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Marcus Wiegand

`marcus.wiegand@tu-dresden.de`

TU Dresden <https://orcid.org/0009-0002-0591-9422>

Philipp Kiendl

TU Dresden

Ronald Mailach

TU Dresden

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Recalibrated Nitrogen-Oxide (NO_x) Emission-Index Model for Hydrogen Combustion Aircraft Engine Performance Analysis

Marcus Wiegand^{§a,*}, Philipp Kiendl^{§a}, Ronald Mailach^a

^a*Technische Universität Dresden, Institute of Fluid Mechanics, Chair of Turbomachinery and
Flight Propulsion, George-Bähr-Str. 3c, Dresden, 01069, Saxony, Germany*

Abstract

Aviation contributes to climate change through both CO₂ and non-CO₂ effects. Hydrogen can eliminate direct in-flight CO₂ emissions, but its combustion still produces nitrogen oxides (NO_x). Reliable NO_x prediction during early engine development remains challenging because detailed models are computationally demanding, whereas reduced-order models have limited validation. This study evaluates and recalibrates an existing p3T3-based NO_x emission-index model using combustor-inlet pressure, temperature, and equivalence ratio as inputs. Additional experimental and computational data compiled from the literature reveal substantial deviations in the original model across different combustor designs and operating conditions. Recalibration increases the cross-validation coefficient of determination (R^2) from 0.54 to 0.77. A lognormal uncertainty distribution is also derived to quantify variability in the model predictions. The updated model is implemented in MAPLE and applied to a representative hydrogen-powered A320 mission. The recalibrated model predicts higher NO_x emissions than the original model, although the predictions remain lower than those for kerosene combustion under corresponding conditions. Substantial uncertainty remains, highlighting the need for broader validation data. The proposed model provides a computationally efficient approach for uncertainty-aware NO_x estimation in hydrogen aircraft-engine performance analyses.

*Corresponding author. Email address: marcus.wiegand@tu-dresden.de

§These authors contributed equally to this work and share first authorship.

1. Introduction

Hydrogen combustion is a promising pathway for reducing the climate impact of future aircraft because it eliminates in-flight carbon dioxide emissions. However, hydrogen-fueled gas turbines still produce nitrogen oxides (NO_x), which are an important non- CO_2 emission species in aviation [1, 2, 3, 4, 5, 6]. Aviation NO_x affects atmospheric ozone and methane concentrations, and its climate impact depends strongly on emitted NO_x mass, release altitude, and background concentrations [1, 2, 7, 8]. Therefore, engine performance studies of hydrogen aircraft engines require computationally efficient methods for estimating NO_x emissions along altitude-resolved mission profiles, particularly when these models are used in early design studies.

Hydrogen combustion can reduce NO_x emissions relative to kerosene combustion because it enables lean operation, high mixing intensity, and combustor concepts specifically designed to suppress high-temperature regions and long residence times, such as the micromix combustion chamber concept [5, 9, 10, 11, 12]. Nevertheless, NO_x emissions remain significant. The emitted mass does not depend directly on fuel composition but is primarily governed by combustor design and operating conditions, including pressure, temperature, equivalence ratio, and residence time [2, 13]. High-fidelity experiments, computational fluid dynamics simulations, and detailed chemical-kinetic models can resolve these effects and the underlying NO_x formation pathways [14, 15]. However, their application requires local thermochemical and mixing properties, residence times, and detailed combustor-flow information, which are generally unavailable in early engine design phases. Furthermore, they are too expensive for repeated use in engine performance studies, mission analyses, or design optimization. Reduced-order models are therefore needed to provide operating-condition-dependent NO_x estimates from quantities available in engine performance models used during early engine design studies. This work focuses on this reduced-order modeling level rather than high-fidelity chemical-kinetic modeling.

