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Analytical formulations for NOx emissions prediction of a SABRE engine

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Abstract

With an expected global revenue exceeding 1 trillion USD by 2040, the space industry is one of the world's fastest-growing sectors. Given the booming investment in the space industry and the anticipated space tourism era, it is crucial to assess the impact of already operative launch assets as well as to adopt design-to-sustainability strategies for the under-development and future launchers. This paper discloses novel analytical formulations to estimate nitrogen oxide emissions of a hydrogen-fueled air-breathing concept using a Synergetic Air Breathing Rocket Engine technology. Throughout the paper, the Skylon spaceplane and its Synergetic Air Breathing Rocket Engine are used as a case study. The methodology described specializes in updating the classical formulation of the Boeing Fuel Flow Method 2 (BFFM2) for estimating Nitrogen Oxide (NO_x) emissions. This method currently enables the estimation of NO_x emissions for any subsonic aircraft powered by traditional fuels. The objective is to derive new mathematical formulations applicable in the case of high-speed engines and hydrogen fuel. The proposed updating strategy is correlation-based and is generally applicable for modifying any analytical method for estimating emissions, including BFFM2. Through the analysis of correlations between the engine's propulsion and emission variables and its NO_x production, a series of parameters are derived to integrate into the original formulation of BFFM2 to adapt it to the case study. The input parameters required for the application and validation of the method, both in its original form and in the proposed variations, are obtained through high-fidelity propulsion and emission modeling of the engine, representative of various on-ground and in-flight operating conditions. To this end, 0D chemical-kinetic air/hydrogen combustion numerical simulations are employed. The methodology disclosed allows proving the high competitiveness of these air-breathing space launchers with respect to famous past and current competitors, such as the Space Shuttle and the Falcon 9.

Keywords: Reusable launchers; Air-breathing propulsive technologies; Nitrogen oxides emission estimation; Synergetic Air-Breathing Rocket Engine; Fuel Flow Method.

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Nomenclature

δ – Pressure ratio between FL and SL standard conditions	ICAO – International Civil Aviation Organization
θ – Temperature ratio between FL and SL standard conditions	LEO – Low Earth Orbits
CC – Combustion Chamber	LES – Large Eddy Simulations
CO – Carbon monoxide	LH2 – Liquid Hydrogen fuel
CO2 – Carbon dioxide	LOx – Liquid Oxygen propellant
DNS – Direct Numerical Simulations	M – Mach number
EI – Emission Index	NOx – Nitrogen Oxides
FAR – Fuel to Air Ratio	PB – Preburner
FFM – Fuel Flow Method	PBratio – Ratio between PB air mass flow and total air mass flow
FL – Flight Level	RANS – Reynolds-Averaged Navier-Stokes
GHG – GreenHouse Gases	REL – Reaction Engines Limited
H – Air humidity factor	SABRE – Synergetic Air Breathing Rocket Engine
H2O – Water Vapour	SL – Sea level
H2–FFM – Hydrogen and High-speed FFM formulation	T_3 – Temperature at the inlet of the combustion chamber
HE ratio - Ratio between He mass flow at the He turbine inlet and total air mass flow at the air compressor inlet powered by the He turbine	USD – United States Dollars
HX – Heat Exchanger	WFR – Water to Fuel Ratio at the inlet of the combustion chamber
	p_3 – Pressure at the inlet of the combustion chamber

1. Introduction

With an expected global revenue exceeding 1 trillion USD by 2040 [1], [2], the space industry is one of the world's fastest-growing sectors. Given the booming investment in the space industry and the anticipated space tourism era, it is crucial to assess the impact of already operative launch assets as well as to adopt design-to-sustainability strategies for the under-development and future launchers [3]. Complementary, the fast-growing request to access to space is pushing the research activities of the aerospace sector to develop breakthrough technologies and innovative products capable to meet design-to-sustainability strategies. In this complex and very challenging scenario, this paper aims at suggesting how to anticipate pollutant and Green House Gases (GHG) emissions prediction for reusable access to space vehicle since the conceptual design phase, specifically focusing on nitrogen oxides emissions. To unlock the possibility to anticipate the environmental sustainability assessment, the authors couple simplified but accurate propulsive systems models with 0D chemical-kinetic combustion models. To make these models useful for the conceptual design stage, they shall require a minimum set of input data (in line with the information usually available at this stage) and minimal computational resources (to be compatible with the fast design loops). Moreover, they shall be highly reliable (to support decisions with very high committed costs). In this context, the paper starts with an in-depth assessment of nitrogen oxides (NO_x) emission prediction techniques, clearly stating the benefits and showstoppers of their exploitation for high-speed air-breathing engines using hydrogen. A comprehensive review of emissions estimation techniques and their applicability beyond traditional subsonic aeroengines and fuels is reported in Section 2. Among all the available methods, the Fuel Flow method is selected as starting point, considering its applicability since the early design phases. Then, Section 3 provides the readers with useful insights on the case study: the Synergetic Air Breathing Rocket Engine (SABRE) technology is described and propulsive and emissive database available from previous authors publications are discussed. Furthermore, this section proposes a strategy for upgrading the propulsion and emissions modeling of the case study. The modifications made to the reference models aim to ensure the cohesion of the generation process of the two databases, thereby enhancing their reliability. Finally, Section 4 provides an in-depth description of the methodology used to derive new formulations of the Fuel Flow Method for high-speed aircraft using hydrogen (H2-FFM) in a step-by-step approach. Once the two databases are updated, the enhancement of the FFM is conducted by introducing additional parameters compared to the original formulation, selected based on a correlation-based approach, and utilizing the curve-fitting functionalities of Matlab. The updated mathematical formulations (H2-FFM) applied to the case study are presented. A discussion regarding the chemical-physical justifications for the mathematical contributions to the formulations for $EINO_{xFL}$ of the new introduced parameters is also provided. Finally, the results of the new formulations are compared with the NO_x Emission Indices evaluated from the engine emissions modeling to verify their estimation effectiveness.

2. State of the Art in NO_x Emissions Modeling for Aeronautical Applications

According to [3], nitrogen oxides emission prediction techniques can be grouped in five main families: (i) correlation-based models, (ii) P3T3 methods, (iii) fuel-flow methods, (iv) simplified physics-based models, and (iv) high-fidelity simulations. Following thorough investigations, the authors selected the FF method, specifically its Boeing Fuel Flow Method 2 (BFFM2) variant, as a foundational framework for developing innovative predictive analytical formulations. Simplified physics-based models and high-fidelity simulations are considered unsuitable for the study's objectives due to their demand for detailed knowledge of combustor geometry and their excessive computational cost within the context of conceptual design. For informational purposes, a brief overview is presented below for correlation-based models, P3T3 methods, and the BFFM2. The latter has been selected as the optimal candidate for applying the methodology of updating and tailoring to the case study. To clarify the rationale behind selecting the BFFM2, the suitability of each method category in the conceptual design phase of high-speed aircraft propelled by liquid hydrogen is discussed.

