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THEORETICAL PERFORMANCE ANALYSIS OF HYBRID ROCKET PROPELLANTS AIMING AT THE DESIGN OF A TEST BENCH AND A PROPULSIVE SYSTEM

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Abstract

The current project aims at the understanding of the propulsive parameters of hybrid rocket motors. Computational simulations using the software CEA-NASA were carried out. The fuels paraffin wax, hydroxyl-terminated polybutadiene (HTPB) and polymethyl methacrylate (PMMA) were combined with three oxidizers: liquid oxygen (LOX), nitrous oxide (N_2O) and hydrogen peroxide (H_2O_2). The propulsive parameters examined were the characteristic velocity, specific impulse and adiabatic flame temperature. The propellant pair paraffin-LOX provided the highest performance for all parameters studied. This work was shown effective as a basis for the design of a static test bench and a hybrid propulsion system.

1. Introduction

Although liquid rocket engines have an efficient system and are more controllable, they are highly complex and are subjected to operational problems due to power systems. In the case of solid rocket motors this problem is non-existent because the fuel and the oxidant are stored in a compact and solid way. However, the disadvantages include the lack of control and the risk of bursting by cracking the grain. The hybrid propulsion is presented as an alternative due to its advantages of greater safety in the manufacture, storage and operation, besides being an inexpensive system in comparison with systems of liquid propulsion of equivalent thrust [1,2].
The main advantage over solid systems is meeting the requirements of missions with variable thrust, serial firing and storage of non-toxic propellants. Some of the applications also include boosters and upper stages for launch vehicles and satellite maneuvering systems [3]. The fuel configuration of a hybrid engine can be either solid fuel and liquid or gaseous oxidant, or vice versa [2]. The combination of a solid fuel with a liquid oxidant is the most studied combination nowadays, thus it was the choice configuration for the present project.
The first steps in the direction of the hybrid propulsion date back to 1930, concomitantly with the first works in liquid and solid propulsion. In the period between 1937 and 1943, O. Luts and W. Noeggerath performed tests of a hybrid 10KN thrust motor using coal and nitrous oxide and, just like Obberth in their experience with LOX and graphite, were not successful in their results due to low burning rate due to the high heat of sublimation presented by the carbon [1].
In the middle of 1940, the first significant effort was made by the Pacific Rocket Society regarding a hybrid rocket capable of being operated safely. However, it was only in 1960 that investments in research into hybrid propulsion systems began in the United States, when at least six organizations entered this field of research [4].
In the 1950s, it was demonstrated by G. Moore and K. Berman in General Electric's laboratory the use of liquid oxidant in hybrid engines using hydrogen peroxide containing 90% H_2O_2 as oxidizing agent and polyethylene as fuel. The results showed that there was uniform grain burning and that cracks in the internal walls did not impact the burning rate, while the oxidant flow could be controlled by the combustion chamber intake valve [5]. In the mid-1960s, more tests and theoretical investigations on high-energy hybrid propellants were performed at the German Space Center (DLR), among which combinations of propellants can be highlighted liquid fluoride and lithium (FLOX / Li) and lithium hydride (FLOX / LiH). More firing tests were performed between the 1970s and 1980s, in which other types of extensible fuels were made, such as N_2O_4, HNO_3, H_2O_2, polymers without and with mixtures of metals [5,6].

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Between 1980 and 1990 AMROC (American Rocket Company) developed the largest hybrid rockets ever. The propellant pair used in the developed engine was LOX and HTPB (hydroxylated polybutadiene), which generated a thrust of approximately 312kN with 70 seconds of firing. The projects were improved and the thrust value reached 1MN. The same propellant pair was used in sounding rockets launched by the American Air Force (USAF) in January 1994 [5].
In 2001, in a joint effort between NASA and researchers at Stanford University, a hybrid engine test facility was built at the NASA Ames Research Center as a result of ground-breaking research on the use of paraffins as fuel. This new fuel had regression rates two to three times higher than other fuels previously studied. Since the 2000s, there has been an increasing amount of research on hybrid propulsion systems, mainly in the United States and in other parts of the world such as China, Germany, Canada and Italy [6].
The hybrid propellant tests in Brazil began within the research institutes INPE, IAE / DCTA and ITA in the 2000s. Several propellants were used in theoretical and experimental researches such as paraffin, polyethylene, hydrogen peroxide, nitrous oxide and oxygen [3,6].
In this view, the present project consists in the execution of a detailed theoretical study, aiming the understanding of the propulsive parameters of hybrid rocket motors. Computational simulations using the chemical equilibrium software CEA-NASA were carried out with the purpose of analyzing and comparing the performance of several propellant pairs and diverse thermodynamic conditions in the combustion chamber. Finally, the results were used as a basis for a preliminary study of the design of a test bench and a system of propulsion for educational purposes.