For conventional kerosene engines, several reduced-order NO_x prediction methods exist and are often based on certification data for existing engines [16, 17, 3, 18]. Equivalent data are not available for hydrogen aircraft engines, because hydrogen-fueled aircraft engines are not currently represented in a unified emissions databank. Consequently, while high-fidelity models for NO_x formation in hydrogen combustion are available [14, 15], reduced-order hydrogen NO_x prediction methods remain limited, and their validation and uncertainty quantification are challenging. Some studies, e.g. in Ref. [19], assume a constant relative reduction compared to kerosene, which cannot capture operating-condition-dependent effects. Recent progress includes the p3T3 method of SINGH et al. [9], which predicts the nitrogen-oxide emission index

EI_{NO_x} from combustor inlet pressure p_3 , combustor inlet temperature T_3 , and equivalence ratio ϕ . This form is attractive for engine performance analysis and preliminary engine design because all three variables are available from cycle calculations. However, the original model was calibrated using computational fluid dynamics results for a single hydrogen micromix combustor design and lacks extensive uncertainty quantification, which limits its broader applicability. Other recent approaches, such as the physics-based model of GARCIDUEÑAS-CORREA et al. [20], include additional combustor-specific quantities such as swirl number, residence time, and flame temperature. These quantities can improve physical fidelity, but they are often unavailable in performance models used during early aircraft-engine design.

This work addresses the need for a simplified hydrogen NO_x emission-index model with quantified prediction uncertainty for preliminary engine performance and emission analysis. The p3T3 formulation of SINGH et al. [9] is first evaluated against a broader dataset compiled from experimental and numerical hydrogen-combustion studies. Because the original coefficients show limited agreement outside the training dataset, the model coefficients are refitted using the compiled literature data. The recalibrated model improves the cross-validation coefficient of determination from $R^2 = 0.54$ to $R^2 = 0.77$. In addition, a relative-error distribution is derived to support uncertainty propagation in mission-level emission and climate-impact analyses. Finally, the updated model is implemented in the engine performance and climate impact assessment tool MAPLE (*Modular Aircraft Engine Performance for Sustainable Aviation*) [21, 3, 6] and demonstrated for a representative hydrogen-powered single-aisle aircraft mission.

2. Data Compilation and Emission-Index Conversion

Experimental and numerical hydrogen-combustion NO_x data are compiled from the literature for model evaluation and recalibration [10, 22, 23, 9, 24, 25, 26, 27, 11]. The compiled dataset includes different combustor concepts, operating conditions, and data types. For each data point, the combustor inlet pressure p_3 , combustor inlet temperature T_3 , equivalence ratio ϕ , and nitrogen-oxide emission index EI_{NO_x} are required for the p3T3 model evaluation after SINGH et al. [9].

In gas-turbine combustors, NO_x formation is promoted by high temperatures and long residence times, mainly through oxidation of atmospheric nitrogen [15, 13]. In this work, NO_x refers to the sum of nitric oxide (NO) and nitrogen dioxide (NO_2). Emissions are expressed as the nitrogen-oxide emission index,

$$EI_{\text{NO}_x} = \frac{m_{\text{NO}_x}}{m_{\text{fuel}}} \quad (1)$$

where m_{NO_x} is the emitted NO_x mass and m_{fuel} is the burned fuel mass. The emission index is reported in $\text{g}_{\text{NO}_x}/\text{kg}_{\text{fuel}}$.

The reported quantities in the literature are heterogeneous. Some studies provide EI_{NO_x} directly, whereas others report NO_x concentrations corrected to a reference oxygen content. For gas-turbine applications, this reference is commonly 15 % O_2 [24, 28]. Therefore, concentration-based values $C_{\text{NO}_x, 15\% \text{ O}_2}$, given in ppmV, are converted to emission indices using

$$EI_{\text{NO}_x} = C_{\text{NO}_x, 15\% \text{ O}_2} \frac{M_{\text{NO}_x}}{M_{\text{air}}} \frac{\dot{m}_{\text{air}}}{\dot{m}_{\text{fuel}}} \frac{Z_{\text{O}_2, \text{air}} - Z_{\text{O}_2, \text{exhaust}}}{Z_{\text{O}_2, \text{air}} - 0.15} \cdot 10^{-3} \quad (2)$$

where M_{NO_x} and M_{air} are the molar masses of NO_x and air, respectively, $\dot{m}_{\text{air}}/\dot{m}_{\text{fuel}}$ is the air-to-fuel ratio, and $Z_{\text{O}_2, \text{air}}$ and $Z_{\text{O}_2, \text{exhaust}}$ are the oxygen volume fractions in ambient air and exhaust gas. The factor 10^{-3} accounts for the conversion from ppmV and kg/kg to g/kg.

