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Authors: Giulia Babazzi, Pierre Q. Gauthier, Parash Agarwal, Jonathan McClure, Vishal Sethi

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NO_X EMISSIONS PREDICTIONS FOR A HYDROGEN MICROMIX COMBUSTION SYSTEM

Giulia Babazzi
Centre of Propulsion Engineering
Cranfield University
Cranfield, Bedfordshire MK430AL, UK
Email: g.babazzi1@gmail.com

Pierre Q. Gauthier*
Royal Academy of Engineering
Visiting Professor in Low Emissions
Combustion System Modelling
SATM Cranfield University
Cranfield, Bedfordshire MK43 0AL, UK
Email: p.gauthier@cranfield.ac.uk

Parash Agarwal†,
Jonathan McClure, Vishal Sethi
Centre of Propulsion Engineering
Cranfield University
Cranfield, Bedfordshire MK430AL, UK
Email: p.agarwal@cranfield.ac.uk,
mcclure@td.mw.tum.de,
v.sethi@cranfield.ac.uk

ABSTRACT

Being free from carbon content, hydrogen has been considered as a promising candidate to reduce pollutant emissions in Gas Turbine Combustion Systems. Due to hydrogen's significantly different burning characteristics, its implementation requires adjustments to the design philosophies of traditional combustion chambers. The micromix concept offers an alternative diffusive combustion injection system, improving the mixing characteristics without the risk associated with pre-mixing, thereby reducing the likelihood of hotspots forming.

The importance of turbulence-chemistry interaction modelling, particularly for highly diffusive flames such as hydrogen, has been widely addressed. A turbulence-chemistry interaction study on such a micromix injector was performed investigating the coupling between the Flamelet Generated Manifold (FGM) combustion model and different hydrogen reaction mechanisms. This methodology correctly reproduces the typical micromix micro-flame behaviour and the analysed mechanisms are shown to be in good agreement in terms of flow characteristics prediction.

A comparative study between two reduced order emissions prediction models was then carried out: a CFD post-processing technique for NO_x emissions calculations and a hybrid CFD-CRN approach were explored. Due to the coupling between accurate turbulence-chemistry interaction modelling and the ability to handle detailed chemistry, the hybrid CFD-CRN approach gives valuable results with a modest computational cost and it could be used as an optimising tool during the injector geometry design process.

NOMENCLATURE

CFD Computational Fluid Dynamics
CO Carbon monoxide
CRN Chemical Reactor Networks
FGM Flamelet Generated Manifold
H_2 Hydrogen molecule
LES Large Eddy Simulation
NO_x Nitrogen oxides
OH Hydroxyl
PDF Probability Density Function
RANS Reynolds-Averaged Navier-Stokes equations
SO_x Sulphur oxides
TRL Technology Readiness Level

*Also a Senior Key Combustor Expert at Siemens Energy, Dorval, QC, H9P1A5, Canada.

†Address all correspondence to this author.

1 INTRODUCTION

Flightpath 2050 very ambitiously targets the substantial reduction of emissions impact with a 75% reduction in CO_2 and 90% reduction in NO_x relative to year 2000 technologies [1]. These targets will be extremely challenging to meet with carbon containing fuels, despite large research efforts on advanced, and in many cases disruptive, airframe and propulsion technologies, even when coupled with improved asset and life cycle management procedures [2].

Therefore, alternative fuels are a major field of investigation. Despite the negative public perception, hydrogen is a promising candidate being the most abundant element in the universe and free of carbon and other impurities. However, there are a number of key challenges which must be addressed, including the cost of infrastructure development and the economic sustainability.

Hydrogen combustion will yield zero carbon or SO_x emissions and has the potential of yielding ultra-low NO_x. One of the challenges associated with facilitating lean combustion, i.e. reducing flame temperatures to reduce NO_x emissions, is the relatively narrow stability band of natural gas or other hydrocarbon fuels, which can result in lean blow-out and combustion instabilities. Combustion systems that are highly optimized to reduce emissions are much more likely to suffer from thermoacoustic oscillations. H_2 as a fuel is more attractive in this respect as it has wider stability limits.

Customising fuel flow in individual injectors (fuel staging) for low emissions is by no means a novel technology for liquid fuelled aero-engine combustors. Combustor concepts such as the CFM56-DAC (Double Annular Combustor) and the GE TAPS (Twin Annular Premixing Swirler) have already reached TRL9 [3]. Advanced, staged, lean direct injection conceptual combustors such as the SAFRAN MSFI (Multiple Staged Fuel Injectors) have reached TRL4 [4]. However, such concepts are limited to liquid fuels only.

Micromixing offers miniaturised diffusive combustion which improves the mixing characteristics (without the risks associated with pre-mixing) relative to lean direct injection systems, thereby reducing the presence of high temperature, stoichiometric, combustion zones.

A large number of analytical and experimental studies on hydrogen micromix combustors for industrial gas turbines have been performed by RWTH Aachen [5]. Their work mainly focused on single-injector and a four injector-array to analyse NO_x emissions, flow fields and flame structure as a function of varying geometrical parameters via a combination of experimental and numerical (RANS CFD) research and development. However, these RANS simulations tend to under-predict NO_x production as a result of the averaging algorithm it uses thereby under predicting the presence of the local hot spots.

Preliminary studies at Cranfield University have shown that hydrogen micromix combustors can offer several extra benefits that extend beyond NO_x reduction [6–13]. These show that it may be possible to eliminate the dilution zone altogether and better control the combustor outlet radial and circumferential temperature profiles, by customising the fuel distribution between multiple injectors. This will yield benefits for turbine life and performance and result in a shorter combustor. Customising the fuel scheduling via micromixing is also expected to reduce combustor thermoacoustic problems.

To this end, Computational Fluid Dynamic (CFD) has been largely used as a standard predicting tool to explore the combustion design space.

An understanding of the influences of fluid dynamics on the flame development is of crucial importance for the design of new combustion technologies. Particularly, the role of turbulence has a major impact on the flame shape, wrinkling and stretching the flame surface and thus increasing the extent of diffusive mixing between the burned and unburned mixture. Simultaneously, the heat released during the combustion process and the changes in kinematic viscosity, with associated temperature variations, modify the turbulence field. This turbulence-chemistry interaction results in an acceleration of the flow through the flame front and its modelling is one of the most challenging aspects of combustion CFD today, especially for highly diffusive flames such as hydrogen.

The first part of this paper presents an assessment of the predictive capability of state of the art CFD models (Section 2). A turbulence-chemistry interaction study on a micromix injector was performed addressing the coupling between the FGM combustion model and different hydrogen combustion mechanisms.

