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Kinetic Combustion Modelling for Aero-thermodynamic Coupled Code Applied to Scramjet Vehicles

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Abstract

The Italian Aerospace Research Centre – CIRA in collaboration with several European organizations, coordinated by Politecnico di Torino contributed to an international project, called Stratospheric Flying Opportunities for High-Speed Propulsion Concepts – STRATOFLY and financed by EC Horizon 2020 programme. This project regarded the field of air-breathing hypersonic scramjet vehicles design and development and was pursued in order to improve the enabling technologies for realization of a commercial hypersonic aircraft able to flight at Mach 8, at 30÷35 km of altitude, for at least 4 hours with a minimum environmental impact and especially low NOx emissions In this framework, an enhanced comprehension of the multidimensional, supersonic, turbulent, combustion processes occurring during scramjet operations is of paramount importance. For this purpose, a thorough 0D/1D kinetic assessment of hydrogen oxidation and reaction with air was carried out by means of both the open-source Cantera software and the CIRA in-house aero-thermodynamic/aero-propulsive code, denominated Scramjet PREliminary Aerothermodynamic Design – SPREAD. The first tool was used for the identification of the most suitable kinetic mechanisms, able to predict with a satisfactory accuracy the ignition delay times and the NOx emissions at the most relevant scramjet operating conditions. Otherwise, the second was aimed to study in real-time several engine/aircraft configurations of air-breathing, hypersonic scramjet vehicles and to model either in a single approach either as a whole the main tail-to-nose components of the aircraft The kinetic assessment was validated by means of comparison of the ignition delay times predicted using three chemical models especially conceived for hydrogen/air supersonic combustion with the experimental measurements accomplished in shock tubes. Instead, 1D SPREAD results were computed to reproduce with satisfactory reliability vehicle performances at nominal conditions. Special emphasis was paid on physical-chemical modelling of hydrogen-air combustion, through preliminary identification and implementation of suitable detailed, skeletal and reduced mechanisms for hypersonic combustion, by means of zero-dimensional, kinetic analysis.

Keywords: *aero-thermodynamics, scramjet, hydrogen-air combustion, zero-dimensional kinetic analysis.*

Nomenclature

c_p	- specific heat at constant pressure
h	- enthalpy
m	– mass
$\dot{m}$	- total mass flow rate
M_w	– molar amount
NR	– number of reactions
NRS	– number of the chemical reacting species in the mixture

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p – pressure
$\dot{Q}$ – heat transfer rate
R – reaction rate
T – temperature
S – shift of the injection point
t – time
V – volume
Greek Symbols
v – stoichiometric coefficient
ρ – density
Subscripts
i – i^{th} chemical species
j – j^{th} forward reaction
-j – j^{th} backward reaction
mix – referred to the overall reacting mixture
Superscripts
` – reactants
“ – products

1. Introduction

In the field of air-breathing hypersonic scramjet vehicles design and development, the Italian Aerospace Research Centre – CIRA contributed to an international project, called Stratospheric Flying Opportunities for High-Speed Propulsion Concepts – STRATOFLY, in collaboration with several European organizations, coordinated by Politecnico di Torino under the EC Horizon 2020 programme financial support. Aim of this project is the improving of enabling technologies for realization of a commercial hypersonic aircraft able to flight at Mach 8, and 30÷35 km of altitude, for at least 4 hours with a minimum environmental impact and especially low NO_x emissions.
In hypersonic vehicles the separation between the engine and the aircraft is not so evident as for the conventional subsonic and supersonic configurations. In fact, as shown in Figure 1, the whole lower surface of the forebody can be used as an intake and the burned gases exiting the combustor can expand along the entire afterbody, thus providing the necessary thrust for flight.

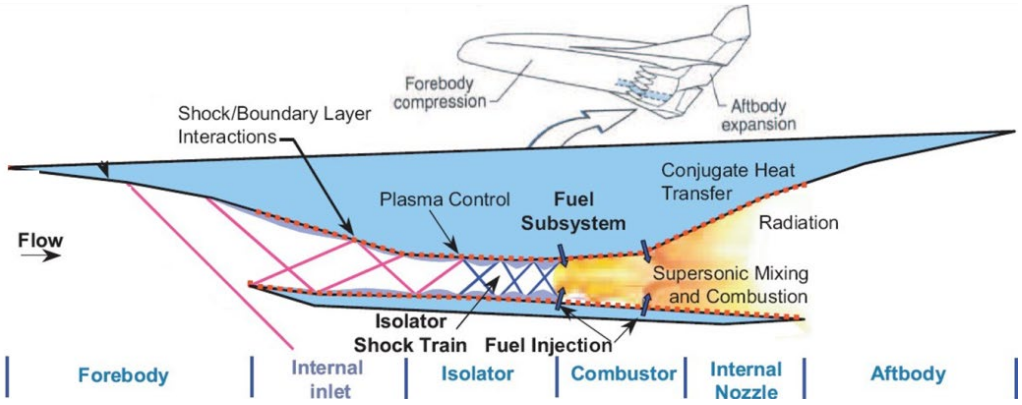

Fig 1. Schematic view of a hypersonic air-breathing engine vehicle

Due to the strong coupling between the aerothermodynamic and propulsive flow fields, an accurate prediction of the engine’s performance can only be attained by means of CFD simulations and wind tunnel testing of the integrated configuration.
Nevertheless, less expensive and time-consuming methods can provide a useful support to the preliminary analysis and design of the vehicle’s configuration engine. In this scenario, SPREAD code is a simplified procedure which allows a real-time screening of several engine/aircraft configurations and the identification of the most promising one/s with respect to user-defined constraints and requirements. The outcome of this procedure defines the base-line for further analyses with more

