

ENCIT-2018-0181 CHEMICAL REACTIONS MODEL APPLIED TO SUPERSONIC COMBUSTION

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Abstract. *A two-dimensional hydrogen powered generic scramjet, designed at the Universidade Federal do Rio Grande do Norte (UFRN), based on the technological demonstrator scramjet 14-X S in development at the Instituto de Estudos Avançados (IEAv), has been considering to demonstrate, in atmospheric flight, a supersonic combustion, of atmospheric air (in supersonic speed) with hydrogen, on an acceleration mission to 2050 m/s (Mach number 6.8) at 30 km geometric altitude. Scramjet technology offers substantial advantages to improve performance of aerospace vehicle that flies at hypersonic speeds through the Earth's atmosphere, by reducing onboard fuel. Basically, scramjet is a fully integrated airbreathing aeronautical engine that uses the oblique/conical shock waves generated during the hypersonic flight, to promote compression and deceleration of freestream atmospheric air at the inlet of the scramjet. Fuel, at least sonic speed, may be injected into the supersonic airflow just downstream of the inlet. Right after, both atmosphere air and on-board hydrogen fuel are mixing. The combination of the high energies of the fuel and the oncoming hypersonic airflow the combustion at supersonic speed starts. The scramjet engine is divided into several components based on key design parameters to assess the engine performance as a function of these parameters. One of the most important design aspects is the temperature at the entrance of the combustion chamber because the compression must provide enough high temperature, higher than ignition temperature of the hydrogen, for supersonic combustion with the supersonic atmospheric air, at the combustion chamber. In this work the conditions after burning hydrogen H_2 and air (O_2 and N_2), at stoichiometric chemical reaction, are presented.*

Keywords: *scramjet, supersonic combustion, hypersonic airbreathing propulsion, chemical reactions.*

1. INTRODUCTION

Advanced propulsion concepts and technologies needed to be integrated at aerospace vehicles to fly in hypersonic velocities above the correspondent Mach number 4 are in developing in several research centers around the world, using the airbreathing propulsion system based on supersonic combustion (scramjet technology).

The recent flight-test successes demonstrating the viability to use the supersonic combustion concept, through the X-43 Aerospace Vehicle flights in 2004, where a hydrogen scramjet-powered was operated during about 10 s at Mach numbers 7 and 10 (McClinton; Rausch; Reukauf, 2001; Moses et al., 2004; Marshall et al., 2005a; 2005b) and the X-51 Aerospace Vehicle flight in 2010, where a hydrocarbon scramjet-powered was operated during about 140 s at Mach number 5 (Hank; Murphy; Mutzman, 2008) provided the new U.S. hypersonic strategy formulated (after NASP

program) by U.S. Government agencies for the next generation of space transportation systems and gave a fresh renaissance in hypersonic flight.

In addition, in 2000's The University of Queensland, Australia, demonstrate the feasibility of scramjet engine concept through the HyShot flights (Paull; Alesi, 2005). After the lessons learned, The University of Queensland and his partners are now pursuing the same goal as those of the X-43 and X-51 aerospace vehicles, through the HIFiRE (Dolvin, 2008) and SCRAMSPACE (Tirtey et al., 2011) projects, that is, flying at Mach 8 a hypersonic airbreathing vehicle based on scramjet propulsion.

In 2007, Brazilian researchers, from Laboratório de Aerodinâmica e Hipersônica Prof. Henry T. Nagamatsu, at Instituto de Estudos Avançados (IEAv), proposed to design, to develop, to manufacture and to demonstrate, in free flight, a technological demonstrator using: i) waverider technology to provide lift to the aerospace vehicle, and ii) scramjet technology to provide hypersonic airbreathing propulsion system based on supersonic combustion.

The fully airframe-integrated scramjet 14-X waverider (Fig. 1) and the scramjet 14-X S (Fig. 2) are being designed to demonstrate supersonic combustion during atmospheric flight in about 30 km of altitude, in hypersonic speeds corresponding to the numbers of Mach 10 (approximately 3000 m/s) and 7 (approximately 2100 m/s), respectively.



Figure 1. Demonstrator scramjet 14-X waverider.