2. Hybrid Propellant Pairs Analysis

In this work, several propellant pairs were tested and the main fuels analyzed were HTPB, paraffin wax and PMMA. These fuels were combined with oxidants such as LOX, N_2O and H_2O_2 in order to compare and study the propulsive performance parameters.
The hydroxylated polybutadiene polymer, commonly called HTPB, is based on the 1,3-butadiene alkene, which polymerizes through a mixture of butadiene base resin and polyisocyanate curing resin, forms the polymer chain [7]. HTPB has been considered one of the most promising solid fuels for applications in hybrid propulsion systems due to its low cost, easy processing and high heat of combustion when reacting with oxidants.
Paraffin wax (C_nH_{2n+2}) is an alkane hydrocarbon whose structure consists of a straight or branched straight chain. Among the advantages of using paraffin as fuel, it can be mentioned that the gases emitted from its combustion are non-toxic [6].

Polymethyl methacrylate (PMMA), also known as acrylic, has a methyl methacrylate repeat unit of $C_5H_8O_2$, and is a non-toxic substance. PMMA has a lower regression rate than the other fuels considered, but because it is transparent in the solid phase, it represents an interesting alternative for didactic purposes [8,9].
The wide use of liquid oxygen (LOX) by the space launch industry is due to the fact that it is a relatively safe oxidant and has a high performance at a low cost. Nitrous oxide (N_2O) is a substance that is considered non-toxic and presents high chemical energy. In addition, it presents advantages such as operational safety and low cost [6].
Another well studied oxidant due to its high performance is hydrogen peroxide (H_2O_2). When passing through a catalyst, the peroxide decomposes exothermically [3]. This causes it to reach temperatures high enough to ignite the fuel, which can be considered a great advantage.
One of the most important parameters for predicting the performance of a hybrid rocket engine is the regression rate. The regression rate is the rate at which the surface of the fuel recedes along a firing. This impacts directly on the configuration and performance of the engine (eg length and diameter of the combustion chamber) [6]. The regression rate can be obtained experimentally. However, there is no complete theory that can reliably measure that amount. Due to the fact that regression rate measurement is difficult to obtain, the data obtained experimentally have a high degree of dispersion, experiments effects of scale and are generally considered as secret material by those who perform the experiments. Therefore, there is little information on various combinations of propellants [10].
In order to compare the different propellant pairs, to size a grain and to predict the performance of a hybrid propellant, obtaining the accurate regression rate is of paramount importance. Figure 1 shows the comparison of the regression rate between some typical fuels of hybrid propulsion systems, using oxygen gas as oxidant, adapted from [10].