An effective NO_x molar mass is estimated from the NO/NO_2 composition

$$M_{\text{NO}_x} = M_{\text{NO}}X + M_{\text{NO}_2}Y \quad (3)$$

with $X = 0.9$ and $Y = 0.1$, based on the dominance of NO observed in hydrogen-combustion studies [9, 23]. This gives $M_{\text{NO}_x} = 31.60$ g/mol. A mean dry-air molar mass of $M_{\text{air}} = 28.966$ g/mol is used [29].

The oxygen correction in Eq. (2) converts the reported 15 % O_2 -corrected concentration back to the exhaust oxygen content of the corresponding operating point. The exhaust oxygen fraction is estimated from hydrogen combustion stoichiometry. Complete combustion of 1 kg of hydrogen consumes 8 kg of oxygen [30], so that

$$\dot{m}_{\text{O}_2, \text{consumed}} = 8\dot{m}_{\text{fuel}} \quad (4)$$

and

$$\dot{m}_{\text{O}_2, \text{in}} = \omega_{\text{O}_2, \text{air}} \dot{m}_{\text{air}} \quad (5)$$

with $\omega_{\text{O}_2, \text{air}} = 0.232$ [31]. The residual exhaust oxygen volume fraction is then approximated as

$$Z_{\text{O}_2, \text{exhaust}} = Z_{\text{O}_2, \text{air}} \left(1 - \frac{\dot{m}_{\text{O}_2, \text{consumed}}}{\dot{m}_{\text{O}_2, \text{in}}} \right) \quad (6)$$

using $Z_{\text{O}_2, \text{air}} = 0.209$ [29]. The conversion procedure was validated against the approach of GARCIDUEÑAS-CORREA et al. [20]. The resulting EI_{NO_x} values differ by approximately 0.1 g/kg, mainly due to different assumptions for the NO_x composition

and molar mass.

The full compiled dataset is provided as supplemental material. It includes the original reported NO_x quantities, converted EI_{NO_x} values, operating conditions, combustor concept, data type, source reference, and conversion assumptions. This dataset makes the recalibration reproducible and enables future extension of the model when additional hydrogen-combustion NO_x data become available.

3. Original and Recalibrated p3T3 Model

SINGH et al. [9] presented one of the first p3T3-based models for predicting EI_{NO_x} in hydrogen micromix combustion systems. The model was derived from a CFD-generated database obtained from RANS simulations of a fixed-geometry hydrogen micromix combustor under representative aircraft engine operating conditions. It relates EI_{NO_x} to combustor inlet pressure p_3 , combustor inlet temperature T_3 , and equivalence ratio ϕ :

$$EI_{\text{NO}_x} = a \left(\frac{p_3}{1000 \text{ Pa}} \right)^b \exp \left(\frac{T_3}{c} \right) \phi^d \quad (7)$$

where EI_{NO_x} is given in $\text{g}_{\text{NO}_x}/\text{kg}_{\text{fuel}}$, p_3 in Pa, and T_3 in K.

The form of Eq. (7) is attractive for engine performance analysis because p_3 , T_3 , and ϕ are available from engine performance calculations. The pressure exponent represents the commonly observed increase of EI_{NO_x} with combustor pressure [9, 11, 32]. Reported pressure exponents vary between studies and combustor designs. SINGH et al. [9] obtained $b = 0.40$, SUDA et al. [11] reported $b = 0.70$, and MASUDA et al. [32] reported values between 0.40 and 0.83. The exponential temperature dependence and power-law equivalence-ratio dependence are also consistent with the expected increase in thermal NO_x formation at higher reactant and flame temperatures [13, 9, 11].