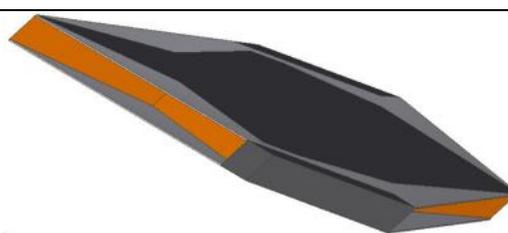


Figure 2. Demonstrator scramjet 14-X S.

Scramjet is a fully integrated airbreathing aeronautical engine, with no moving parts, that uses the oblique/conical shock waves generated during the hypersonic flight, to provide compression and deceleration of freestream atmospheric air at the inlet of the scramjet, which are pushed to combustion chamber. Fuel, at least sonic speed, may be injected into the supersonic airflow just downstream of the inlet or at the beginning of the combustion chamber (combustor). Right after, both oxygen (from the atmospheric air) and on-board hydrogen fuel are mixed. The combination of the high energies of the fuel and of the oncoming supersonic airflow starts the combustion at supersonic speed. Finally, the divergent exhaust nozzle at the afterbody vehicle accelerates the exhaust gases, providing thrust.

In consequence of the nature of the scramjet engines, scramjets are unable to produce thrust while stationary. Solid-rocket engines may be used to accelerate the scramjet to a speed such that the shock waves produced by the air intake are able to compress the atmospheric air achieving the operational conditions (Hass et al., 2005). Such approach may provide an affordable path for maturing Brazilian hypersonic airbreathing components and subsystems in flight. The Brazilian hypersonic accelerator vehicle which is composed by two-stage (S31 and S30) solid rocket engines, unguided, rail launched, is able to accelerate the 14-X S to the predetermined flight test conditions of the scramjet operation (30 km altitude at Mach number 7) from one of the Brazilian Launch Centers (Centro de Lançamento de Alcântara, CLA, or Centro de Lançamento da Barreira do Inferno, CLBI).

2. METHODOLOGY

2.1 Scramjet characteristics

First, it is necessary to establish a nomenclature to be used in the scramjet design. Heiser and Pratt (1994) present the terminology of the scramjet, which may be divided in three main components (Fig. 3): external and internal compression section (inlet), combustion chamber (combustor), and internal and external expansion section (outlet).

Stations 0 and 1 are the leading edges of the scramjet and of the cowl, respectively. Stations 3 and 4 are the entrance and exit of the combustion chamber. Stations 9 and 10 are the trailing edges of the cowl and the scramjet, respectively.

The external compression section is governed by incident shock wave, while the internal is governed by reflected shock wave. The internal and external expansion section is governed by expansion wave, Prandtl-Meyer Theory, and area ratio. The constant area section of the combustion chamber is called as isolator and is used to uniformize the flow from the compression section. Fuel is injected right after the isolator used to expand the gases from burning the fuel and the oxygen. In general, one-dimensional flow with heat addition, Rayleigh flow, is used to simulate the burning the fuel and the oxygen.

An important feature of the scramjet is a highly integrated system, where engine and vehicle are indistinguishable. This tight integration is caused by the fact that the front section of the vehicle contributes to the compression of atmospheric air, while the rear contributes to the generation of thrust. The net thrust produced by the scramjet is the difference between the thrust (force that propels the vehicle) generated by the expansion of exhaust gases from the rear

of the engine and the total drag (force that resists the movement of the vehicle). These forces may produce thrust to the flight of the vehicle or not depending on the balance of these forces in engine design in question.

Therefore, the operation of the scramjet engine obeys the (closed) Brayton thermodynamic cycle. Note the correspondence of Brayton cycle points (Fig. 4) with the reference stations of scramjet (Fig. 3). Observe that the heat addition should be evaluated as constant pressure section, because it avoids the possibility of boundary-layer separation and the necessity to design the structure to withstand the peak pressure. In order to obtain constant pressure section after fuel injection the area in this section should be divergent (Fig. 3). Also, the static pressure at the exit, station 10, of the scramjet expansion section (trailing edge) should be very close of the freestream static pressure, station 0 (Fig. 4).

