



Methods and tools for chemical emissions prediction for space launchers

Alessio Ricca¹, Valeria Borio², Roberta Fusaro³, Nicole Viola⁴, Guido Saccone⁵

Abstract

The present work aims to investigate the methods for estimating the chemical emissions generated by space launchers. After providing an overview of the current scenario of access to space in terms of technology and propellants employed, the work is focused on reviewing the emissions estimation tools available in the literature and on bridging their inherent shortcomings by developing new formulations. As a matter of fact, the majority of the available prediction methods are semi-empirical and they require a great number of input variables, some of which may not be yet known in the early design stage. Therefore, the objective of this work is to develop the propulsive model preparatory to derive novel emissions estimation formulations for space launchers, building from emissions estimation methods used for other categories of aerospace vehicles.

Keywords: *reusable access to space, emissions estimation, conceptual design*

Nomenclature

| | |
|--|---|
| Al ₂ O ₃ – Aluminium Oxide | LOX – Liquid Oxygen |
| BC – Black Carbon | LRE – Liquid Rocket Engine |
| C _D – Drag coefficient | MMH – Monomethylhydrazine |
| Cl - Chlorine | N ₂ - Nitrogen |
| CO – Carbon Monoxide | N ₂ H ₄ – Hydrazine |
| CO ₂ – Carbon Dioxide | N ₂ O – Nitrous Oxide |
| CH ₄ - Methane | NH ₄ ClO ₄ – Ammonium Perchlorate |
| EI – Emission Index | NO _x – Nitrogen Oxides |
| F – Wake growth factor | PBAN – Polybutadiene Acrylonitrile |
| H ₂ – Hydrogen | RF – Radiative Factor |
| H ₂ O – Water Vapour | RP-1 - Kerosene |
| HCl – Hydrochloric Acid | SRM – Solid Rocket Motor |
| HTPB - Hydroxyl-Terminated Polybutadiene | UDMH – Unsymmetrical Dimethylhydrazine |
| LH ₂ – Liquid Hydrogen | |

1. Introduction

In the last decade, access to space has become more and more frequent, with the number of annual launches increasing exponentially as shown in Fig 1 [1]. The Boom of the Space Economy [2] will lead to the construction of new satellite constellations and the advent of space tourism, likely causing a steady increase in the demand for access to space. In this scenario, it is of utmost importance to evaluate and minimize the environmental impact of rocket launches, both concerning emissions and the life cycle impact of the assets involved. Regarding chemical emissions, the products resulting from the combustion inside the rocket chamber can be divided into climate-altering substances and pollutants

¹ Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Turin, Italy, s291398@studenti.polito.it

² Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Turin, Italy, valeria.borio@polito.it

³ Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Turin, Italy, roberta.fusaro@polito.it

⁴ Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Turin, Italy, nicole.viola@polito.it

⁵ Italian Aerospace Research Centre, Via Maiorise, 81043 Capua, Italy, g.saccone@cira.it

based on their effect on the environment. Climate-altering substances act as greenhouse gases directly contributing to global warming and their impact is measured through the Radiative Factor (RF), which is the variation in energy flux in the atmosphere caused by natural or anthropogenic factors. On the contrary, pollutants affect the local air quality posing a potential threat to human health. Currently, the space sector is responsible for a limited contribution to global emissions compared to the aviation sector. For example, the impact of climate-altering emissions from the space sector is $16 \pm 8 \text{ mW m}^{-2}$ of the global Radiative Factor [3] whereas the contribution of aircraft emissions amounts to $149,1 \pm 79 \text{ mW m}^{-2}$ [4]. As a consequence, the environmental impact of rockets is often neglected with respect to other aviation emissions. However, differently from emissions from subsonic aviation which are confined to the upper troposphere, rocket emissions are distributed through the entire atmosphere, especially above the tropopause. In the upper layers, climate-altering substances and pollutants cannot be neglected anymore as they represent the only forms of pollution caused by humans and their effect on climate can vary significantly with respect to the lower altitudes.

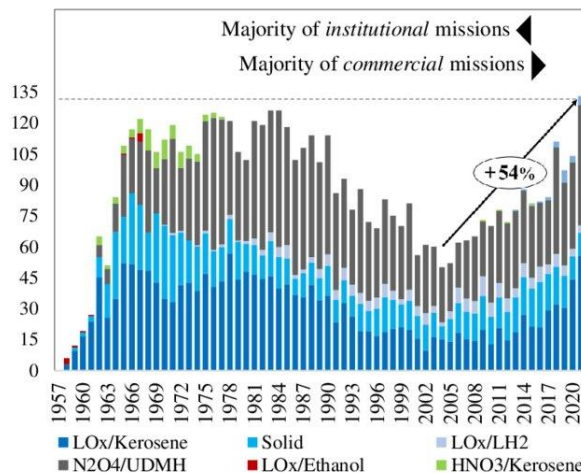


Fig 1. The trend of annual launches [1].