To assess the broader applicability of the original model, Eq. (7) was evaluated against the compiled experimental and numerical dataset described in Section 2. Figure 1 (a) compares predicted and reference EI_{NO_x} values. The original model gives a cross-validation coefficient of determination of $R^2 = 0.54$. Agreement is best for the dataset of SINGH et al. [9], which is expected because those data were used to derive the original model. Larger deviations occur for other combustor designs and operating conditions, indicating limited applicability beyond the original calibration dataset.

Several factors contribute to these deviations. First, the original model was derived for one micromix combustor geometry, whereas the compiled dataset contains

different combustor concepts and design features. Second, some literature data were obtained outside typical aircraft engine operating conditions, including atmospheric-pressure test-rig conditions and comparatively high equivalence ratios [24, 26, 23, 22, 27]. Third, NO_x formation also depends on quantities not included in Eq. (7), such as injector momentum flux ratio, injection velocity, mixing distance, residence time, and detailed combustor geometry [10, 25, 12]. These dependencies cannot be resolved by a three-parameter reduced-order model.

Because the original coefficients show limited agreement with the broader literature dataset, the coefficients a – d in Eq. (7) were refitted. The optimization was performed in Python using SciPy. The objective was to maximize the coefficient of determination between modeled and reference EI_{NO_x} values. The original and recalibrated coefficients are listed in Table 1.

Table 1: Original and recalibrated p3T3 coefficients

Model	a	b	c in K	d
SINGH et al. [9]	0.0864	0.40	190.89	1.95
Present recalibration	0.2127	0.61	403.51	1.83

The pressure exponent increases from 0.40 to 0.61 and remains within the range reported for hydrogen combustors in the literature [9, 11, 32]. The temperature coefficient increases from 190.89 to 403.51 K, corresponding to a weaker effective temperature sensitivity for the broader compiled dataset. The equivalence-ratio exponent changes only moderately, from 1.95 to 1.83.

The recalibrated model improves the cross-validation coefficient of determination from $R^2 = 0.54$ to $R^2 = 0.77$, as shown in Figure 1 (b). The improvement is most pronounced for intermediate emission-index values. However, the recalibrated model still shows considerable scatter and tends to overpredict some low-emission cases. This remaining error is expected because the model intentionally excludes combustor-specific geometric and mixing parameters that are often unavailable during preliminary engine design.

The present recalibration is point-weighted rather than study-weighted. This preserves the operating-condition distribution of the compiled dataset, but gives larger influence on the fitted coefficients to studies reporting many operating points. This limitation should be considered when applying the model outside the range of the compiled dataset and should be reevaluated when additional hydrogen-combustion NO_x data become available.