accurate tools. The accuracy and reliability of the developed coupled code were evaluated by comparing SPREAD results with CFD simulations, available literature results and/or aero-propulsive databases.
In particular, the SPREAD tool was applied to the nose-to-tail analysis of the LAPCAT-II Mach 8 MR2.4 vehicle configuration under hypersonic flight conditions [1], demonstrating its capability to rapidly predict reliable performance values at nominal design condition. Within the EC H2020 STRATOFLY project, the tool was further refined and the new developments will be presented in this paper.
The limits highlighted in the LAPCAT-II project were indeed addressed, including the modelling of the isolator module, an improvement in modelling of the injection module, as well as a greater flexibility in evaluating performance along the entire trajectory (not only in cruise, i.e., in ramjet mode) and, more generally, in all off-design conditions.
The first step toward this modelling activity was the preliminary assessment of the complex, supersonic, turbulent, combustion process. Therefore, zero-dimensional, kinetic analysis was carried out by means of the open-source Cantera software [2] under Python interface and the most suitable chemical mechanisms, able to predict with a satisfactory accuracy the ignition delay times, the adiabatic flame temperatures and the NO_x production, at the relevant scramjet operating conditions, were identified and compared among them. Several kinetic schemes were investigated and the best agreement was achieved using the kinetic mechanism formulated by Zettervall and Fureby [3]. Moreover, for taking into account also generation of NOx, through the thermal route, also the three fundamental reactions of Zel'dovich were implemented [4], obtaining in this way a new skeletal scheme consisting in 25 elementary reactions and 13 chemical atomic, radical and/or molecular species.
The final step was the application of SPREAD to a realistic hypersonic propelled vehicle as STRATOFLY MR3 for the calculation of the air-hydrogen combustion characteristics inside the combined dual-mode ramjet propulsive system using the kinetic schemes analysed in the first part of the present paper.

2. 0D kinetic analysis

Several literatures available, hydrogen-air, kinetic mechanisms were considered and among them the three most promising ones were analysed i.e., Jachimowski – 1988 [5] suitably conceived for scramjet applications, Keromnes – 2013 [6] and Z22 [3] developed by Zettervall and Fureby at the Swedish Space Research and Defence Agency (FOI). Subsequently this kinetic mechanism was further improved with the inclusion of a detailed H/O/N kinetic sub-mechanism of NOx generation reactions involving not only the three fundamental, thermal NO production steps by Zel'dovich [4], but also the low-temperature chemical paths leading to NOx through formation of NH_3 and HNO intermediates.

2.1. Jachimowski – 1988

This is a detailed mechanism, consisting in 13 chemical species and 33 reactions.
It was based on experimental data acquired in shock-tube and laminar flame tests, carried out at NASA - Langley Research Center in the framework of the American National Aero-Space Plane – NASP with the aim to investigate hydrogen/air combustion for propulsion systems of vehicles able to operate at flight speed up to Mach 25 [5].
It includes all the main atomic, radical and molecular species of the hydrogen-oxygen-nitrogen system relevant at elevated Mach number conditions (M > 12) i.e., H_2, O_2, H, O, OH, H_2O, HO_2, H_2O_2, N, NO, HNO. Moreover, this mechanism was refined, through comparison between calculated and experimental kinetic data.
Comparison of the computed ignition delay times, calculated as sudden increase of pressure in isochoric conditions, with the reflected shock-tube data of Slack and Grillo [6], reveals that, at pressures of 0.5, 1 and 2 atm for stoichiometric hydrogen/air mixtures, induction times are very sensitive to the rate coefficients, assigned to the second and ninth reactions of the whole scheme:

[RJ-2] $H + O_2 \rightarrow OH + O$

[RJ-9] $H+O_2 + M \rightarrow HO_2 + M$

Furthermore, it was worth noting that at high flight Mach numbers (M > 12) conditions, reactions involving nitric oxide become greatly important. Indeed, experimental data by Slack and Grillo [6] show that a limited addition of nitric oxide to stoichiometric hydrogen/air mixtures decreases the ignition delay times because NO converts the chain-terminating species HO_2 to the very reactive OH radical, according to the following reactions:

[RJ-30] $HO2 + NO \rightarrow NO_2 + OH$

[RJ-31] $H + NO_2 \rightarrow NO + OH$

2.2. Kéromès – 2013

This is a detailed kinetic mechanism suitably conceived for investigating the oxidation of syngas mixture consisting in $H_2/CO/O_2/N_2/Ar$ at pressures from 1 to 70 bar, over a temperature range from 900 to 2550 K and equivalence ratios from 0.1 to 4 [7]. It involves 10 chemical species comprising also the excited radical OH* and interacting among them through 31 reversible reactions.
Several reactions were identified in the most relevant literature as being important for hydrogen oxidation concluding that its reactivity is mainly controlled by the competition between the chain-branching reaction:

[RK-1] $H + O_2 \rightleftarrows O + OH$

and the pressure-dependent chain-propagating reaction:

[RK-9] $H + O_2 (+M) \rightleftarrows HO_2 (+M)$

For this reason, [RK-1] and [RK-9] reactions were extensively investigated and it was noticed that, at high-pressure conditions, the thermal decomposition of hydrogen peroxide (H_2O_2) through the pressure-dependent reaction:

[RK-15] $H_2O_2 (+M) \rightleftarrows OH + OH (+M)$

becomes the dominant chain-branching step. Moreover, as for most fuels, at intermediate temperatures the following reaction between the fuel, i.e. hydrogen, and the radical HO_2

[RK-17] $H_2 + HO_2 \rightleftarrows H + H_2O_2$

is important in the prediction of accurate ignition delay times.
At the low-to-intermediate temperatures (< 1000 K), usually encountered in the Rapid Compression Machines (RCM), hydrogen oxidation is predominantly governed by reaction [RK-9], which leads to production of hydroperoxyl radical i.e., HO_2. It reacts with molecular hydrogen thus generating H_2O_2 according to reaction [RK-17]. Finally, oxygenated water decomposes into two OH radicals as prescribed by reaction [RK-15].
Instead, at the high temperatures experienced by shock tube equipment, the competition between [RK-1] and [RK-9] leads to a pressure dependence of ignition delay times. Indeed, depending on the pressure, at high temperatures the oxidation process is mainly controlled by reaction [RK-1]. Due to the pressure dependence of reaction [RK-9], the temperature range in which the competition between the kinetic steps [RK-1] and [RK-9] occurs depends on the operative pressure.
The authors [4] investigated the effects of the reaction rate constants on ignition delay times by means of sensitivity analysis over a wide range of pressures between 1 and 100 bars and temperature between 850 and 1200 K. They concluded that at low temperatures (<1000 K) and relatively low pressure (1 bar) the reaction kinetics is mainly controlled by the competition between the chain-branching reaction [RK-1] and the chain-terminating one [RK-9], while at more elevated temperature (>1000 K) the reactivity is only governed by the chain-branching reaction [RK-1]. Instead, under high pressure and intermediate temperature conditions, the reaction kinetics is determined by the sequence first identified by Pitz and Westbrook of steps [RK-15] and [RK-17], involving H_2 and the HO_2 radical producing and consuming H_2O_2 that subsequently decomposes to release two OH radicals leading to the chain branching reaction.
The Kéromnes – 2013 [7] mechanism includes also the OH* sub-mechanism in order to more accurately predict the experimental ignition delay times measured in shock tube tests recording the onset, the maximum rate of increase or the peak of the chemiluminescence emission of OH*.

2.3. Z22 - 2018

This is a detailed, hydrogen/oxygen kinetic mechanism consisting in 9 species and 22 irreversible elementary reactions [3].
Analogously to Kéromnès et al. [7], also Zettervall and Fureby [3] highlight the importance of the competition between the chain-branching reaction [RZ-4]: $H + O_2 \rightarrow OH + O$ and the chain-propagating reaction [RZ-12]: $H + O_2 (+M) \rightarrow HO_2 (+M)$.
The first creates a pool of radical species effectively decreasing the ignition time, while the second produces the hydroperoxyl radical, which inhibit the chain-branching combustion process and therefore increases the induction time.
The competition between these reactions, and the consequent distribution of fast O, H and OH radicals and the slow radical HO_2, is strongly temperature dependent. Furthermore, in the P-T explosive hydrogen/air diagram illustrated in Fig. 2, a region of rapid ignition corresponding to chain-branching explosion at high temperatures and a region of slow ignition, associated to the thermal explosion at low temperatures are separated by a crossover region, corresponding to intermediate temperatures and dominated by extremely complex chemical processes.