2.1. Correlation-based Models

Correlation-Based models utilize thermodynamic and emissive data obtained from engine tests conducted under ground-level conditions. These data are integrated into mathematical formulations to estimate the NO_x Emission Index, utilizing combinations derived from the analysis of correlations between the engine's chemical-propulsive parameters and its NO_x emissions. These methods are divided into two categories, empirical and semi-empirical, depending on the type of variables included in the final mathematical formulations. Empirical correlation-based methods employ primary engine parameters, such as combustion chamber inlet temperature (T_3) and pressures (p_3), end-of-combustion temperature, Fuel-to-Air Ratio (FAR), or Water-to-Fuel Ratio (WFR). Semi-empirical methods, on the other hand, require a detailed knowledge of the combustion chamber configuration as they involve the use of specific combustor variables, such as primary zone temperature, flame temperature, combustor volume, and residence time in the chamber. Correlation-based methods can also be classified based on how the variables are incorporated into the mathematical formulations to derive NO_x Emission Index ($EINO_x$): direct methods involve the direct use of these variables, while ratio methods employ them in the form of dimensionless ratios between flight-level and sea-level conditions. These methods offer the advantage of a wide range of variables to investigate when generating mathematical formulations for estimating $EINO_x$, with some of these variables being easily estimable or readily available. Consequently, they are recognized as one of the most easily applicable types of methods in conceptual design. On the downside, achieving an acceptable accuracy in estimations with these methods necessitates using a considerable number of variables. However, considering that each variable is subject to detection or estimation errors, this leads to an accumulation of errors, which becomes more significant with an increasing number of variables considered. Furthermore, these methods are highly specialized for the specific engine and combustor under study, and thus cannot provide generalized formulations for different aircraft. At most, they can be adapted to suit specific cases.

2.2. P3T3 Method

The P3T3 method stands as the most used approach for estimating NO_x emission indices. This method directly stems from Correlation-Based Models, focusing on a limited range of parameters of interest, which include the inlet temperature and pressure to the combustor (P_3, T_3), and the Fuel-to-Air Ratio. These variables are included in the compact mathematical formulation provided below:

$$EINO_{xFL} = EINO_{xSL}\left(\frac{p_{3FL}}{p_{3sL}}\right)^n\left(\frac{FAR_{FL}}{FAR_{SL}}\right)^m exp(H) \tag{1}$$

$$H = 19 * (h_{SL} - h_{FL}) \tag{2}$$

where H represents the humidity factor, introduced to consider humidity's impact on NO_x formation in the combustion chamber. As humidity rises, combustion temperature decreases, reducing NO_x production. The H factor is calculated based on the relative increase in specific humidity due to altitude gain. Despite not being explicitly included, the inlet temperature to the combustor T_3 implicitly influences the method's application and serves as the determining parameter. This is evident in the method's application procedure described in [3]:

- As an initial step, access to specific proprietary engine data is required, corresponding to the four throttle conditions outlined in [4] for the Landing Take-Off cycle (LTO). This data encompasses pressure and temperature at the combustor inlet (p_{3SL}, T_3) and Fuel to Air Ratio (FAR_{SL}), all assessed under Sea Level conditions. These data can be directly provided by the engine manufacturer rather than being estimated through propulsion modeling. Additionally, access to $EINO_{xSL}$ emissions data is necessary, which can be obtained from the ICAO Aircraft Engine Emissions Databank rather than being estimated using dedicated software. Subsequently, the parameters p_{3SL}, FAR_{SL}, and $EINO_{xSL}$ must be plotted as functions of T_3 and appropriately interpolated to achieve a satisfactory fit.
- The same propulsion parameters as in the previous step need to be derived under flight level conditions (p_{3FL}, T_{3FL}, and FAR_{FL}). Once again, this information should be obtained directly from the engine manufacturer rather than through propulsion modeling.
- Starting from the values of T_{3FL} obtained in step 2, it is possible to deduce the parameters $EINO_{xSL}$, p_{3SL}, and FAR_{SL} using the fits obtained in step 1. Once these parameters are known, as the P3T3 method operates as a ratio-method, ratios between FL and SL conditions need to be constructed.
- Finally, the method's formulation can be applied to evaluate $EINO_{xFL}$ based on corrected $EINO_{xSL}$, considering the evolution ratio of p_3, FAR, and the humidity factor.

The generalized formulation typically employs exponent coefficients (n=0.4 and m=0), but optimized coefficients can be used for specific cases to enhance accuracy. Despite the accuracy in estimating Emission Indices that this method offers, it requires access to proprietary engine data. If these data are not available, they must be estimated with an accuracy level that is on the verge of compatibility with conceptual design.

2.3. Fuel-Flow Method

The fuel-flow methods are developed using the P3T3 method as a basis, but with the objective of using only non-proprietary engine information, even if at the cost of the prediction accuracy. The main parameter considered by these prediction methods is the fuel flow, which represents the engine power setting and is publicly available. In addition, these methods take into account the effect of ambient pressure and temperature, humidity, and Mach number. Three fuel-flow methods are presented in the literature: the Boeing fuel-flow method 2 developed by Boeing (BFFM2) [5] and its applications [6, 7], and the sustainable supersonic fuel-flow method [8]. This family of methods can be very useful for a preliminary estimation of the emissions even if the achievable accuracy is lower than those attainable from P3-T3 formulations. The variations of the fuel-flow method differ only in the introduced coefficients in the mathematical formulations. Therefore, it is decided to refer only to the BFFM2 below, as it is more commonly used in literature. The BFFM2 is selected as the baseline for the proposed update methodology for adapting to the estimation of NO_x for high-speed aircraft powered by hydrogen, similar to what was proposed in [8] for a supersonic speed regime scenario and the use of Sustainable Aviation Fuel (SAF). Analogously to the P3T3 method, the $EINO_{xFL}$ is derived from a correction of the $EINO_{xSL}$. However, for the BFFM2 method, this correction is performed based on the profiles of environmental conditions, the fuel flow profile W_f, and the Humidity Factor H. Unlike the P3T3 method, the BFFM2 involves an additional intermediate step concerning the fuel flow parameter. To derive this parameter under SL conditions from that under FL conditions, a mathematical formulation is provided which includes the Mach number. Although the fuel flow parameter is not directly included in the final mathematical formulation of the method used for evaluating $EINO_{xFL}$, it serves as the parameter based on which $EINO_{xSL}$ are plotted and interpolated. These interpolated values are then used for environmental correction, leading to $EINO_{xFL}$. The complete procedure for applying the original BFFM2 can be summarized in the following steps:

- As a first step, it is necessary to derive the fuel flow values at sea level corresponding to the four throttle settings prescribed in [4] for the Landing Take-off (LTO) cycle by applying the following correction to the fuel flow values in FL conditions.

$$w_{fSL} = w_{fFL} \frac{\theta_{amb}^{\mathrm{a}}}{\delta_{amb}^{b}} \exp\left(\mathrm{c} * M^{\mathrm{d}}\right) \tag{3}$$

$$\theta_{amb} = T_{amb}[K]/288.15 \tag{4}$$

$$\delta_{amb} = p_{amb}[Pa]/101325 \tag{5}$$

  It is possible to use exponential coefficients specifically tailored for the engine under study, although the original formulation of the method prescribes the following values: *a*=3.8, *b*=1, *c*=0.2, *d*=2.

