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NUMERICAL INVESTIGATION INTO THE IMPACT OF OPERATING BOUNDARY CONDITIONS ON NOX FORMATION IN HYDROGEN MICROMIX COMBUSTION SYSTEM

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ABSTRACT

Hydrogen micromix combustion is a promising technology for achieving zero mission-level carbon emissions with ultra-low NOx potential. A reduced-order NOx emissions prediction model is essential for preliminary hydrogen engine cycle design space exploration and optimization studies.

Hence, this paper investigates the influence of key operating conditions, including equivalence ratio (Φ), combustor inlet temperature (T_3) and pressure (P_3) on NOx emissions in a hydrogen micromix combustion. The assessments were performed using steady Reynolds-Averaged Navier-Stokes (RANS) simulations with thermal NOx model at various power conditions representative of the aircraft mission. The RANS model constants were calibrated against Large Eddy Simulations (LES) conducted previously by the group. The comprehensive numerical database was developed from these assessments to derive a NOx emissions correlation as a function of the operating conditions defined above.

The study demonstrates that the LES-calibrated RANS models can predict NOx emissions trends, which agrees with the known physics of NOx formation. When experimental data is not yet available, the resulting correlation can be used at the preliminary stage of the design process to identify low NOx engine cycles that merit (more resource-intensive) higher fidelity numerical simulations or experiments. The methodology is flexible and extensible and may be applied to future low-emissions hydrogen combustion technologies.

Keywords: CFD; Hydrogen; Hydrogen Micromix; Momentum Flux Ratio; NOx Correlation; Low Emission.

NOMENCLATURE

BPR	Bypass Ratio
CO ₂	Carbon Dioxide
EINOx	Emission Index of NOx (g/kg)
FGM	Flamelet Generated Manifold

H ₂	Hydrogen
ISA	International Standard Atmosphere
JICF	Jet-In-Crossflows
LES	Large Eddy Simulation
MFR	Momentum Flux Ratio
NOx	Nitric Oxide emissions
OPR	Overall Pressure Ratio
P	Pressure (kPa)
SLS	Sea Level Static
T	Temperature (K)
Φ	Combustor Equivalence Ratio
$\dot{m}$	Mass flow (kg/s)
ω	Specific humidity (kgH ₂ O/kg _{air})
Subscripts	
3	Station 3 combustor inlet
4	Station 4 combustor outlet
f	Fuel
Alt	Altitude

1. INTRODUCTION

The aviation industry is under increasing pressure to reduce its environmental impact and meet ambitious emission reduction targets set by aviation agencies, government organizations, and environmental NGOs. For instance, the Advisory Council for Aerospace Research in Europe (ACARE) aims to reduce CO₂ emissions by 75% and NOx emissions by 90% relative to year 2000 technologies in its Flightpath 2050 plan [1]. Radical technological advancements in low-emission combustion technologies are required to achieve these ambitious goals. Hydrogen (H₂), a carbon-free fuel, holds great promise as an alternative to Jet A-1, as it can deliver zero mission-level CO₂ and potential ultra-low NOx emissions. Jet A-1 has relatively narrow combustion flammability limits which presents several challenges for low NOx combustion technologies. H₂ is a promising fuel as it has much wider flammability limits enabling leaner (lower flame temperature) combustion. Additionally, the molecular diffusivity and high flame speed of H₂ offer good mixing and lower residence times, therefore significant reductions in thermal NOx are possible.

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One promising technology for achieving ultra-low NO_x H₂ combustion is micromix (diffusion) combustion in a jets-in-crossflow (JICF) configuration, as envisioned by Aachen University [2]. The microinjector in this configuration miniaturizes the mixing length scale and the JICF configuration enhances mixing intensity, resulting in a large number of lean burning micromix flames. This technology improves fuel-air mixing without the risks of auto-ignition and flashback associated with premixing, reducing local high-flame temperature regions and leading to ultra-low NO_x emissions [3].

The Momentum Flux Ratio (MFR) is a dimensionless quantity that characterizes the penetration and mixing quality of the JICF micromix injector, as described by **Equation (1)**. Previous studies [4–8] have identified a complex design space of H₂ micromix combustors relative to state-of-the-art Jet A-1 combustion systems. They have shown that small changes in either injector design parameters and/or combustor operating boundary conditions may significantly impact the MFR, i.e., the flame interactions, and hence the NO_x emissions.

$$MFR = \frac{\rho_j v_j^2}{\rho_{CF} v_{CF}^2} \quad (1)$$

Where ρ_j is the density of H₂ jet in kg/m³, v_j is the velocity of H₂ jet in m/s, ρ_{CF} is the density of air crossflow in kg/m³, v_{CF} is the velocity of air crossflow in m/s.

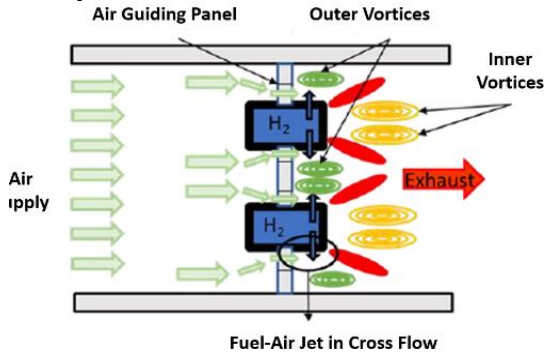


FIGURE 1: H₂ MICROMIX INJECTION IN JETS-IN-CROSSFLOW AND THE IDEAL POSITIONS OF THE FLAMES WITH RESPECT TO THE INNER AND OUTER VORTICES (ADAPTED FROM [9] WITH AUTHORIZATION).

Figure 1 shows the ideal configuration of the JICF micromix injector. The flame is located in the shear layer between the two contrarotating vortex pairs: the inner recirculating zone (IRZ) and the outer recirculation zone (ORZ). To minimise NO_x emissions, keeping flame-to-flame interaction to a minimum (with acceptable pressure loss) is critical to avoid the increased residence time of hot combustion products. Two types of radial flame-to-flame interactions observed in a JICF micromix configuration are shown in **Figure 2**. The first type of interaction (**Figure 2 (a)**) occurs when flames emerging from the same fuel feed merge downstream of the H₂ feed. This is caused by the under-penetration (relatively lower momentum flux ratio) of the H₂ jet in the crossflowing air, which results in fuel reaching the IRZ. The second type of interaction (**Figure 2 (b)**) occurs when two opposing flames

originating from adjacent fuel feeds merge due to the over-penetration (relatively higher momentum flux ratio) of the H₂ jet. This leads to H₂ penetrating into the ORZ and the flames merging downstream of the air gate between the two neighbouring H₂ feeds.