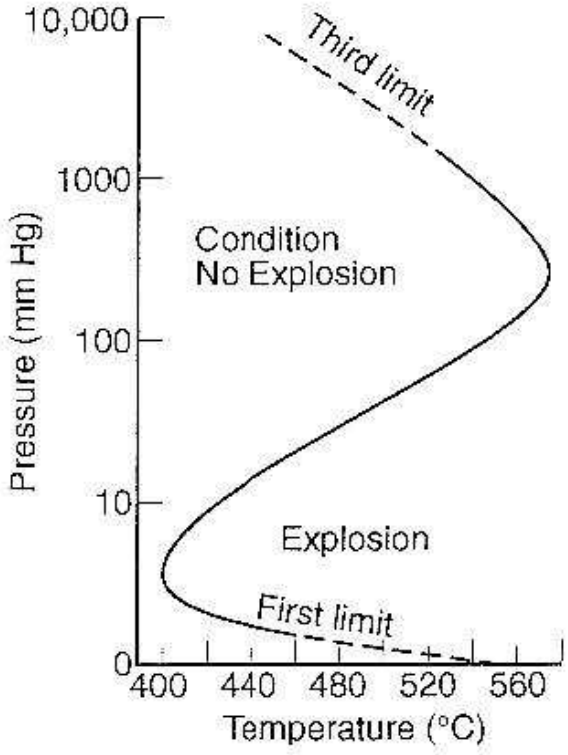

Fig.2. Explosion limits of a stoichiometric hydrogen/oxygen mixture [8]

However, for instance, several ramjets, scramjets and dual mode engines operate exactly in this connecting, critical zone.
Z22 [3] includes reactions important for the complete temperature spectrum, below and above the crossover region. In the mechanism development, authors spent particular efforts for improving its capability to match the ignition experimental behavior also in the intermediate connecting region, because it is extremely useful for ensuring flame anchoring and the stabilization within the supersonic combustion engines [9].
At low temperatures, reaction [RZ-12] predominates over reaction [RZ-4], the HO_2 concentration enhances and new reaction paths become more important i.e., [RZ-16]: $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$ and [RZ-20]: $H_2O + HO_2 \rightarrow H_2O_2 + OH$.

These reactions increase the concentration of H_2O_2, which main consumption route is carried out by means of reaction [RZ-17]: H_2O_2 (+M) → OH + OH (+M), that produces two OH radicals, which in turn generate H radical through [RZ-8]: H_2 + OH → H_2O + H.

2.4. 0D Kinetic Modelling

0D time-dependent simulations of perfectly stireed, isochoric and adiabatic batch reactors, filled with premixed gaseous reacting hydrogen/oxygen mixtures were carried out by means of the kinetic and thermodynamic open-source Cantera software [2] under Python interface. The 0D simulations were performed using implementing the three investigated mechanisms at fixed internal energy and at the initial combustion chamber pressure, temperature and equivalence ratio (listed in Table 1) belonging to operative box most representative of the real working conditions of scramjet vehicles:

Table 1. Operative conditions for Cantera simulations

Temperature [K]	**~750**	**~1050**
Pressure [atm]	1.2	5.2
Equivalence ratio	0.5	1

The mathematical-chemical model consists in the following fundamental both total and partial mass balance equations coupled with the energy conservation law:

$$m_{mix} = \sum_{i=1}^{NRS} m_i = const. \Leftrightarrow \frac{dm_{tot}}{dt} = 0 \qquad (1)$$

$$\frac{dm_i}{dt} = VR_i M_{w,i} \qquad (2)$$

$$c_{p,mix}\frac{dT}{dt} + v \cdot \sum_{i=1}^{NRS} h_i \cdot R_i \cdot M_{w,i} = 0 \qquad (3)$$

where m stands for the mass, V for the volume M_w for the molar amount, h for the enthalpy, T temperature, c_p the specific heat at constant pressure, t the time and R the reaction rate and NRS the number of the chemical reacting species in the mixture, while the subscript *mix* refers to the overall reacting mixture and i to a single i^{th} chemical species.
Numerical results were compared with two-literature available shock tube's experimental datasets acquired by Snyder and co-workers [10] and by University Turbine Systems Research (UTSR) [11] at different operative conditions ranging from atmospheric pressure to 5.2 atm and composition spanning from the stoichiometric ratio to the fuel lean regime.

2.5. Kinetic Results and Discussion

In the plots from Fig. 3 to Fig. 6, the ignition delay time profiles in function of the inverse of the initial temperature are shown.

