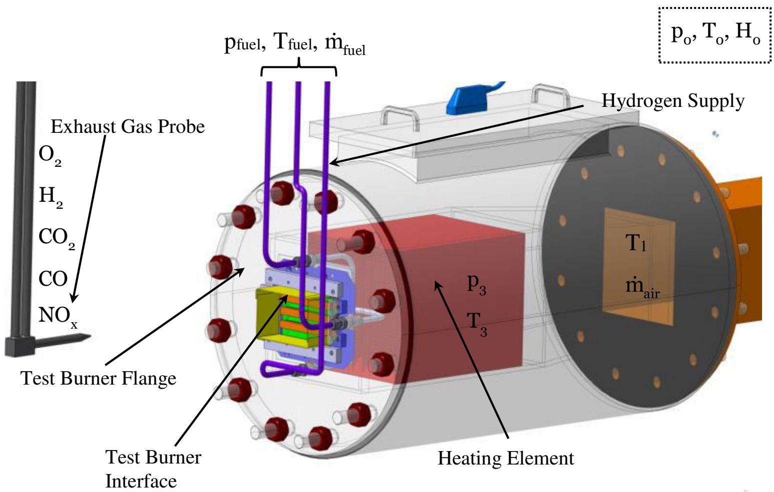

Figure 20: Atmospheric combustion chamber test-rig

The test burners are ignited by a high-energy ignition spark plug. An active heated probe, fully adjustable in three axes, takes samples from a defined measuring area within the test burner, covering representative flow phenomena of the combustion process. In order to compare the obtained results for different test-burner configurations, the measuring area is always placed and adjusted to cover the same location of important combustion phenomena for different test-burners.

4.3 Measurement Equipment and Data Acquisition

The technical data of the measurement equipment and data acquisition are summarize in the appendix. Table 13 presents the data of the equipment used at the combustion chamber test rig for the experimental test-burner investigations (Figure 20); in Table 14, the data of the gas turbine test rig equipment is given (Figure 21); the technical data of the applied exhaust-gas analysis-system is shown in Table 15.