- The $EINO_{xSL}$ values must be obtained from the ICAO Aircraft Engine Emissions Databank or estimated using appropriate modeling software. These values must then be curve-fitted as a function of the corrected fuel flow in SL conditions obtained in the previous step, W_{fSL}.
- Starting from the considered flight condition and the corresponding fuel flow at FL, it is possible to derive its value at SL using Eq. 3, and thus the corresponding value of $EINO_{xSL}$ based on interpolation from the previous step. Once $EINO_{xSL}$ is determined, it is possible to estimate $EINO_{xFL}$ using the following formulation:

$$EINO_{xFL} = EINO_{xSL} \left(\frac{\delta_{amb}^{d}}{\theta_{amb}^{e}}\right)^{f} \exp\left(H\right) \tag{6}$$

  Similar to the P3T3 method, it is possible to use exponent coefficients specifically tailored for the engine under study, although the original formulation of the method prescribes the following values: d=1.02, e=3.3, f=0.5. H is the humidity factor introduced previously for the

P3T3 method. Please note that, despite the BFFM2 appearing as a direct method, it is actually a ratio method because the parameters delta (δ) and theta (θ) represent the ratios between environmental conditions at varying altitudes and those under SL standard conditions.

3. Case study: Synergetic Air Breathing Rocket Engine fueled with Hydrogen

The Synergistic Air-Breathing Rocket Engine (SABRE) is the key component of the Skylon single-stage-to-orbit vehicle, enabling it to transition between air-breathing and rocket propulsion modes. This unique engine concept operates like a turbojet, utilizing hydrogen as fuel alongside atmospheric air, from take-off until reaching an altitude of 25 km, where it achieves a Mach number of 5. Once this speed regime is reached, the engine transitions to rocket mode, during which air is replaced by liquid oxygen (LO_x), ensuring optimal energy release during combustion to facilitate ascent to low Earth orbit. The transition to rocket mode occurs at an altitude where sustaining LH_2-Air combustion becomes impractical due to atmospheric conditions. The air-breathing mode reduces the onboard propellant requirement for Skylon, thereby enhancing payload capacity. The environmental benefits of this engine are evident as it produces no carbon emissions. However, it is important to assess the non-CO_2 emissions of this engine, particularly NO_x emissions, due to the potential effects of such emissions at high altitudes characteristic of high-speed and space access operations. This study focuses on the critical air-breathing phase of this engine, for which a brief summary is provided in Section 3.1 regarding the original state of the art in propulsion and emission modeling available to the authors. These models serve as references and are subsequently refined where necessary in Section 3.2, to generate updated propulsion and emission databases for the adaptation of the BFFM2 for estimating NO_x emissions from the engine.

3.1. State-of-the-Art in Propulsion and Emission Modeling

The propulsion model available to the authors was developed by G. Grimaldi [9] using Matlab to simulate the engine's operation during its air-breathing phase. The engine consists of four thrust chambers, two preburner-reheater units, two hydrogen turbo-pumps, two regenerators, and two helium circulators, each driven by a hydrogen turbine. To simplify, the model scales down the propulsion system by a quarter, representing only one unit of each component in the Matlab model, equivalent to 1/4 of the actual engine. Two fundamental assumptions are made: no incoming air is directed to the ramjet burners of the Skylon throughout the mission profile, and the intake maintains nominal pressure recovery while matching the mass flow required by the air compressor. Fig. 1 illustrates the model [9], featuring three distinct thermodynamic cycles: the complete air cycle, represented in blue, the hydrogen cycle in purple, and the regenerative helium cycle in green.

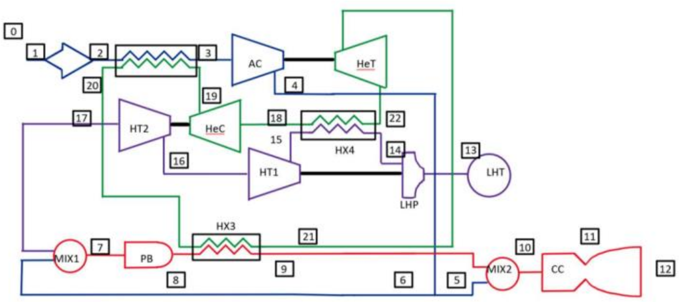


Fig 1. Cycle scheme of the complete model [9]

Regarding the emission modeling of the engine, the study reported in [10] has been used as a reference. This study [10] includes, in addition to a set of evaluated $EINO_x$ for the SABRE varying with

Mach, a strategy for updating the original formulation of the P3T3 method and its application to the SABRE case study. The proposed approach involves utilizing the propulsion database resulting from the model [9] to simulate the mixing and combustion processes using dedicated software. Specifically, Cantera, an open-source software for 0D/1D mathematical-chemical modeling, is employed under the Python interface. Cantera conducts 0D time-dependent simulations of homogeneous, isochoric, and adiabatic batch reactors with premixed gaseous reacting hydrogen/oxygen mixtures. For this purpose, the kinetic mechanism i.e., the Z24_NOx20 developed by the Swedish Defense Research Agency FOI modeling group was effectively utilized [10]. The 0D simulations of the preburner combustion were conducted under isobaric conditions, while the simulations for the combustion chamber were executed assuming isochoric conditions. Additionally, the composition of the exhaust gases leaving the preburner was employed as input for the combustion chamber after being mixed with the additional air stream from the intake. Consequently, a chemical kinetic Emission Inventory was compiled. The trend of the $EINO_x$ as a function of the calculated Mach, as computed in [10], is presented in Fig. 2.

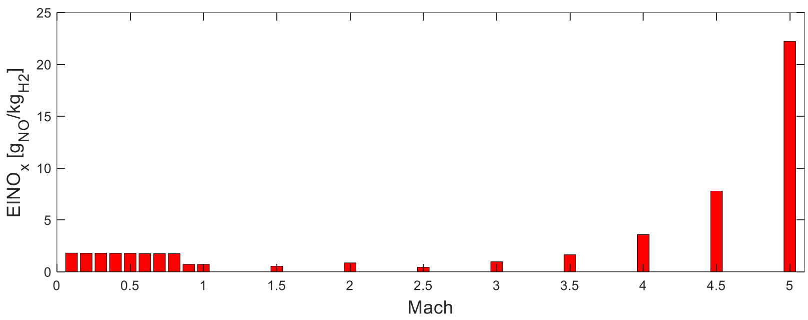


Fig 2. $EINO_x$ from Cantera 0D kinetic-chemical simulations [10]

3.2. Upgraded Propulsion and Emission Modeling

The Matlab propulsion model accessible to the authors [9] presents several potential areas for improvement to refine its sophistication. Specifically, it needs to be updated to integrate three main modifications: (i) the incorporation of the regenerative thermodynamic cycle of helium, (ii) an increase in sophistication in modeling thermodynamic equilibrium in the combustion chambers, and (iii) a new modeling approach for mixing processes that takes into account their chemical nature. The reference model [9] effectively encompasses and describes the primary engine cycle, specifically the air cycle. However, it does not incorporate the study and implementation of the helium auxiliary thermodynamic cycle. The regenerative helium cycle, crucial for thermal balance among gas flows in the engine, is particularly significant for deeply precooled combined cycles like the SABRE. Therefore, (i) the regenerative helium cycle has been integrated into the main model with the support of the Cantera software for studying the thermodynamic characteristics of the helium gas. Additionally, the reference model [9] adopts a conventional approach for modeling mixing and combustion processes within the SABRE, relying on enthalpy balances under isobaric and isochoric conditions. Although this enthalpy-based modeling yields reasonably accurate results, substantial enhancements can be achieved by integrating specialized software to address thermodynamic balance and equilibrium issues. The second modification, therefore, involved (ii) integrating the Matlab interface of the Cantera software into the propulsion model for evaluating chemical equilibrium in the combustion chamber. Finally, considering the high reliability of modeling through Cantera, (iii) mixing processes were also modeled using the Cantera software via its Python interface, which is more developed than its Matlab counterpart. The following figure presents propulsive parameters relevant for modifying the fuel flow method and input propulsive parameters for the emissive modeling of the engine. Specifically, emissive modeling requires as input the temperature and pressure profiles of the mixture entering the main combustion chamber. The trends of these two parameters resulting from the updated propulsion modeling are plotted as a function of Mach and compared with those resulting from the original propulsion model [9].