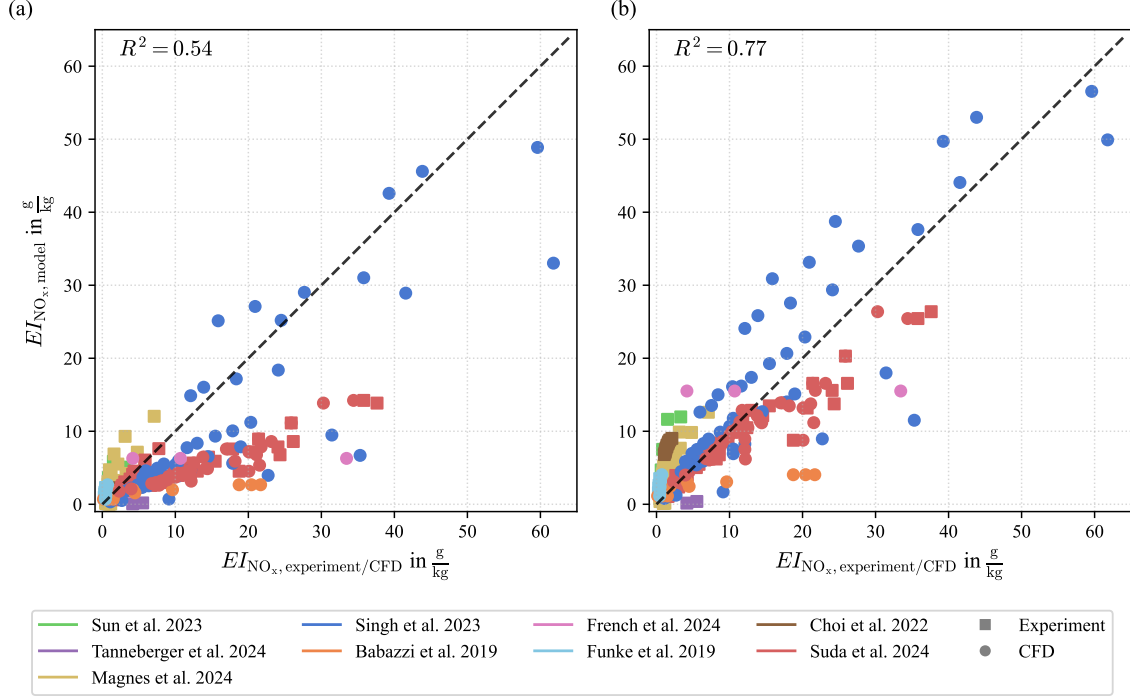


Figure 1: Comparison of (a) original and (b) recalibrated p3T3 predictions with experimental and numerical hydrogen-combustion data. The dashed line indicates exact agreement.

4. Relative-Error Uncertainty Model

The recalibrated p3T3 model provides a deterministic estimate of EI_{NO_x} . For mission-level emissions assessment and subsequent climate-impact analysis, the prediction uncertainty of this reduced-order model should also be quantified. The uncertainty is represented using the ratio between the reference emission index and the modeled emission index:

$$r_{\text{fit}} = \frac{EI_{NO_x, \text{experiment/CFD}}}{EI_{NO_x, \text{model}}} \quad (8)$$

where $EI_{NO_x, \text{experiment/CFD}}$ denotes the experimental or CFD reference value and $EI_{NO_x, \text{model}}$ is the corresponding model prediction. A value of $r_{\text{fit}} = 1$ indicates exact agreement. Values larger than one indicate model underprediction, whereas values smaller than one indicate model overprediction.

For the original p3T3 model, the distribution of r_{fit} shows substantial scatter and a median value of 1.85, indicating that the original model tends to underpredict the compiled literature data. After recalibration, the median of the corresponding ratio

r_{fit} decreases to approximately 1.00, see Figure 2, confirming the reduced systematic underprediction. Nevertheless, the distribution remains broad because the compiled data include different combustor designs, operating conditions, and data sources.

A parametric distribution was fitted to r_{fit} to enable uncertainty propagation in engine performance and early design studies. Candidate distributions were evaluated using the Kolmogorov–Smirnov distance between the empirical and fitted cumulative distribution functions [33]. A lognormal distribution provided the best practical representation among the tested distributions. Although a single parametric distribution cannot reproduce all features of the empirical histogram, especially local peaks caused by uneven data coverage across references, Figure 2, the lognormal distribution is adopted as an engineering uncertainty model because it preserves positivity and enables the model error to be expressed multiplicatively.

The fitted lognormal distribution parameters are summarized in Table 2. The parameters μ_{rel} and σ_{rel} describe the mean and standard deviation of $\ln(r_{\text{fit}})$. The 5% and 95% quantiles are 0.434 and 2.302, respectively, showing that the prediction uncertainty remains large despite the improved deterministic fit.

Table 2: Parameters of the fitted lognormal relative-error distribution

Parameter	Distribution	μ_{rel}	σ_{rel}	$Q5 / Q95$
Value	lognormal	0.0	0.507	0.434 / 2.302

For uncertainty propagation, the nominal emission index is first computed using Eq. (7) with the recalibrated coefficients. A probabilistic emission-index sample is then obtained by multiplying the nominal value with a random sample from the fitted relative-error distribution:

$$EI_{\text{NO}_x, \text{prob}} = r_{\text{fit}} EI_{\text{NO}_x, \text{model}} \quad (9)$$

This produces a distribution of possible EI_{NO_x} values instead of a single deterministic estimate. The same approach can be applied independently at each mission operating point to propagate NO_x model uncertainty through aircraft-engine performance and emissions calculations.