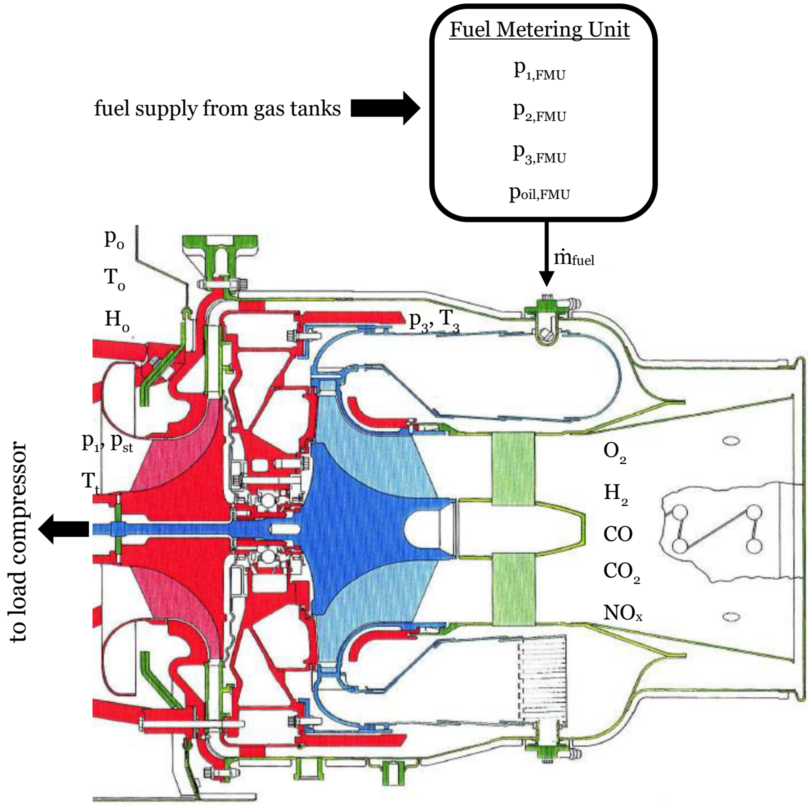

Figure 21: APU GTCP 36-300 measurement parameter definitions

The extracted samples are supplied via probes to the analysis modules of the gas analysis system ABB Advanced Optima AO2020 by heated tubing (180°C), which is designed to avoid concentration changes of the different components within the exhaust gas sample, and condensation of water in the tubing that could influence the analysis results. In the combustion chamber test rig, a probe that is moveable in three axes is used to extract samples; at the gas turbine test rig, a rotating isokinetic[9] probe is applied. In the gas analysis system, the gas sample is directed through a gas-dehydrator to each analyzing module by heated tubes and hoses under controlled pressure (1.01325 bar) and temperature (180°C) conditions. The Advanced Optima exhaust gas analysis system determines the amount of unburned hydrogen (ABB Caldos 27), the concentration of O_2 (ABB Magnos 206) and the amount of CO and CO_2 (ABB URAS 26). For the determination of NO_x (i.e. NO and NO_2), an Eco Physics CLD 700 EL is used and directly connected to the hot exhaust gas sample. Internal hot tubing and particle filters in the Eco Physics CLD 700 EL allow analyses without pre-processing of the gas sample and prevent water condensation.

Before each test campaign, all exhaust gas analyzer devices are calibrated using zero-point calibration gases and defined reference-point calibration gases.

The gas analyzer Caldos 27 uses the physical principle of heat conductivity to measure the amount of hydrogen [113]. The thermal conductivity detector (TCD) is one of the main detectors in gas

[9] The exhaust gas stream over the cross-section of the gas turbine exhaust duct is not homogeneous (temperature distribution, fluid velocity, turbulences due to rotating turbine disc etc.). Taking a large number of samples from points across the duct helps to minimize influences due to inhomogeneity. The isokinetic sampling system consists of a probe that rotates over the complete section of the exhaust duct using multiple fixed nozzles sized to get isokinetic flow conditions in each nozzle. This gives an isokinetic sample at each measuring point, i.e. the flow of the sample at the sampling nozzle has the same velocity as the velocity of the exhaust gas at that point.

chromatography and is used to measure permanent and noble gases. The TCD is made of a temperature-controlled metal block, which has a measurement cell and a micro-structured silicon sensor. The sample gas is continuously flowing through the measuring cell. A tungsten wire in the cell is heated to 200°C, the cell wall-temperature is 60°C. As a result, a continuous flow of heat flows through the measuring cell, which depends on the thermal conductivity of the gases in the exhaust sample. The actual measuring element consists of two heated measuring resistors, which are applied in thin-film technology on a silicon sensor. When the resistors are exposed to the exhaust gas sample, their temperature change. The resistors are part of a Wheatstone-bridge. If there are thermal conductive components in the sample, a voltage can be measured over the Wheatstone-bridge. The voltage is proportional to the amount of heat-conductive components in the sample. However, there are other gases besides H_2 that are thermally conductive as well, e.g. oxygen. Therefore, the data acquisition considers this cross-sensitivity and uses the amount of oxygen obtained by the Magnos 206 in its calculation routine.

The Magnos 206 is a thermomagnetic oxygen analyzer, which gives the amount of oxygen in the exhaust gas [114]. The measurement method is based on the behavior of paramagnetic gases in a magnetic field. Most gases are diamagnetic and can therefore be manipulated in a magnetic field. Oxygen and nitrogen are paramagnetic and the magnetization of paramagnetic materials decreases with increasing temperature. Inside the thermomagnetic oxygen analyzer, a dumbbell-shaped hollowware is implemented. The gaseous sample is magnetized by permanent magnets. If oxygen is present in the sample, a force is applied on the rotatable hollowware by the magnetized oxygen atoms. The hollowware is suspended by thin straps, which are used simultaneously as circuit paths. The hollowware is displaced around its axis and a torque is generated. A compensation-current in a torque-motor generates a counter-torque, which acts against the torque generated by the magnetized oxygen atoms. The compensation-current is delivered by two photo-elements, which are illuminated by an infrared beam. A mirror is located on the rotation axis of the hollowware. Smallest rotations of the body produce a deviation at the photo-elements, which generate the compensation current. The compensation current is thus a direct measure of the amount of oxygen in the exhaust gas and is converted into a linear output signal.