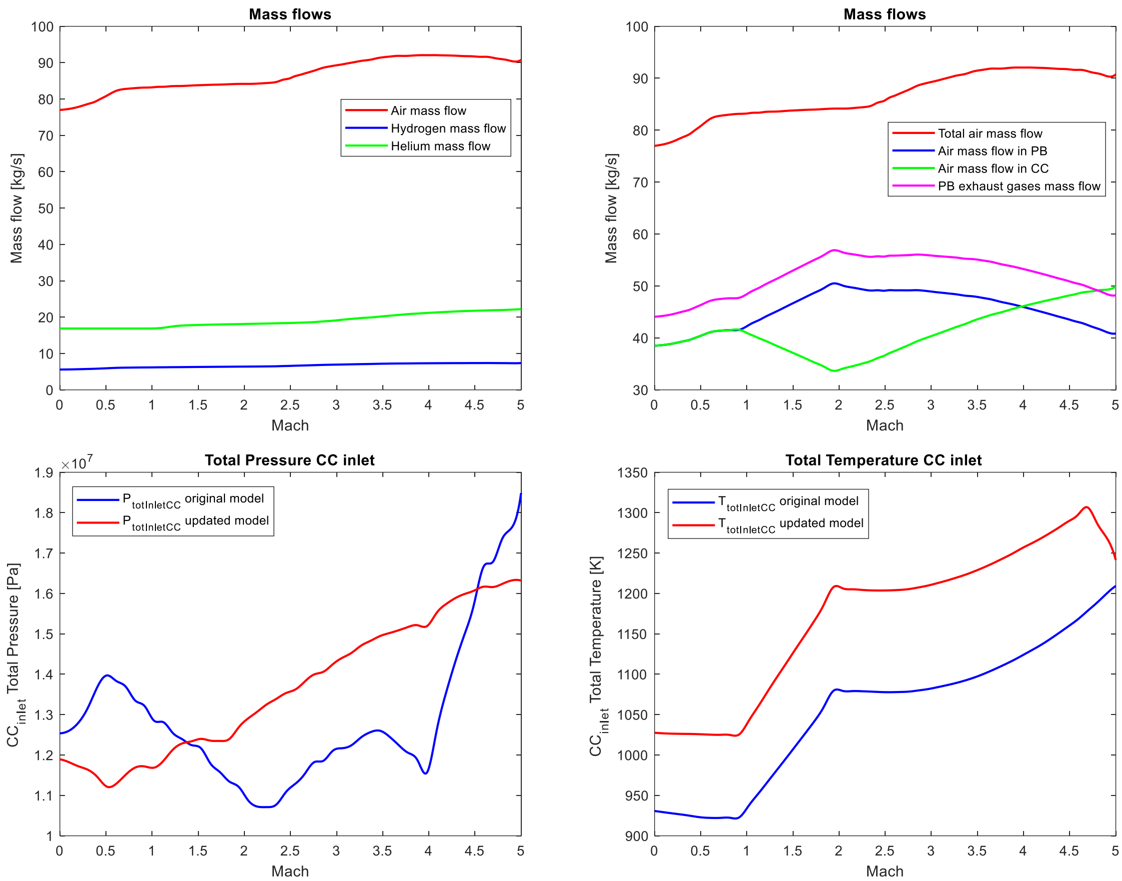


Fig 3. Propulsive parameters useful for emissive modeling and for modifying the Fuel Flow Method

In the case of emission modeling, what needs updating is not the modeling technique itself, which is considered correct and accurate for conceptual design, but rather the emissive database resulting from the application of this technique based on the propulsion database formulated using the model [9]. Regarding the upgraded chemical-emissive modeling of the engine, it is conducted via Cantera under the Python interface and remains unchanged from what was reported in [10]. In this case, as well, the kinetic mechanism i.e., Z24_NOx20 was successfully used. This mechanism is specialized for evaluating NO_x emissions resulting from hydrogen-air combustion. For the mixing processes, the attainment of chemical equilibrium conditions is simulated, while for combustion, both the chemical equilibrium of the mixed gases and their time-dependent kinetic-chemical evolution within ideal reactors are simulated. The $EINO_x$ values pertaining to the updated emissive database, derived from the recalculated input data using the proposed new propulsion model, are provided for comparison purposes in Fig. 4. An additional area of intervention in this context is the spacing of the evaluated $EINO_X$ over the Mach number. A homogeneous and denser spacing of the reference $EINO_X$ as the Mach number increases is indeed very useful, considering the involvement of curve-fitting functions in the update process of the FF method for estimating NO_x emissions. For this reason, in accordance with what has been implemented in the propulsion model for performance analysis, it has been decided to study fifty equispaced Mach conditions ranging from Mach 0.1 to Mach 5, also in the case of emissive modeling.

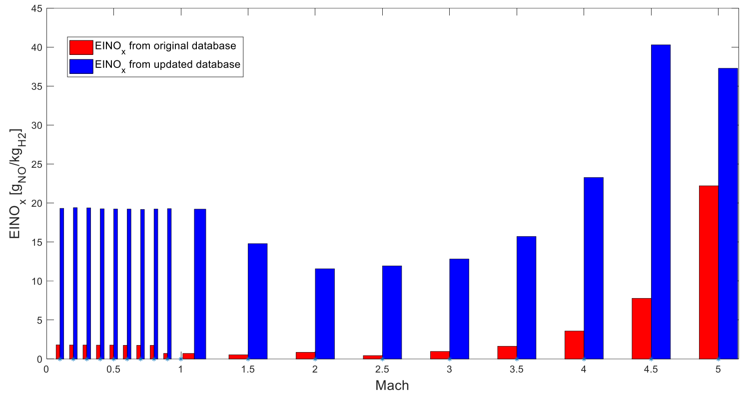


Fig 4. Comparison between $EINO_x$ from the original [10] and updated emissive databases