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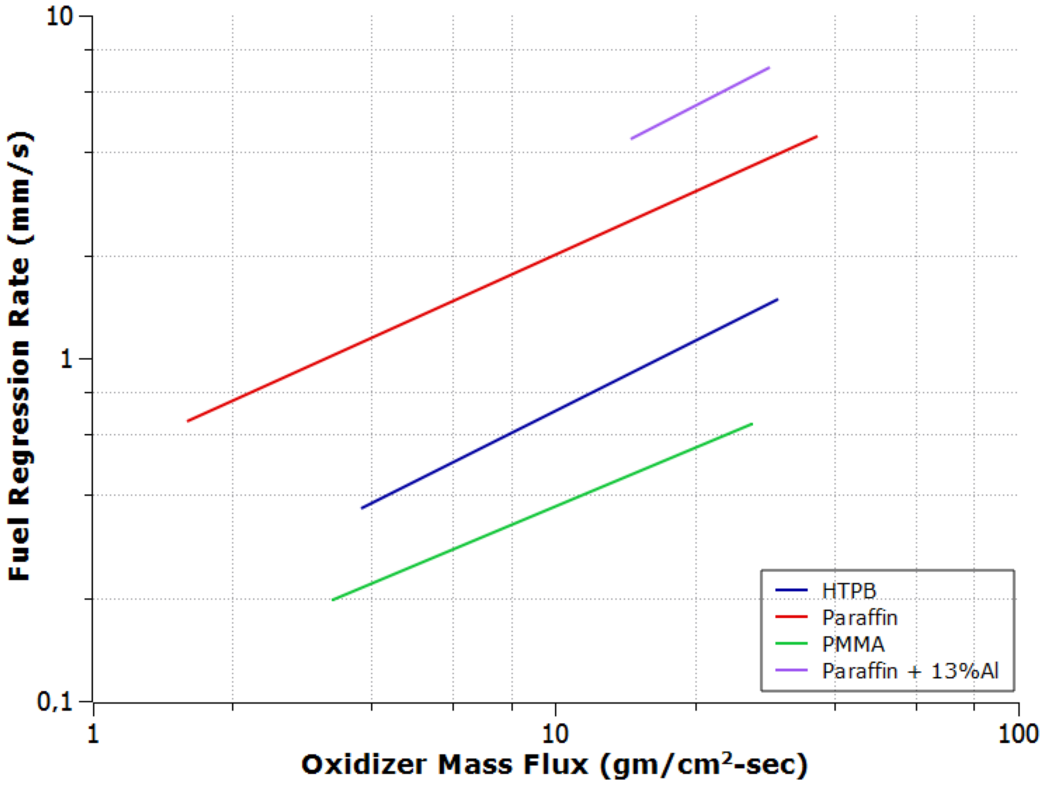

Figure 1: Relation between the fuel regression rate and mass flow of oxidant for various fuels used in hybrid rocket engines, adapted from [10].

When comparing the fuels used, PMMA has the lowest regression rate, which implies limited real applications. Fuels composed of hydroxyl-terminated polybutadiene (HTPB) have relatively high regression rates and are the most applicable fuels in the aerospace industry when it comes to hybrid propulsion.
In addition, it is interesting to note that paraffin-based fuels have a regression rate around three times higher than other fuels. During the paraffin combustion process, a thin liquid layer is created on the surface of the fuel, which has low viscosity and low surface tension. The flow of the gaseous oxidant provides the displacement and inflow of fuel droplets into the gas stream, that generates an instability of that thin layer. In this way, the mass transfer rate of fuel increases considerably [3]. The droplet transfer is not restricted by diffusion heat transfer from the combustion zone to the fuel, both processes occur in parallel. That is why paraffin-based hybrid fuels have a much higher regression rate than conventional fuels, which depends exclusively on evaporation of the grain surface. Due to this fact and a low complexity required in the grain geometry, the use of paraffin for propulsive purposes has been the subject of several researches recently.

3. Thermochemical Simulations

Thermochemical simulations were run through the free distribution software NASA Chemical Equilibrium With Applications (CEA-NASA). The calculation of rocket motor performance parameters involves a number of assumptions such as zero velocity at the inlet of the combustion chamber, a homogeneous mixture, complete combustion and no heat loss. In addition, a one-dimensional flow and isentropic expansion of the gases along the nozzle is considered. The equilibrium condition is based on the hypothesis that there is instantaneous chemical equilibrium during expansion in the nozzle. The frozen condition considers that there is no chemical variation during the expansion process, in other words, it keeps the concentrations of reagents and products constant after the freezing point.
The fuels chosen to be analyzed were paraffin, HTPB and PMMA, each fuel was combined with the oxidizers LOX, N_2O and H_2O_2. The main properties of the fuels used as input data for the simulation are shown in Table 1.

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Table 1: Properties of the fuels paraffin, HTPB and PMMA.