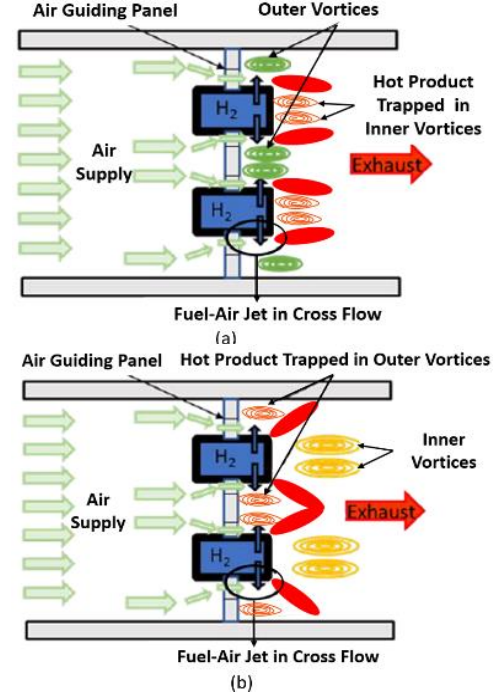


FIGURE 2: (a) FIRST TYPE OF RADIAL FLAME INTERACTIONS OCCURRING IN IRZ AND (b) SECOND TYPE OF RADIAL FLAME INTERACTIONS OCCURRING IN ORZ IN H₂ MICROMIX INJECTORS (ADAPTED FROM [9] WITH AUTHORIZATION).

Indeed, only a few experimental and numerical studies have been conducted to assess the influence of the combustor operating boundary conditions on the NO_x emissions of H₂ micromix injectors. Kroniger et al. demonstrated the influence of combustor inlet pressure P_3 as a power law function ($\text{NO}_x \sim P_3^X$) and of combustor outlet temperature T_4 as an exponential function ($\text{NO}_x \sim \exp T_4^X$) on NO_x emissions of H₂ micromix injector [10,11]. Marek et al. also demonstrated similar pressure-NO_x relation with a variation in selecting combustor inlet temperature T_3 instead of T_4 and extending the influence of other parameters such as residence time, pressure loss and equivalence ratio on NO_x emissions of H₂ micromix injectors [12]. Much of these studies were limited to small rig-scale injector arrays at low to mid-power conditions and do not represent the technology's scaling up for the future ultra-high bypass ratio (UHBR) engine combustion systems.

Hence, the aim of this research is to numerically analyze the influence of inlet boundary conditions, namely equivalence ratio (Φ), combustor inlet temperature (T_3) and pressure (P_3) on the NO_x emissions of a sector of hydrogen micromix combustor designed for the UHBR aero engine, while keeping the injector design parameters fixed. The assessments were performed using Reynolds-Averaged Navier-Stokes (RANS) CFD

simulations at different power conditions representative of a full aircraft mission. The model constants for the RANS CFD models were calibrated and verified based on best modelling practices established in previous work by Cranfield University via higher fidelity (LES) CFD and preliminary experiments [3,13]. The outcome of this analysis was then used to derive a correlation-based NO_x emissions prediction reduced order model (ROM) from higher fidelity (CFD) simulations that capture these effects. The ROM can be used at the preliminary stage of the design process, to identify low NO_x engine cycles that merit (more resource-intensive) higher fidelity numerical simulations or experiments, ultimately saving time and cost. For instance, for preliminary engine cycle design space exploration and optimisation, as well as aircraft trajectory optimisation (i.e., Techno-Economic, Environmental Risk Assessment (TERA) type studies), a reduced-order NO_x emissions prediction model is essential for which the more computationally expensive, higher-fidelity CFD models would not be suitable.

ROMs can help define engine cycle architecture and trade-offs and determine the feasibility of disruptive aircraft and propulsion technologies at the early design stage. E.g., while engines with higher overall pressure ratios and turbine inlet temperatures will have higher thermal efficiency and reduce fuel burn, they will also generate more thermal NO_x. ROMs can be employed in multi-disciplinary optimisation studies to quantify trade-offs between mission-level fuel burn and NO_x emissions. Traditionally correlation-based NO_x emissions prediction models are derived from experiments and are used to assess NO_x emissions for higher TRL concepts. However, for preliminary design studies, no experimental data is available. Therefore, the authors note that this work is unique as it developed an extensible methodology to derive and generate a correlation from RANS-based CFD simulations for preliminary design studies of a novel H₂ micromix combustion system. This work is also unique in that the NO_x emissions were assessed on a full-scale sector of the H₂ micromix combustor sized for Ultra-high Bypass Ratio (UHBR) aero engine that incorporates the preferred ultra-low NO_x H₂ micromix injector at representative high-pressure, high temperature conditions.

2. NO_x FORMATION IN H₂ MICROMIX COMBUSTION SYSTEM

Oxides of Nitrogen (NO_x) comprise Nitric Oxide (NO) and Nitrogen Dioxide (NO₂). Typical aircraft NO_x emissions comprise 90-92% NO and 8-10% NO₂. The formation of NO_x occurs through five primary mechanisms: thermal NO_x, prompt NO_x, fuel-bound NO_x, NNH NO_x, and N₂O NO_x. Glarborg et al. [14] have explained that hydrocarbon (CH) fuels containing organically bound nitrogen produce fuel-bound NO. Fenimore [15] has shown that prompt NO_x is formed early in CH flames, near the spray front, when smaller CH radicals react with N₂. Therefore, in pure H₂-air combustion, it can be inferred that prompt NO_x and fuel-bound NO_x is not a significant concern [16]. The NNH route to NO formation, described by Bozzelli and Dean in ref. [17], involves N₂ reacting with an H atom to form NNH, which then reacts with an O atom to form NO and

NH. Konnov [18] has demonstrated that NO formation via the NNH route is significant in hydrogen combustion at lower temperatures between 1400-1560K. The N₂O route to NO formation is described by Rutar and Malte in ref. [19] as a third body stabilised reaction between N₂ and O leading to NO formation, increasing with residence times. Thermal NO_x formation is a well understood endothermic process explained by the extended Zeldovich mechanism, predominant in flames above 1850K, and increasing with increased residence time.

