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AUTOMATED DESIGN SPACE EXPLORATION OF THE HYDROGEN FUELED "MICROMIX" COMBUSTOR TECHNOLOGY

Anis Haj Ayed, Constantin J. D. Striegan, Karsten Kusterer
B&B-AGEMA GmbH
ayed@bub-agema.de
Aachen, Germany

Harald H.-W. Funke
Aachen University of Applied Sciences
funke@fh-aachen.de
Aachen, Germany

M. Kazari, A. Horikawa, K. Okada
Kawasaki Heavy Industries, Ltd.
Akashi, Japan

ABSTRACT

Combined with the use of renewable energy sources for its production, Hydrogen represents a possible alternative gas turbine fuel for future low emission power generation. Due to its different physical properties compared to other fuels such as natural gas, well established gas turbine combustion systems cannot be directly applied for Dry Low NO_x (DLN) Hydrogen combustion. This makes the development of new combustion technologies an essential and challenging task for the future of hydrogen fueled gas turbines.

The newly developed and successfully tested "DLN Micromix" combustion technology offers a great potential to burn hydrogen in gas turbines at very low NO_x emissions. Aiming to further develop an existing burner design in terms of increased energy density, a redesign is required in order to stabilise the flames at higher mass flows and to maintain low emission levels.

For this purpose, a systematic design exploration has been carried out with the support of CFD and optimisation tools to identify the interactions of geometrical and design parameters on the combustor performance. Aerodynamic effects as well as flame and emission formation are observed and understood time- and cost-efficiently. Correlations between single geometric values, the pressure drop of the burner and NO_x production have been identified as a result.

This numeric methodology helps to reduce the effort of manufacturing and testing to few designs for single validation campaigns, in order to confirm the flame stability and NO_x emissions in a wider operating condition field.

INTRODUCTION

Aviation and power generation industry has need of efficient, reliable, safe and low-pollution energy conversion systems in the future. Gas turbines will play a decisive role in long-term high power application scenarios, and hydrogen has great potential as renewable and sustainable energy source derived from wind- or solar power and gasification of biomass substituting the limited resources of fossil fuels (Lieuwen et al. [1]). Hydrogen affects the operation of common gas turbine systems due to its high reactivity requiring combustion chamber modifications to guarantee efficient, stable, safe and low NO_x combustion. Besides optimised combustion technology and related exhaust gas emissions, modifications of the gas turbine control and fuel metering system have to be applied to guarantee safe, rapid and precise changes of the engine power settings (Dahl et al. [2], [3], Funke et al. [4] - [7]).

Against this background the Gas Turbine Section of the Department of Aerospace Engineering at Aachen University of Applied Sciences (AcUAS), B&B-AGEMA and Kawasaki Heavy Industries work in the research field of low-emission combustion chamber technologies for hydrogen gas turbines and related topics investigating the complete system integration of combustion chamber, fuel system, engine control software and emission reduction technologies. The hydrogen gas turbine research started at AcUAS during the European projects EQHHPP (Shum et al. [8]) and CRYOPLANE (Westenberger et al. [9]) where the low NO_x Micromix Hydrogen combustion principle was invented. When hydrogen is burned as fuel with air, nitric oxide emissions occur, but Dahl et al. [2], [3] & Funke et al. [10], [11] have shown that the combustion process has to be modified and optimised in order to achieve low NO_x emissions. Because of the large difference in the physical properties of hydrogen compared to other fuels such as kerosene and natural gas, well established gas turbine

combustion systems have to be modified for Dry-Low-NO$_x$ (DLN) combustion. Thus, the development of DLN hydrogen combustion technologies is an essential and challenging task. The DLN Micromix combustion principle for hydrogen is being developed and optimised for years to reduce NO$_x$-emissions significantly by miniaturising the combustion zone, reducing the residence time of reactants in the combustion zone, and enhancing the mixing process using a jet in cross-flow design. A review of the previous research activities at AcUAS is presented in Funke et al. [12].