For measurements with hydrogen fuel, these two analyzers are sufficient. Since also syngas is used as fuel, CO and CO_2 need to be analyzed as well by the URAS 26 analyzer module [115]. It uses the adsorption characteristics of carbon monoxide CO and carbon dioxide CO_2. The detector is comprised of a small, closed test chamber. The URAS uses a non-dispersive infrared absorption measuring method that is based on the characteristic absorption of infrared radiation by CO and CO_2. The test chamber consists of a source of infrared radiation, radiographed tube-cells, through which the gas sample streams, a wavelength filter and an electro-optical infrared detector. The concentration of CO and CO_2 in the gas sample is measured by the extent of the absorption of their specific wavelengths in the infrared spectrum compared to the reference gas nitrogen N_2. The light from the infrared source radiates through the gas in the tube-cell and the filter, and then affects the IR-sensor. The filter lets pass only a defined part of the light-spectrum through the test chamber. This has the advantage that there is only a very narrow spectrum of light to be analyzed. As a result, the IR-sensor produces a current signal, which is evaluated by the exhaust gas analysis and proportional to the amount of CO and CO_2.

The amount of NO and NO_2 in the exhaust, is measured by the CLD analyzer [116]. It analyzes the chemiluminescence of the reaction between nitrogen monoxide and ozone according to the equation

$$NO+O_3 \leftrightarrow NO_2+O_2+h\nu \tag{13}$$

Ozone is generated by the CLD itself and made available for the reaction with NO. O_3 is delivered to two reaction chambers, one for NO and one for

NO_2. Their chemical reaction results in an optically measurable radiation (chemiluminescence). The intensity of this radiation is a direct measure of the concentration of the nitrogen oxides in the exhaust gas sample. After the analysis, the residuals of ozone are thermally destroyed, so that no harmful gases can escape into the environment.

For the monitoring of the operational conditions of the test burners, the test rig is equipped with mass-flow-, temperature-, pressure- and humidity-sensors (Table 13). The same applies for the gas turbine test rig; the data of the installed sensory is summarized in Table 14.

For the recording of the measurement data, a data acquisition system is used that was already built during earlier hydrogen research programs [7, 8] and that was extended to syngas. The measurement ranges of the applied equipment is fitted to the operational conditions of the tested burners. The output currents and voltages of the different sensors and analyzers are forwarded to the data acquisition system that translates the output signals into measuring data using zero-to-reference-point linearization. The system allows real-time monitoring of the operational conditions and the measurement- and analysis-data. Simultaneously, additional parameters like the fuel-air-equivalence ratio, the utilization of H_2 and CO during combustion, the overall combustion efficiency and the combustion temperature are calculated immediately out of the measurement data using the equations of the global reaction mechanism and of the energy balance [117, 118]. During all test campaigns, measurement data is recorded only when all parameters have reached stable conditions; measurement of transient conditions is not possible.

The research focuses on industrial gas turbine applications. Therefore, all NO_x-data is related to 15% O_2-content in the exhaust gas stream using the usual calculation [119]:

$$NO_x(15\%\ O_2) = NO_{x,measured} \cdot \left(\frac{20.95\% - 15\%}{20.95\% - O_{2,measured}}\right) \quad (14)$$

Between ten and twelve measuring points are taken for each operation point and are equally distributed in the circumferential (x-axis) and radial (y-axis) direction (Figure 22).

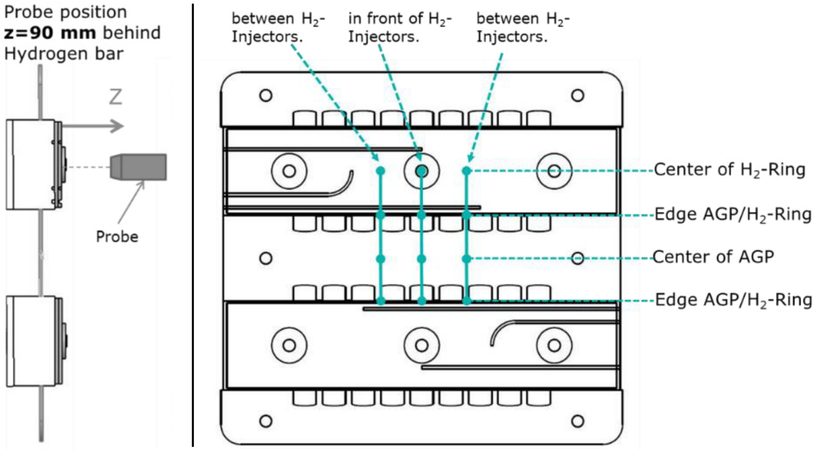

Figure 22: Illustration of measurement grid, probe location [120, 143]