At high pressure high temperature conditions prevalent in gas turbine combustor, NO formation via the N₂O and Zeldovich mechanisms is the majority contributor to NO_x formation, increasing with residence times [19]. Therefore, reducing temperature, minimizing the time spent at high temperatures, and minimizing the reaction zone volume can help reduce NO_x emissions. Micromix flames offer the best possible reduction in reaction zone volume by miniaturizing the flame length scale, limited only by manufacturing capabilities. Consequently, in H₂ micromix combustion systems, thermal NO_x is deemed the primary concern.

3. NO_x CORRELATION REQUIREMENT

NO_x emissions formation is a complex process that is affected by numerous cycle parameters, including inlet pressure, inlet temperature, combustion zone equivalence ratio, outlet temperature, and fuel composition, as well as design choices such as degree of premixing, fuel injector and swirler design, and fuel staging strategy, among others. Accurately quantifying NO_x emissions requires precise information on all these parameters, which is often not the case in the early stages of engine design. As a result, the most important requirement for a correlation-based NO_x emissions prediction ROM was that it should be simple to use with preliminary engine-cycle performance data, enabling NO_x trends estimations with reasonable accuracy in the absence of precise design and sizing data. Traditionally, NO_x emissions prediction correlations are derived from either experimental data and/or engine certification data. The correction for environmental factors such as humidity is occasionally included to match the emissions measurements from the testbed [20].

In the absence of experimental data, this study presents a novel methodology for deriving a ROM for predicting thermal NO_x emissions using computational fluid dynamics (CFD) simulations. In the following section, we discuss the selection and relevance of key operating boundary condition variables that impact thermal NO_x formation in the H₂ micromix combustion system. The analysis is performed under the assumption of fixed geometry for the variables of interest.

3.1 NO_x Emissions Correlation Variables

For a typical gas turbine combustors thermal NO_x emissions are a function of flame temperature (linked to the reaction rate), residence time and mixing homogeneity. NO_x emissions can therefore be derived as a function of the variables shown in **Equation (2)** which influence the mixing homogeneity, reaction rate and residence time [10,21].

$$NOx \propto f(P_3, T_3, \Delta P_c, \Delta P_{fa}, Geo, T_4, T_{ft}) \quad (2)$$

Where P_3 is the combustor inlet pressure, T_3 is the combustor inlet temperature, ΔP_c is the combustor fractional pressure loss, ΔP_{fa} is the fractional differential in pressure between the fuel and air, Geo is the combustor geometry, T_4 is the combustor outlet temperature, and T_{ft} is the adiabatic flame temperature. If the geometry and design of the combustor is fixed, then the simplified NOx correlation relating only to its inlet boundary conditions can be developed as shown in **Equation (3)**.

$$NOx \propto f(P_3, T_3, T_4, T_{ft}) \quad (3)$$

However quite often when running an experimental campaign for deriving NOx emissions correlations some of this data may not be measurable (such as T_{ft}) or challenging and costly to measure (such as T_4). NOx emissions may be therefore correlated to other parameters that can be easily measured in the rig such as FAR or equivalence ratio which implicitly capture the effect of the variables T_{ft} and T_4 as shown in **Equation (4)** [12].

$$NOx \propto f(P_{in}, T_{in}, \Phi) \quad (4)$$

Where Φ is the equivalence ratio. The preliminary design and sizing of the H₂ micromix combustor was first undertaken to determine the appropriate size for a representative H₂ micromix combustor for a ultra-high bypass ratio turbofan engine used in the ENABLEH2 Year 2050 blended wing body long-range aircraft (LR BWB 2050) [22], performance data shown in **Table 1**. Subsequently, a sector of the combustor was used for numerical assessment.

4. MICROMIX COMBUSTOR GEOMETRY

For the conceptual H₂ micromix combustor, the following assumptions and design choices were made (primarily due to the unique difference in the burning and flame characteristics of H₂) based on the best engineering judgements. These assumptions primarily relate to the combustor architecture.

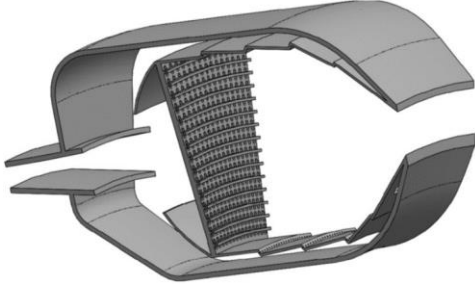


FIGURE 3: CONCEPTUAL H₂ MICROMIX COMBUSTOR CAD [23].

In the preliminary design phase, the H₂ micromix combustor was designed without primary, secondary, or dilution holes as shown in **Figure 3**. Conventional combustors employ primary and secondary air jets to enhance flow recirculation to stabilize the flame and complete the CH combustion. However, this is not necessary in the H₂ micromix combustor. The temperature profile can be regulated through active fuel scheduling.

TABLE 1: DESIGN POINT (TOP OF CLIMB) ENGINE CYCLE DATA.

Parameter	Data
Net Thrust (kN)	64.1
Altitude (m)	9754
Flight Mach Number	0.82
Delta Temperature (ISA)	10.0
BPR	20.4
OPR	83.3
Compressor Outlet Mach Number	0.272
Combustor Inlet Mass flow (kg/s)	30.22
Fuel Mass flow (kg/s)	2.77E-01
Combustor Inlet Pressure (kPa)	3073
Combustor Inlet Temperature (K)	962
Combustor Liner Inlet Mach Number	0.025
Combustor Inlet Static Pressure (kPa)	2918
Combustor Inlet Static Temperature (K)	948
Combustor Outlet Pressure (kPa)	2950
Combustor Outlet Temperature	1775
Combustor Outlet Static Pressure (kPa)	2906
Combustor Outlet Static Temperature (K)	1768
Combustor Outlet Mach Number	0.15

In the near future, high-temperature-resistant materials such as Ceramic Matrix Composites (CMCs) will be used in liners, as evidenced by GE's TAPS-III [24] and Rolls-Royce's Phase 5 combustors, which have implemented CMCs and tiled walls[25]. Furthermore, improvements in cooling technology such as enhanced impingement-effusion cooling are expected to decrease the cooling air requirement.

The primary purpose of air entering the liner is for lean H₂ combustion. A small fraction of this air will be utilized for cooling the mating surface between the liner and injector plate, which will be introduced into the combustor through cooling jets from the top and bottom unfuelled air gates. This will provide protection to the liner surface in the primary zone, where the highest temperatures are anticipated. Downstream the air will mix with the combustion products, leading to a reduction in the equivalence ratio in the combustor.