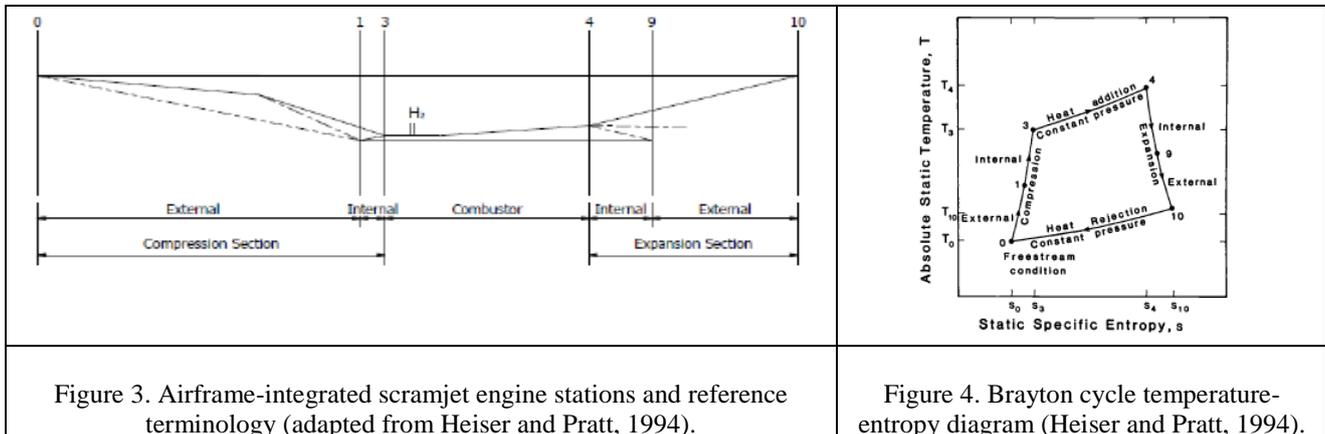


Figure 3. Airframe-integrated scramjet engine stations and reference terminology (adapted from Heiser and Pratt, 1994).

Figure 4. Brayton cycle temperature-entropy diagram (Heiser and Pratt, 1994).

2.2 Scramjet inlet design

Toro et al. (2018) has been designed the scramjet inlet (Fig. 5) applying the one-dimensional compressible flow (shock wave) theory, considering no boundary layer (non-viscous) effects and the atmospheric air flow behaves as calorically perfect gas. The scramjet flies at 30 km altitude with velocity of 2051.6 m/s (corresponding to Mach number 6.8). After the atmospheric air flow are compressed and decelerated through the inlet of the scramjet (stations 0 to 3, Fig. 3), the atmospheric air flow is pushed to combustion chamber.

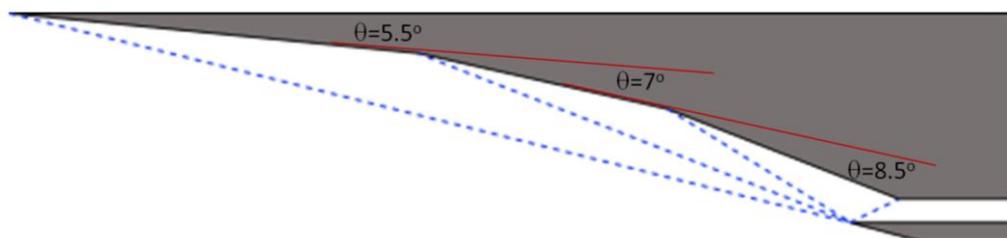


Figure 5. Cross section of the scramjet inlet.

Thermodynamic properties and the velocity (and corresponding Mach number) of the supersonic atmospheric air flow at the entrance of the combustion chamber (Tab. 1) are estimated by Toro et al. (2018), which are adequate to burn the gaseous fuel inside of the combustion chamber.

Table 1. Thermodynamic properties at the entrance of the combustion chamber.