Whilst CFD codes provide valuable assistance in resolving complex flow fields, they are still not capable of an accurate prediction of pollutant emissions. A valid assessment of pollutant emissions requires the use of detailed chemical reaction mechanisms which would lead to very high computational costs. Therefore, given the finite availability of computational resources, the flow field resolution usually has priority over detailed chemistry fidelity and the combustion reaction mechanism is therefore reduced to a few species and fundamental reactions.

As pollutant emissions assessment is important during the design process, new methodologies for a rapid and reliable estimation have been developed. A possible approach would be to couple CFD with Chemical Reactor Networks (CRN). This approach has the potential of delivering high fidelity solutions of the flow field (from the CFD simulations) coupled with high fidelity chemistry analysis using the CRN method.

The second part of this paper assesses the predictive capability of two lower order models for emissions prediction (Section 3). The resulting NO_x emissions levels were compared against experimental measurements performed at Aachen University [14].

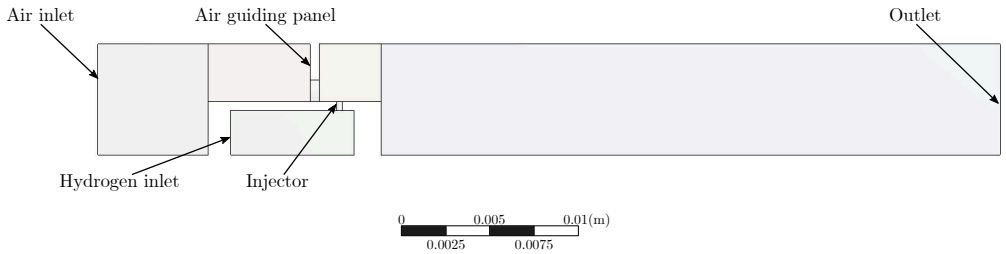

FIGURE 1. MICROMIX INJECTOR GEOMETRY MODEL

TABLE 1. INVESTIGATED HYDROGEN-AIR REACTION MECHANISMS

Author	Number of species	Number of reactions
Kéromnès [15]	12	33
ÓConaire [16]	10	21
Konnov [17]	10	33
Naik [18]	12	105

The aim is to find a CFD modelling approach with improved chemistry interaction, coupled with an emission tool that can provide a good compromise for rapid design space exploration without compromising significantly the accuracy of the simulations and allow the assessment of performance and emissions at preliminary stages of the design process.

2 TURBULENCE-CHEMISTRY INTERACTION STUDY

First, a selection process was undertaken to choose the reaction mechanisms that could accurately represent hydrogen/air kinetics over a range of operating conditions, especially at high pressures conditions (15-45 atm) present in typical gas turbine combustors.

Taking into consideration their level of validation as well as their frequency referrences [19], four hydrogen reaction mechanisms (Table 1) were selected and used in our comparative study.

Each one of these mechanisms was put into a Chemkin format file to be imported into the commercial CFD software ANSYS Fluent [18]. RANS simulations, of a simplified injector design, were performed taking advantage of its symmetric design to reduce computational expenses (Fig. 1). Therefore, only half of the real injector was modelled and simulated with symmetric boundaries.

The computational model used in this study is based on previous work carried out at Cranfield University where the

TABLE 2. BOUNDARY CONDITIONS SETTINGS

Boundary	Specification
Air inlet	Temperature 560 K Mass Flow 1.64×10^{-5} kg/s
H_2 inlet	Temperature 300 K Mass Flow 2.07×10^{-7} kg/s
Operating Conditions	Pressure 101325 Pa

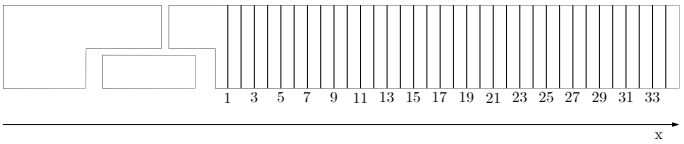

FIGURE 2. PLANES DISTRIBUTION ALONG THE DOMAIN FOR PROPERTIES EVALUATION

injector jeometry was investigated through two dimensional and three dimensional CFD simulations [20]. This gemetry derives directly from the injector configuration developped by Aachen University, where the computational model was validated experimentally [21].

A hexahedral mesh consisting of about 920,000 computational cells was created with a refinement in critical regions, such as the ducts where air and fuel are injected and the flame region. More details relative to the mesh sensitivity study on the same geometry can be found in [20].

The $k-\omega$ SST model was selected as the turbulence model for all the simulations. The turbulence-chemistry interaction approach selected was the Flamelet Generated Manifold (FGM) model [22, 23]. This approach interprets a multi-dimensional turbulent flame as an ensemble of distinct steady laminar flames called flamelets. It offers the possibility of notably reducing the computational cost by pre-processing and tabulating the

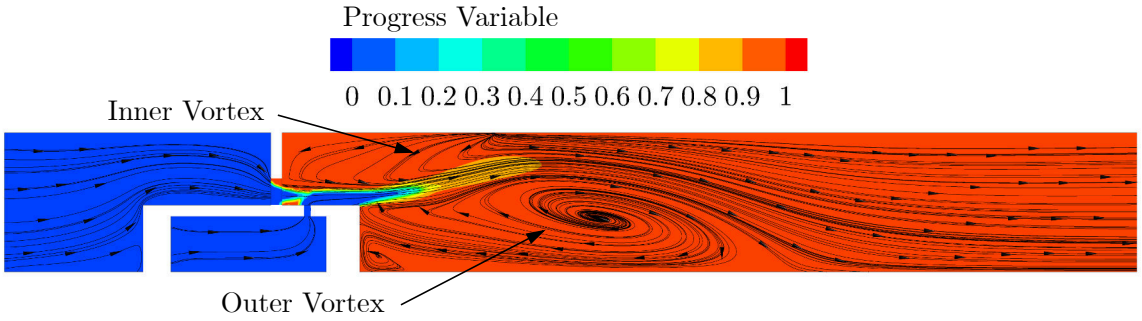

FIGURE 3. STREAMLINES OF VELOCITY AT THE SYMMETRY PLANE

chemistry, and statistically integrating the chemical kinetics effect into the flow calculations. Employing this approach, the chemistry is tabulated parametrically using mixture mass fractions and scalar dissipations, which are then stored in look-up tables. During CFD simulations, differential equations are solved for the controlling variables and the required thermochemical values are retrieved by interpolation from the stored FGM table. However, this model is taking advantage of the assumption of relatively fast chemistry, so it is not able to capture strong non-equilibrium effects such as ignition, extinction and slow chemistry like NO_x formation [18].