Especially the flame anchoring - mostly dominated by the resulting recirculation zones and vortices within the Micromix burner geometry (Funke et al. [10]) and by the momentum flux ratio of the jet in cross-flow (Funke et al. [11]) - is most essential to the Micromix low NO$_x$ characteristics. Based on previous investigations a Micromix combustion chamber with about 1600 miniature injectors (Figure 1) was designed for a small size Auxiliary Power Unit APU GTCP 36-300 and successfully tested (Funke et al. [13]).
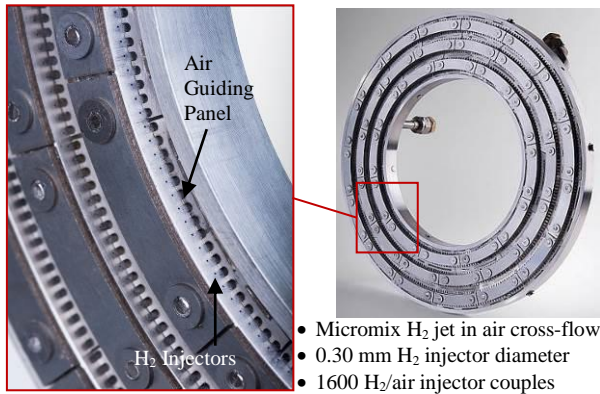

- Micromix H$_2$ jet in air cross-flow
- 0.30 mm H$_2$ injector diameter
- 1600 H$_2$/air injector couples

Figure 1: Micromix Prototype Combustor for Gas Turbine Honeywell/Garrett Auxiliary Power Unit APU GTCP 36-300

The GTCP 36-300 requires about 1.6 MW thermal energy converted to shaft power generating electrical and pneumatic power up to 335 kW. The combustion section consists of an annular reverse flow combustion chamber in which the Micromix combustor is to be integrated.

The Micromix hydrogen combustion research is done using an interactive optimisation cycle including experimental and numerical studies on test burners, full-scale combustion chamber investigations and the feasibility is proven in real gas turbine operation.

Based on these studies the impact of different geometric parameters on flow field, flame structure and NO$_x$ formation are identified and the Micromix combustion principle is continuously optimised.

Within the present study, the impact of different geometric parameters of a high energy density Micromix burner on its flame structure and NO emission is studied within an automated numeric design exploration. Thereby, a systematic variation of three major geometric dimensions is performed within a geometrically feasible range. 3D CFD simulations of the reacting flow have been performed for the different Micromix burner variations in order to evaluate the resulting flow field, flame structure and NO emissions and understand the influence of the single parametric variations on the complex reactive flow field of the Micromix burner. The observations resulting from this study will reveal optimisation potentials of the Micromix combustion technology in terms of NO emissions, especially concerning increased energy densities.

MICROMIX HYDROGEN COMBUSTION

Micromix Burning Principle

Gaseous Hydrogen is injected through miniaturised injectors perpendicularly into an air cross-flow through small air guiding panel (AGP) structures. This leads to a fast and intense mixing, which takes place nearly simultaneously to the combustion process. As a result, miniaturised micro flames develop and anchor at the burner segment edge downstream of the injector nozzle. Multiple micro flames instead of large scale flames lower the residence time of the NO$_x$ forming reactants and consequently the averaged molar fraction of NO$_x$ can be reduced significantly as has been shown in Funke et al. [6].
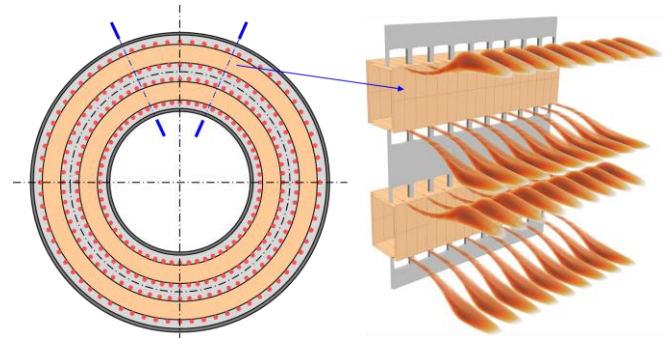

Figure 2: Schematic front view and curved section of Micromix annular burner

Figure 2 shows a schematic front view of the Micromix ring combustor with two rings and four rows of hydrogen flames. A curved section is cut out and the full-symmetric CFD-results indicate ideally equal and separated flames.

The main influence on the low NO$_x$ characteristic can be ascribed to the key design parameters blockage ratio BR of the air guiding panel AGP (Figure 3) and injection depth y of the fuel into the oxidizer cross-flow (Figure 3b). The blockage ratio BR represents the ratio between the air guiding height and the height of the air guiding panel (AGP).