Here, the lifetime of the chemical compounds emitted reaches 3-5 years [5], thus enhancing the risk of particle accumulation [6]. Moreover, depending on the propellant used, rocket launches can emit more than a hundred more soot than traditional aircraft engines. Although they do not directly contribute to global warming, these types of pollutants impair air quality, potentially harming human health. Given the projected boom of the Space Economy [2], it is necessary to adopt a more sustainable approach to accessing space, both concerning the reusability of assets and the minimization of climate-altering emissions. Regarding the latter, it is of utmost importance to predict the chemical emissions generated by every launch, in order to assess their environmental impact since the conceptual design stage.

The target of this paper is to offer an extensive examination of the methodologies and tools presented in the literature for estimating rocket emissions. Additionally, the research endeavours to address existing gaps by introducing a novel semi-empirical formulation, with a specific focus on utilizing the SABRE engine in rocket mode as a case study. The work presented focuses in particular on the development of the propulsive model of the SABRE engine in rocket mode, which is preparatory for emission estimation, since the thermodynamic variables related to the engine cycle are required as input for the analytical predictive formulations. Furthermore, the work seeks to conduct a thorough analysis of a space mission, exploring its various aspects and considering multiple perspectives.

2. Overview of propulsive technologies and propellant combinations for space launchers

The emissions generated from launchers are dependent on the propulsive technology and on their chemical composition. For this purpose, space launchers can be divided into four categories based on the physical state of the oxidizer and fuel and the type of reaction between them. Solid Rocket Motor (SRM) launchers employ a solid grain formed with a mixture of powdered aluminium, which is the fuel, powdered ammonium perchlorate (NH_4ClO_4), as oxidizer, and a binder usually consisting of hydroxyl-terminated polybutadiene (HTPB) or polybutadiene acrylonitrile (PBAN). The advantages of this solution

are represented by its low complexity and ease of storage, while a major limitation is imposed by the difficulty in thrust throttling and the inability to shut down the engine once it is ignited. Liquid Rocket Engines (LRE) employ both fuel and oxidizer in their liquid state. Usually, the oxidizer consists of liquid oxygen (LOX), while different options are available in terms of fuel. The most common fuel is liquid hydrogen (LH₂), which is the best in terms of performance, but it can be substituted with kerosene (RP-1) or methane (CH₄). The latter is still being studied and tested in innovative engines. In the past years, hydrazine (N₂H₄) was largely employed as a fuel both as monomethylhydrazine (MMH) or unsymmetrical dimethylhydrazine (UDMH) [7], but it has gradually been abandoned since this substance has been proven to be potentially carcinogenic [8]. LREs allow to operate at different throttle levels but against a higher complexity of the technology involved. A possible solution seeking to combine the advantages of the above technologies is hybrid-propellant rocket engines, which involve the use of a liquid oxidant and a solid fuel. However, these engines are still under development. Finally, an additional solution in terms of propellant is represented by hypergolic propellants, which spontaneously ignite when fuel and oxidant come into contact [7]. The propulsive technology involved is very simple, but their performance is not optimal [6].

3. Overview of rocket emissions and their potential atmospheric impact

Various chemical emissions are obtained depending on the type of propellant used, as can be observed in Table 1, where the main products of each combustion process have been listed. In order to carry out a more detailed and precise analysis, it is necessary to take into account black carbon (BC), also known as soot, resulting from incomplete combustion of carbon-based propellants, unburned hydrocarbons and impurities in addition to the compounds listed in Table 1.

Table 1. Major primary emissions species for common rocket propellants [7].

| Type | Oxidizer | Fuel | Major Primary Emissions |
|--------|--|---|---|
| Liquid | LOX (O ₂) | Hydrogen (H ₂) | H ₂ O, H ₂ |
| | LOX (O ₂) | RP-1 (kerosene) | H ₂ O, CO ₂ , CO, H ₂ |
| | LOX (O ₂) | Methane (CH ₄) | H ₂ O, CO ₂ , CO, H ₂ |
| Solid | Ammonium perchlorate (NH ₄ ClO ₄) | Aluminum (Al) & HTPB or PBAN | Al ₂ O ₃ , CO, HCl, H ₂ O, N ₂ , CO ₂ , H ₂ , Cl, NO _x |
| | | Hydrazine (N ₂ H ₄), MMH or UDMH | N ₂ , CO ₂ , H ₂ O, CO, NO _x |
| Hybrid | Liquid (e.g., N ₂ O) | Solid (e.g., HTPB) | Varies (e.g., H ₂ O, CO ₂ , CO, H ₂ , N ₂ , NO _x) |