Considering the knowledge acquired during previous studies at Cranfield University [10, 11, 20], a Prandtl number of 0.85 and a Schmidt number of 0.5 were chosen for this work.

In order to correlate the time-averaged values of the fluctuations of the turbulent flow and the instantaneous properties captured through the flamelet model, the Probability Density Function approach (PDF) is employed to capture the turbulence-chemistry interaction. Through this model time-averaged values of mixture fractions, temperature and density can be calculated and stored in a look-up table [18].

During the comparison, the modelling approach and the boundary conditions (Table 2) were kept constant for the analysis of the reaction mechanisms. An arbitrary equivalence ratio of 0.43 was chosen for this first part of the study.

2.1 Results

In order to analyse and compare the temperature distributions and flame shape predictions, 34 planes were created across the injector domain together with a symmetry plane that cuts longitudinally the geometry (Fig. 2). On each plane, mass weighted averaged static temperatures and hydroxyl mole fractions were calculated to capture the flame shapes and positions.

Aerodynamic characteristics In Figure 3 streamlines of velocity are displayed on a contour showing the reaction progress variable on the symmetry plane. The two main

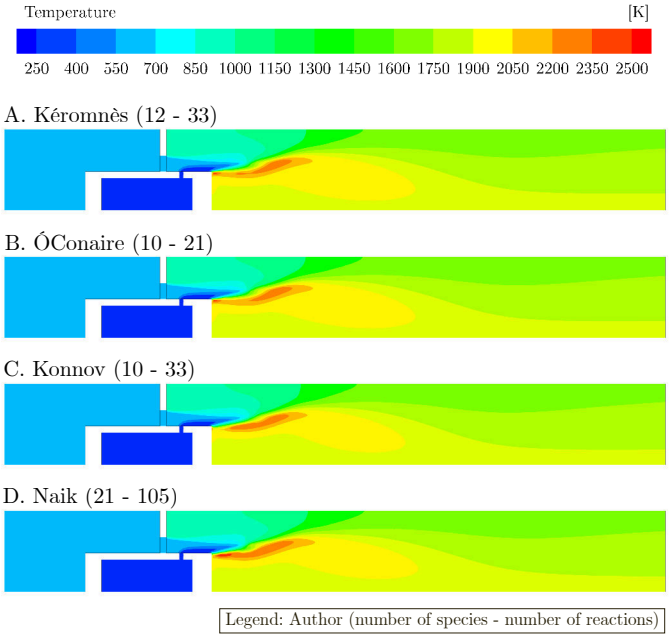

FIGURE 4. TEMPERATURE CONTOUR AT THE SYMMETRY PLANE

recirculation zones, which are characteristic of the micromix jet-into-cross-flow injection feature [21], are correctly captured. The inner vortex comes from the recirculation of colder air from the air stream inlet, whereas the outer vortex arises from the hot gas recirculating downstream the hydrogen injection. These vortices are fundamental for the flame anchoring and are responsible for the preservation of the flame shape and position. The shear layer arising from the vortex interaction is stabilizing the reaction zone and giving a structure and shape to the flame.

The vortex interaction intensifies the mixing process and leads to the development of micro flames, which allow for a lower residence time of the NO_x forming reactants and consequently a reduced NO_x averaged molar concentration.

However, recirculation zones are generally associated with pressure losses. Therefore, an optimisation process should

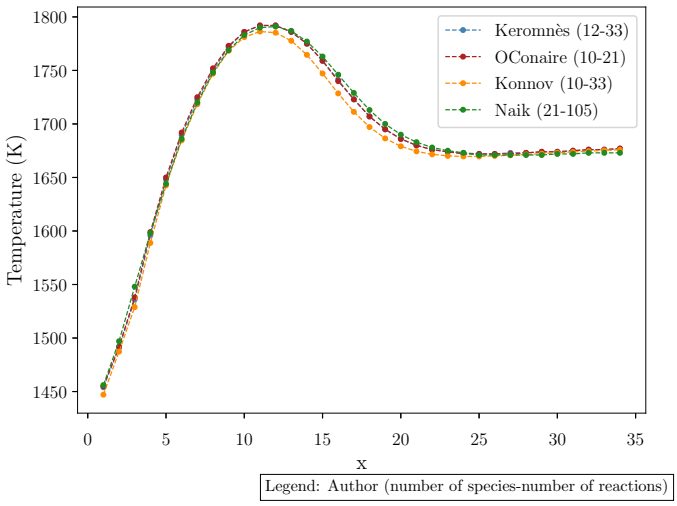

FIGURE 5. AREA AVERAGED STATIC TEMPERATURE ALONG THE DOMAIN FOR THE ANALYSED MECHANISMS

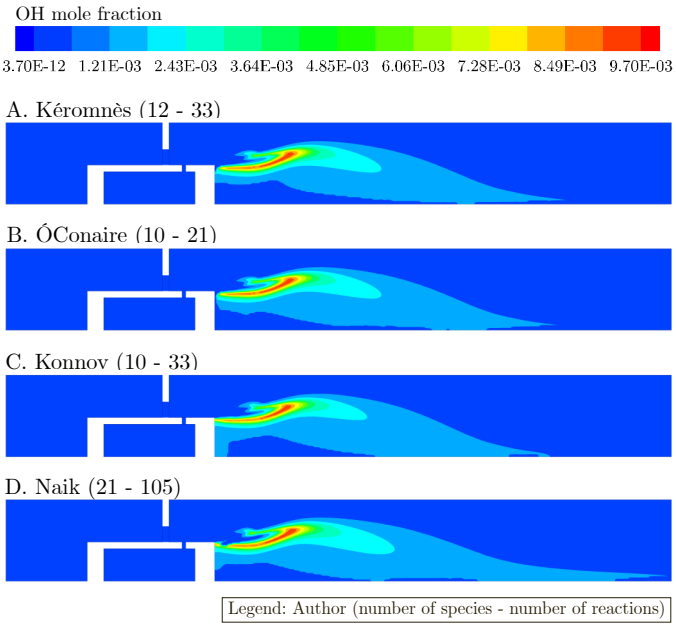

FIGURE 6. OH MOLE FRACTION CONTOUR AT THE SYMMETRY PLANE

be performed to achieve enough recirculation for the shear to constrain the flame shape with minimal pressure drop.

Temperature comparison The proposed simulation settings are able to create the flame shapes characteristic of the micromix concept. In Figure 4, the temperature contours along the symmetry plane are displayed for the mechanisms being considered.

Overall the different reaction mechanisms are all in good agreement for the temperature field predictions, as well as for the peak temperatures, which reaches around 2400K.