The blockage ratio influences shape, position and size of the flame stabilising vortices downstream of the air guiding panel and the burner segment. The jet-in-cross-flow mixing of fuel and air stabilizes the low NO$_x$ emission characteristics of the combustion principle as long as the injection depth y (Figure 3b) is not penetrating the shear layer of the AGP-Vortex (critical injection depth y_{crit}). A recirculation of the

fuel/air mixture into the AGP vortex leads to raised NO_x emissions (Funke et al. [13]).
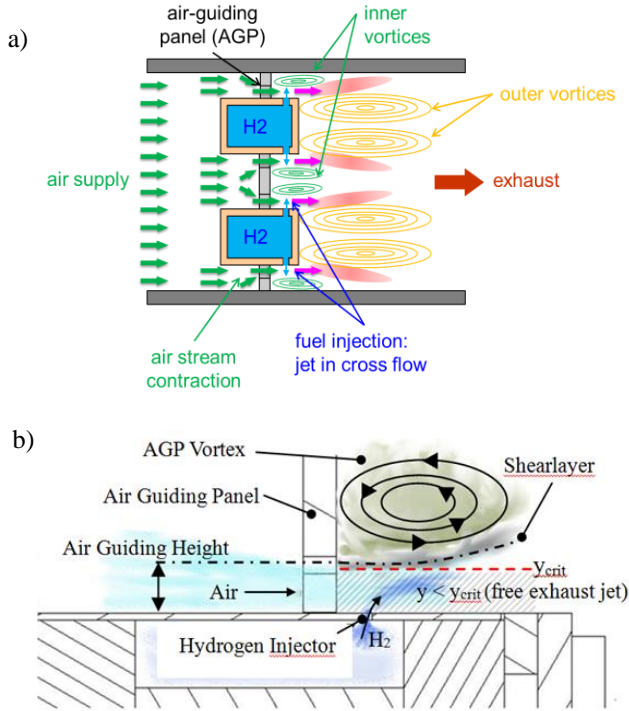

Figure 3: a) Schema of aerodynamic flame stabilisation principle and b) Hydrogen injection depth definition

CFD STUDY & DESIGN EXPLORATION

For the numerical simulation of the different burner variations, a simplified numerical approach is applied. It uses the 3D numerical simulation of the flow field within the test-burner based on a RANS solver, reduced combustion reaction mechanism and thermal NO formation models to analyse flow-field-structures, temperature distribution, tendencies of flame-anchoring, flame-structure and emission behaviour. In this section of the paper, the simplified numerical approach is described, and its application to calculate the reactive flow in the burners is presented. The aim of the numerical analysis is to understand the basic flow phenomena and qualitatively identify tendencies of the different design parameter influences with respect to flow- and flame-structure, and resulting thermal NO emissions. The emission calculation includes only thermal NO via the three Zeldovich equations, because it is a good and fast indicator of the burner configuration emission behaviour and very useful for the numerical prediction of the test-burner emission characteristics prior to testing. Therefore, the calculated NO emissions are expected to be generally slightly below the real values, but provide a qualitative evaluation possibility for the intended numerical design exploration of the high energy density Micromix combustion technology. In order to justify the selected models, simulations with a more elaborated chemical combustion model for hydrogen and nitric oxides are carried out in advance. The results are in very good agreement with experimental measurements of nitric oxides in case of an enlarged Micromix design (compare Figure 7) [14].

Computational Domain

The numerical analysis has been carried out using a commercial CFD code (CD-adapco [16]) and has been based on simplified geometric models derived from the different burner configurations to be investigated. The geometric model is shown in Figure 4 and covers a longitudinal burner slice, which makes use of the symmetric nature of the burner in both lateral and vertical directions. The symmetric boundaries along the lateral direction are set on the cross section through the centre of one hydrogen injection hole and on the cross section between two hydrogen injection holes, respectively. Along the vertical direction, the symmetry planes are set on the centre section through one air-guiding panel and on the centre section through one hydrogen segment. Thus, the slice model contains one-half of a hydrogen injection hole and one-half of an air-guiding gate.
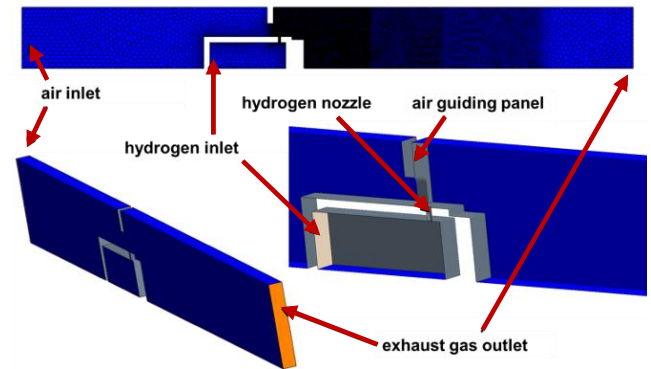