Rockets stand as the sole anthropogenic source of pollution in the upper layers of the atmosphere. Diverse effects emanate from these launches, with notable consequences including the depletion of the ozone layer and alterations to the atmospheric energy balance, contributing to climate change. The ozone layer is essential in absorbing most of the ultraviolet radiation from the Sun, yet it is a highly sensitive component of the atmosphere. Its depletion is attributed to interactions with nitrogen oxides (NO_x), as well as chlorine (Cl_x), bromine (Br_x), and hydroxyl (OH) radicals [6]. These combustion by-products are predominantly generated by Solid Rocket Motors (SRMs), which, being integral to the Space Shuttle as boosters, have been the focus of numerous studies examining their impact on the ozone layer, while other propulsion technologies have received less attention. Although Liquid Rocket Engines (LREs) have a significantly lower impact compared to solid propellants, the effects of LREs must also be considered since many current launch vehicles employ this technology. Research has been conducted on a local scale, analyzing these interactions. The presence of launch vehicles and the interaction of their exhaust with the surrounding atmosphere have a pronounced effect on atmospheric chemical composition changes: for example, the Delta II, utilizing liquid oxygen and kerosene, results in a 70-100% ozone depletion in the vicinity of its exhaust plume for approximately forty minutes, whereas the Ariane 5 can affect the ozone layer for up to four days [1]. Observations also indicate direct ecological impacts on wildlife and plant life in the vicinity of launch sites, particularly with the Space Shuttle emissions [6]. Beyond direct interactions with the ozone layer due to high temperatures in the exhaust plume, LREs indirectly affect the ozone through combustion products like Black Carbon (BC) and nitrogen oxides (NO_x). Global effects largely depend on the number of launches and, crucially, the ascent trajectories of the vehicles since combustion products may accumulate in specific regions of

the upper atmosphere, triggering mechanisms that alter its composition. An additional observed effect is the interaction between emissions, both gaseous and particulate, with solar radiation and Earth's infrared radiation. These substances can induce Radiative Forcing: a change in the planet's heating or cooling. Specifically, certain compositions of particles emitted into the atmosphere can aggregate and form a layer that induces a positive RF. For instance, black carbon causes warming in the troposphere but cooling in the stratosphere, with a net effect of warming the Earth's atmosphere [1].

One combustion by-product that cannot be overlooked is water vapor. While it poses no issue in the troposphere, its impact is significantly greater at higher altitudes, where it contributes to cloud formation in regions where clouds are particularly rare, consequently impacting climate and potentially obstructing communication with satellites [9]. A commonly adopted solution in launch vehicles involves the use of liquid oxygen and liquid hydrogen (LOX/LH₂) in the upper stages to achieve maximum performance, generating only water in the combustion process, excluding unburned components. In the case of the Space Shuttle, a single launch has been observed to cause a 10-20% increase in the mass of mesospheric clouds in the polar region. This aspect should not be disregarded, especially considering the expected rise in the number of launches in the near future. A recent study investigated a potential scenario with 10⁵ flights per year for the Skylon vehicle, analyzing the impact of water vapor on high-altitude clouds [10]. A 10% increase of water vapour concentration in the stratosphere and a 100% increase in the mesosphere are predicted, leading to a significant variation in RF.

The chemical substances described above are labelled as primary emissions, meaning they are formed as a direct product of the combustion process and subsequently released into the atmosphere. However, a proper emission assessment should consider also the chemical species formed due to the interaction between the rocket's wake and the atmosphere, which are usually referred to as secondary emissions [7].

4. Emission estimation techniques

Various simulation tools have been developed for emission estimation. One of the most widely known is the Chemical Equilibrium with Application (CEA) developed by NASA [11]. It is a software capable of analysing different problems, including those related to combustion, in launchers and rockets. Once some input parameters are provided, this tool is able to simulate the combustion process. As output, the software will provide the thermodynamic performance at various stations inside the rocket and the chemical composition expressed in molar fractions at the end of combustion. A major limitation of this software is represented by the fact that the simulation of the combustion process is performed under the assumption of reaching a sequence of chemical equilibrium states. This hypothesis makes the tool unable to consider the formation of compounds such as BC, which are generated from non-equilibrium situations and non-homogeneous mixing. Furthermore, this software does not consider the interaction effects between the high-temperature wake and the surrounding atmosphere. A solution to make up for these shortcomings was implemented in [7] by considering secondary emissions, with whom the values obtained from CEA are corrected, providing therefore a more complete solution. However, in [7], secondary emission indexes (EI) are obtained by fitting experimental data found in literature. Consequently, the final relations obtained are semi-empirical, and therefore dependent on high-fidelity or experimental data.