Fuel	**Formula**	**Enthalpy of formation (kJ/mol)**	**Temperature (K)**
Paraffin	$C_{20}H_{42}$	-594.572 [6]	298
HTPB	$C_{3.8462}H_{5.8077}O_{0.0385}$	23.99 [11]	298
PMMA	$C_5H_8O_2$	-348.7[12]	298

A total of nine combinations were made and the propulsive parameters of each pair were studied. The propulsive parameters considered in the scope of this project are characteristic velocity, specific impulse and adiabatic flame temperature.

The equilibrium condition was adopted for the simulation analysis, which in most of the cases presents overestimated values. Since the HTPB and PMMA combustion takes place in the gas phase, which means a very quick reaction, the approximation to the frozen model is quite plausible (reference missing). However, regarding the paraffin, it is important to consider the post combustion region to reach a more complete combustion process of paraffin droplets in the oxidizing flow, therefore an equilibrium model would better describe the process. For the purposes of this work, the equilibrium condition was chosen for representing an acceptable approximation to establish upper limits of performances expected for the analyzed propellants.

In order to obtain the values of the specific impulse, adiabatic flame temperature and characteristic velocity, a mixing ratio O/F ranging from 1 to 8.5 was considered. All the simulations were run at a pressure of 10 bar in the combustion chamber, a combustion temperature of 2800 K was estimated and contraction and expansion ratios of 2 and 4, respectively, have been considered for all the propellants.

Characteristic velocity, c^*, is basically a function of the propellant pairs chosen and the efficiency of the combustion. Thus, it is a parameter frequently used to compare the performance of various combinations of propellants, since each propellant pair presents a different adiabatic temperature as well as different specific heats involved. The ideal value of c^* is given in Eq. (1) showing that it is a function of the ratio of specific heats, k, chamber temperature, T, and effective molecular mass, $\mathfrak{M}$, [2]:

$$c^* = \frac{\sqrt{\frac{kRT}{M}}}{k\sqrt{\left(\frac{2}{k+1}\right)\frac{k+1}{k-1}}} \tag{1}$$

For the same ratio of specific heats, the highest characteristic velocity is obtained when maximizing the $T/\mathfrak{M}$ ratio.

The ideal values of characteristic velocity, obtained in the thermochemical simulation for all propellants, can be observed in Figure 2.

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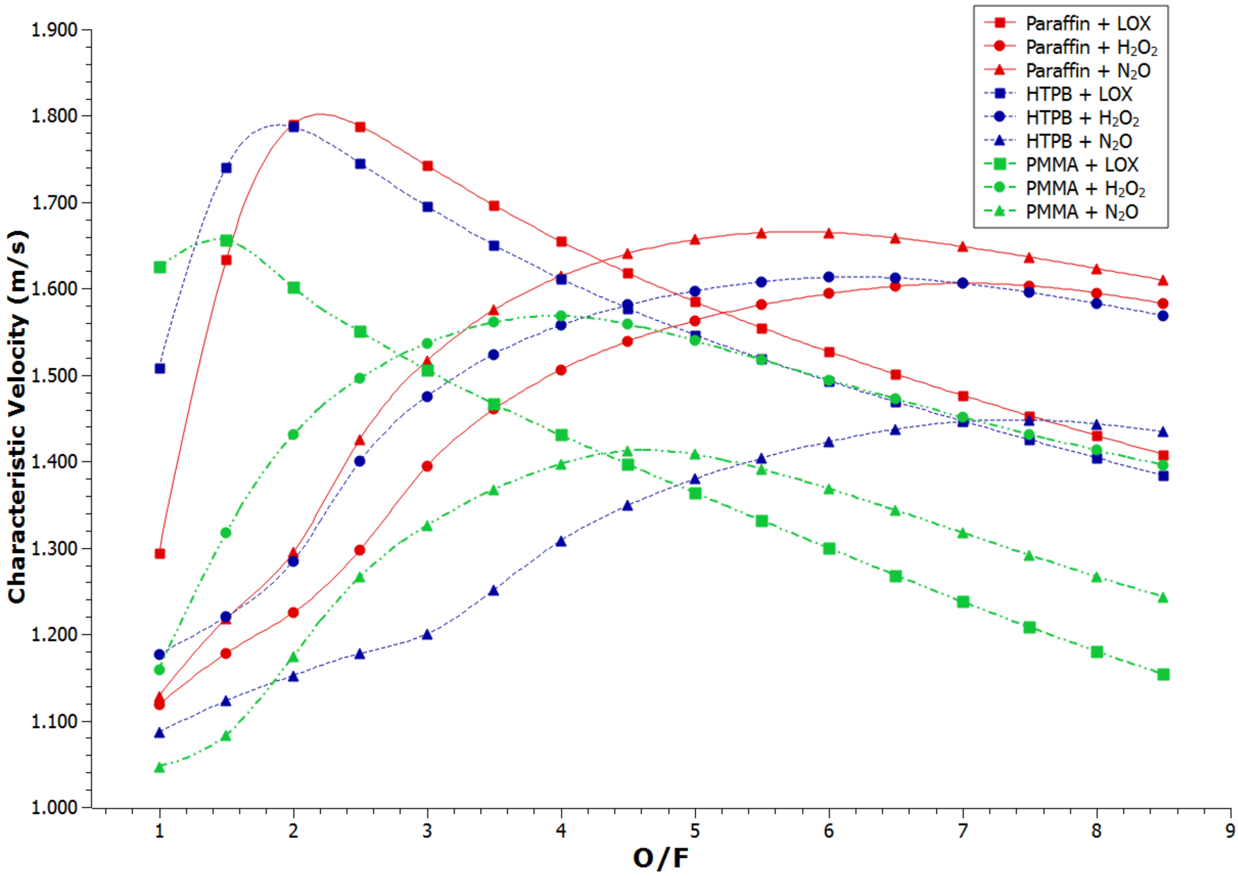