Figure 4: Computational Domain

The spatial discretisation has been performed using the STAR-CCM+ surface remesher and polyhedral mesher resulting in an unstructured polyhedral mesh. The polyhedral cell shape is especially advantageous as it helps minimising the total number of cells while maintaining mesh resolution quality and thus, helps saving calculation time and cost. Progressive mesh refinement has been performed along the reaction and hot gas zone starting from the hydrogen injection surrounding. There, the smallest volume cell size has been selected to get a sufficient resolution inside the mixing and the reaction zone. The refinement process has been performed iteratively within a reference calculation until a mesh independent solution could be obtained. The final mesh includes approx. 1 million volume cells in total.

3D-steady state RANS calculations have been performed. The realizable k-ε turbulence model with all y+ wall treatment has been applied. The wall treatment is decided depending on the local dimensionless wall distance y+ values. For high y+ values the wall function approach is used. For low y+ values (below or not much larger than 1) no

wall function is required, since the boundary layer is well discretised by the numerical mesh.

Combustion model

The hydrogen combustion process is simulated based on a reduced hydrogen combustion reaction model including a one-step hydrogen combustion reaction, where the reaction rate has been calculated by the hybrid EBU combustion model described in Funke et al. [11]. This model combines the turbulent mixing driven reaction rate and the chemical kinetic reaction rate (finite chemistry). The turbulent mixing driven reaction rate is calculated via the EBU (Eddy Break Up) combustion model formulation [16], which assumes that reactants are directly burnt after mixing. The chemical kinetic rate is calculated based on the Arrhenius formulation and considers a chemical time scale that is needed to burn the mixed reactants. By application of the hybrid EBU approach, both reaction rates (turbulent mixing driven rate and chemical kinetic rate) are calculated and compared. The smallest rate is assumed as reaction limiting.

By applying the reduced hydrogen combustion reaction model the calculation time is reduced significantly and large number of parameter variations can be achieved within a reasonable numerical effort. If detailed hydrogen combustion reaction mechanisms were considered, the calculation time would exceed an acceptable time for the present design exploration. A more detailed combustion model can validate the accuracy of the chosen combustion model with regard to the flame shape and length. It considers 19 elemental equations for the hydrogen combustion [17] and over 200 equations containing a chemical compound of different NO-pathways [18]. This model is applied for one enlarged Micromix design in direct comparison to experimental test burner results.

Thermal NO formation is implemented by application of the extended Zeldovich NO formation mechanism. A corresponding numerical model is provided by the applied CFD code. Its activation adds NO to the transported species within the solution domain. This allows the evaluation of NO distribution within the reaction zone and the full hot gas path as well as the evaluation of NO concentrations at the burner outlet boundary (calculate the NO emission).

Boundary conditions

The fuel and the air jet are introduced separately into the burner model via two inlet boundaries as shown in Figure 5. The inlet boundaries are set far enough from the air guiding panel and the fuel injection hole in order to avoid any boundary influence on the key flow phenomena in the mixing and combustion regions. No-slip wall boundaries represent the air guiding panel and the hydrogen segment walls.

Since contact with hot gas is limited to the front surface of the H_2 segment and the surfaces surrounding the reaction and exhaust gas zone are symmetry planes, heat transfer from the hot gas into the burner wall has been neglected and has not been considered within the numerical simulations for all burner configurations.

The air and fuel inlet parameters for the design space exploration simulation are defined according to the conditions in the gas turbine. The air inlet pressure is 10.5 bar and a temperature of 621 K. The fuel enters the domain with an inlet temperature of 300 K. The fuel mass flow has been selected according to the design operating point ($\Phi = 0.31$).
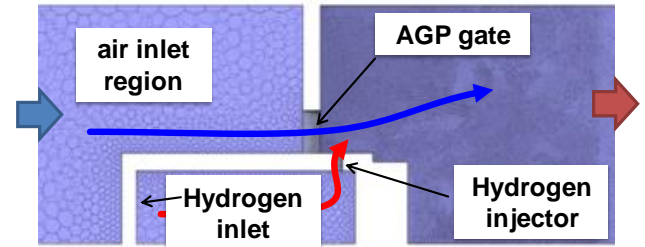