The sizing methodology used in this study is adapted from the Lean Partially Premixed (LPP) combustor sizing approach described in other studies [26,27]. The proposed methodology accounts for the inlet boundary flow conditions and geometric constraints as inputs and calculates the combustor liner and casing dimensions based on the air split and flow velocities. The flow velocity ranges of 7-12 m/s for the liner and 35-60 m/s for the passage have been recommended for Jet A-1 fuelled combustors. However, the flow velocity for the H₂ micromix combustor liner was deduced based on the flow requirements downstream of the air gate based on the single-injector numerical studies available in the literature [7,8]. The liner flow velocity of 15 m/s (Mach number of 0.025) was chosen. The outcome of the sizing task is shown in **Figure 4**.

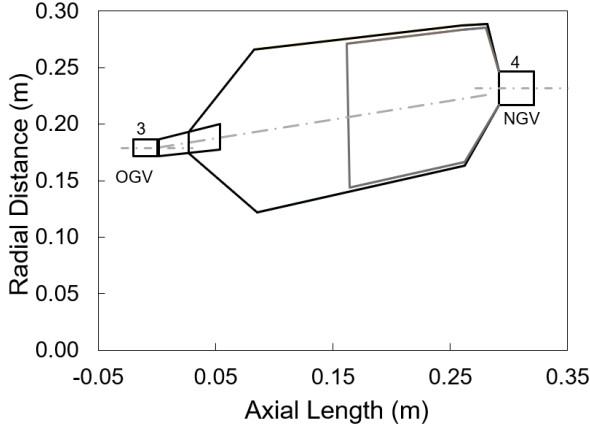


FIGURE 4: HYDROGEN MICROMIX COMBUSTOR GEOMETRY.

Based on the sized combustor, the micromix injector sector comprising 52 injectors arranged in a 26x2 matrix is chosen for numerical investigation.

5. NUMERICAL DOMAIN AND TEST CONDITIONS

The injector geometry chosen for analysis is the result of extensive numerical and experimental research conducted in project ENABLEH2 [28] as shown in **Figure 5**. Cranfield University (CU) has taken the lead in the development of H₂ micromix combustion technology to deliver zero mission-level CO₂ ultra-NO_x H₂ combustion system.

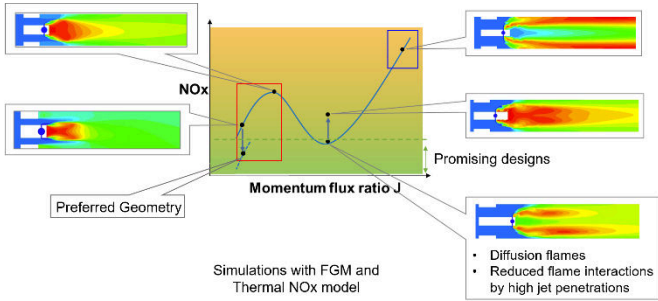


FIGURE 5: H₂ MICROMIX INJECTOR DESIGN VARIABLES INFLUENCE ON NO_x EMISSIONS [3].

The “preferred geometry” is shown in **Figure 6** and the shape and dimension is available in **Table 2** and it is the one that has pure diffusion flame without flame-to-flame interactions shown in **Figure 5** as “preferred geometry”. The domain started 5 mm upstream of the airgate channel entrance and extended to 60 mm downstream of the flame anchoring position at the bluff edge of the H₂ injector.

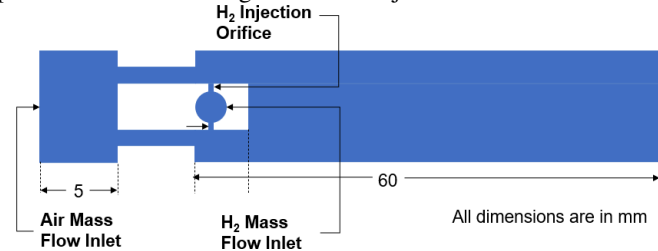


FIGURE 6: HYDROGEN MICROMIX INJECTOR GEOMETRY.

TABLE 2: CHOSEN H₂ MICROMIX INJECTOR GEOMETRY.

Design Parameter	Value
Shape	
Air Gate Diameter (mm)	2.11
Air Gate Height (mm)	1.055
Aspect Ratio (AR)	0.5
H ₂ Injection orifice Diameter (mm)	0.3
Momentum Flux Ratio (MFR)	0.5-0.55

The geometry shown in **Figure 6** is of a pair of two opposing injectors fed from the same H₂ fuel manifold. The numerical domain consisted of 12 such pairs of injectors arranged in radial direction times two in the circumferential direction, i.e., a 24x2 injector array with 48 injector orifices and 48 airgates. Another four airgates that were not fuelled, two at the bottom of geometry in Main 1 and two at the top of the geometry in Main 2, as shown in **Figure 7**, serving as film cooling air flows, are also incorporated in the domain.

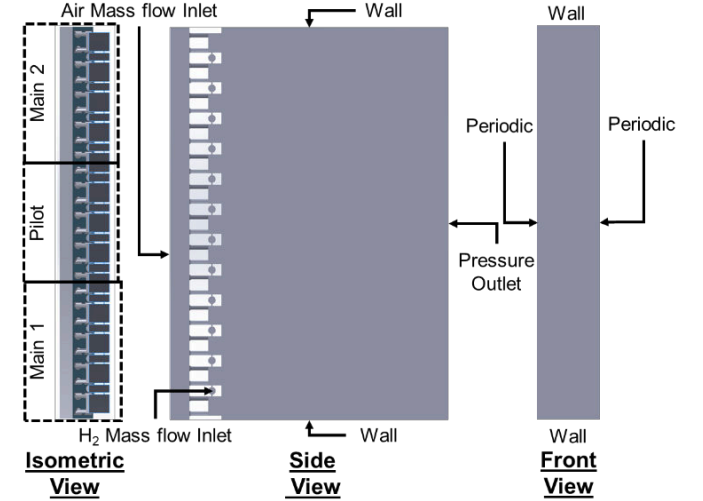


FIGURE 7: NUMERICAL DOMAIN AND BOUNDARY CONDITIONS.