Figure 2: Characteristic velocity of the combination of the fuels with different oxidants as a function of O/F.

The combination of LOX with any fuel provides the highest values of characteristic velocity. The performance of the fuels HTPB and paraffin in combination with LOX are similar with slightly displaced O/F, providing approximately 1800 m/s for an O/F close to 1.8 and 2.2, respectively. On the other hand, the lowest values are presented for HTPB and PMMA when using N_2O as oxidizer. The main reason for this trend should be found in the combustion products composition containing nitrogen which doesn't contribute to the oxidation process while retaining part of the released heat, thus reducing the value of $T/\mathfrak{M}$.

Another essential parameter for the performance analysis of any rocket propulsion system is the specific impulse, which is directly associated with the variation of the amount of movement per unit weight of the propellant [3,6]. The higher the I_{sp} value is, the less amount of propellant the engine requires to function at a given total impulse, the better the performance. Figure 3 shows the simulated specific impulse trend of the propellant pairs versus O/F.

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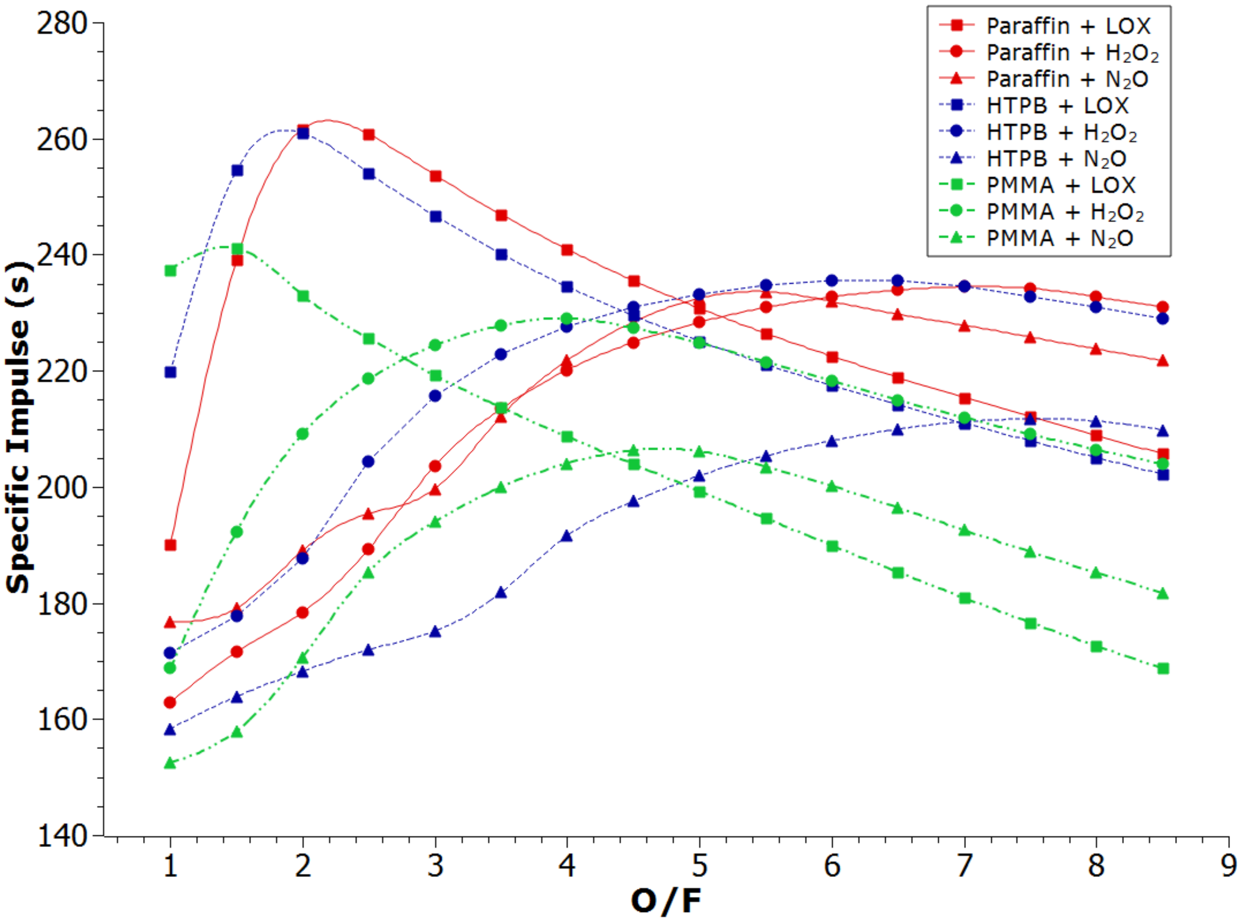

Figure 3: Specific impulse of the combination of the fuels with different oxidants as a function of O/F.

The highest values of Isp are observed for the combination of HTPB-LOX and paraffin-LOX, in which the peak of 262s occurs for an O/F ratio of approximately 1.7 and 2, respectively. When PMMA reacts with LOX, it provides the highest value, 242s for a 1.5 mixture ratio. The highest values of Isp obtained with LOX compared to the other oxidizers is explained by the high oxidation potential of LOX [1].

HTPB and PMMA reacting with N_2O provides the lowest values of Isp, whereas for paraffin the N_2O-curve has a tendency similar to that of H_2O_2. Storable oxidizers, H2O2 and N2O, tend to optimize at a high O/F ratio, whereas LOX optimizes at O/F close to 2.

Furthermore, specific impulse values presented by the hybrid propellant pairs are considerably lower when compared with the conventional alternatives, liquid rocket propellants, with Isp varying between 200-460s. Therefore, the main idea is to study a combination of propulsion pairs in order to maximize values for better engine performance, so that they are comparable to conventional rocket motor.

During a combustion process, the released chemical energy is lost as heat to the vicinity or can be used to raise the temperature of the combustion products within the chamber. When there is no loss of heat to the environment, the temperature of the products reaches its maximum value, called the adiabatic flame temperature. The adiabatic flame temperature depends on the reactants, the degree of completion of the reaction and the amount of air used, and its maximum value occurs when there is complete combustion with a close to stoichiometric amount of air. In addition, it is an important design parameter for combustion chambers and nozzles. In general, temperatures within these devices do not reach the theoretical flame temperature because combustion is incomplete, there is loss of heat to the vicinity and a part of the flue gases dissociate at high temperatures [13].