Figure 5: Computational Domain, Close up to fuel injection region

Experimental test burner results

The department of Aerospace Engineering of AcUAS executed an experimental campaign at an atmospheric test rig. Experimental tests and numerical analyses with a detailed elemental combustion model have been performed for a burner design with a hydrogen injector of 1.0 mm at different equivalence ratios and are explained in Funke et al. [14]. Thereby, the Micromix flames were found very stable and well in accordance with the typical Micromix structure, despite of the increased energy density. Figure 6 shows the experimentally observed flame structure at an equivalence ratio of 0.4 (design point at the test rig).
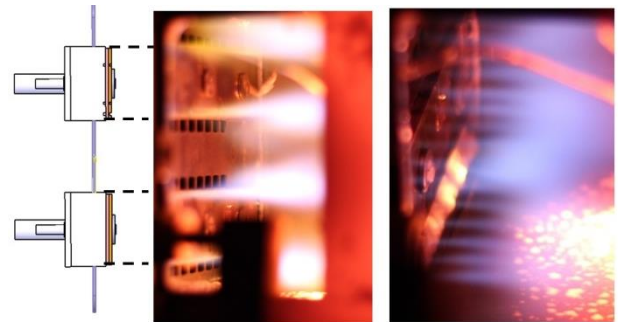

Figure 6: Optical flame appearance of established Micromix flamelets at design point $\Phi = 0.40 - 1.0$ mm injector burner

The corrected NO_x emissions (corrected to 15% O_2 fraction at the outlet) obtained experimentally and numerically are given against the equivalence ratio in Figure 7. At the design equivalence ratio of $\Phi = 0.4$ the NO_x emission was measured to approx. 2.2 ppm. The simulation with the detailed combustion model is able to achieve the nitric oxide results at atmospheric conditions. The simplified hybrid EBU-model with thermal NO_x consideration results in a value of only about 0.5 ppm at $\Phi = 0.4$. The discrepancy can be mainly referred to the simplified combustion

calculation, but the overall tendency of the values shows the same trend as for the more advanced model.

This experimental test burner is considered as reference case within the present study for the design exploration under gas turbine conditions.
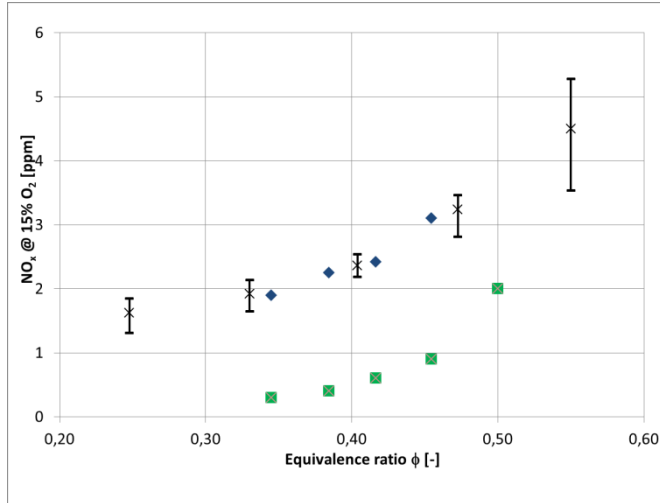

Figure 7: Experimental results of NO$_x$ emission (crosses) in comparison to numerical results of detailed combustion (blue) and EBU model with thermal NO$_x$ (green)

Numerical results & Parametric Study

The Micromix burning principle is characterised by distinct reaction zones, anchoring near the edge of the H$_2$ segment and stabilised by the inner and the outer vortex pairs as shown in Figure 8. Both vortex pairs result from the flow conditions due to the channel widening when the flow recirculates downstream the air-guiding panel after the contraction in the air gate. Due to the axial shift in the position of the H$_2$ segment front face and the air guiding panel, an inclined shear layer is established in-between the vortices and combustion reaction takes place and is stabilised along this inter-vortex shear layer. Under operating conditions, the inner vortex pair is dominated by a cold air stream due to the lean combustion mixture. Whereas the outer vortex pair is fed by a recirculating of hot gas downstream the H$_2$ segment.

The structure and orientation of the Micromix flame is depending on the structure of the mentioned shear layer, which is in turn defined by the size, position and intensity of the stabilisation vortices.

Figure 9 shows the calculated temperature distribution (bottom part) and the calculated thermal NO mass fraction (top part) in the reference Micromix burner (reference geometry). The Micromix flames are clearly separated from each other, well anchored and stabilised according to the Micromix burning principle.