4. H2-FFM - New Formulations of the Fuel-Flow Method

Once both databases have been updated, it is possible to proceed with modifying the classical formulation of the fuel-flow method to adapt its applicability to the characteristics of the case study. As mentioned earlier, this adaptation and upgrade process from the original BFFM2 is carried out through two modifications: the addition of new parameters in the form of ratios between FL and SL conditions, along with the curve-fitting of the resulting mathematical formulations. The Mach, FAR, WFR, PBratio, and HEratio parameters are selected to be included in the mathematical relationship that calculates the $EINO_{xFL}$ as a correction of the $EINO_{xSL}$. In particular, (i) the Mach parameter is introduced to account for the effects of high speed, (ii) the FAR ratio is introduced to consider the decrease in the temperature reached during the fuel-rich combustion as a function of the increase in the fuel percentage, (iii) the PBratio parameter is introduced to account for the decrease in the temperature reached in the combustion chamber due to the segmented combustion of the SABRE, (iv) the WFR ratio, closely related and with the same trend as the PBratio, is introduced to consider the effect of decreasing temperature reached during combustion due to the presence of a water fraction at the inlet of the main combustion chamber resulting from the combustion stage in the PB, and (v) the HEratio parameter introduced to consider the increase in temperature reached in the chamber as a function of the thermal power that the engine must manage through the helium regenerative cycle. An increase in the temperature reached in the combustion chamber results in an increase in NO_x produced by the engine, as also demonstrated by the trends of the $EINO_x$ in Fig. 4, which faithfully mirror the trends of the adiabatic flame temperatures reached during combustion. Different combinations of parameters result in different curve-fitting optimization coefficients, calculated using the *lsqcurvefit* function in Matlab and referencing the updated emissive database's $EINO_{xFL}$. Each unique parameter combination thus yields different errors for the modified formulations. Considering the absence of certified standards for fuel flow and $EINO_x$ values at sea level conditions for the SABRE, the steps required for the application of the updated H2-FFM formulations to the case study can be summarized as follows.

As a first step, it is necessary to derive the fuel flow values at sea level by applying the following correction to the fuel flow values in FL conditions. The relationships are the same as those employed in the original version of the fuel-flow method. The equations are recalled below as Eq. 3, Eq. 4, and Eq. 5.

$$w_{fSL} = w_{fFL} \frac{\theta_{amb}^{\mathrm{a}}}{\delta_{amb}^{b}} \exp\left(\mathrm{c} * M^{\mathrm{d}}\right) \tag{3}$$

$$\theta_{amb} = T_{amb}[K]/288.15 \tag{4}$$

$$\delta_{amb} = p_{amb}[Pa]/101325 \quad (5)$$

The trend of the fuel flow profile at sea level, evaluated using the classical formulation of the BFFM2, exhibits an exponential increase with rising Mach numbers. Consequently, an initial correction is undertaken by recalculating the exponents of the original mathematical formulation through Matlab's curve-fitting functionalities. Given the absence of a standardized sea level fuel flow reference, a linear fit is created interpolating the first 4 fuel flow values corresponding to Mach conditions ranging from 0.1 to 0.4, representing the engine's operation at sea level altitudes. This fit is depicted in Fig. 5 alongside the values of W_{fSL} from the propulsive database. Evaluating the value of this linear fit for each Mach condition from 0.1 to 5, it is possible to recalculate the exponents *a, b, c* and *d* from Eq. 3 using the *lsqcurvefit* function in Matlab. The original and updated exponents are listed in Table 1. The profile of W_{fSL} as a function of Mach resulting from the application of the W_{fFL} correction with the updated coefficients is presented in Fig. 5.

Table 1 Original and updated exponents for fuel flow correction

	a	b	c	d
Original w_{fSL}= f(θ_{amb}, δ_{amb}, M)	3.8	1	0.2	2
Updated w_{fSL}= f(θ_{amb}, δ_{amb}, M)	0.0084	0.0207	0.0089	1.4917

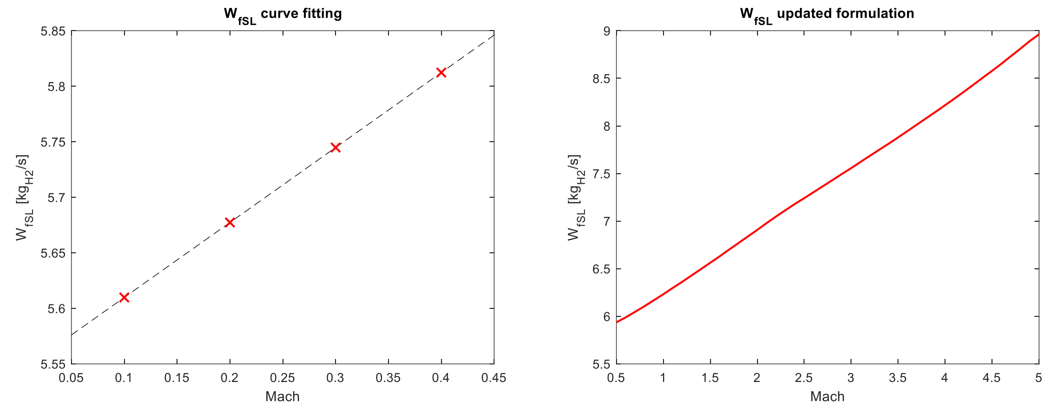


Fig 5. W_{fSL} linear fit and recalculated profile as a function of Mach

Once the correct profile of W_{fSL} varying with Mach is known, the second step of the methodology involves interpolating the parameters $EINO_{xSL}$, FAR_{SL}, $PBratio_{SL}$, WFR_{SL}, and $HEratio_{SL}$ as a function of the corrected W_{fSL}. Since certified standards for these values are not available, it is necessary to create linear fits of the data from the updated propulsive and emissive databases for the first three or four Mach conditions. For Mach conditions less than or equal to 0.4, the mission profile involves altitudes comparable to Sea Level. These fits for the sea level conditions are plotted in Fig. 6.