The local measurements cover representative flow phenomena of the combustion process at the edges between AGP- and burner-segment, in front of AGP- and burner-segment, directly in front of an air/fuel-nozzle and between adjacent air/fuel-nozzles. Therefore, all relevant areas influencing the combustion and mixing process are covered during the measurements. The probe is positioned in a distance of 90 mm behind the burner segment downstream (z-axis). This ensures a homogeneous exhaust gas distribution over the complete burner cross-section, even for increased flame length for burners with increased power density. The application of a completely sealed flame tube that surrounds the combustion area rules out atmospheric influences from the outside. The test burner investigations are used to identify flow-, emission- and combustion-phenomena influencing the Micromix combustion process. To generate significant and comparable results, that are important to draw conclusions from for the later APU operation, the inlet air is always heated to meet the compressor discharge temperature of the APU. Since the combustion chamber test-rig operates under atmospheric conditions, the air mass flow is adjusted under the consideration of equal airflow velocities in the test burner and in the APU. This correlation is done by calculation of the corrected air mass flow for one single injector in the APU, multiplied with the ratio of test-rig and gas turbine inlet pressures, APU combustion chamber and test-rig inlet temperatures and the number of total injectors n_{fuel} applied to the test burner according to the following equation:

$$\dot{m}_{air_{Test-Rig}} = \dot{m}_{air_{APU}} \cdot \frac{p_{3_{Test-Rig}}}{p_{3_{APU}}} \cdot \frac{T_{3_{APU}}}{T_{3_{Test-Rig}}} \cdot n_{fuel} \qquad (15)$$

During testing, the air mass flow and air inlet temperature are kept constant. The investigated operation point is adjusted by variation of the fuel-air-equivalence ratio. In general, the fuel-air-ratio is varied from part-load-conditions to the design point of the combustion chamber and beyond to off-design conditions.

4.4 Numerical Investigations

The aim of the numerical analyses is to visualize and identify basic phenomena, and to understand the influences of various design parameters in terms of flow- and flame-structure. The creation and research of the numerical models and their properties are not part of this doctoral thesis. In the applied approach, the numerical results are used to explain phenomena, which are discovered by the measurements during testing, and to visualize these phenomena. Detailed information about the numerical research can be found in [98, 100, 120-124].

The chosen simplified numerical approach uses RANS-solver-based 3D simulations of the flow field in the MMX test burners with reduced and detailed reaction mechanisms and thermal NO formation models. The flow field structure, the temperature distribution, trends in flame anchoring, the flame structure and the emission behavior are analyzed; the emission calculation includes thermal NO only. In reality, several different NO_x formation mechanisms are active (chapter 1.5.1.1), but the sole consideration of the thermal NO formation allows fast and reliable assessments and tendencies of the emission behavior of various test burners. The calculated NO-levels in the numerical evaluation are then indeed underestimated compared to the expected experimentally measured NO_x, but deliver a reliable trend for a phenomenological review. The phenomenological analysis allows the visualization of the main parameters influencing the DLN MMX process for SG 90/10 and H_2 as they are reflected in the experimental data.

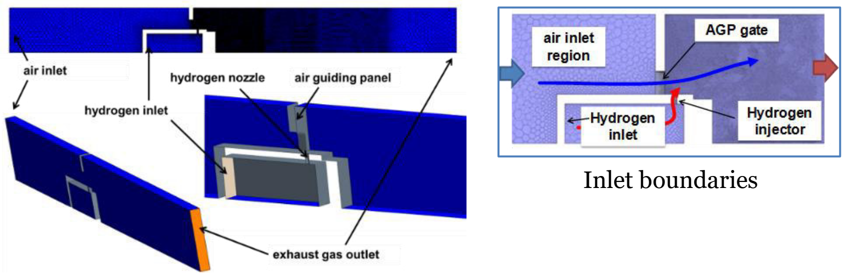

Figure 23: Test burner model and boundary conditions [98]

The numerical analyzes are performed using the commercial software CD-adapco STAR CCM+ based on simplified geometric models that are derived from the actual test burners (Figure 23). The symmetrical configuration of the test burners allows simulating a simplified slice model, which consists:

- in the horizontal direction of one half of a fuel nozzle and one half of an air-guiding-panel gate only,
- in the vertical direction of half an air-guide-panel and one half of a burner segment.

Fuel and air are fed into the model by two separate boundary conditions within the model. The entry borders are set far enough from the defined air guiding panel position and the fuel nozzle location to avoid any border influences on the main flow phenomena in the mixing and combustion areas. No-slip wall boundaries represent the air guiding panels and the burner segments. The air and fuel intake parameters are scaled according to the experimental conditions of the gas turbine to the atmospheric test burner operation. The corresponding air inlet pressure in the simulation is 1 bar; the air temperature is 560 K; the fuel inlet temperature is 300 K. The fuel-air-ratio is adjusted by adjusting the fuel mass flow according to the examined operating point. Stationary 3D-RANS calculations are performed and the realizable k,ε-turbulence-model is applied with all y+ wall treatment. The boundary layer modeling is done as a function of the local, non-dimensional wall distance y+. For high y+ values a wall function is used; for small y+ values (below or not much greater than 1), no wall function is required.