Observing the temperature distribution, two peak temperature regions can be distinguished. The first is found along the first flame fragment, which is stabilised in-between the inner and outer recirculation vortices along the inter-

vortex shear layer. This zone is thin, but shows a significant temperature gradient across the flame, which is typical for this kind of flames.
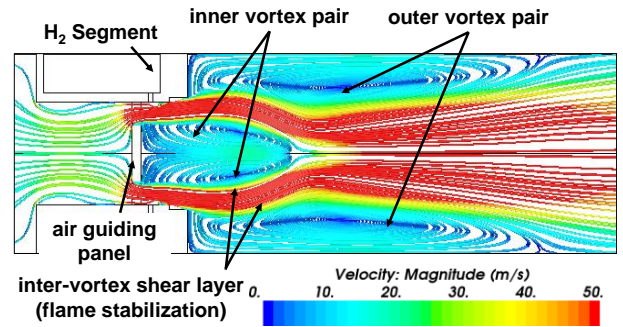

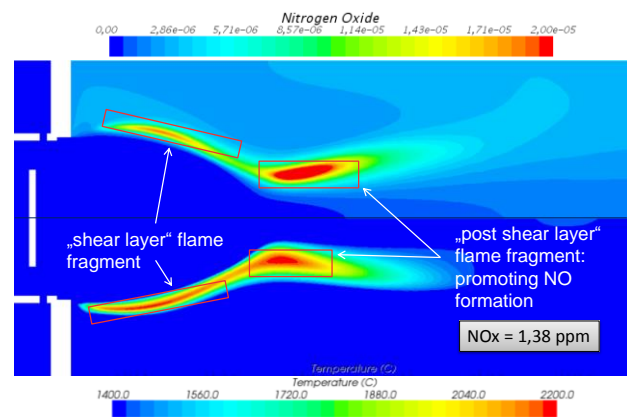**Figure 8: Typical recirculation and vortex structure of the Micromix burning principle**

Figure 9: Calculated temperature (bottom) and NO mass fraction (top) distributions for the reference burner

The second peak temperature zone is found downstream of the inter-vortex shear layer (as marked in Figure 9). Here, the remaining fuel that was not burnt along the first flame fragment continues its consumption and the main heat release of the injected fuel takes place. In this zone, a higher peak temperature is found and the flame expands, indicating an increased concentration of heat release. Since the angular momentum of the inner vortex pair decreases further downstream and its impact on the flame is reduced, the flame gets the possibility to extend its shape in this "post shear layer" zone.

The present flame structure due to the increased energy density of the considered burner is not typical for the Micromix burning principle, which aims to burn all the injected fuel along the thin inter-vortex shear layer, avoid high fuel concentrations, high temperature peaks and thus, reduce NO$_x$ emissions. It is to be noted that the injector size of the burner in question is 1mm, which leads to an 11 times higher energy density compared to the originally invented burner, having an injector size of 0.3 mm). Since the overall burner dimensions are not scaled with the same factor as the injectors (due to combustor integration issues), the length of the inter-vortex shear layer becomes not sufficient to

accomplish all the heat release (or to accommodate the whole flame). The fuel that could not be burnt along the shear layer starts to burn further downstream, creating the aforementioned second flame fragment.

The calculated NO mass fraction for the reference burner (shown in the top part of Figure 9) reflects the flame structure well and clearly shows two distinct high NO zones: inside the first and the second hot flame fragment. Thereby, a significant NO mass fraction peak and concentration is found in the second flame fragment. It means that the new flame structure, which is dividing the flame into a "shear layer" and a "post shear layer" part, has a negative influence on the NO_x emission level of the burner.

It is expected to reduce the burner's NO_x emissions by reducing the extent of the "post shear layer" part of the flame. This could be achieved by increasing the shear layer length, so that a higher amount of the heat release can take place within the thin "shear layer" part of the flame. Observations are made to lower the nitric oxide emissions by an adaption of the geometry, e.g. an increasing of the air-guiding panel (AGP) height. An enlargement of the AGP height would extend the cross-section behind the air gate and consequently enlarge the inter-vortex shear layer.
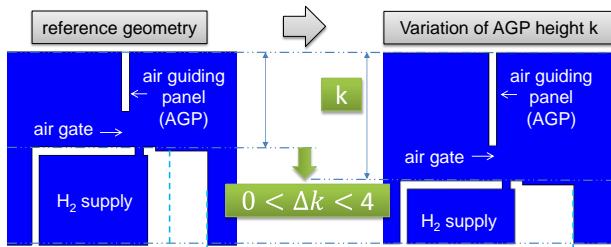

Figure 10: Variation of the AGP (air guiding panel) height by variation of the k parameter