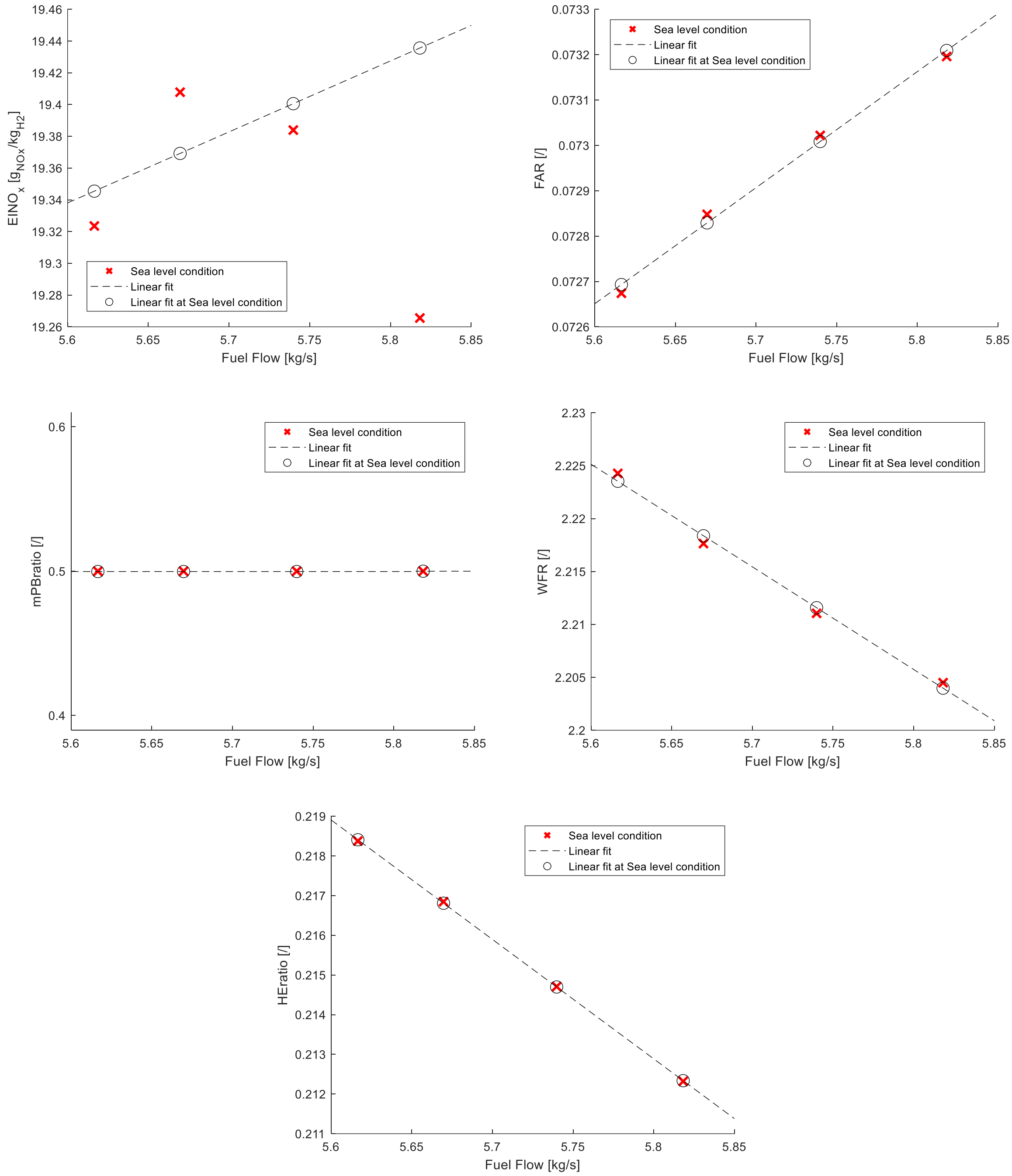


Fig 6. Fits at sea level conditions

Starting from the fits related to sea level (SL) conditions and drawing from the propulsive and emissive databases for the flight level (FL) conditions, it is possible to construct the ratios between SL and FL conditions. Once the ratios are determined, it is possible to evaluate the $EINO_{xFL}$ by correcting the values resulting from the $EINO_{xSL}$ fit using one or more of the ratios between SL and FL conditions. As an example, below are two of the mathematical formulations studied. The first one in Eq. 7 introduces the Mach parameter, which is the only parameter not expressed in the form of a ratio. The second one in Eq. 8 is the most complete formulation containing all the constructed ratios. All coefficients appearing in the formulations are optimized for the case study using the *lsqcurvefit* function in Matlab and the $EINO_{XFL}$ from the emissive database as a reference.

$$EINO_{FL} = k * EINO_{SL} \left(\frac{\delta_{amb}^{a}}{\theta_{amb}^{b}}\right)^{c} * M^{d} * \exp\left(H\right) \quad (7)$$

$$\mathrm{EINO_{FL}} = \mathrm{k} * \mathrm{EINO_{X\,SL}} \left(\frac{\delta^{a}_{amb}}{\theta^{b}_{amb}}\right)^{c} \left(\frac{\dot{m}_{HEratioFL}}{\dot{m}_{HEratioSL}}\right)^{r} \left(\frac{WFR_{FL}}{WFR_{SL}}\right)^{s} \left(\frac{FAR_{FL}}{FAR_{SL}}\right)^{t} \left(\frac{\dot{m}_{PBratioFL}}{\dot{m}_{PBratioSL}}\right)^{u} M_0^{d}\, e^{H} \tag{8}$$

What can be done is to add in the original formulations one, two, three, or all of the ratios of the new parameters introduced. As the number of ratios introduced in the formulations increases, one can expect an improvement in the accuracy of estimation. For each different combination of introduced parameters, it is possible to recalculate the exponent coefficients of the mathematical formulation starting from the initial guess of the original BFFM2 method, ensuring the best possible estimation of the reference $EINO_{xFL}$. The optimized coefficients, along with a discussion on their physical-chemical justification and the estimation results of the updated formulations, are reported in the next section.

4.1. Results and Discussion

The following tables report the optimized coefficients for the formulations given in Eq. 7 and Eq. 8. For comparison, the coefficients of the original BFFM2 formulation and those optimized without the introduction of any parameters are also included. All combinations of Mach with one, two, or three additional ratios have been tested, and generally, an increase in estimation accuracy is observed with the increase in the number of introduced ratios. Please refer to the first column of the tables to identify the corresponding mathematical formulation.

Table 2 $EINO_{xFL}$= f($EINO_{xSL}$, δ_{amb}, θ_{amb}, Mach)

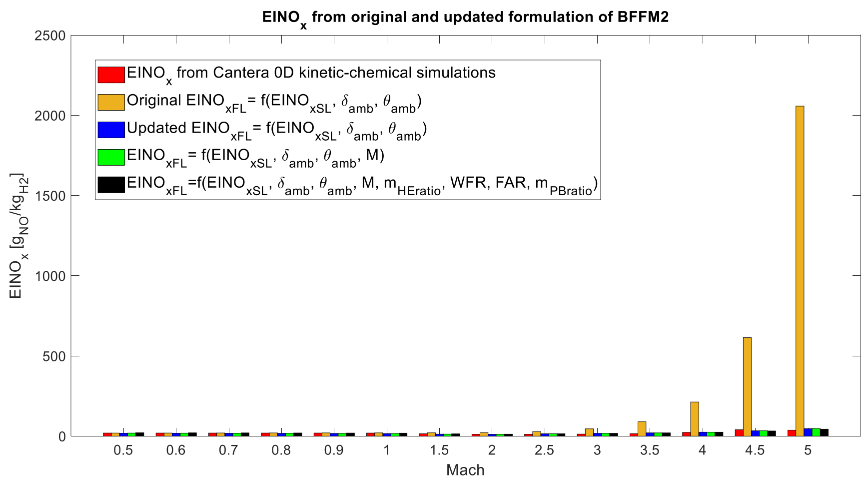
	k	a	b	c	d
Original $EINO_{FL}$= f($EINO_{SL}$, δ_{amb}, θ_{amb})	1	1.02	3.3	0.5	-
Updated $EINO_{FL}$= f($EINO_{SL}$, δ_{amb}, θ_{amb})	0.9541	0.3490	3.3380	-1.6738	
$EINO_{FL}$= f($EINO_{SL}$, δ_{amb}, θ_{amb}, M)	0.9429	0.2669	2.3982	-2.3701	-0.0943

Table 3 $EINO_{xFL}$= f($EINO_{xSL}$, δ_{amb}, θ_{amb}, Mach, $\dot{m}_{HEratio}$, WFR, FAR, $\dot{m}_{PBratio}$)

k	a	b	c	d	r	s	t	u
1.0000	0.2110	1.9797	-1.8745	-0.1714	0.4039	-0.9982	-0.0157	-0.8152