The boundaries for H₂ and the air inlet are set as mass flow inlets. The left and right sides are set to periodic boundaries, and the exit of the domain is set to a pressure outlet. For all the cases, hydrogen fuel injection is set at 450K and the inlet conditions as shown in **Table 3**. The equivalence ratio (Φ) is calculated assuming 10% of the incoming air ($\dot{m}_3$) is used for cooling and the stoichiometric fuel air ratio for hydrogen is 0.029. The equivalence ratios were incrementally stepped up from the minimum values to the maximum values specified in **Table 3**. The sector was segregated into three zones, namely Pilot, Main 1 and Main 2, for fuel scheduling at different power conditions, as shown in **Figure 7**. The centre 16 injector were attributed as pilots, the 16 closest to the shaft were called Main 1, while the 16 farthest from the shaft were Main 2. The key criterion in staging was to keep the pilot injectors at an equivalence ratio of 0.40 at all power conditions to ensure flame stability. At the lowest power condition, all the fuel goes to the pilot only, while at other power conditions, while the pilot is maintained at 0.40, the leftover fuel goes either to Main 1 only

or equally to both Main 1 and Main 2. The pattern of injectors that were lit at different power conditions is shown in **Table 3**.

TABLE 3: NUMERICAL CAMPAIGN DATASETS.

P ₃ (kPa)	T ₃ (K)	Φ		Injectors lit		
		Min	Max	Main 1	Main 2	Pilot
400	446	0.13	0.20	No	No	Yes
	546					
1500	646	0.19	0.28	Yes		
	746					
2500	646		0.30			
	746					
3500	646		0.31			
	746					
4000	846	0.22	0.31			
	946					
6200	896	0.28	0.32			
	996					

The polyhedral mesh with a base size of 0.4 mm, surface growth rate of 1.15 and volumetric growth rate of 1.12 is applied to the whole domain. The zone-based custom refinement using volumetric and surface control on areas of particular interest is exercised to refine the mesh in these regions such as for the flame stretch zone, the element base size is set to 0.08 mm, for hydrogen feed and airgate channels, it is 0.07 mm and for injection orifice, it is set to 0.03 mm. 6 prism layers were used near the walls, with prism layer stretching of 1.1 and prism layer thickness of 0.08mm. A mesh independence study was carried out to determine the optimal mesh size while maintaining a satisfactory balance between computational time cost and result accuracy.

Three-dimensional steady 2nd-order segregated flow Reynolds Averaged Navier Stokes (RANS) analysis is performed for all the cases using Simcenter STAR-CCM+. The shear stress transfer (SST) formulation based on the k- ω SST turbulence model is used, which enables integration through viscous sublayers down to the wall for more precise wall treatment [8,29]. The all-y+ wall treatment attempting to emulate the high- wall treatment for coarse meshes and the low-y+ wall treatment for fine meshes is used. To model H₂ combustion and turbulence-chemistry interaction, a Flamelet Generated Manifold (FGM) kinetic rate model with diffusion flamelets is used. According to this model, the rate of a chemical reaction is substantially faster than the turbulent flows integral time scale [30]. The turbulent flame can be viewed as a differential set of laminar flames if even the smallest scale of eddies has no impact on the chemical reactions. The chemistry is defined by mixture fraction and progress variable so that the scalars can be pre-tabulated. A Probability Density Function (PDF) is used to mimic the effect of turbulence on chemistry. Zghal et al. compared the predictions obtained using the less computationally expensive FGM combustion model to the higher-fidelity Complex Chemistry (CC) model for H₂ micromix flames under high pressure conditions (15 bar) using

both RANS and Large Eddy Simulations (LES) [31]. The effect of different turbulence-chemistry interaction models was assessed with LES by coupling the CC model with the Eddy Dissipation Concept (EDC) model and the Thickened Flame Model (TFM). The prediction trends of both combustion models were shown to be affected by the turbulence approach used, especially in terms of flame length as they reported an absolute relative difference from the RANS predictions of 11% with the FGM model and of 28% with the CC-EDC models. Moreover, compared to the latter, the FGM model predicted flame lengths on average 22% when using RANS. It was also shown that with RANS, the FGM model tends to predict a lower flame temperature compared to the CC-EDC model. Since different solutions were obtained with LES and RANS for the same combustion model, the predictions need to be validated in the future with experimental data. However, the ability of the FGM model to accurately model H₂ combustion within reasonable tolerances was not invalidated. While it is acknowledged that using RANS-FGM could result in underestimation of NO_x values, the primary focus of this study was to examine the influence of operating boundary conditions on NO_x formation trends rather than establishing absolute values. Therefore, RANS-FGM was deemed appropriate for this investigation due to its lower computational cost.

The diffusion feature is modified for the hydrogen-air mixture by varying the PDF Schmidt number to accommodate hydrogen's much higher mass diffusivity than hydrocarbon fuels. Lopez et al. investigated the calibration of the model constant, namely turbulent Schmidt number (Sc_t) for RANS against the LES FGM combustion model; the study recommended the Sc_t of 0.2 for the H₂ micromix combustion system [13]. A 9-species 25-steps mechanism is used for hydrogen reaction [32]. Previous work has proven that it is a good compromise between accuracy and computational cost [7,33]. The concentration of thermal NO_x was calculated using the Zeldovich mechanism as a post-processing step by freezing the flow field employing temperature and species concentration values for NO_x calculation [34]. The numerical setup follows the best practices developed from previous work done by the research team, and further details of the numerical models used can be found in the literature [8,13,31].

6. METHODOLOGY

To develop a correlation over a desired range the utmost important requirement is the availability of data covering the entire range. In this study, in absence of experimental data the numerical campaign was run over a wide range of parametric values covering a typical aircraft mission profile Idle, End of Runway (EoR), Top of Climb (ToC), and Cruise as shown in **Table 3**. The numerical simulations comprised two campaigns.

The first campaign examined the influence of variation of individual parameters T₃ and P₃ while maintaining all other boundary conditions constant. This was repeated for multiple incremental-step changes in all the parameters. The second campaign assessed the combined variation of Φ , T₃, and P₃, representative of the aircraft mission profile, again repeating the

process for multiple incremental-step changes.

The database was then created from these simulations and split into training data (80%) and numerical test data (20%). The NOx correlation was then derived using the regression in python and “Generalised Reduced Gradient (GRG) Non-Linear (multi-start)” solver in MS Excel. The developed correlation was verified against the test data. The numerical simulations were conducted assuming the composition of dry air and the resulting correlation for EINOx was subsequently corrected assuming 60% relative humidity at ISA-SLS conditions. The methodology adopted is shown in **Figure 8**. The following section presents the numerical campaign results and highlights the key findings of the work.