Alternatively, the emissions estimation for space launchers can be carried out through high-fidelity simulations of the rocket operations. The results of these simulations are the most reliable, but they are not feasible in the conceptual design stage as they require information that is typically not yet available at the early stages of the design process.

As presented, the current literature offers very limited methodologies for assessing rocket emissions. To address these gaps, a potential approach would involve expanding existing methodologies for preliminary emissions estimation developed for the aeronautical field to the space access domain. Specifically, the novel formulations should be derived by considering both the flight altitude and the chemical composition of the atmosphere. Among the existing prediction methods, the P₃-T₃ method and the fuel flow method are the most widely used due to the simplicity of their formulations and they have therefore been selected to be upgraded. In particular, the P₃-T₃ method is the most accurate of the analytical predictive models, allowing the calculation of emission indices (EI) in operational conditions based on those calculated at ground level, leveraging the conditions at the combustor inlet for both datasets. Specifically, as illustrated in Fig 2, according to the original P₃-T₃ formulation, the sea level values of combustor inlet pressure (p_3), Fuel-to-Air Ratio (FAR), and EINO are extracted from

the ICAO database and they are plotted against the combustor inlet temperature (T_3). The profiles resulting from the interpolation of these data are then used to obtain the values of p_3 , T_3 , and FAR at flight conditions. Knowing the sea level and flight level data, the flight level NO_x emission indices can be determined using the formulation:

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

where H represents the humidity factor, which depends on the atmospheric conditions at flight altitude. The main issue raised by the implementation of the P_3 - T_3 method is that it requires the knowledge of proprietary data, which is usually difficult to obtain especially in the early design stages. A solution to this problem is provided by the Boeing Fuel Flow Method 2 (BFFM2), which is a predictive method derived from the P_3 - T_3 which does not require proprietary data. The original formulation of the BFFM2 method is:

$$EINO_{FL} = EINO_{SL} \left(\frac{\delta_{amb}^{1.02}}{\theta_{amb}^{3.3}} \right)^{0.5} \exp(H) \quad (2)$$

where δ_{amb} and θ_{amb} are the ratio of ambient temperature and pressure with respect to standard conditions [12].

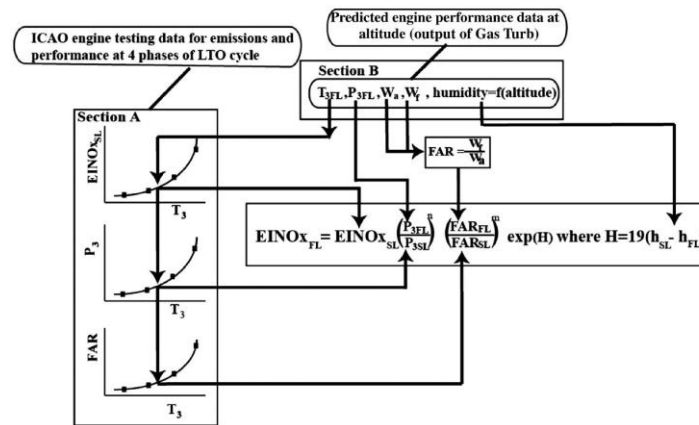


Fig 2. Schematic representation of the operational methodology for the P_3 - T_3 method [12].

In both the P_3 - T_3 and the BFFM2 methods, an emissive database is required in order to extract the values of EINO at sea level conditions to be used as a parameter in the formulations. Moreover, in the context of extending these methods formulations to access-to-space vehicles, the emissive database also serves as a target for deriving the upgraded formulations. Since the emissions of a general engine are directly related to the combustion efficiency, it is necessary to estimate the propulsive performance through experimental campaigns or mathematical/numerical modelling. The simulation of the thermodynamic cycle is also useful to extract the input variables of the P_3 - T_3 method, i.e. the conditions at the inlet of the combustion chamber.

5. Methodology

The methodology proposed to develop new emissions estimation methods is shown in Fig 3 and it is tailored on the Synergetic Air Breathing Rocket Engine (SABRE) in rocket mode, considered here as the case study [13]. In accordance with the conceptual framework depicted in Fig 3, the objective of this paper is to develop a propulsion system model for the SABRE engine in rocket mode, from which a propulsive database will be built. This step is preparatory for the creation of the emissive database, which in this work will be computed with the Cantera software [14]. Cantera is an open-source software capable of performing 0D/1D chemical thermodynamic/kinetic simulations in several kinds of reactor models including homogeneous, isochoric and adiabatic batch reactors. Since for the case study the combustion process does not produce NO_x, the Cantera software is employed in this work to model the interaction between the rocket exhaust gases and the atmospheric air, providing as input the data contained in the propulsive database. Employing this tool, we will develop a systematic approach for

generating a comprehensive emissions database, which in turn will be essential to develop new emissions estimation methods.