Overall, it is possible to observe a nearly constant trend in the optimized exponents as the number of parameters and ratios introduced in the new formulations increases. With the addition of each new ratio, the optimized coefficients for the ratios evaluated in the previous formulation are therefore validated by the non-oscillation of the recalculated coefficients. Considering the most complete formulation (Eq. 8), whose optimized coefficients are reported in Table 3, it is possible to derive some chemical-physical conclusions and justifications about the numerical values of these coefficients. Considering the ratios of temperature and pressure between ambient conditions and standard sea level (SL) conditions, the coefficients *a* and *b* result in positive values, while the coefficient *c* is negative. Regarding the pressure ratio, its value is less than one and it decreases with increasing Mach. Therefore, the combined effect of coefficients a and c results in an increasing contribution from the pressure ratio to the increase in EINOx as Mach increases. Concerning the temperature ratio, its value is less than one and it decreases with increasing Mach. In this case, the combined effect of coefficients b and c results in a decreasing contribution from the temperature ratio to the increase in $EINO_x$ as Mach increases. As Mach increases, the pressure and temperature at the engine inlet decrease according to the ISA standard, consequently reducing the respective ratios between FL and standard SL conditions. The increasing mathematical contribution of the pressure ratio with increasing Mach in the formulation for $EINO_{xFL}$ is not physically coherent. Indeed, a decrease in the pressure and temperature of the air entering the engine compared to standard SL conditions ideally translates to a decrease in temperature and pressure in the combustion chamber and therefore a decrease in the $EINO_x$ produced by the engine. However, in the case of the SABRE, its deeply precooled configuration, which involves a high compression ratio air compressor, means that the pressure and temperature conditions of the air entering the engine are not felt at the combustion chamber level. This justifies the unexpected contribution of the pressure ratio in the mathematical formulation, as well as the optimized negative coefficient of Mach that appears in almost all the formulations studied. Despite an expected increasing mathematical contribution of Mach with increasing speed in the updated formulations for $EINO_x$, such contribution instead decreases when the exponent d is less than 0. Again, the lack of memory of the flow in the combustion chamber with respect to the inlet conditions justifies the loss of information regarding the speed regime. Examining the FAR ratio term, the negative exponent value, along with the ratio between FL and SL conditions itself being below one and uniformly decreasing, mathematically demonstrates that this ratio term positively contributes to the formulation for calculating $EINO_x$ as Mach increases. This mathematical result is not consistent with what is expected physically. Indeed, as the Mach number increases, the FAR rises, leading to an increase in the hydrogen fraction in the combustion chamber. Since combustion occurs under conditions of FAR beyond stoichiometric, the adiabatic flame temperature decreases as the hydrogen fraction increases, consequently reducing NO_x emissions, at least ideally. The increasing contribution of the FAR ratio, which appears in the formulation in Eq.8 but not in all the studied formulations, may be due to the purely mathematical optimization performed in Matlab, which can result in sign oscillations for the optimized exponents as the number of introduced ratios in the formulations increases. Another justification for this unexpected contribution lies in the opposite trends presented by the FAR and the corresponding ratio between FL and SL conditions as the Mach number increases. As Mach and FAR increase, the FAR ratio decreases. This inconsistency may therefore originate from a superposition of errors in the various estimated SL fits involved in the evaluation of this ratio. On the contrary, the positive exponent of the ratio between FL and SL conditions of the parameter HEratio, combined with the ratio itself being above one and uniformly increasing with Mach, aligns with the physical expectations. An increase in the HEratio reflects a higher thermal load managed by the engine, thus leading to a higher temperature reached in the chamber and an increase in NO_x production. Regarding the ratio between FL and SL conditions of the parameter PBratio, its negative exponent, coupled with the value of the ratio itself above one and its segmented trend as a function of Mach that faithfully mirrors that of the parameter PBratio, is in line with physical expectations. An increase in the air flow to the preburner results in greater segmentation of combustion, leading to a reduction in the temperature reached in the main combustion chamber and consequently a decrease in NO_x production. The same reasoning applies to the ratio between FL and SL conditions of the parameter WFR, which exhibits a value above unity coupled with a negative exponent and demonstrates a segmented trend that faithfully mirrors that of the parameter PBratio. This configuration leads to a decreasing mathematical contribution in the formulation for $EINO_x$ as Mach increases up to Mach 2, followed by a decreasing mathematical contribution up to Mach 5. This behavior aligns with physical expectations and is attributed to the decrease in temperature reached in the chamber due to the presence of a significant fraction of water vapor in the incoming flow.

Finally, Fig. 7 compares the predictions from the various formulations reported in Table 2 and 3, illustrating the incremental reduction of error compared to the original method.