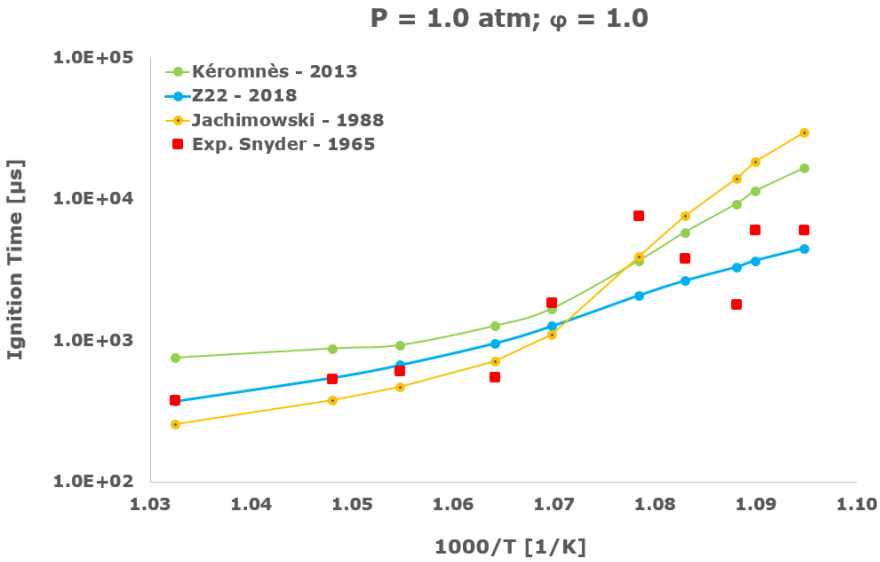

Fig 3. Comparison among experimental data of Snyder and co-workers [10] at atmospheric pressure and stoichiometric conditions with Cantera [2] predictions using three different kinetic mechanisms

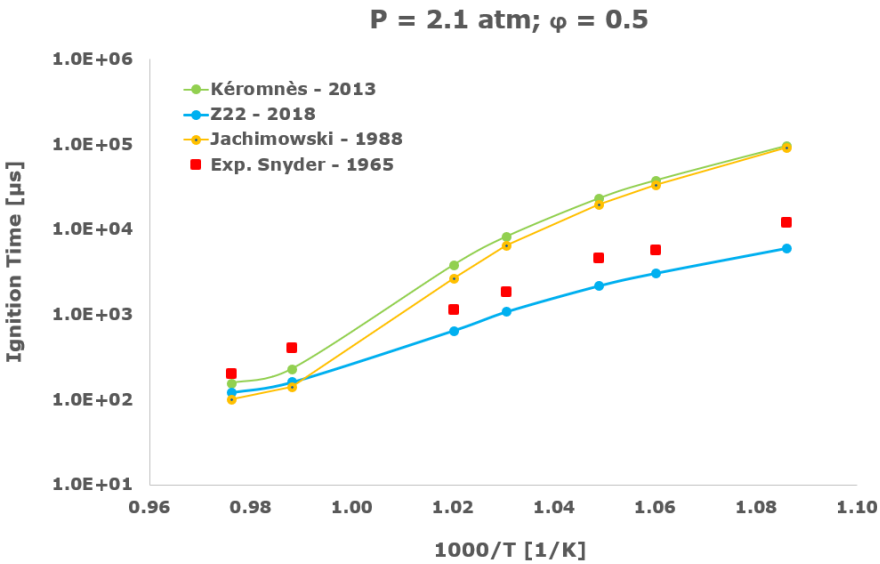

Fig 4. Comparison among experimental data of Snyder and co-workers [10] at pressure equal to 2.1 atm and fuel lean conditions with Cantera [2] predictions using three different kinetic mechanisms

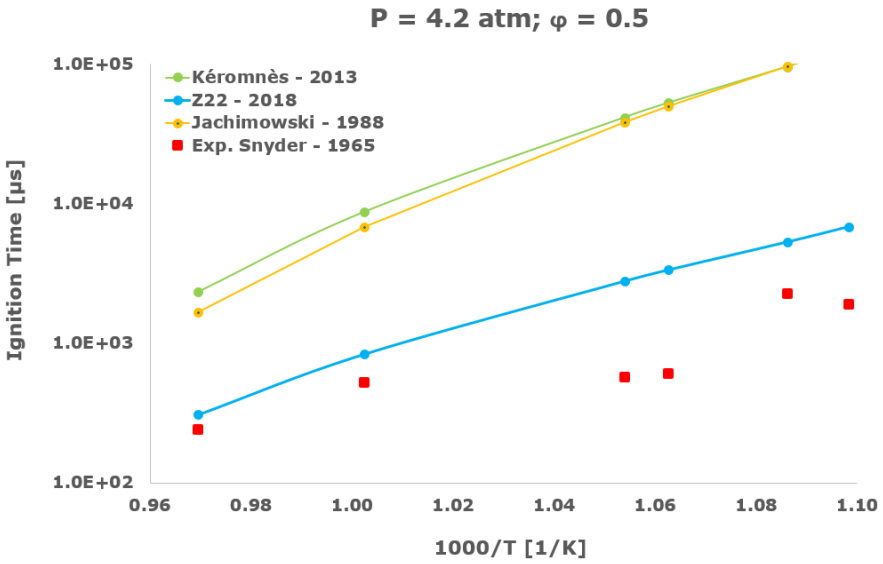

Fig 5. Comparison among experimental data of Snyder and co-workers [10] at pressure of 4.2 atm and fuel lean conditions with Cantera [2] predictions using three different kinetic mechanisms