The spatial discretization is done with the STAR-CCM+ Surface Remesher and an unstructured polyhedral mesh. The polyhedral cell shape helps to minimize the total number of cells at high-resolution quality and reduced computing time. To improve the mesh quality in the near-wall areas and for improved modeling of the phenomena appearing there, additional prism layers are used. A progressive mesh refinement is applied in the range along the reaction- and hot-gas-zone propagating from the fuel nozzle. There, the smallest volume of the cell size is located to obtain sufficient resolution in the mixing- and reaction-zone. The refining process for the mesh is performed iteratively within a reference calculation to obtain a grid independent solution. Finally, the applied mesh consists of approximately 1.3 million volume cells.

The simulation of the hydrogen combustion process is mainly based on a reduced reaction model with the following one-step hydrogen-combustion reaction:

$$2H_2 + O_2 \rightarrow 2H_2O \quad (16)$$

The calculation of the reaction rate is described by a Hybrid Eddy-Break-Up-(H-EBU)-combustion model [98], which combines the reaction turbulent mixing driven rate and the chemical kinetic rate (finite chemistry). The turbulent mixing driven rate of the reaction is formulated via the EBU combustion model. This model assumes that the reactants burn immediately after mixing. The chemical kinetic reaction rate is determined based on the proposed Arrhenius formulation by Fernández-Galisteo [125].

$$r = 2.05E14 \frac{m^3}{kmol\, s} exp\left(-\frac{1.6629E8 \frac{J}{kmol\, K}}{RT}\right)[H_2]^2 \quad (17).$$

It determines the amount of time that is required to burn reactants when they are fully mixed. After applying the Hybrid-EBU approach, both reaction rates are calculated and compared; the smallest rate is assumed to limit the reaction. To evaluate the results obtained with the Hybrid-EBU model, combustion simulations are performed based on a detailed H_2/O_2 reaction mechanism. For this purpose, the reaction models described by Li et al. [126] are used which consist of 19 reversible elementary reactions and 11 species.

The general combustion topology of the test burners has been studied experimentally and are reproduced very well by both the Hybrid-EBU- and by the detailed mechanisms. Minor discrepancies only exist in the prediction of the NO concentrations. The formation of thermal NO is modelled using the extended Zeldovich mechanism. The calculation is done by the NO-model implemented in STAR CCM+ and by including the underlying equations as user-defined functions. A calculation of the concentration of oxygen radicals is necessary; it is derived by an internal assessment in Star-CCM+ when the EBU model is used, or by direct calculation, when the detailed mechanism is applied. The activation of the provided NO-model adds NO to the transported species within the reaction zone. This allows an assessment of the NO-distribution within the reaction zone, along the hot-gas flow and the NO concentration at the burner outlet. Concluding, the NO concentration is underestimated by the EBU model and more precisely predicted by the detailed mechanism. Since NO represents only a subset of nitrogen oxides (see chapter 1.5.1.1), the trend to underestimated NO by the numerical simulation is reasonable. Therefore, for the complimentary calculations as part of the extensive experimental parametric study and due to the significantly reduced computational effort, the Hybrid-EBU model is used.

To simulate syngas SG 90/10, only the detailed reaction mechanism has been used because of the complexity of the underlying reactions. Two reaction mechanisms are established that provide comparable results with respect to the experimental studies. The built-in Star-CCM+ combustion mechanism based on a detailed H_2/CO-mechanism by Hawkes et al. [127] has been derived for application in direct numerical simulations of three-dimensional unsteady turbulent flames. The mechanism consists of 21 reversible reactions and contains 11 species. In addition, the mechanism created by the Chemical Reaction Engineering and Chemical Kinetics (Creck) Group of the Politecnico di Milano [128] is used. It consists of 34 reversible reactions and 14 species. Both reaction mechanisms provided nearly identical results of the main exhaust gas components (H_2O, O_2 and CO_2) in relation to the experimental studies. Regarding the CO- and H_2-concentrations, the qualitative trend of the emissions is well reproduced as a function of the fuel-air-ratio. Each mechanism obtains comparable results, but because of the significantly less computational effort due to the smaller number of species, the Star-CCM+

integrated reaction mechanism is used for the presented simulations of the syngas combustors.