		Atmospheric freestream airflow	Entrance of the combustion chamber
M_{in}		6.8	2.55
p_{out}	Pa	1197	106991.30
T_{out}	K	226.5	1008.64
ρ_{out}	kg/m ³	0.01841	0.36952
a_{out}	m/s	301.7	636.67
u_{out}	m/s	2051.6	1624.01

2.3 Atmospheric air molar composition

The molar composition of air is important to evaluate the combustion. Its molar composition at 30 km is the same at sea level and its value as follows:

Table 2. Atmospheric air molar composition at the entrance of the combustion chamber.

Composition	Values%
O ₂	20,59
N ₂	77,48
H ₂ O	1,90
CO ₂	0,03

2.4 Fuel data for hypersonic vehicle range

Due to high heats of reaction (Tab. 3) hydrogen is the only fuel that might deliver net positive thrust up to Mach number 24, near orbital velocity. However, due to high density (Tab. 3) hydrocarbon fuels may result in superior overall performance for Mach number below 8 (Fig. 6). Hydrogen will be used for the present case study of Mach number 6.8.

Scramjet is a reaction jet engine with high specific impulse used for airbreathing hypersonic flight that may provide higher the specific impulse than the conventional rockets by burning hydrogen fuel in a supersonic atmospheric compressed airflow (Fig. 7). Also, safety, storage and handling of hydrocarbon (except for cryogenic methane) are easier than the hydrogen (Fig. 7).

Table 3. Ignition temperature and heats of reaction for typical gaseous hydrogen and gaseous hydrocarbon fuels reacting with air at the standard reference state.

Fuel	Chemical Formula	Ignition temperature	(heats of reaction)		Density	γ	Gas constant
		T_{ig}	h_{pr}	f_{st}			
		CRC (1985)	Heiser e Pratt (1994)				
	C _x H _y	(K)	(MJ/kg)	-	kg/m ³	-	(J/kg.K)
Hydrogenic	H ₂	845.15	119.954	0.0291	82	1.404	4124.16
Methane	CH ₄	810.15	50.010		424	1.32	518.35
Ethane	C ₂ H ₆	745.15	47.484			1.183	276.5
Hexane	C ₆ H ₁₄	498.15	45.100				96.48
Octane	C ₈ H ₁₈	479.15	44.786	0.0664	703	1.044	72.79
JP-7	C ₁₂ H ₂₅	514.15	43.90325		790		
JP-10	C ₁₀ H ₁₆	518.15	42.100				

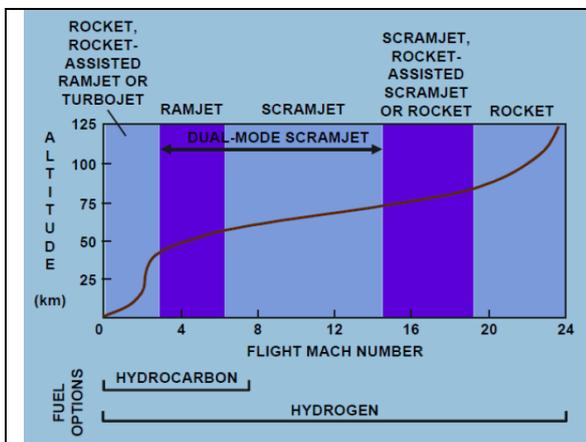


Figure 6. Airbreathing engines function of mach number (Fry, 2011).

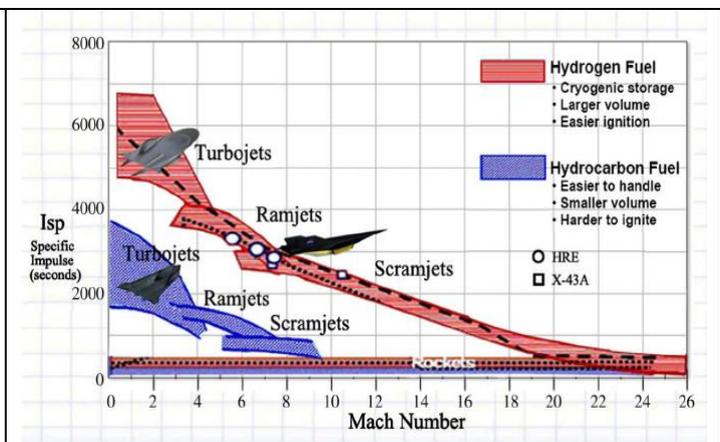


Figure 7. Specific impulse as function of the Mach number (Moses et al., 2004).