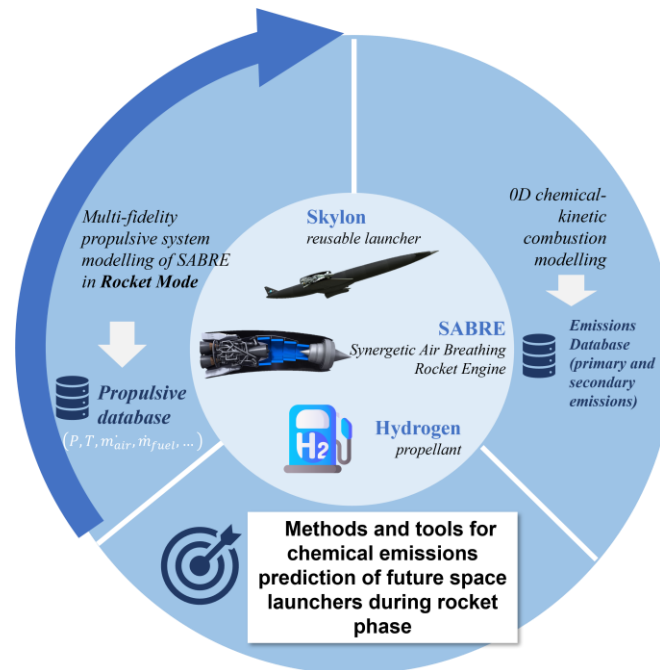


Fig 3. Methodology proposed for the development of new methods and tools for rocket emission estimation.

6. Case study

The Synergetic Air-Breathing Rocket Engine (SABRE) is used as case of studies for this paper. Developed by Reaction Engines Ltd in the United Kingdom, this cutting-edge propulsion system is set to propel the Skylon spaceplane, an innovative concept for a fully reusable Single Stage To Orbit (SSTO) spaceplane. A distinctive feature of Skylon is its ability to take off and land on an extended runway, akin to conventional airplanes. This characteristic simplifies its operational management, allowing for preparation in hangars and easy transportation without the need for complex and expensive ground equipment typical of other launch vehicles. In contrast to conventional spaceplane designs, Skylon features a pronounced division between its slim fuselage and wing. While this design optimizes weight, lift, and volume factors, it introduces challenges during re-entry, resulting in elevated localized heat fluxes. To address this, an active cooling system has been implemented. The core of the Skylon development project is the SABRE engine, an acronym for Synergetic Air-Breathing Rocket Engine, which is conceived to be the primary propulsion system for the Skylon vehicle [15]. The propulsive concept of SABRE engine evolves from the British Aerospace HOTOL and from the Liquid Air Cycle Engine (LACE), eliminating the need for air liquefaction [16]. The engine's unique capability lies in the possibility of performing the entire ascent phase with the same engine operating in different modes. As a matter of fact, the SABRE functions as an air-breathing engine during the initial ascent phase, up to an altitude of approximately 25 km and a velocity corresponding to Mach 5. As the air becomes too rarefied, the SABRE engine transitions to a pure rocket mode, where both fuel and oxidizer are onboard consumables. This advanced propulsive concept aims at combining the advantages of air-breathing and rocket engines, offering low propellant consumption in the first phase and high delivered thrust, leading to a substantial reduction in total weight. The SABRE engine uses liquid hydrogen (LH₂) as a fuel in both operating modes while the oxidizer changes from atmospheric air in airbreathing mode to liquid oxygen (LOX) in rocket mode [15].