The uncertainty model should be interpreted as a practical approximation rather than a universal statistical description of hydrogen-combustion NO_x behavior. The available data are unevenly distributed across references, and studies with many data points influence the empirical distribution more strongly than smaller datasets. In addition, the relative-error distribution contains uncertainty from both the reduced-

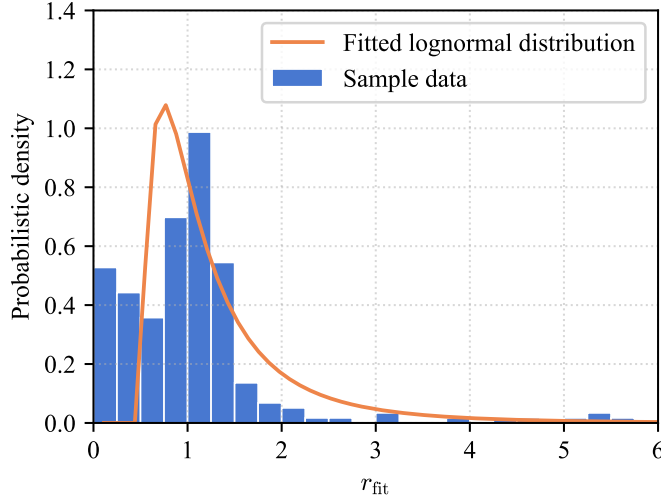


Figure 2: Empirical distribution of the relative-error ratio r_{fit} and fitted lognormal distribution.

order model and the underlying experimental or numerical reference data. Future experimental data at aircraft engine-relevant pressures and temperatures should therefore be used to update both the recalibrated coefficients and the relative-error distribution.

5. Mission-Level Demonstration in MAPLE

To demonstrate the use of the recalibrated model in an aircraft-engine performance analysis, the model was implemented in MAPLE [21, 3, 6]. MAPLE is a modular zero-dimensional aircraft-engine performance framework for performance, emission, and climate impact estimations along flight missions [21, 3]. Its conventional engine performance calculations have been validated against GasTurb with design-point deviations below 0.1 % and off-design deviations below 2 % [21]. The hydrogen-aircraft mission modeling used here builds on the previously published MAPLE hydrogen-combustion framework, which includes hydrogen fuel-system integration and mission-level emission assessment for an A320-class aircraft [6].

In the present work, MAPLE is used to provide the combustor operating conditions required by Eq. (7), namely combustor inlet pressure p_3 , combustor inlet temperature T_3 , and equivalence ratio ϕ , at each mission operating point. The recalibrated model can therefore be evaluated directly along an altitude-resolved flight profile.

The demonstration case considers a representative medium-range mission of a

hydrogen-adapted A320-like aircraft equipped with two CFM56-like engines, following the MAPLE setup described in Ref. [6]. The resulting EI_{NO_X} values are compared with predictions from the original p3T3 model of SINGH et al. [9] and with those of a comparable kerosene-powered engine. In addition, Figure 3 shows the 90 % confidence interval obtained by multiplying the deterministic EI_{NO_X} values from the recalibrated model with the fitted relative-error distribution from Section 4.