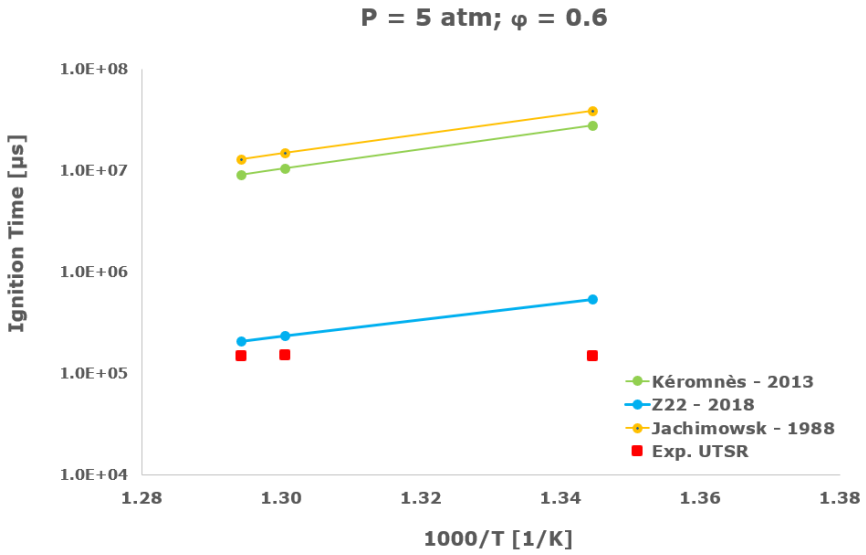

Fig 6. Comparison among experimental data of UTSR [11] at pressure of 5 atm and fuel lean conditions with Cantera [2] predictions using three different kinetic mechanisms

Although at atmospheric pressure (see Fig. 3), all the investigated mechanisms show a fairly good matching to the experimental data, especially for high temperatures, increasing the pressure up to 5 bars, only the Z22 [3] scheme remains able to accurately capture the complex and strongly non-linear behaviour of the hydrogen/air ignition also at low temperatures i.e., in the critical crossover region (see Fig. 2).

Kinetics of hydrogen/air confirms to be extremely sensitive to operative conditions, emphasized by the competition between chain-branching and pressure dependent chain propagation reactions, where the hydrogen combustion switches between the first flammability limit, dominated by the thermally activated radical initiation steps, to the third limit governed by the pressure-dependent wall radical recombination reactions, passing through the critical complex zone represented by the second limit region. Thus, a single, even detailed, mechanism, able to describe with sufficient accuracy the H_2/air chemical kinetics, is still difficult to develop.

3. SPREAD results

The SPREAD (Scramjet PREliminary Aerothermodynamic Design) code is a powerful tool to draw a preliminary design of a propulsion system, such as scramjet, ramjet or turbojet. This software was preliminary developed in the frame of the LAPCAT-II project [12], but was then upgraded to overcome some important limitations. The main idea behind SPREAD is that a complex system, such as an airbreathing propulsive system, may be divided into its main components, as compressor, combustor, heat exchanger, nozzle, etc., each of them modelled as a black-box with inputs, outputs and ad-hoc mathematical models to link the outputs to the given inputs. Each mathematical model, that describes the performance and capabilities of the corresponding engine's component, can be implemented with different levels of accuracy, from a just theoretical one, to one tied to empirical correlations, to a merely numerical model. Therefore, a generic propulsion system can be built up by connecting the involved modules (black-box) through nodes, each of them described by appropriate thermodynamic and geometric variables.
As regards specifically the combustor of an air-breathing scramjet vehicle, the velocity *V* of the gas stream has to be computed along with the composition, temperature, density and pressure. In the frame of SPREAD solving system, the following assumptions were made for the combustor module:

- steady, inviscid, one-dimensional flow of a chemically reacting ideal-gas mixture in a duct;
- variables uniform across any cross section but varying with distance along the duct (Q1D: quasi 1D flow);
- negligible diffusion of mass and energy;
- heat transfer between the reacting gas mixture and its surroundings allowed;
- Distance *x* as independent variable;
- Area profile as a function of distance assigned (area assigned problems).

In order to solve for ρ, *T*, *p* and *V*, appropriate forms of the continuity, momentum balance and energy conservation equations (i. e., 1D Euler equations) are derived, and they read:

$$\frac{dT}{dx} = -T\left\{\frac{\gamma-1}{M^2-1}\left[M^2\left(\frac{1}{A}\frac{dA}{dx} - M_w\sum_{j=1}^{NRS}\frac{d\sigma_j}{dx}\right) + \frac{\gamma M^2-1}{\gamma}M_w\left(\sum_{j=1}^{NRS}\frac{\bar{h}_j}{\bar{R}T}\frac{d\sigma_j}{dx} + \frac{\frac{\dot{Q}'}{\dot{m}}}{\bar{R}T}\right)\right]\right\} \quad (4)$$

$$\frac{d\rho}{dx} = \frac{\rho}{\gamma M^2-1}\left(\frac{1}{T}\frac{dT}{dx} + M_w\sum_{j=1}^{NRS}\frac{d\sigma_j}{dx} - \frac{\gamma M^2}{A}\frac{dA}{dx}\right) \quad (5)$$

$$\frac{dV}{dx} = \frac{-V}{\gamma M^2-1}\left(\frac{1}{T}\frac{dT}{dx} + M_w\sum_{j=1}^{NRS}\frac{d\sigma_i}{dx} - \frac{1}{A}\frac{dA}{dx}\right) \quad (6)$$