7. The modeling of the SABRE engine in rocket mode

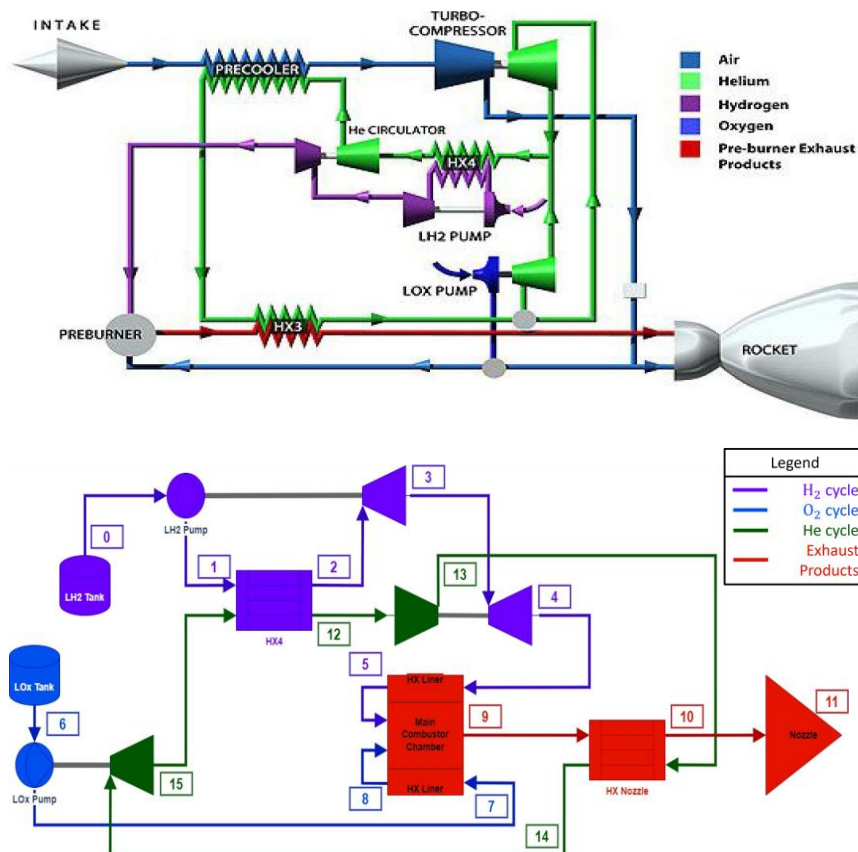


Fig 4. Combined cycle of SABRE engine [17] (top) and working cycle for the rocket mode (bottom).

In the air-breathing phase, the airflow entering the engine is channelled into the intake and then into the pre-cooler, which is expanded the operational envelope by extracting heat from the incoming flow and simultaneously transferring it to the helium. With the pre-cooler and heat exchanger HX3, the helium has sufficient energy to self-power its circuit and provide the necessary energy to the air compressor. The pre-cooled air can be compressed to high enough pressures to be fed into a rocket combustion chamber, divided into a pre-cooler and main chamber. The exhaust gases are then expelled through the nozzle. When the transition to rocket mode occurs, the engine cycle changes: the intake is closed, and the airflow from the external environment is replaced by the oxygen stored in the tanks. The pre-cooler is removed, as well as the turbo-compressor [18].

Due to the limited descriptions of the rocket phase in the official documents released by Reaction Engines Limited, the rocket mode cycle has been modelled by assuming typical rocket operations. The development of the propulsive model of the SABRE engine in rocket mode is preliminary for the creation a propulsive database and consequently of an emissive database. A 0D thermodynamic model has been developed based on the combined cycle considered for the air-breathing phase of the same engine [19]. In the selected rocket cycle, shown in Fig 4, particular attention has been paid to the modelling of the heat exchangers. Specifically, with respect to the air-breathing mode, a nozzle heat exchanger has been introduced in the rocket cycle, with the tasked transferring the heat from the nozzle walls to the helium, in order to control the nozzle temperature and prevent component damage. Additionally, the combustion chamber liner is cooled by the propellants. The mixing and combustion processes have been simulated both through a purely thermodynamic approach, i.e., with a simple power balance, and by using the Cantera software. The latter solution provides a more accurate assessment of the behaviour of these components because it considers the chemical kinetics of the process, whereas the thermodynamic approach is easier to use when no data is available. Furthermore, the entire helium circuit was modelled through the implementation of the Cantera software in Matlab. Liquid hydrogen and liquid oxygen were managed using a thermodynamic model also implemented in Matlab [20].

Considering the initial conditions of the LH₂, LOX, and helium inside the tanks, the thermodynamic cycle was simulated and the propulsion database was populated. In addition, some variables were assumed in order to proceed to cycle resolution, such as pressure in the combustion chamber and temperatures straddling the heat exchangers: the latter were assumed from the results obtained in [18] under the transition conditions between the air-breathing and rocket phases. A parametric analysis was conducted based on the mixture ratio. In particular, a series of simulations have been run with the mixture ratio varying between 3 and 8, which represents respectively the optimal mixture ratio for effective exhaust velocity (*c*) and the stoichiometric ratio that maximizes the flame temperature.