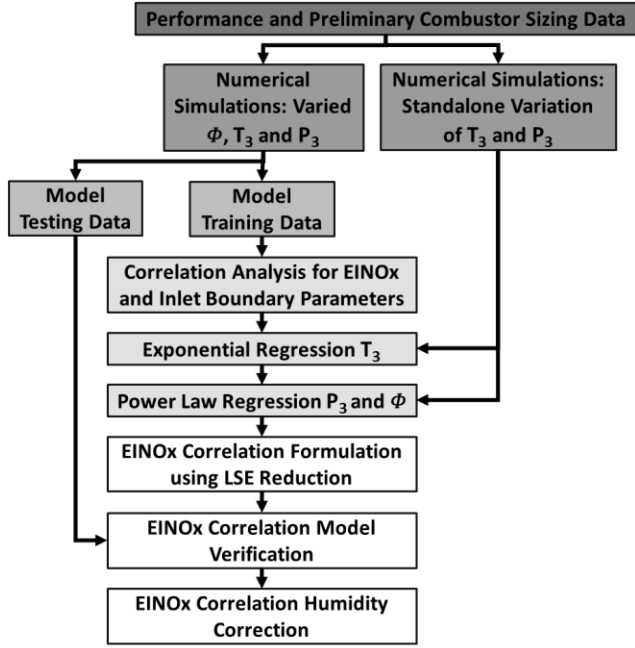


FIGURE 8: CORRELATION DEVELOPMENT METHODOLOGY.

7. RESULTS

The numerical campaign extended over a wide range of operating conditions to analyse the NOx formation in the H₂ micromix combustion system. The results are in agreement with the general scientific understanding of NOx formation in H₂ micromix combustion systems [10–12]. The EINOx (g NOx/kg H₂) was calculated using **Equation (5)**.

$$EINOx = (MF_{MFA} NOx) \frac{\dot{m}_4}{\dot{m}_f} \quad (5)$$

Where MF_{MFA} is the mass flow averaged mass fraction of thermal NOx calculated at the exit of the combustor, $\dot{m}_4$ is the total mass flow at the exit of the combustor in g/s, $\dot{m}_f$ is the mass flow of fuel in kg/s.

Before formulating the EINOx correlation using the data obtained from the numerical simulations, the influence of T₃ and P₃ were independently analysed as a standalone variable. The purpose of these analyses was twofold:

1. To establish the influence of these variables and EINOx.
2. To deduce the mathematical functions and establish initialisation values for the regression coefficients to reduce computational time.

7.1 Effect of Inlet Temperature

As shown in **Figure 9** and **Figure 10**, for a given pressure, EINOx increases exponentially as a function of inlet temperature, and this is consistent with the trends reported by Marek et al. [12] for H₂ micromix combustion. This establishes the exponential relation shown in **Equation (6)**.

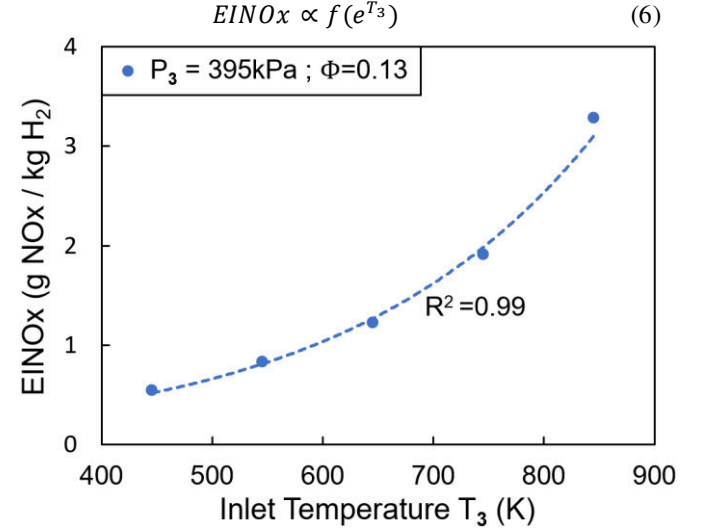


FIGURE 9: INFLUENCE OF INLET TEMPERATURE ON NOx FORMATION AT LOW POWER CONDITIONS (CONSTANT COMBUSTOR INLET PRESSURE AND EQUIVALENCERATIO).

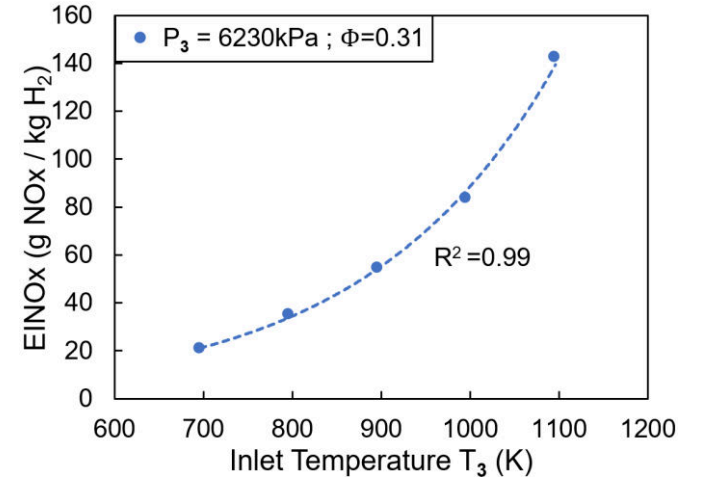


FIGURE 10: INFLUENCE OF INLET TEMPERATURE ON NOx FORMATION AT HIGH POWER CONDITIONS (CONSTANT COMBUSTOR INLET PRESSURE AND EQUIVALENCERATIO).

7.2 Effect of Inlet Pressure

For a given temperature, the relationship between EINOx and pressure is a power law function as shown in **Figure 11**. This is consistent with the findings reported by various studies available in the literature [10–12] for H₂ micromix combustion.

This establishes the power law relation shown in **Equation (7)**.

$$EINOx \propto f(P_3^x) \quad (7)$$

Where x is the exponent coefficient of pressure.

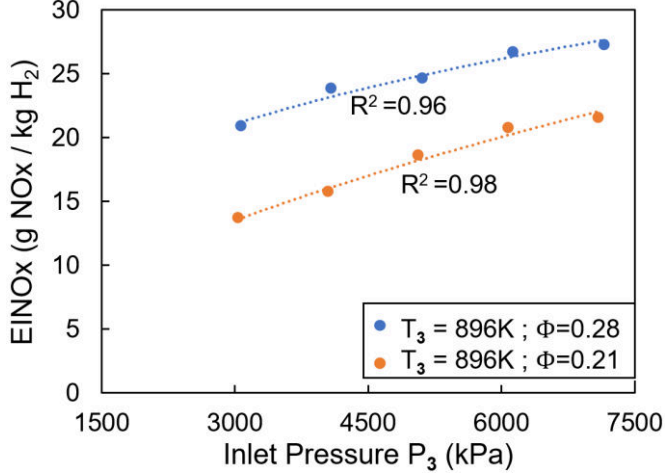


FIGURE 11: INFLUENCE OF INLET PRESSURE ON NOx FORMATION (CONSTANT COMBUSTOR INLET TEMPERATURE AND EQUIVALENCE RATIO).