$$\frac{d\sigma_i}{dx} = \frac{1}{V}\frac{d\sigma_i}{dt} = \frac{1}{\rho\cdot V}\sum_{j=1}^{NR}\left(\nu_{ij}^{''} - \nu_{ij}^{'}\right)\cdot\left(R_j - R_{\_j}\right) \quad (7)$$

where NR the number of reactions, $\dot{Q}'$the heat transfer rate per unit area and $\dot{m}$ the total mass flow rate, $\nu_{ij}^{''}$and $\nu_{ij}^{'}$are the stoichiometric coefficients of the i^{th} reactant species and product species, respectively, whereas R_j and$R_{_j}$ are the forward and backward molar reaction rates per unit volume of j^{th} reaction, expressed according to the classical Arrhenius formulation. In order to carry out such an analysis SPREAD incorporates LSENS solver [12]. LSENS, which stands for Lewis General Chemical Kinetics and Sensitivity Analysis Code, is a software developed at NASA Lewis Research Center in the early 90's which performs complex chemical kinetics computations for any chemical system and several different reaction types, including static and one-dimensional flow reaction, shock-initiated chemical reaction, and the fully back mixed perfectly stirred reactor.
In the work here reported, the chemical model implemented in SPREAD is based on the Z22 kinetic mechanism [3]. Indeed, it demonstrated to be the most accurate at the end of the kinetic analysis and validation up to 5 bars against shock tube's experimental data of ignition delay times, as described in more details in the previous section.

Provided that the injection scheme for the STRATOFLY vehicle was derived from the LAPCAT-II MR2.4 vehicle and consists in a multiple full-strut configuration with a V-shape placement of the struts (see Fig. 7), a proper 1D model of the combustor has been developed.

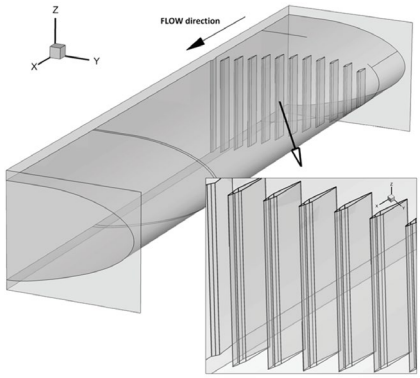

Fig 7. Combustor strut array arrangment (3D view)

That is, the whole combustor injection strut array system (i. e., the array of the 21 vertical bar designed for the STRATOFLY MR3) is modelled as a set of $N_i = 21$ single 1D combustors (one per strut bar), linked in parallel one to the each other (same inlet conditions from the air intake and common outlet towards the outside of the nozzle), but each with its specific injection point S_j: by properly shifting the S_j injection point for each single 1D combustor any kind of axial displacement of the array of struts could be analysed, as the one sketched in Fig. 8, which resembles the actual configuration of the STRATOFLY combustor.

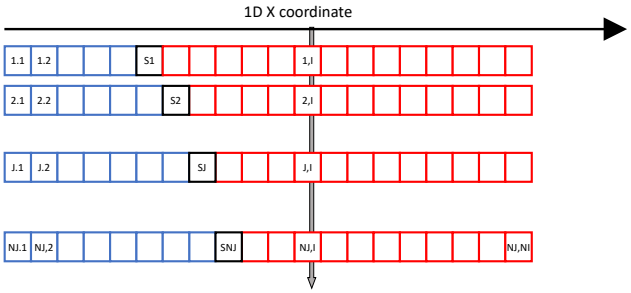

Fig 8. Combustor strut array layout

Then, at a given x position, the overall thermodynamic state of the system is obtained by adiabatically and frictionless mixing the corresponding states of the N_i single 1D combustors.
Along the STRATOFLY project, several analyses were carried out by adopting the approach so far described, in particular the flow-field inside the combustor was characterized in four specific conditions, which corresponds to four specific freestream flight Mach number. Table 2 reports the combustor inlet conditions, in term of local Mach number, temperature and pressure, corresponding to the four selected freestream Mach number, namely M=5, 6, 7 and 8, provided by the SPREAD air intake module (here not described for the sake of brevity).

Table 2 Combustor inlet conditions

	$\mathbf{M_\infty = 8}$	$\mathbf{M_\infty = 7}$	$\mathbf{M_\infty = 6}$	$\mathbf{M_\infty = 5}$
Mach	2.63	2.55	2.47	2.39
Pressure [Pa]	26349	43781	47085	43198
Temperature [K]	1147	992	886	784