8. Re-entry Phase

As mentioned above, nitrogen oxides are not only generated by primary and secondary combustion emissions but also during the re-entry phase, which therefore plays a crucial role in this analysis. Due to the high orbital velocities reached by the Skylon vehicle during the descent phase, particle collisions upon impact with the atmosphere raise the temperatures downstream of the vehicle to values exceeding 1800 K, which Zeldovich has identified as the threshold between the formation or non-formation of nitrogen oxides according to the thermal route [21]. The Zeldovich NO_x formation mechanism has been selected in this case study as it is the prevalent one at high temperatures and lean mixture conditions. However, two other routes for NO_x formation are available, namely the Fenimore mechanism and the formation through N₂O, which become relevant for high-temperature rich mixtures and low-temperature lean conditions respectively [22]. This temperature is determined by the energy required to break the triple bond present in the nitrogen molecule (N₂), which then allows the formation of nitrogen oxides. In an effort to estimate the emissions produced during re-entry, this work aims to reproduce the analysis conducted by Park on the Space Shuttle re-entry phase updated to the re-entry of the Skylon [23, 24]. The analytical methods considered in the original paper are the *trailing edge-freezing* and the *wake-freezing* model. The first one assumes that chemical reactions terminate at the leading edge of the aircraft due to the strong expansion generated. However, this method is thought to be overly simplistic. Therefore, the *wake-freezing* model is preferred in this analysis, as it considers that reactions can continue downstream of the spaceplane's leading edge. As a matter of fact, the strong expansions that occur are countered by recompressions and turbulent motions that in turn generate heat, allowing the reactions to proceed. At a certain distance from the aircraft, the temperature will reach a characteristic value such that the reactions will stop: this point is known as the *freezing-point*. The *wake-freezing* method is a two-step process: the first step defines the molar fraction of nitrogen oxides generated at the *freezing-point* downstream of the aircraft's passage. The second step calculates the entire volume of air encountered by the aircraft and within which the reactions take place. This quantity must be multiplied by the wake growth factor (*F*), which takes into account the increase in the frontal section due to the turbulent motions generating mixing between the wake and the surrounding atmosphere.

The validity of the method presented by Park depends on the fact that the vehicle is treated as a triangular flat sheet with an area equal to the exposed surface of the aircraft during the re-entry phase, which depends on the angle of attack maintained during the trajectory. The air swept by the vehicle can be estimated by considering the energy conservation, equating the contribution of the drag on the vehicle to the variation of its kinetic energy:

$$\frac{1}{2} C_D \rho U^2 A ds = \frac{1}{2} M d(U^2)$$

Isolating the frontal area (*A*) and the density (ρ) and integrating the expression on the descent segment, the following expression is obtained:

$$\int_{s_1}^{s_2} \rho A ds = 2 \frac{M}{C_D} \ln \frac{U_1}{U_2} \quad (3)$$

where *M* indicates the mass of the aircraft in the descent phase which is assumed to be constant while *U*₁ and *U*₂ are the velocities at the initial and final instants respectively. The result of the integral of Eq. (3) gives the air swept by the aircraft. The drag coefficient (*C*_D) is obtained using Newton's approximation in the hypersonic field:

$$C_D = 2 \sin^2 \alpha$$

The freezing point is selected corresponding with the distance that maximises the mole fraction of nitrogen oxides, in order to consider the worst-case scenario. Furthermore, the NO_x mole fraction is assumed to remain constant throughout the descent phase and equal to 1.951% [23]. The product of the air swept by the aircraft, the wake growth factor and the mole fraction of the nitric oxide provides an estimate of the emissions generated during re-entry. Considering the hypotheses presented above, two boundary trajectories with incidence angles of 25 and 40 degrees are considered, resulting in a NO_x production of 4215 and 5056 kg per Skylon flight, respectively.

9. Conclusions and future development

Thanks to the propulsive model developed, the performance of the SABRE engine in rocket mode has been evaluated and the related propulsive database has been obtained. This is preparatory for the creation of an emissive database. As a matter of fact, the rocket performance determines the composition of the exhaust gases, which in turn influences the NO_x emissions level resulting from the recombination of the rocket plume with the atmospheric air. In order to perform a more exhaustive assessment, the emissions generated in the re-entry phase should also be included. The approach presented provides a preliminary NO_x estimation for the re-entry phase, which could be further investigated considering a specific descent trajectory, if the related data would be available.