A further measure that could reduce NO_x emissions of the burner is to increase the mixing path length (way between injection and flame anchoring) by changing the jet in cross-flow (JICF) mixing conditions. Previous investigations of H. Ayed et al. [15] have shown an influence of the gate size and the injector distance. Accordingly, the shape and the velocity of the air flow downstream the air gate is changed that interacts with the central injected hydrogen jet. Funke et al. [14] and Ayed et al. [15] point out the importance of an adequate fuel and oxidizer mixing. The flame shape and the flame extension in the first shear layer are dominated by the intensity and size of the inner vortex pair. In the case when the injector distance is too large under a certain mass flow condition, the intensity of the inner vortex pair decreases and the ability to cool the flame is reduced. The numerical results in [15] indicated an excess of air penetrating the zones between the flames so that a lateral flow connection between the inner and outer vortex pair is achieved. This connection can be disturbed in case of too wide or small injector distances.

Figure 11 shows possible shapes of the gate when the height and the width are varied. The variation ranges are limited by the ability of manufacturing and flow velocity in the air gate. Experimental tests indicated that the area of the

gate should not fall below or exceed certain values. Results in this paper indicate that high velocities increase a total pressure drop, whereas low velocities reduce the capability of mixing and increase the flame length and NO_x emission.
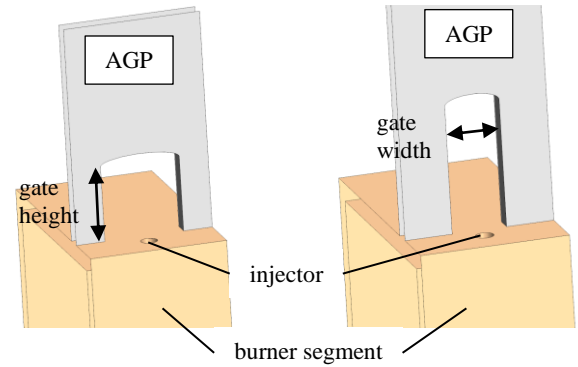

Figure 11: Modifications of gate height and width

Automated design space exploration

Starting with the geometry parameters of a base design, single lengths shall be adapted with the intent to optimise the flame structure and guarantee low nitric oxide emissions. Achieving the application of the Micromix module in a defined gas turbine configuration, the main parameters of the burner height and width are set as constant. This determines the outer diameter of the ring burner and specifies the number of gates in the ring burner module at steady air mass flow conditions.

With the intend to modify the flame structure in order to reduce the maximum temperature in the first and second shear layer zone, the geometry of the gate shall be adapted for an improved fuel and oxidizer mixing. Further on, the hot "post shear layer" shall be diminished by an extended inner vortex pair in the wake of an enlarged AGP height.

Accordingly, three variables are defined: the gate height (the shape of arc is kept constant, see Figure 11), the gate width and AGP height. The fact that the gate area is influenced by the gate height and width, it is necessary to define not only ranges for each variable, but also for the resulting area size, so that the air velocities adjust in between 70 and 110 m/s.

Aim of the design optimisation is the minimisation of the produced NO_x considering a tolerable total pressure drop range of about 2 to 3 %.

The optimisation study is carried out by the commercial software of Optimate+ [16] using the multi-objective SHERPA algorithm. It uses different search algorithms simultaneously and consists of self-learning methods, which decide over the extent to use the single search approaches.

RESULTS AND DISCUSSION

In Figure 12 the result of about 250 successful optimisation steps is illustrated. Each point indicates a feasible or unfeasible evaluated design by the optimisation approach in plotting the value of NO_x emission over the total pressure drop. The size of each bubble shows the molar

fraction of unburnt hydrogen at the burner outlet boundary. Bigger bubble sizes indicate a higher amount of unburnt fuel and a lower burning performance. The range of 2-3 % total pressure drop means the required zone for the application in the gas turbine.

Mainly two trend lines are visible in the results. There are well performing "usual" Micromix flames with a nearly complete combustion process, which show increasing NO_x emissions with a reduced total pressure drop (see Figure 12-A). Further on, the optimiser tested designs in a feasible pressure range with gate geometry, which impaired the mixing, and combustion process negatively. The temperature and the NO_x emission especially in the "post shear layer" increase strongly to intolerable high values (Figure 12-B).

Finally, a second trend line at very low NO_x levels can be recognised which seems to be independent of a pressure loss value. The optimisation showed such flame results for the first time, since previous experimental designs followed different design laws. These "unusual" flame shapes can be numerically achieved when the AGP burner height is high. As previously investigated, the inner vortex pair can be increased when the AGP height is enlarged, but its high angular momentum destabilises the normal vortex structure. The flames are pressed together (Figure 12-C) as the outer vortices diminish. The flame temperature is very low, which is the reason of the low nitrogen oxide emission. Due to the extent of the inner vortex, the shear layer at which the combustion can take place is enlarged as well. This fact can be the reason why the second shear layer does not show an increased heat release.