The hottest region predicted by Konnov mechanism (Fig. 4 C) is slightly smaller compared to the other ones. This discrepancy also results in a shorter flame region. On the contrary, the more detailed mechanism by Naik (Fig. 4 D) estimates higher temperatures especially in the region close to the injector wall. However, care should be taken when analysing near wall regions considering that walls were modelled as adiabatic surfaces. Hence, no heat transfer between the flow and the surroundings is considered.

Considering that all the other parameter were kept constant for the comparison, an explanation of the discrepancies could be found in the reaction mechanisms development. Reaction mechanisms are usually generated for a range of temperature and pressure conditions. They are often derived and validated through experiments, therefore reactions and reaction coefficients have an inherent degree of uncertainty.

In order to provide an overview of the overall temperature field development, the mass averaged static temperature was evaluated across the planes created along the length of the domain (Fig. 5). The temperature plot highlights the lower temperature resulting from Konnov mechanism in the central region of the injector domain. This is a reflection of the lower flame temperature prediction and the shorter flame shape previously shown in Fig. 4. A lower peak temperature in the flame zone also results in a slightly lower temperature in the post-flame region.

A limitation on the temperature predictions comes from the use of symmetric boundary conditions and the fact that only one injector is modelled. The injector-injector interactions are therefore not captured, making it difficult to estimate the true maximum temperatures and flame zones that would be achieved in such an injection system.

Overall, the analysed mechanisms are all in good agreement in terms of temperature field prediction, both qualitatively (trends) and quantitatively (absolute values).

OH mole fraction comparison The flame front position is captured by means of hydroxyl values, which are widely employed as a flame marker [24].

Hydroxyl mole fraction contours are showed at the symmetry plane in Fig. 6. From these figures it can be seen that, reasonable agreement is observed between the different chemistry mechanisms. The higher values of hydroxyl mole concentrations are correctly constrained in the region of higher heat release. Only with the last mechanism (Fig. 6 D), a slightly higher hydroxyl mole concentration appears at the end of the injector suggesting a longer reaction zone.

As for the temperature, some discrepancies arise near the

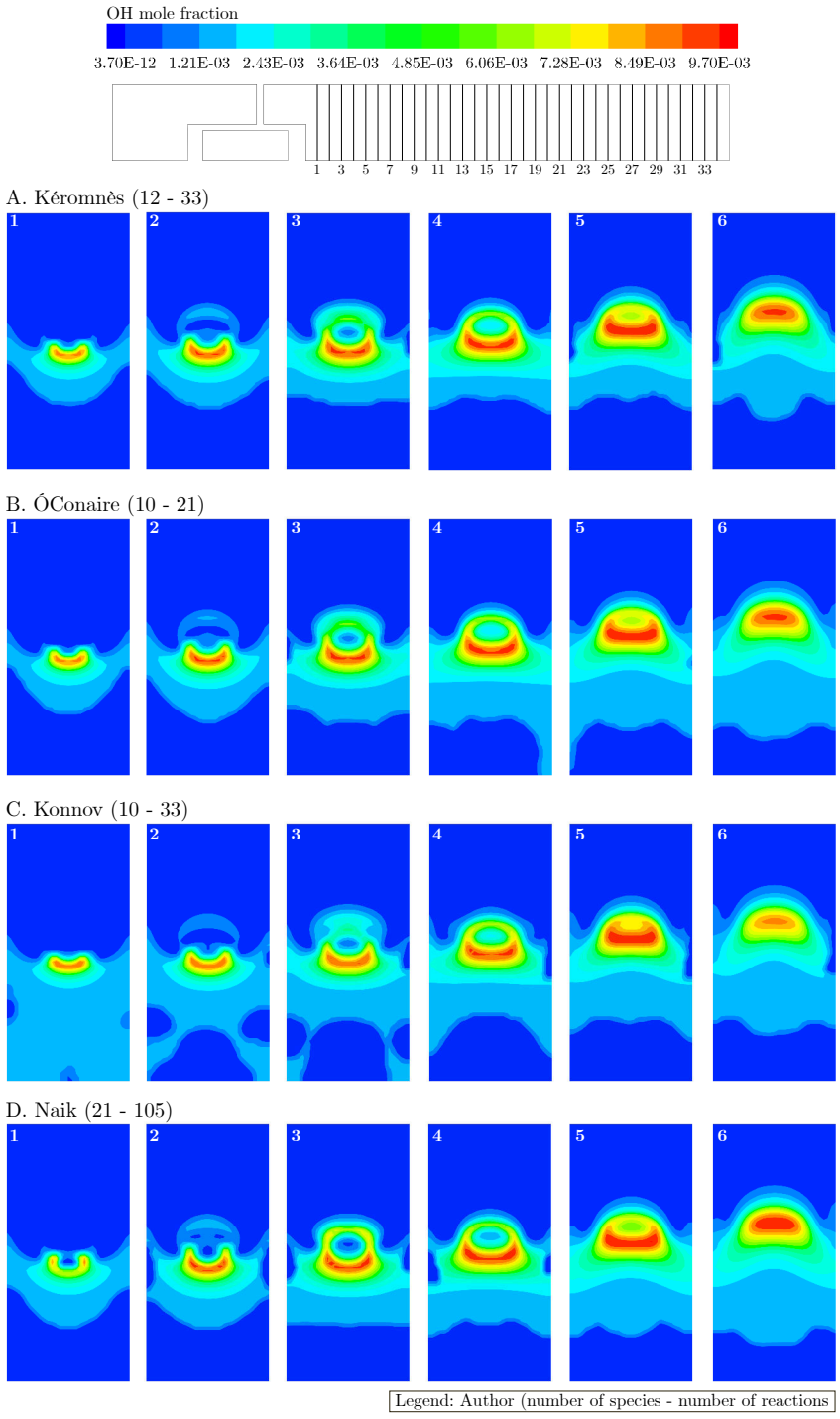

FIGURE 7. OH MOLE FRACTION CONTOUR AT DIFFERENT PLANES ALONG THE DOMAIN IN THE FLAME REGION

injection site walls, most likely due to the imposition of adiabatic wall boundary conditions during the simulation process.

In Figure 7, the hydroxyl mole concentrations are displayed at different planes in the flame region. Starting from plane 2, a typical phenomenon arising from the cross-flow injection characteristics can be noticed. As a result of the impulse of the jet on the crossflow [25], a counter-rotating vortex pair is formed to enhance the mixing between fuel and air. Its formation begins around the first plane and it is responsible for the horseshoe shape distribution of the hydroxyl that can be mainly noticed in plane 2 and 3. From plane 4 onwards, the effect of the pair vortex is vanishing and the hydroxyl distribution is more homogeneous.