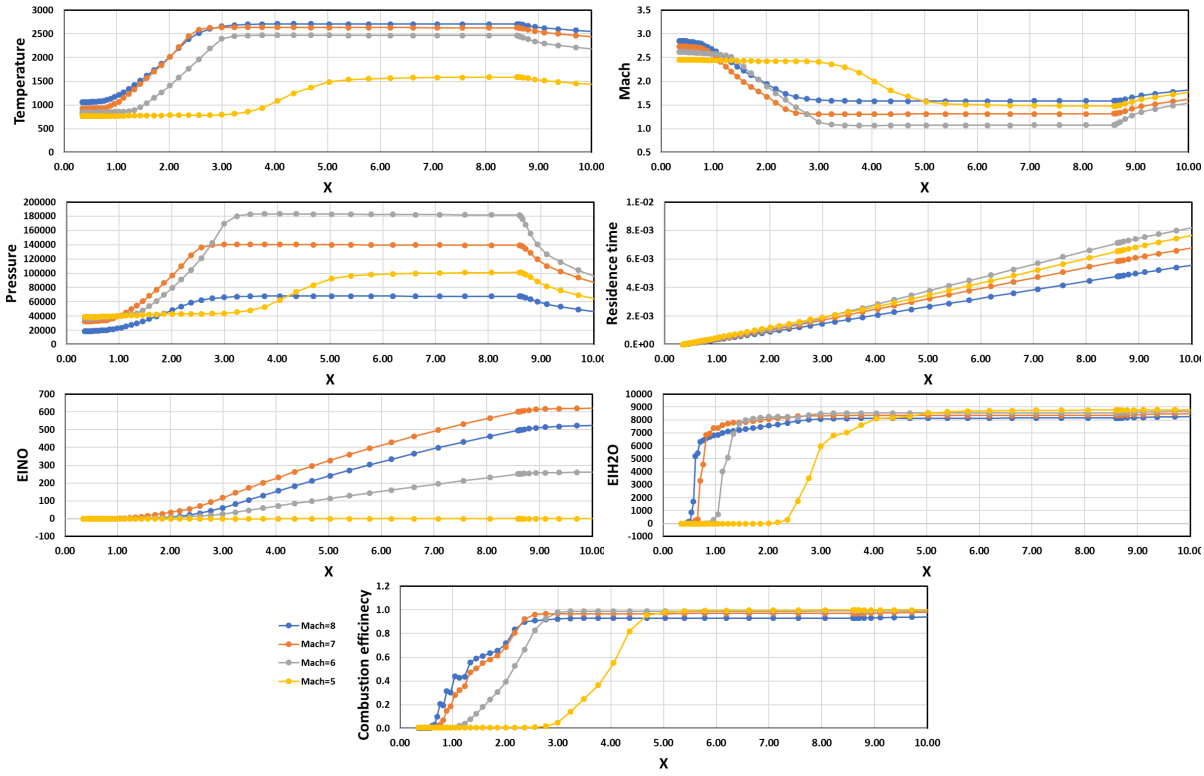

Fig 9. 1D profile of main termodynamic and emission-related quantities

Fig. 9 reports the main thermodynamic and emission-related quantities profiles along the streamwise direction inside the scramjet combustor for the four considered cases. Depending on the specific equivalent ratio used and the local velocity (and corresponding residence time), the temperature reaches, and in some cases exceeds, the value of 2500 K. This ensures a good combustion efficiency, but leads to an increased production of NOx, which are sub-sequentially released in the atmosphere. These results refer to the initial combustor design of the STRATOFLY aircraft, which was subsequently improved, but this is out of the scope of the present paper.
However, particular care must be taken in the design of a combustor for a scramjet aircraft e.g., STRATOFLY MR3, and tools such as SPREAD can be useful since they allow for the analysis of various configurations in conceptual design requiring only a very short time. Moreover, SPREAD can be easily integrated into optimization loops.

4. Conclusions

The CIRA in-house 0D/1D SPREAD code was further improved and successfully used as very promising, powerful and predictive tool for design and development of the propulsive system of airbreathing, stratospheric, supersonic, scramjet vehicles fuelled by liquid hydrogen.
It includes the chemical model for hydrogen/air ignition and combustion arising from a thorough kinetic assessment. It was carried out analysing the ignition behaviour of reacting mixtures by means of 0D simulations of perfectly stirred, isochoric, adiabatic batch reactors resembling the chemical processes occurring within the engine's combustion chamber. For this purpose, three literature available kinetic schemes were selected and investigated and their reaction kinetics performance was assessed through comparison between the 0D computational predictions and the experimental measurements collected in two shock tube's datasets belonging to the operative box defined by the extremes listed in the Table 1.
Kinetic analysis clearly shows that among the considered kinetic mechanisms, only Z22 [3] provides a very good agreement with the experimental values in the overall studied operative envelope including the low temperature and medium pressure conditions belonging to the critical crossover region. Instead, the other two schemes i.e., Jachimowski [5] and Kéromnès [7] exhibit a satisfactory matching only near atmospheric pressure.
This kinetic model was suitably implemented in the aerothermodynamic and propulsive SPREAD code and effectively applied to calculation of the main physical fluid dynamic and thermodynamic parameters

e.g., combustion efficiency, Mach, residence time, NO emission indexe along the whole STRATOFLY vehicle's propulsive flow path, thus demonstrating the good design potentiality of the several modules embedded in the SPREAD tool.

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