2.5 Stoichiometric fuel/air ratio

The fuel/air mass flow ratio f_{st} is defined based on the ratio of fuel mass flow rate to air mass flow rate, given by

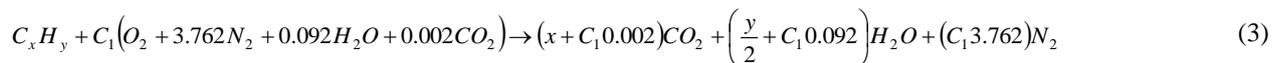
$$f = \frac{\dot{m}_{fuel}}{\dot{m}_{air}} = \frac{\text{Fuel mass flow rate}}{\text{Air mass flow rate}} \quad (1)$$

However, the stoichiometric fuel/air mass flow ratio f_{st} based on the products of burning (Tab. 3) hydrocarbon C_xH_y or hydrogen H_2 and humid air (O_2 , N_2 , H_2O and CO_2), which include only carbon dioxide and water, is the upper ideal limit for the complete mutual combustion of all the oxygen present in the air with all the reactants available in the fuel, which can be calculated from the basic principles of chemical reactions using

$$f_{st} = \frac{36x + 3y}{104.3(4x + y)} = \frac{36x + 3y}{M_{Air_F}(3/4)(4x + y)} \quad (2)$$

where, M_{Air_F} is the air mass per kmol of fuel ($1M_{O_2} + 3.762M_{N_2} + 0.092M_{H_2O} + 0.002M_{CO_2} = 139.1$ kg of Air). The atomic weights of the participating elements have been incorporated: H = 1, C = 12, O = 16 and N = 14. The constants are the ratio of molar composition of the air component to oxygen molar composition as ($3.762 = 77.48/20.59$); ($0.092 = 1.90/20.59$) and ($0.002 = 0.03/20.59$). The values are based on molar air composition.

The general chemical equation for the complete combustion of all carbon, hydrogen and oxygen atoms are consumed in the stoichiometric chemical reaction is given by



where: $C_1 = \left(x + \frac{y}{4}\right)$ is the stoichiometric theoretical air.

Burning hydrogen and air the stoichiometric fuel/air ratio is $f_{st} = 0.0291$, where $x = 0$ and $y = 2$ for H_2 . Therefore, the fuel mass flow rate may be calculated as $\dot{m}_{fuel} = f_{st} \dot{m}_{air}$, where $\dot{m}_{air} = \rho_0 u_0 A_0$, considering shock on-lip and shock on-corner. The rate at which the chemical reactions make energy available to the engine cycle is given by (Heiser and Pratt, 1994)

$$\text{Chemical energy rate} = \dot{m}_{fuel} h_{pr} \quad (4)$$

However, the amount of heat added per kilogram of air is proportional to the fuel to air mass flow ratio and the heat of reaction h_{pr} of the fuel, which may be evaluated by

$$q = \dot{m}_{fuel} h_{pr} = f_{st} \dot{m}_{air} h_{pr} \quad (5)$$

where, the heat of reaction h_{pr} for H_2 is 119.954 MJ/kg (Tab. 3).

2.6 Freestream mass flow rate

The mass flow rate of air captured by the scramjet inlet (Fig. 5) and enter at the combustor chamber, considering shock on-lip and shock on-corner design conditions, is given by

$$\dot{m} = \rho_0 u_0 A_0 = \rho_{1st} u_{1st} A_{1st} = \rho_{2nd} u_{2nd} A_{2nd} = \rho_{3rd} u_{st} A_{3rd} = \rho_3 u_3 A_3 \quad (6)$$

2.7 Combustion of fuel

The first law of thermodynamics for reacting system at steady-state system is used to evaluation of energy balance. It is given as follows according to (Borgnakke and Sonntag, 2009; Moran and Shapiro, 2009).

$$Q_{VC} + \sum_R n_{in} (\bar{h}_f^0 + \Delta\bar{h})_{in} = \sum_P n_{out} (\bar{h}_f^0 + \Delta\bar{h})_{out} + W_{CV} \quad (7)$$

where: n is the number of moles of the combustion reaction; \bar{h}_f^0 is the enthalpy of formation and $\Delta\bar{h}$ is the variation of enthalpy of formation. The subscript R and P are Reagent and Product, respectively. The enthalpy of formation of hydrogen is 0, it is standard reference state according to (Borgnakke and Sontag, 2009).