3 EMISSIONS ASSESSMENT

The results of the initial reaction mechanisms comparative study were employed to carry out a NO_x emissions assessment where two different emissions prediction tools were investigated. The first is a post-processing technique applied directly to the CFD simulations performed in the first part of the analysis; whereas the second approach used the Reactor Network model found in ANSYS Fluent coupled with a detailed hydrogen/air reaction mechanism developed at Eindhoven University of Technology [26]. Both methodologies were tested for different mixture equivalence ratios keeping the fuel mass flow constant.

The resulting NO_x emissions values were then compared with the experimental measurements performed at Aachen University [14]. In the experimental campaign, each data point was determined as the arithmetic mean of the measured values within the measuring window. More details about the experimental campaign can be found in [14, 27].

Considering that the experimental measurements are obtained as an average along the measuring window, it is expected that the inclusion, in this average, of the regions at the edge of the injector domain in the NO_x assessment would not significantly affect the results. Hence, when compared against the present work, a closer relative-fit to the experimental values will be judged as positive result in the discussion sections.

For both methodologies the NO_x values are calculated as a weighted average along the outlet plane and then a correction for the dry basis is applied ($15\%O_2$).

3.1 CFD approach

As previously discussed, the FGM modelling approach adopted for the turbulence-chemistry interaction study assumes fast chemistry. Therefore, this model is not suitable for capturing complex non-equilibrium effects such as the slow chemistry involved in NO_x formation. Under the majority of circumstances, only NO_x trends can be correctly predicted whereas quantitative predictions are not as reliable. Such investigations are still quite useful and may be used to narrow down, or guide, the number of experimental testing required for the certification of engine emissions.

A decoupled approach for NO_x calculations was used for this case study. That is, for each of the reaction mechanisms investigated, the solutions obtained from a reacting flow simulation was frozen and used as a starting point for the NO_x calculations. In this approach, a simple Zeldovich NO_x mechanism is used [28]:

$$O_2 \rightleftharpoons 2O \tag{1}$$

$$N_2 + O \rightleftharpoons NO + N \tag{2}$$

$$N + O_2 \rightleftharpoons NO + O \tag{3}$$

$$N + OH \rightleftharpoons NO + H \tag{4}$$

Concentrations of O_2, N_2, O, OH and H are therefore necessary for the solution to be calculated. However, the chemistry involved in thermal NO_x formation happens at much slower rates compared to the high energy-releasing reactions. Therefore, this approach assumes that NO_x formation reactions can be decoupled from the combustion process [29]. The Zeldovich mechanism is then solved using the frozen temperature, velocity fields and species concentrations obtained from the converged CFD simulations.

As stated in Section 2, the mechanism by Konnov results in different flow prediction compared to the other analysed mechanisms, in particular the shorter flame and lower temperature prediction has led to the decision to not further analyse this mechanism from an emissions point of view as it would lower the NO_x emissions prediction. Therefore the CFD approach for emissions prediction was only applied to the Kéromnès, ÓConaire and Naik mechanisms.

In Figure 8, the amount of calculated NO_x, for the investigated range of equivalence ratios, are plotted together with the average temperature measured at the exit of the domain.

Due to uncertainties regarding the measurement area in the experimental research, a sensitivity analysis on the simulation measurement locations was carried out. Three concentric rectangular areas were used to assess the influence of wall interaction on the emissions prediction. However, as a result of the NO_x emissions distribution across the outlet plane, no significant changes in the area averaged NO_x values were detected. Indeed, along the outlet plane, NO_x amounts increase from the upper part of the domain to the lower one. Hence, limiting the measurement zone to a smaller central region does not impact the averaged values.

Even though the discrepancies between calculated and measured NO_x emissions are fairly reasonable, it was found that the CFD approach has underestimated the amount of NO_x emissions for the majority of the cases.

For the lower equivalence ratios, the Naik detailed mechanism does not correctly represent the trend of emissions.

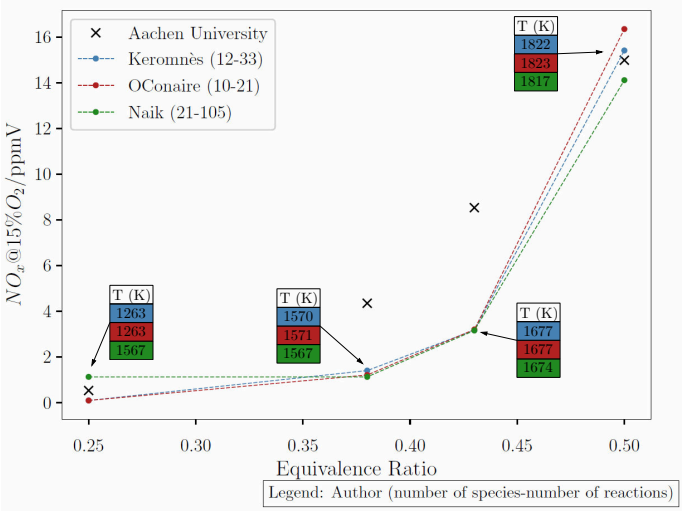

FIGURE 8. CORRECTED NO_x EMISSIONS AND CORRESPONDENT AREA AVERAGE TEMPERATURES PLOTTED AGAINST THE EQUIVALENCE RATIO

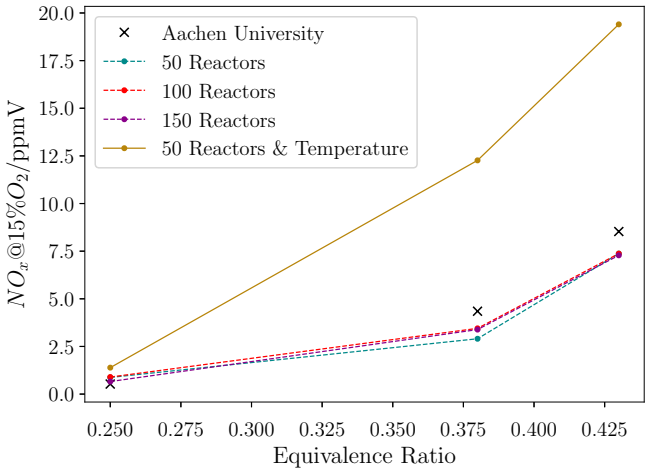

FIGURE 9. CORRECTED NO_x EMISSIONS AS A FUNCTION OF THE EQUIVALENCE RATIO. THE TEMPERATURE VALUES ARE RETRIEVED FROM CFD (DASHED LINES) OR CALCULATED BY THE REACTOR NETWORK (SOLID LINE)

Indeed, increasing the equivalence ratio from 0.25 to 0.38 the amount of NO_x remains constant instead of presenting the expected incremental growth. This is also reflected in a higher temperature measured at the injector outlet.