Due to the changed flame structure of the "unusual" designs which leads to lower nitric oxide emissions but is not in accordance with proven Micromix flame shapes, such designs will be subject to validation testing at atmospheric conditions in order to confirm their lowest NO_x ability, stability and combustion efficiency.
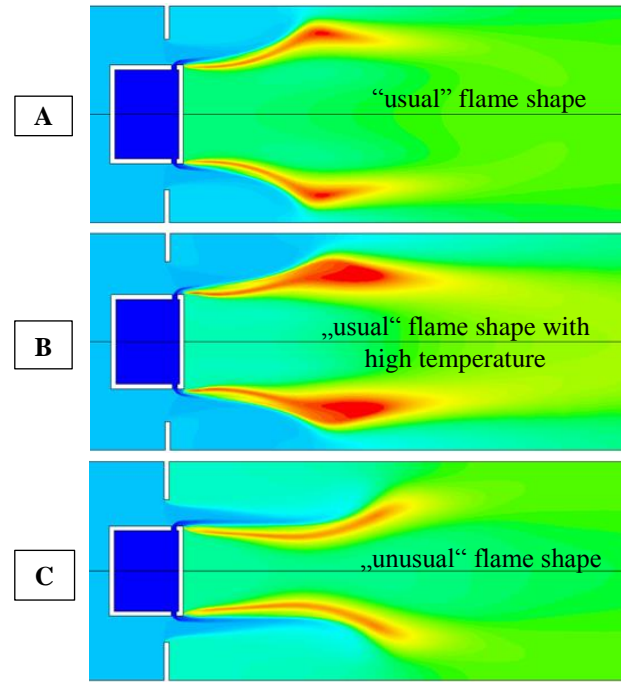

Figure 12: Results of the design space exploration: corrected NOₓ depending on total pressure drop and characteristic flame shapes

CONCLUSIONS

An automated parametric study and numerical exploration of the high energy density Micromix burner revealed that it is well possible to positively influence the flame shape by a stabilisation of the vortex pairs and the mixing path length. An adequate selection of the burner geometric parameters allows adjusting flame length and inter-shear layer length to suppress the NO rich "post shear layer" flame fragment. This has been found to decrease the NO emissions of the burner in question significantly. This offers a great potential of further increasing the Micromix energy density while maintaining low NO_x emissions. Especially the consideration of elevated pressure conditions (for integration in real gas turbine combustors) leads to thicker and longer Micromix flames. The design of adequate burners for real gas turbine applications can make use of the present findings to balance the design requirements in terms of energy density, manufacturability, stability and emission behaviour.
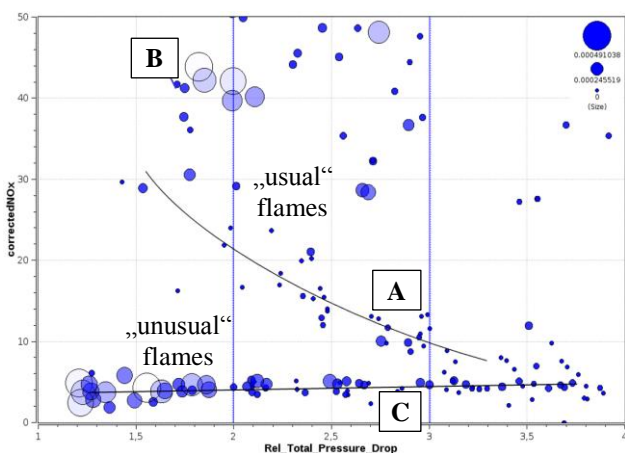
NOMENCLATURE

A	area (unit: mm^2)
BR	blockage ratio (unit: -)
c	velocity (unit: m/s)
d	diameter / inner diameter (unit: mm)
D	outer diameter (unit: mm)
ED	energy density (unit: MW/(m² bar))
k	AGP height (unit: mm)
$\dot{m}$	mass flow (unit: kg/s)
p	pressure (unit: bar)
s	distance between H_2 injectors (unit: mm)
T	temperature (unit: K)
y	Injection Depth (mm)
Φ	equivalence ratio (unit: -)
AGP	air guiding panel
H_2-Seg.	hydrogen burner

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