7.3 Effect of Equivalence Ratio

Figure 12 shows the effect of simultaneous variation of equivalence ratio, combustor inlet temperature, and pressure on NOx emissions at different engine power settings. The results follow the expected trends i.e., NOx emissions increase with increasing equivalence ratio, combustor inlet temperature, and pressure. The trends highlight certain observation listed below-

1. For the range of conditions that were numerically investigated as shown in **Table 3** the NOx emissions have an exponential dependence on the flame temperature in the combustion zone in the combustor.
2. The influence of pressure is more significant at higher equivalence ratio.

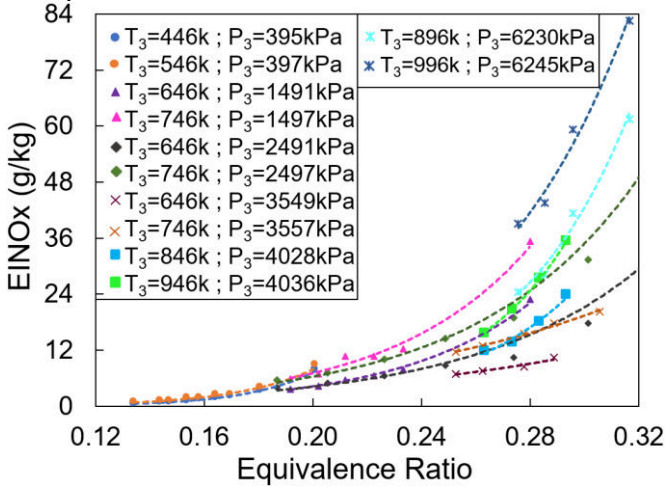


FIGURE 12: INFLUENCE OF EQUIVALENCE RATIO ON NOx FORMATION (CONSTANT PRESSURE DROP).

Figure 13 highlights the observed influence of MFR on the

flame interactions i.e., the NOx emissions, and the results are consistent with the expected trends as illustrated in **Figure 2**, the values are normalized over the range of the selected scale.

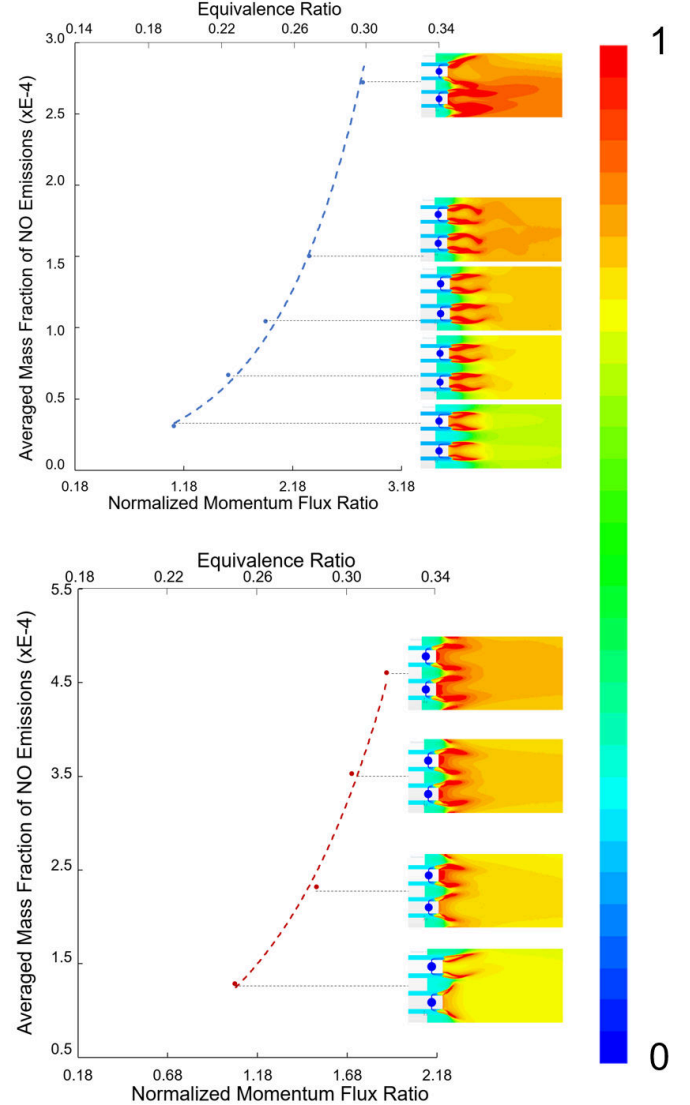


FIGURE 13: MOMENTUM FLUX RATIO AND TEMPERATURE CONTOURS AGAINST THE AVERAGED MASS FRACTION OF NO EMISSIONS AT TWO DIFFERENT POWER CONDITIONS (CONSTANT COMBUSTOR INLET TEMPERATURE AND PRESSURE).

7.4 H₂ Micromix NOx Correlation Coefficients

The NOx correlation coefficients are now derived for the variables down selected in **Section 3.1** using the numerical simulations database that was created under two campaigns described in **Section 6** methodology. As presented in **Section 7**:

1. NOx emissions have an exponential dependence on temperature.
2. The relationship between EINOx and pressure is a power law function.

3. The relationship between EINOx and equivalence ratio is a power law function.

Using these relationships, the correlation for EINOx described in **Equation (8)**, was developed.

$$EINOx = a(P_3^b) \left(e^{\frac{T_3}{c}} \right) (\Phi^d) \quad (8)$$

Where a is the coefficient of proportionality, b is the combustor inlet pressure (P_3) exponent coefficient, c is the combustor inlet temperature (T_3) exponential coefficient, and d is the combustor equivalence ratio (Φ) exponent coefficient.

First, the exponential coefficient of temperature “c” was obtained for a fixed pressure and equivalence ratio based on the dataset for standalone inlet temperature variation described in **Section 7.1**. Similarly, the coefficient “b” was derived using results from **Section 7.2** accounting only for the pressure variation. Finally, the coefficient “d” was derived using the results from **Section 7.3** varying both the combustor inlet temperature, and the pressure.