Looking at mid-range equivalence ratios, the different mechanisms have similar behaviours, representing a proper trend. Despite some differences in the temperature predictions, the NO_x values are consistent. A higher outlet temperature is not always directly linked to higher NO_x emissions at the same equivalence ratio.

As for the highest equivalence ratio, all the three mechanisms represent the measured trend. However, Kéromnès mechanism predicts higher NOx emissions compared to the ÓConaire and Naik mechanisms, which is the lowest one. Once again the temperatures arising from the different mechanisms are similar, but more pronounced differences in terms of emissions values are displayed.

As stated before, nothing can be said in terms of absolute values since the assessment is based on weighted average values along the outlet plane.

3.2 Hybrid CFD-CRN approach

The second methodology used is another hybrid approach that consists of the use of CFD in conjunction with Chemical Reactor Networks (CRN) and it is based on three main steps:

1. The reactive flow field is predicted through CFD simulations

2. The CFD results are then used as a starting point and post processed. A set of criteria is used to split the combustor domain in physically and chemically homogeneous regions

3. The cells of the domain that satisfy the same criteria are clustered together to form reactors in the reactor network. The reactors are then linked together computing the mass fluxes between zones. Finally, the reactor network is solved using a detailed reaction mechanism to achieve a precise emissions prediction

The reactor network is therefore constructed from a converged Fluent simulation and the volume is automatically split into a certain number of reactors specified by the user.

This procedure of clustering reactors is performed by the software and is done considering temperature and mixture fraction distribution resulting from the CFD simulations. Additional user-specified parameters, such as the turbulent kinetic energy or dimensional coordinates, can be applied to further refine this clustering [18]. A more detailed chemistry file than the ones used for the flow computations can be imported. This is one of the main advantages of this hybrid method since it decouples flow calculations from emissions calculations. For the present work, the detailed hydrogen reaction mechanism developed at Eindhoven University, which involves 32 species and 237 reactions, was employed [26].

The mass fluxes between reactors are computed directly from the CFD simulations and the energy equation is not solved, whereas the temperature of each reactor can be either fixed or calculated. In the first case, temperature values are retrieved from the CFD solutions. Using the temperature calculation option, temperatures are estimated from the pressure field available from

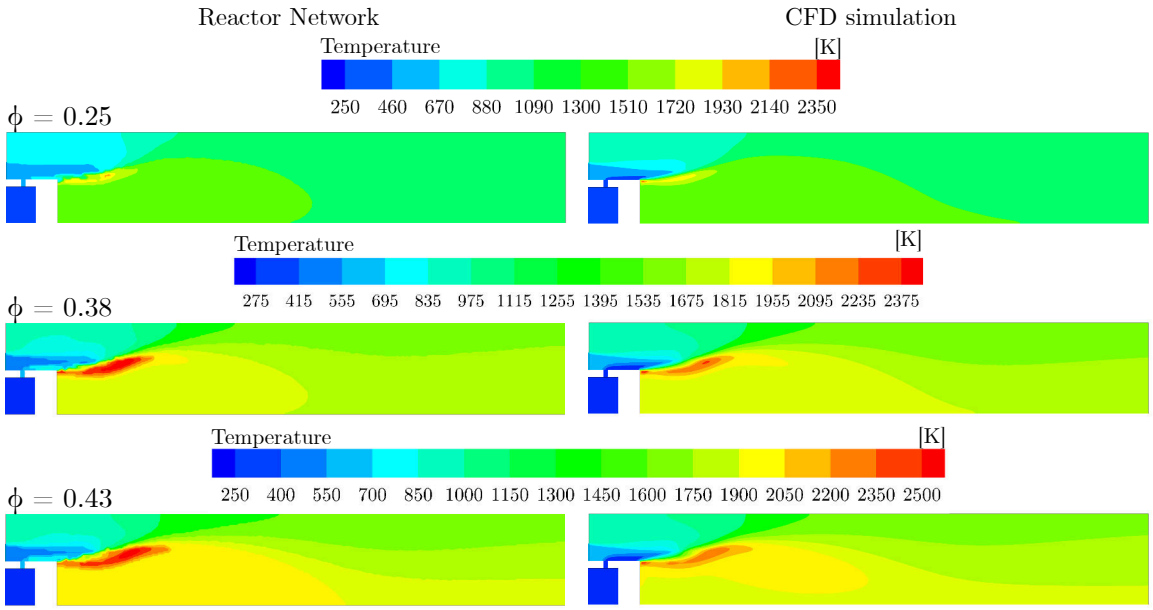

FIGURE 10. CONTOUR OF TEMPERATURE FOR THE TEMPERATURE OPTION OF THE REACTOR NETWORK COMPARED WITH THE CFD TEMPERATURE PREDICTION

the CFD simulations by solving an equation of state.

However, the user cannot specify the type of reactor and each identified zone is represented by a perfectly stirred reactor. This is a primary limitation of the reactor network solver, as for most pollutant the typical residence times in aero-engines combustors are usually much shorter than the time necessary to reach the chemical equilibrium. This could result in an over-prediction of pollutant amount and in an inappropriate modelling of some regions, such as recirculation and post-flame zones.

For this case study, each mixture equivalence ratio was tested with an increasing number of reactors and the detailed reaction mechanism developed by Goswami [26] was employed. As discussed in Section 2, the different reaction mechanisms used for the CFD simulations all have a good agreement in terms of flow property predictions. Hence, the chosen CFD results to be used for the reactor network creation will not have a great impact on the final emissions prediction. The solutions obtained with the Kéromnès [15] mechanism were chosen for this section.

As it was previously done for the CFD approach, the NO_x mole fractions were calculated as an average along the outlet to the domain. A sensitivity analysis on the locations where the simulation measurements are taken was performed. As discussed in the previous section, no considerable changes are encountered in the averaged values due to the NO_x emissions being well distributed across the outlet of the computational domain.

The number of reactors was increased from 50, which is the recommended starting value in the ANSYS User Guide [18], to 100 and then to 150 reactors. In addition, one calculation was performed by activating only the temperature equation with 50 reactors.

In Figure 9, the NO_x values corrected to $15\%O_2$ are plotted against the equivalence ratios for the different options of the CRN tool. The emissions curve trend is correctly reproduced by all options, while the calculated points get closer to the experimental values when increasing the number of reactors, as expected. The recirculation zones become better covered by the reactor network when increasing the number of reactors: the injector domain is split into smaller and smaller volumes, therefore smaller scale phenomena can be leading to improved capturing of the slow chemistry effects involved in NO_x formation. However, the activation of the temperature option brings the emissions to much higher values. The trend is once again correctly reproduced, but solving the state equation instead of retrieving the temperature values from the CFD solution leads to an overestimation of the temperature field and therefore to higher NO_x emissions (Fig. 10).