4.5 Possible Sources of Error and Data Illustration

During the several measurement campaigns, the utilized measurement equipment was checked and calibrated daily before testing. Nevertheless, the measurement results are affected by the accuracy of the used measurement devices, the analyzers (Table 13) and the tolerances of the reference gases[10].

The probing conditions can have an effect on the measurement results. The existence of a certain amount of NO_2 in the exhaust gas emissions of turbulent diffusion type flames is characteristically (chapter 1.5.1.1). Inside the probe, NO can be converted to NO_2 by wall reactions and pressure conditions in the probe. However, the general amount of NO_x is not affected by this effect [23, 129-132]. Therefore, only the overall NO_x-emissions are discussed within the framework of the investigations.

To identify low NO_x key drivers in the investigations, a phenomenological approach is chosen. All figures in this work show NO_x-emissions that are related to 15% O_2-content (chapter 4.3) [9]. The data regarding equivalence ratios and combustion temperatures are calculated by the data acquisition system and are based on data from the exhaust-gas-analysis-system. Each data point in the diagrams represents the arithmetic mean value[11] of all the measuring points in the chosen measuring grid (Figure 22). The equivalence ratio is calculated in the data acquisition system using the measured O_2-and H_2-values. Consequently, the equivalence-ratio-

[10] Resulting accuracy of NO_x is ±0.3 ppm; of the equivalence ratio ±3% [11].

[11] The measurements cover all influencing phenomena of the combustion process (chapter 4.3). The arithmetic mean of all obtained values is feasible and give representative mean data. The data on equivalence ratios and combustion temperatures are checked against the theoretical calculations based on the measured overall fuel- and air-mass-flow. The calculated values and the measured mean values showed to be in a good agreement.

calculation is influenced by the analyzer-accuracy of the Magnos- and the Caldos-device (Table 13). However, the applied measuring equipment has a very high accuracy and a deviation of the measurement values is marginal.

In order to consolidate the quality of the measuring results and reproducibility, a test-series should be performed several times. The hydrogen- and especially the syngas-testing generates high costs. Therefore, most of the tested burner-series are carried out twice. Nevertheless, the predominant physical flow phenomena and their influences are detected in several different test-series and can therefore be stated to be reproducible, Figure 24.

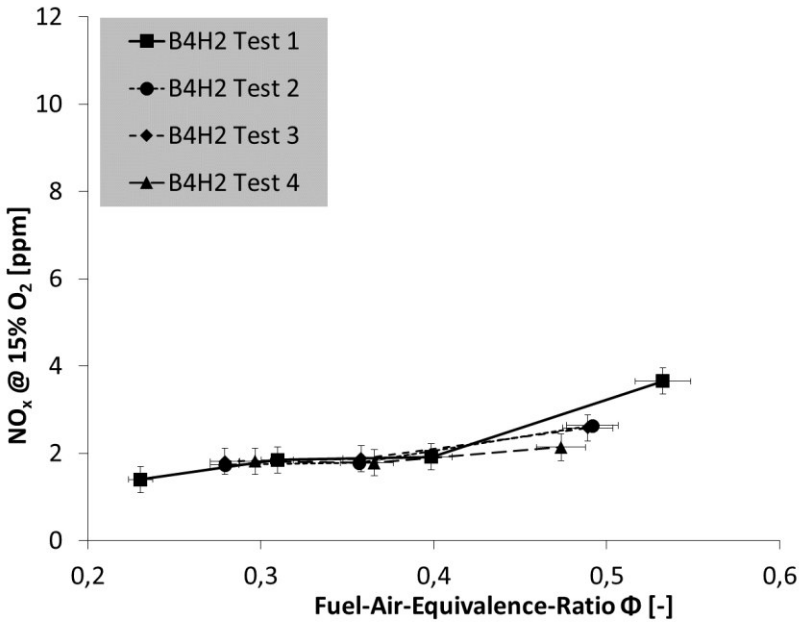

Figure 24: Reproducibility and accuracy shown for B4H2 test series

Concluding, the reproducibility and accuracy of the measuring equipment and the related calculations highlight that the observed flow phenomena and their effects on NO_x-emissions are identified accurately and reproducibly (Figure 24). The research aims for the identification of geometric key design parameters and their influence on the combustion process and the resulting NO_x-formation. Against this background, the applied approach allows an adequate discussion of the obtained results.