3. RESULTS AND COMMENTARIES

First is necessary to define the thermodynamic atmospheric air properties, which the scramjet will perform atmospheric flight, at 30 km geometric altitude (Tab. 3) and speed corresponding to Mach number 6.8.

Table 1. Thermodynamic atmospheric properties at 30 km altitude (U.S. Standard Atmosphere, 1976).

Altitude	Temperature	Pressure	Density	Mean free path	Sound speed	Dynamic viscosity
km	K	Pa	kg/m ³	m	m/s	N s /m ²
30	226.5	1197	0.01841	0.000004413	301.7	0.000014753

Three processes at supersonic combustion of the hypersonic aerospace vehicle were analyzed. They are mixture formation of fuel and air, combustion and expansion at nozzle. The approach used for evaluation is the first law of thermodynamic without and with reacting at steady-state system based at enthalpy of formation. The results are shown as follows:

The first process analyzed is the mixture formation at combustion chamber. The input condition of air and hydrogen are known. The output conditions of air and hydrogen mixture are calculated. The mixture temperature should reach 845K to self-ignition. This process takes place at combustion chamber before the combustion, i.e., it is only the process of mixture formation. Figure 8 shows the effect of fuel air mixture ratio on the speed mixture to achieve the temperature of 845 K.

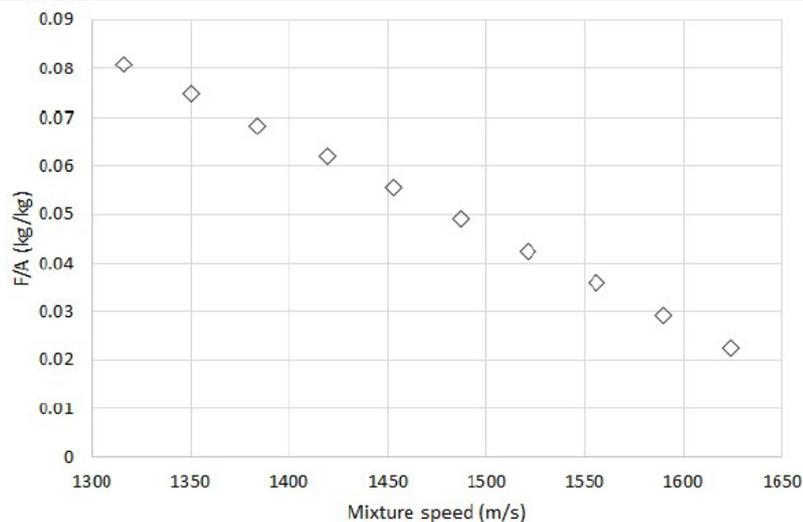


Figure 8. Effect of mixture speed on the mass fuel air ratio.

The speed of mixture affects the fuel air ratio. The fuel is the cold fluid, which cools the mixture due to its low temperature of 300 K. Even though, the air at 1008.64 K heats the mixture. The kinetic energies of working fluids were considered. The hydrogen speed is 1316 m/s (Mach number 1) and the air speed is 1624 m/s (Mach number 2.55). As mixture speed increases, the fuel air ratio decreases. This fact is due to less fuel mass flow rate is necessary to reach the self-ignition temperature and the fuel air decreases. The speed range of mixture was changed from minimum of 1316 m/s (hydrogen speed) to maximum of 1624 m/s (air speed).

The effect of fuel air ratio on the mixture temperature was evaluated at Fig. 9. The mixture speeds were defined as three values: Maximum of 1624 m/s (air), average 1470 m/s and minimum of 1316 m/s (hydrogen).