4 LIMITATIONS

The aim of the comparative study performed in the present work is not a validation, but a primary investigation of the employed models. The limitations due to the assumptions made through the modelling approaches are stated throughout the paper. A brief summary of the limitations related to each section is provided in below.

Combustion modelling

Hydrogen is a fast burning molecule, highly reactive and diffusive. Therefore, the modelling of hydrogen combustion behaviour is extremely challenging.

The general assumption of homogeneous diffusion of all species is not suitable considering hydrogen's fast burning and diffusion characteristics.

The flamelet model's primary assumption is that of infinitely fast chemistry, therefore the flamelets are assumed to have an instantaneous response to the aerodynamic strain. This approach is not well suited for capturing non-equilibrium effects, so the resulting NO_x emissions predictions are not reliable in terms of absolute values [30].

The predicted constant flame temperature results from the fast chemistry assumption and the unity Lewis number assumption. The Lewis number has a major role in the characterisation of the transport process and it affects the propagation, stability and extinction characteristics of laminar flames

The diffusion resulting from a non-unity Lewis number has a significant impact on flame temperature prediction, especially for low molecular weight species such as hydrogen and turbulent flow conditions. Due to the diffusion process, local fuel enrichment leads to the formation of localised hotspots where the flame is burning more intensely [31, 32].

In addition, RANS simulations solve balance equations for mean values only. As a consequence, the use of RANS may result in the over-prediction of the temperature field: larger and hotter regions are predicted affecting both species formation and emissions calculation.

The applied boundary conditions also influence the solution. The adiabatic wall assumption imposes a higher near wall temperature than for a cooled liner wall; and the symmetric boundary condition set for the upper zone of the domain does not correctly replicate the injector-injector interaction. It is then difficult to state a correct value for the maximum temperature and to establish a realistic reaction length with these simplified models.

Reactor network

The reactor network layout is customised from the CFD simulation; hence all the assumptions made during the computational modelling step will also affect the reactor network measurements.

The reactor network developed through ANSYS Fluent is entirely composed of perfectly stirred reactors [18]. This represents a limitation in capturing combustion behaviours such as regions of non homogeneous fuel-air mixing and post flame zones. For these regions, partially stirred reactors or plug flow reactors could be used to better replicate the real phenomenon [33].

In a perfectly stirred reactor, the mixing to the molecular scale is assumed to occur instantaneously compared to chemical reactions. This model is therefore particularly suitable for modelling the primary zone of the combustor, which involves large recirculation regions and high turulence levels [34].

5 CONCLUSIONS

The chosen computational models are able to capture the complex interactions between air and fuel, well representing the typical cross flow injection characteristics. Indeed, the two recirculation zones responsible for the flame anchoring and stabilization are correctly reproduced together with the counter-rotating vortices accountable for the horseshoe shape of OH distribution of Fig. 7.

From the comparison of the results of the investigated mechanisms, small variations are observed in terms of temperature and OH species predictions. All the analysed mechanisms are found to be consistent, apart from Konnov mechanism which leads to lower temperature and therefore to a different OH distribution.

In an attempt to further reduce NO_x emissions, the mechanisms predictive capability should be further investigated for leaner mixtures.

Following an in-depth comparison of the performance of the mechanisms in the first section, different equivalence ratios were tested to highlight any discrepancies in terms of averaged outlet temperature and NO_x emissions.

In terms of emissions trends, both methodologies are able to capture NO_x emissions trends throughout the analysed range of equivalence ratios. Regarding absolute quantitative predictions, the calculation of NO_x through the CFD approach in known to result in a poor performance. Although it has lead to results within a reasonable error range for this work, a closer prediction of NO_x is obtained with the hybrid approach through the reactor network option of Ansys Fluent. Given the fact that a greater number of reactors has not led to a significant benefit in terms of emissions predictions, although this increased the computational expense, 50 reactors are considered as a sufficient number to represent this present case study. In the future, the possibility of a further reduction in the reactors number could be investigated.

Higher fidelity tools for emissions prediction such as ANSYS Chemkin Pro [33] would surely provide a more accurate estimate of pollutant. However, the process to construct a reactor network is rarely performed during the design exploration of a new technology due to the considerable time required to refine the model. With the change in geometrical parameters and therefore flow distribution, the reactor network has to be adjusted and redesigned to correctly reproduce the combustion process.

To this end, the Fluent reactor network option reproduces correctly the trend of NO_x formation and provides an acceptable

estimation of absolute values while being a rapid tool for emissions calculation.

From the results, it can be noticed that the actual geometry creates a large recirculation zone responsible for enhancing NO_x production. The reactor network model assessed in this work can help identify the geometrical parameters driving pollutant formation. It can be a valuable tool to quickly assess the influence of the variation of geometrical parameters, such as the air inlet height, on NO_x formation. Being a lower order model, Fluent reactor network model can be applied for preliminary investigations whereas for advanced research the adoption of dedicated emissions prediction tools is required.

In the later design stages, LES simulations should be used to obtain more accurate temperatures and flow fields. This would increase the fidelity of the CRN creation and results.

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REFERENCES

[1] Darecki, M., Edelstenne, C., Enders, T., Fernandez, E., Hartman, P., Herteman, J.-P., Kerkloh, M., King, I., Ky, P., Mathieu, M., Orsi, G., Schotman, G., Smith, C., and Wörner, J.-D., 2011. Flightpath 2050 Europe's Vision for Aviation. Tech. rep.

[2] International Civil Aviation Organization (ICAO), 2016. ICAO Environmental Report. Tech. rep.

[3] Liu, Y., Sun, X., Sethi, V., Nalianda, D., Li, Y. G., and Wang, L., 2017. "Review of modern low emissions combustion technologies for aero gas turbine engines". *Prog. Aerosp. Sci.,* ***94***(July), pp. 12–45.

[4] Tantot, N., Von der Bank, R., Bourgeois, S., Donnerhack, S., Lundblath, A., Peschiulli, A., Basset, E., Guin, C., Hassa, C., and C. Gebel, G., 2016. "LEMCOTEC : a key project to tackle pollutant emissions by developing new core technologies". In Greener Aviat. 2016.

[5] Ayed, A. H., Striegan, C. J. D., Kusterer, K., Funke, H. H.-W., Kazari, M., Horikawa, A., and Okada, K., 2017. "Automated Design Space Exploration of the Hydrogen Fuelled Micromix Combustor Technology". *Glob. Power Propuls. Soc.,* ***141***, pp. 1–8.