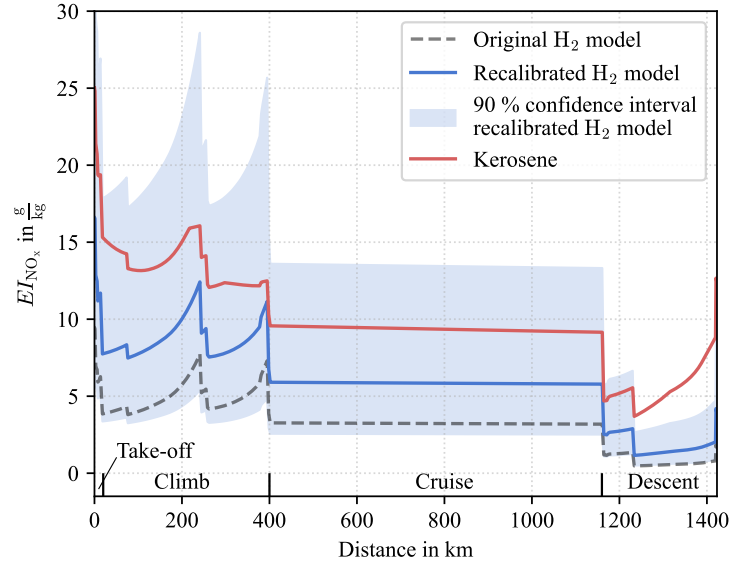


Figure 3: Mission-level EI_{NO_X} prediction and 90 % confidence interval from the recalibrated model and derived relative-error distribution for a representative hydrogen-powered single-aisle aircraft. The recalibrated p3T3 model is compared with the original model of SINGH et al. [9] and a kerosene reference mission.

The recalibrated model predicts higher EI_{NO_X} values than the original model throughout the mission. The difference occurs in all flight phases. The largest absolute EI_{NO_X} values occur during high-power operating conditions, especially takeoff and climb, where combustor pressure, temperature, and equivalence ratio are comparatively high. In lower-emission flight phases, such as descent, the absolute EI_{NO_X} values remain lower, but the relative difference between the original and recalibrated models can be larger.

The uncertainty interval remains wide along the complete trajectory. This reflects the scatter observed in the compiled experimental and numerical dataset and confirms that model uncertainty should be retained when using reduced-order NO_X models for mission-level emission or climate-impact studies. The predictions from the original

model remain within the 90 % confidence interval of the recalibrated model.

A kerosene reference mission is also included in Figure 3 for context, with NO_x emissions calculated using the p3T3 method derived in Ref. [3]. The hydrogen case shows lower EI_{NO_x} values along the mission than the kerosene reference, combined with lower fuel consumption due to hydrogen's higher lower heating value, resulting in a total NO_x emission reduction of 77 %.

6. Conclusions

A recalibrated reduced-order p3T3 model for estimating nitrogen-oxide emission indices EI_{NO_x} from hydrogen-powered aircraft-engine combustors was presented. The model retains the simple structure of the original model of SINGH et al. [9], using only combustor inlet pressure p_3 , combustor inlet temperature T_3 , and equivalence ratio ϕ as input parameters. These quantities are available from engine performance calculations, making this reduced-order model suitable for early aircraft-engine performance, mission, emission, and climate impact studies.

The original p3T3 model was evaluated against a compiled dataset of experimental and numerical hydrogen-combustion NO_x results from the literature. The comparison showed limited agreement outside the original calibration dataset, with a cross-validation coefficient of determination of $R^2 = 0.54$. Therefore, the coefficients of the p3T3 formulation were refitted using the compiled dataset. The recalibrated model improved the cross-validation coefficient of determination to $R^2 = 0.77$.

In addition to the deterministic recalibration, a relative-error uncertainty model was derived from the ratio between reference and modeled emission indices. A log-normal distribution was adopted as a practical multiplicative uncertainty model for engine performance and preliminary design applications. The resulting 90 % confidence interval remains broad, indicating that substantial prediction uncertainty persists even after recalibration. This uncertainty reflects both the limited availability of hydrogen-combustion NO_x data and the simplified structure of the p3T3 model.

The recalibrated model and uncertainty model were implemented in the performance and climate impact assessment tool MAPLE and demonstrated for a representative hydrogen-powered single-aisle aircraft mission. The updated model predicts higher EI_{NO_x} values than the original model throughout the mission, while the original predictions remain within the uncertainty interval of the recalibrated model. In comparison with a kerosene-powered aircraft engine, NO_x emissions are reduced by about 77 %.

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CRedit authorship contribution statement

M. Wiegand: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Resources, Data curation, Writing – original draft, Writing – review & editing, Visualization, Project administration. **P. Kiendl:** Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Resources, Data curation, Writing – original draft, Writing – review & editing, Visualization. **R. Mailach:** Conceptualization, Writing – review & editing, Supervision, Project administration, Funding acquisition.

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