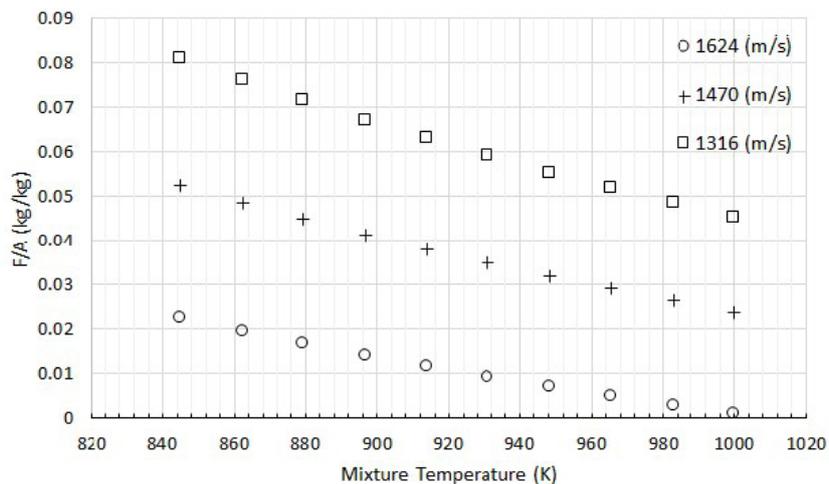


Figure 9 – Effect of mixture temperature on the mass fuel air ratio.

As fuel air ratio increases, the mixture temperature decreases, due to more cool mass flow rate of hydrogen is into mixture. The cool hydrogen reduces the mixture temperature. And as higher is the mixture speed, lower is the fuel air ratio. The reason for this fact is same. The hydrogen fuel has low temperature and low energy (enthalpy). The energies between the input and output of mixture process are the same. The balance energy is constant. In this process the combustion was not considered, however only the mixture of fuel and air.

The second process analyzed is the combustion at combustion chamber. There is a change of chemical composition. In the literature, the exhausted gases can reach at range of 2400 to 2600 K. The fuel air ratio is evaluated considering that the variation kinetic energy is negligible. The speeds at input combustor of mixture air fuel and at output combustor of exhausted gases are similar. The process is considered adiabatic. Figure 10 shows the effect of exhausted gases adiabatic temperature on the fuel air ratio.

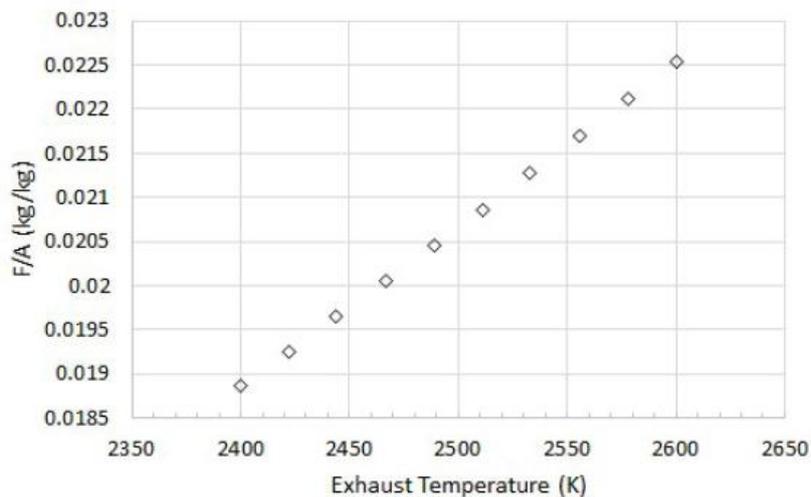


Figure 10 – Effect of exhausted gases temperature on the fuel air ratio.

The values of fuel air ratio change from minimum of 0.0189 to maximum of 0.0225. As fuel air ratio increases, the exhausted gases temperature increase due to more flow ratio of fuel is burned at combustion chamber.

The last process analyzed is the isentropic expansion of the exhausted gases into nozzle. The exhaust gas under pressure should flows into nuzzle increasing the speed to provides a thrust that propels the vehicle in the opposite direction. The output conditions of exhausted gases depend on the input condition of nuzzle. Assuming that the mixture speed is average of 1470 m/s and changing the exhausted gases temperature from 2400 to 2600 K, the temperature and speed of exhausted gases at output of nuzzle could be evaluated. Figure 11 shows the output condition of exhausted gases at nozzle output.