[6] Murthy, P., 2011. "Numerical Study of Hydrogen Micromix Combustors for Aero Gas Turbine Engines". Msc thesis, Cranfield University.

[7] Karakurt, A., 2013. "Parametric Investigation of Combustion Characteristics of a Hydrogen Micromix Combustor Concept". Msc thesis, Cranfield University.

[8] Asanitthong, S., 2014. "Outlet Temperature Distribution Control and Heat Transfer Calculation for a Hydrogen Micromix Combustor". Msc thesis, Cranfield University.

[9] Degroote, A. J., 2014. "Assessment of the Feasibility of Controlling the Outlet Temperature Distribution of a Novel Micromix Combustor". Msc thesis, Cranfield University.

[10] Petit de Bantel, M., 2014. "Comparison Study of Combustion Models for a Conceptual Hydrogen Micromix Combustor". Msc thesis, Cranfield University.

[11] Sabin, R., 2016. "Comparative Perfromance Study of CFD Species Models For Hydrogen Micromix Combustion". Msc thesis, Cranfield University.

[12] Babazzi, G., 2018. "Turbulence-Chemistry Interaction Study for a Hydrogen Micromix Combustion System". Msc thesis, Cranfield University.

[13] McClure, J., 2018. "Preliminary thermoacoustic risk assessment for H2 micromix combustion systems using CFD methods". Msc thesis, Cranfield University.

[14] Haj Ayed, A., Kusterer, K., Funke, H. H., Keinz, J., Striegan, C., and Bohn, D., 2015. "Improvement study for the dry-low-NOx hydrogen micromix combustion technology". *Propuls. Power Res.,* ***4***(3), pp. 132–140.

[15] Kéromnès, A., Metcalfe, W. K., Heufer, K. A., Donohoe, N., Das, A. K., Sung, C. J., Herzler, J., Naumann, C., Griebel, P., Mathieu, O., Krejci, M. C., Petersen, E. L., Pitz, W. J., and Curran, H. J., 2013. "An experimental and detailed chemical kinetic modeling study of hydrogen and syngas mixture oxidation at elevated pressures". *Combust. Flame,* ***160***(6), pp. 995–1011.

[16] Ó Conaire, M., Curran, H. J., Simmie, J. M., Pitz, W. J., and Westbrook, C. K., 2004. "A comprehensive modeling study of hydrogen oxidation". *Int. J. Chem. Kinet.,* ***36***(11), pp. 603–622.

[17] Konnov, A. A., 2008. "Remaining uncertainties in the kinetic mechanism of hydrogen combustion". *Combust. Flame,* ***152***(4), pp. 507–528.

[18] Ansys, 2014. *Ansys Theory Guide*, release 18 ed.

[19] Olm, C., Zsély, I. G., Pálvölgyi, R., Varga, T., Nagy, T., Curran, H. J., and Turányi, T., 2014. "Comparison of the performance of several recent hydrogen combustion mechanisms". *Combust. Flame,* ***161***(9), pp. 2219–2234.

[20] Abdallah, R. B., 2017. "NOx Micromix Hydrogen Combustion System: -Preliminary Design and Performance Assessment of Novel Injectors Using RANS and LES CFD". Msc thesis, Cranfield University.

[21] Funke, H. H.-W., Keinz, J., Kusterer, K., Haj Ayed, A., Kazari, M., Kitajima, J., Horikawa, A., and Okada, K., 2015. "Experimental and Numerical Study on Optimizing the DLN Micromix Hydrogen Combustion Principle for Industrial Gas Turbine Applications". *J. Therm. Sci. Eng. Appl.,* ***9***(June 2017), p. V04AT04A008.

[22] Gauthier, P. Q., 2017. "Comparison of Temperature

Fields and Emissions Predictions Using Both an FGM Combustion Model, With Detailed Chemistry, and a Simple Eddy Dissipation Combustion Model With Simple Global Chemistry". In Vol. 4B Combust. Fuels Emiss., ASME, p. V04BT04A068.

[23] van Oijen, J. A., Donini, A., Bastiaans, R. J., ten Thije Boonkkamp, J. H., and de Goey, L. P., 2016. "State-of-the-art in premixed combustion modeling using flamelet generated manifolds". *Prog. Energy Combust. Sci.,* ***57***, pp. 30–74.

[24] Tinaut, F. V., Reyes, M., Gimenez, B., and Pastor, J. V., 2011. "Measurements of OH and CH Chemiluminescence in Premixed Flames in a Constant Volume Combustion Bomb under Autoignition Conditions". *Energy & Fuels,* ***25***(1), jan, pp. 119–129.

[25] Fric, T. F., and Roshko, A., 1994. "Vortical structure in the wake of a transverse jet". *J. Fluid Mech.,* ***279***, pp. 1–47.

[26] Goswami, M., Volkov, E. N., Konnov, A. a., Bastiaans, R. J. M., and de Goey, L. R. H., 2008. "Updated Kinetic Mechanism for NOx Prediction and Hydrogen Combustion". pp. 1–28.

[27] Funke, H. H., Boerner, S., Keinz, J., Kusterer, K., Kroniger, D., Kitajima, J., Kazari, M., and Horikawa, A., 2012. "Numerical and Experimental Characterization of Low Nox Micromix Combustion Principle for Industrial Hydrogen Gas". *Proc. ASME Turbo Expo 2012*, pp. 1–11.

[28] Lefebvre, A. H., and Ballal, D. R., 2010. *Gas Turbine Combustion, Alternative Fuels and Emissions*, third edit ed.

[29] Liu, Y., 2018. "Development of Preliminary Design and Optimisation Methodology for Aero Engine Low Emissions Combustors". Phd thesis, Cranfield University.

[30] Ramaekers, W., 2011. "Development of flamelet generated manifolds for partially-premixed flame simulations". PhD thesis, Technische Universiteit Eindhoven.

[31] Ishizuka, S., 1982. "An experimental study on the opening of laminar diffusion flame tips". *Symp. Combust.,* ***19***(1), pp. 319–326.

[32] Katta, V. R., Goss, L. P., and Roquemore, W. M., 1994. "Effect of Nonunity Lewis Number and Finite-Rrate Chemistry on the Dynamics of a Hydrogen-Air Jet Diffusion Flame". *Combust. Flame,* ***96***(1-2), pp. 60–74.

[33] Reaction Design: San Diego, 2015. *ANSYS Chemkin Theory Manual 17.0 (15151)*.

[34] Celis, C., 2010. "Evaluation and Optimisation of Environmentally Friendly Aircraft Propulsion Systems". Phd thesis, Cranfield University.

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Babazzi, Giulia

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