References

1. Sirieys, E., Gentgen, C., Jain, A., Milton, J., de Weck, O.: Space sustainability isn't just about space debris: On the atmospheric impact of space launches. MIT Science Policy Review, 3 (2022). <https://doi.org/10.38105/spr.whfig18hta>
2. Morgan Stanley: Space: Investing in the final frontier. Morgan Stanley. <https://www.morganstanley.com/ideas/investing-in-space>. Accessed October 2023
3. Ross, M. N., Sheaffer, P. M.: Radiative forcing caused by rocket engine emissions. Earth's Future, 2 (2014). <https://doi.org/10.1002/2013EF000160>
4. Tait, K.N., Khan, M.A.H., Bullock, S., Lowenberg, M.H., Shallcross, D.E.: Aircraft Emissions, Their Plume-Scale Effects, and the Spatio-Temporal Sensitivity of the Atmospheric Response: A Review. Aerospace, 9 (2022). <https://doi.org/10.3390/aerospace9070355>
5. Waugh, D., Hall, T.: Age of stratospheric air: Theory, observations and models. Rev. Geophys., 40 (2002). <https://doi.org/10.1029/2000RG000101>
6. Dallas, J.A., Raval, S., Alvarez Gaitan, J.P., Saydam, S., Dempster, A.G.: The environmental impact of emissions from space launches: A comprehensive review. Journal of Cleaner Production (2020). <https://doi.org/10.1016/j.jclepro.2020.120209>
7. National Academies of Sciences, Engineering, and Medicine: Commercial Space Vehicle Emissions Modeling. The National Academies Press (2021). <https://doi.org/10.17226/26142>
8. Carlsen, L., Kenessov, B.N., Batyrbekova, S.Ye.: A QSAR/QSTR study on the human health impact of the rocket fuel 1,1-dimethyl hydrazine and its transformation products: Multicriteria hazard ranking based on partial order methodologies. Environmental Toxicology and Pharmacology, 27 (2009). <https://doi.org/10.1016/j.etap.2009.01.005>
9. Ch. Voigt, U. Schumann, K. Graf, K.D. Gottschaldt: Impact of rocket exhaust plumes on atmospheric composition and climate – an overview (2013). <http://dx.doi.org/10.1051/eucass/201304657>
10. E.J.L. Larson, R.W. Portmann, K.H. Rosenlof, D.W. Fahey, J.S. Daniel & M.N. Ross: Global atmospheric response to emission from a proposed reusable space launch system (2017). <https://doi.org/10.1002/2016EF000399>
11. NASA, CEARUN: <https://cearun.grc.nasa.gov/index.html>
12. Chandrasekaran, N., Guha, A.: Study of Prediction Methods for NO_x Emission from Turbofan Engines. Journal of Propulsion and Power 28:1, 170-180 (2012)

13. Reaction Engines Ltd.: SABRE. The engine that changes everything. <https://reactionengines.co.uk/advanced-propulsion/sabre/>. Accessed October 2023
14. Goodwin, D.G., Moffat, H.K., Schoegl, I., Speth, R.L., Weber, B.W.: Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. (Version 2.6.0). Zenodo (2022). <https://doi.org/10.5281/zenodo.6387882>
15. Reaction Engines Limited: SKYLON User's Manual (2014).
16. Borg, K., Matula, E.: The SKYLON Spaceplane, University of Colorado, Boulder, CO, 80309, USA.
17. Aggarwal, R., Lakhara, K., Sharma, P.B., Darang, T., Jain, N., Gangly, S.: SABRE Engine: Single stage to orbit Rocket Engine (2015). https://www.researchgate.net/SABRE_ENGINE_Single_Stage_to_Orbit_Rocket_Engine
18. Villacé, V.F. Master's Degree Thesis: Simulation, Design and Analysis of Air-Breathing Combined-Cycle Engine for high speed propulsion (2013).
19. Grimaldi, G. Master's Degree Thesis: Development of a conceptual design tool to predict performance and pollutant and GHG emissions of high-speed vehicles using liquid hydrogen (2021)
20. Mjaavatten, A.: User guide for matlab class thermo. (2020) <https://github.com/are-mj/thermodynamics>
21. Zeldovich, Y.B., Sadonikov, P.Y., Frank-Kamenetskii, A.: Oxidation of nitrogen in combustion, Academy of sciences of URSS, Institute of Chemical Physics, Moscow, Russia (1947).
22. Warnatz, J., Maas, U., Dibble, R.: Combustion: Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation. Springer (2006)
23. Park, C.: Estimates of nitric oxide production for lifting spacecraft re-entry (1975). [https://doi.org/10.1016/0004-6981\(76\)90171-2](https://doi.org/10.1016/0004-6981(76)90171-2)
24. Park, C., Rakich, J.V.: Technical Note, Equivalent-Cone Calculation of nitric oxide production rate during space shuttle re-entry (1979). [https://doi.org/10.1016/0004-6981\(80\)90011-6](https://doi.org/10.1016/0004-6981(80)90011-6)