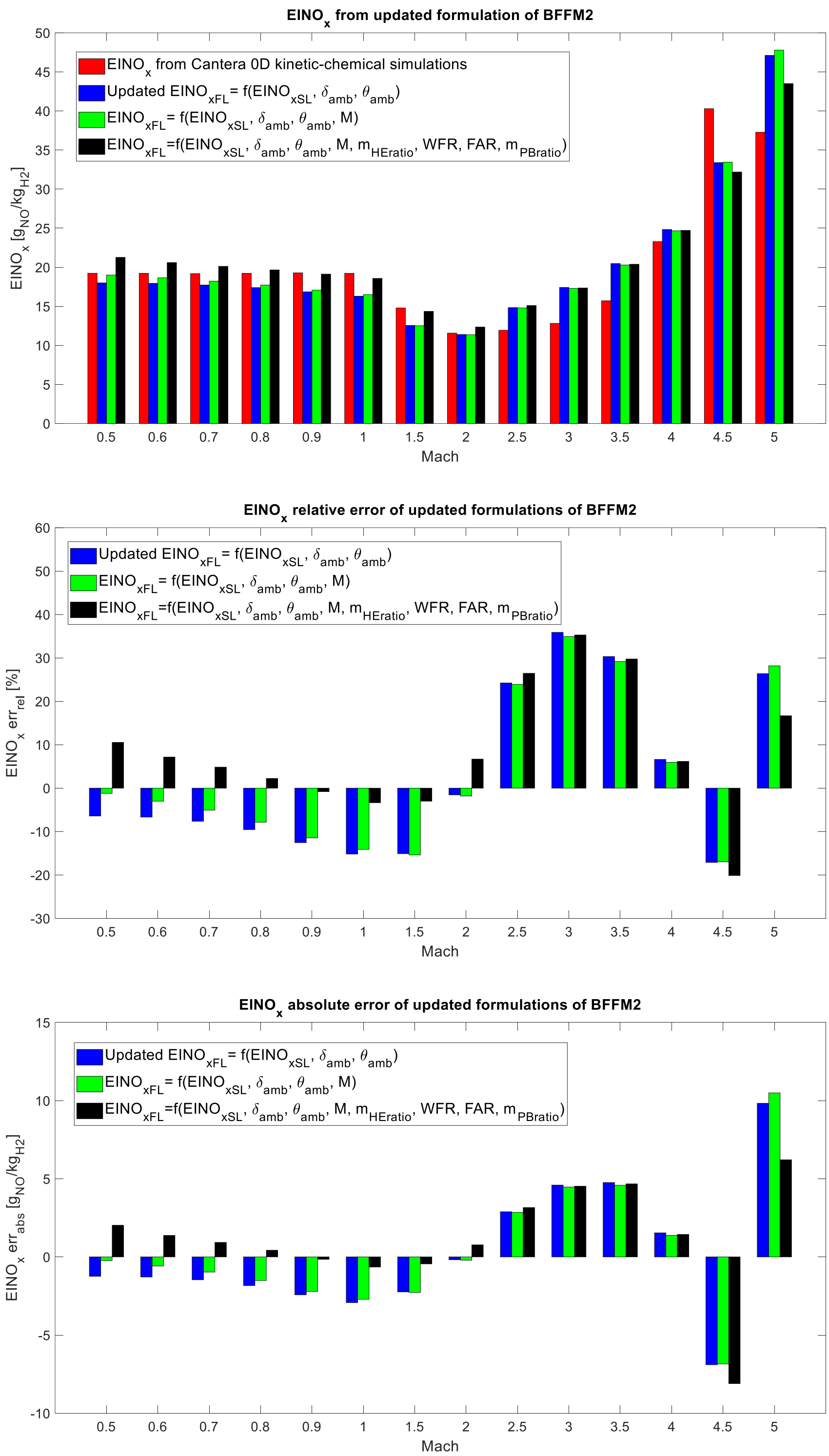


Fig 7. Comparison between $EINO_x$ reference and $EINO_x$ from different formulations of Table 2 and 3

Conclusions

In a context of growing demand for access to space, this paper introduces innovative analytical formulations aimed at estimating non-CO_2 emissions at the outset of the design process, with the goal to meet upcoming environmental requirements. Specifically, to forecast nitrogen oxide emissions during conceptual design, the authors developed the Hydrogen and High-speed Fuel Flow method (H2-FFM), an evolution of the original BFFM2 method, appropriately tailored for (i) advanced air-breathing propulsion systems for high-speed flights and (ii) environmentally friendly fuels, such as hydrogen. The paper outlines the step-by-step approach used to derive these innovative analytical formulations customized for the Synergetic Air Breathing Rocket Engine, revealing the existing correlation between nitrogen oxides production and key parameters including the Mach number, the Fuel-to-Air ratio (FAR), the airflow rate into the PreBurner (PBratio), the water flow rate into the main Combustion Chamber (WFR), and the helium flow rate used for regeneratively managing the engine's thermal load (HEratio).

The key achievements of this work can be summarized as follows:

- The paper introduces a methodology for updating the propulsive and emissive modeling of the SABRE, aimed at refining the fuel flow method for NO_x estimation from the SABRE engine. Currently, this innovative engine concept is still under study, making it particularly useful to generate increasingly accurate estimators for propulsive and emissive variables, given the absence of certified official databases. The accuracy of the data in the two updated databases, propulsive and emissive, is higher compared to that of the original databases.
- The innovative H2-FFM method adopts a methodology similar to the original BFFM2 approach, enabling the forecast of in-flight emissions based on emissions at sea-level conditions and the ratios between flight level and sea level conditions for air pressure and temperature at the inlet of the engine. However, the incorporation of new parameters into the analytical formulations alters the original method, introducing new contributions with the increase of Mach for each combination of parameters.
- The original BFFM2 method offers a single analytical formulation with adjustable parameters to effectively model various engine architectures. In contrast, the new H2-FFM method comprises multiple formulations tailored for the same engine architecture (SABRE). These diverse formulations generally exhibit an increasing level of accuracy across the entire Mach range as the number of introduced parameters increases. Having multiple formulations of the method characterized by varying errors, larger or smaller depending on Mach, allows for the selection of the estimation formulation based on the desired speed regime to be better modeled, thus rendering the method's application more flexible.
- The introduction of new factors to enhance the analytical formulations is based on the analysis of the engine architecture and the correlations between chemical and propulsion parameters with the formation of NO_x within the engine. This analysis is conducted with the aim of minimizing emissions by reducing the temperature reached in the chamber, which proves to be the determining parameter in NO_x formation from hydrogen combustion in high-speed aviation propulsive systems.
- To achieve estimation errors smaller than those characterizing the new H2-FFM formulations, an alternative is to apply the same updating methodology to the P3T3 method. This method, for which an update is currently being developed, originally relies on proprietary engine data, such as temperature and pressure at the inlet of the combustion chamber and is therefore likely to exhibit higher estimation accuracy if appropriately updated.

The proposed methodology can serve as a baseline for adapting analytical formulations to better represent other engine architectures, particularly regarding the integration of the two software used for propulsion and emission modeling. Finally, the developed analytical formulations can quantitatively support trade-off analysis during the propulsive architecture definition phase. Additionally, these new analytical estimation formulations can be valuable for reducing engine emissions even before they occur. In fact, integrating these simple formulations into emission minimization route optimization strategies can lead to emission reduction from the outset of the design process.

References

1. Lai, Y.Y., Christley, E., Kulanovic, A., Teng, C.C., Björklund, A., Nordensvärd, J., Karakaya, E., Urban, F.: Analysing the opportunities and challenges for mitigating the climate impact of aviation: A narrative review. Renew. Sustain. Energy Rev. 156, 111972, ISSN 1364-0321 (2022)
2. Grewe, V., Gangoli Rao, A., Grönstedt, T., Xisto, C., Linke, F., Melkert, J., Middel, J., Ohlenforst, B., Blakey, S., Christie, S., et al: Evaluating the climate impact of aviation emission scenarios towards the Paris agreement including COVID-19 effects. Nat. Commun. 12, 3841 (2021)
3. Chandrasekaran, N., Guha, A.: Study of Prediction Methods for NOx Emission from Turbofan Engines. J. Propuls. Power. 28, 170–180 (2012)
4. ICAO, ICAO. "Annex 16 Volume II Aircraft Engine Emissions." ICAO, Montreal, Canada, (2014)
5. DuBois, D., Paynter, G.C.: 'Fuel Flow Method2' for Estimating Aircraft Emissions. SAE Trans. 115, 1–14 (2006). Available online: https://www.jstor.org/stable/44657657. Accessed on 21 September 2023
6. Dinc, A.: NOx emissions of turbofan powered unmanned aerial vehicle for complete flight cycle. Chin. J. Aeronaut. 33, 1683–1691, ISSN 1000-9361 (2020)
7. Wang, Y., Yin, H., Zhang, S., Yu, X.: Multi-objective optimization of aircraft design for emission and cost reductions. Chin. J. Aeronaut. 27, 52–58, ISSN 1000-9361 (2014)
8. Fusaro, R., Viola, N., Galassini, D.: Sustainable Supersonic Fuel Flow Method: An Evolution of the Boeing Fuel Flow Method for Supersonic Aircraft Using Sustainable Aviation Fuels. Aerospace. 8, 331 (2021)
9. Grimaldi, G.: Development of a conceptual design tool to predict performance and pollutant and GHG emissions of high-speed vehicles using liquid hydrogen. Webthesis. http://webthesis.biblio.polito.it/id/eprint/20930 (2022)
10. Fusaro, R., Saccone, G., Viola, N.: NOx emissions estimation methodology for air-breathing reusable access to space vehicle in conceptual design. Acta Astronautica. 216, 304-317 (2024)