Next based on **Equation (8)**, these coefficients were exported into MS Excel for correlation Least Square Error (LSE) reduction using the Generalised Reduced Gradient (GRG) Nonlinear with Multi-Start solver. The training dataset described in **Section (6)** and **Table 3** was used. Numerical test data was randomly selected and excluded from the training process. The derived coefficients using the training dataset are presented in **Table 4**.

TABLE 4: H₂ MICROMIX EINOx CORRELATION COEFFICIENTS VALUE.

Coefficients	a	b	c	d
Value	0.0864	0.40	190.89	1.95

Figure 14 shows a comparison between the EINOx predictions from the CFD simulations and the derived correlation (for a range of T_3 , P_3 and Φ values) using test dataset.

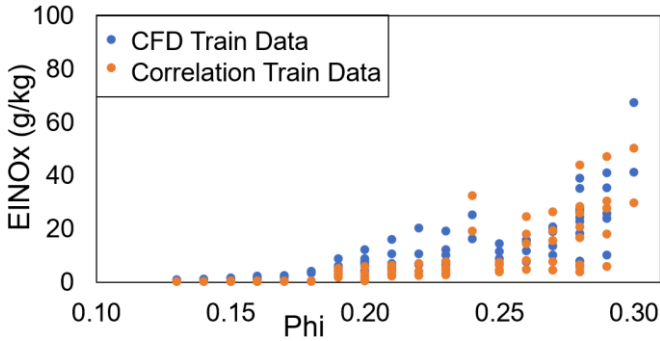


FIGURE 14: THE EINOx CORRELATION COMPARISON AGAINST CFD DATA.

7.5 Humidity Correction for ISA-SLS

Humidity has a significant impact on NOx emissions, primarily due to the reduction in flame temperature resulting from the higher water vapour content. Hence it is important to include corrections in an EINOx correlation to incorporate the effect of varying humidity with altitude.

The standard practice for deriving EINOx correlation is from experimental data obtained at ISA-SLS conditions with a RH of ~60%. However, the correlation and corresponding values of the coefficients presented in **Section 7.4** were based on a dry air assumption in CFD simulations. Hence, the humidity correction factor F_H for typical 60% humidity at ISA-SLS is applied to the correlation based on the study by Norman et al. [35].

The correction factor F_H applied to the correlation displayed in **Equation (9)** to account for ~60% RH at ISA-SLS is shown in **Equation (10)**.

$$EINOx = 0.0864 P_3^{0.40} \left(e^{\frac{T_3}{190.89}} \right) (\Phi^{1.95}) F_H \quad (9)$$

$$F_H = (1 - (e^{RH0} - e^{RH60})) \quad (10)$$

Where e^{RH0} is 1.125 at relative humidity of 0% (completely dry air) at SLS conditions, e^{RH60} is 1 at relative humidity of 60% at ISA-SLS conditions [35]. This results in the correlation shown in **Equation (11)** for ISA-SLS EINOx prediction.

$$EINOx = 0.0756 P_3^{0.40} \left(e^{\frac{T_3}{190.89}} \right) (\Phi^{1.95}) \quad (11)$$

Note, humidity correction to EINOx correlation for ISA-SLS is only necessary if the correlation is derived from CFD simulations with dry air assumption.

7.6 Humidity Correction for Altitude

For the EINOx correlation to be applicable for the entire flight envelope a further correction is required to account for the variation of humidity with altitude. Typically, EINOx increases by ~12.5% in the drier air conditions at the top of climb and cruise [35]. This correction and the final proposed correlation, which accounts for the effects of altitude on relative humidity and consequently NOx, is shown in **Equation (12)**.

$$EINOx = 0.0756 P_3^{0.40} \left(e^{\frac{T_3}{190.89}} \right) (\Phi^{1.95}) e^{H_{Alt}} \quad (12)$$

$$H_{Alt} = -19(\omega_{Alt} - 0.006344) \quad (13)$$

Where ω_{Alt} is the specific humidity at the required altitude in kgH₂O/kg_{air}.

Note, humidity correction to EINOx correlation is only necessary if engine performance is modelled assuming dry air, which tends to overestimate the highest engine gas temperatures at a thrust when compared to more accurate performance calculations taking humidity into account.

7.7 Assumption and Limitations

The NOx correlation has been derived using RANS CFD numerical simulations that were based on best modelling practices and calibration constants derived from higher fidelity LES simulations conducted under other tasks in ENABLEH2 project and published in the studies [8,13,31]. However, the models have not yet been calibrated against experimental data and hence caution must be exercised when using the correlations presented in this report. The NOx emissions are also influenced by parameters such as those listed below, which were not explicitly evaluated in this study, so the absolute NOx

emission values and the EINOx correlations coefficients are specific to the tested geometry.

- Pressure Drop
- Residence Time
- Fuel/Air Mixing (combustor-injector design variations)

8. CONCLUSION

In this study the EINOx correlation (as a function of combustor equivalence ratio, and inlet temperature and inlet pressure) was derived for a fixed geometry of a low-NOx hydrogen micromix combustion system. A correction factor to account for humidity effects was recommended as shown in Equation (12).

The correlation developed was verified against numerical test data. Relative to a fully rigorous CFD analysis, it is estimated that the correlation over-predicts mission-level NOx estimations by 5-8% and provides the NOx emissions trends that would be expected over a typical aircraft mission profile. The methodology developed (including the verification process) is flexible and extensible and may be applied to any future low emissions hydrogen combustion technologies. As experimental data becomes available to validate and calibrate numerical CFD models predicting H₂-air mixing, reactions, and NOx emissions, the resulting ROMs generated through this methodology will become more robust and reliable for future applications. The ROM can be used for the Techno-Economic, Environmental Risk Assessment (TERA) type studies comprising aircraft mission-level design space exploration and multi-disciplinary optimisation studies for which the more computationally expensive, higher fidelity computational fluid dynamics (CFD) models would not be suitable. The following areas of research are recommended for further work:

1. The correlation may be further refined using higher fidelity, experimentally validated, large eddy simulation (LES) CFD models.
2. The correlation can be further developed to include the influence of injector design variables on EINOx e.g., by incorporating pressure drop term in the correlation.
3. This study only focussed on the thermal NOx formation mechanism but for more rigorous calculations one may wish to include an analysis of NNH and N₂O NOx formation mechanisms.

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Numerical investigation into the impact of operating boundary conditions on NO_x formation in hydrogen micromix combustion system

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