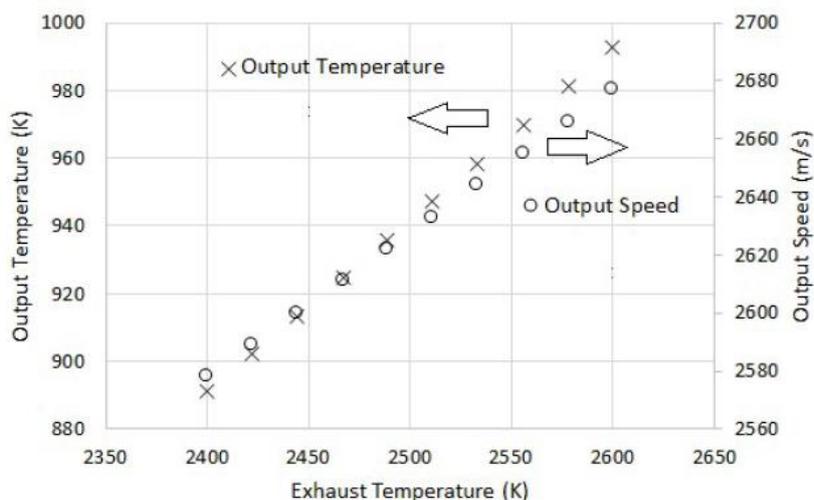


Figure 11. Exhausted gases condition at output nozzle for isentropic expansion with input speed of 1470 m/s.

The maximum condition of temperature and speed of exhausted gases at nozzle output are shown. The range of temperature is 891 to 993 K and the range of speed is 2578 to 2677 m/s. The input and output pressure at nozzle are 106.99 and 1.197 kPa. If there is heat transfer or loss into nozzle, these values will be reduced.

4. CONCLUSION AND OUTLOOK FOR FUTURE PROJECTS

The primary objective of this work is to present a methodology to understand the burning process of hydrogen and air in supersonic speed applying the general chemical equation for the complete combustion of all hydrogen and oxygen atoms consumed at the stoichiometric fuel/air ratio.

This analysis were applied to the generic scramjet, which has been designed at the Universidade Federal do Rio Grande do Norte (UFRN), using analytical theoretical analysis (engineering approach), to fly at Earth's atmosphere at 30 km geometric altitude in Mach number 6.8 (2050 m/s), considering the atmospheric air behavior as a calorically perfect gas, from the tip-to-tail of the scramjet and the flow do not present viscous effects.

The generic scramjet, with three ramps at the compression section, with the turning angles of 5.5°, 7° and 8.5°, flying at 30 km of geometric altitude with speed corresponding at Mach number 6.8 is capable to generate a supersonic velocity corresponding to Mach number of 2.55 and a static temperature higher than 845.15 K, showing the possibility to burn hydrogen.

The First Law of Thermodynamics was applied to obtain the speed of mixture of hydrogen and air, the temperature after burning hydrogen and air, at the condition of fuel air ratio from 0.019 to 0.022 kg hydrogen per kg of air.

The maximum fuel air ratio for self-ignition for three different mixture speeds were analyzed, considering the air and hydrogen speeds of 1624 (m/s) and 1316 (m/s), respectively. After the air and hydrogen are mixture, the air heats the hydrogen and the speed of the mixture reaches 1470 (m/s), and the mixture reaches the equilibrium temperature of 1020 K at stoichiometric hydrogen/air burning.

The results of the analysis reveal that the operational value of fuel air ratio should be from 0.019 to 0.022 kg hydrogen per kg of air, which the flame adiabatic temperature reaches from 2400 to 2600 K. The maximum temperature range at output nozzle is 890 to 990 K and the maximum speed range is from 2580 to 2680 m/s.

This analysis was able to estimate the operational parameters. These parameters as fuel air ratio, pressure, temperature and speed, are important for the performance of supersonic vehicle. A further analysis with new empirical data of combustion chamber and nozzle should be carried out for the evaluation of combustor and nozzle efficiency. The final speed of exhausted gases is useful for estimation of vehicle thrust.

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7. RESPONSIBILITY NOTICE

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