The adiabatic flame temperature in the combustion chamber depends on the oxidant choice. The higher the thermal energy obtained by the combination of the pair, the greater the amount of energy that will be transformed into kinetic

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energy, which will directly affect the performance parameters. Figure 4 shows the adiabatic flame temperature curve for the different propellant pairs versus mixture ratio.

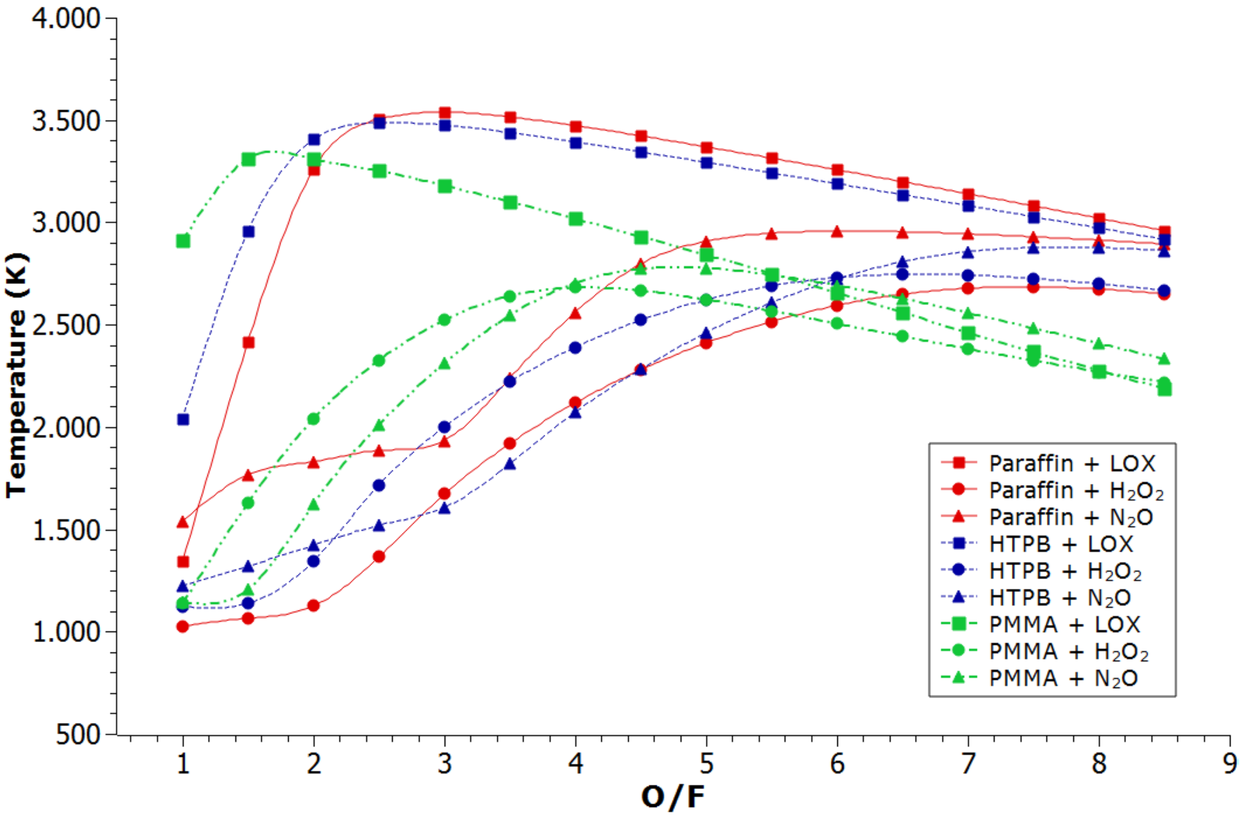

Figure 4: Adiabatic flame temperature in the chamber considering the combination of the fuels with different oxidants as a function of O/F.

The peak temperature occurs when LOX is used as oxidizer in combination with paraffin, at approximately 3520K for an O/F ratio of 2.8. Similarly, the combination of LOX and HTPB provides temperature values with the same trend curve, however, with a peak of 3500K for an O/F of 2.4. For a combination of LOX and PMMA, it is noted that the combustion temperature increases until it reaches an O/F of 1.6.

Adiabatic temperatures of paraffin in combination with H_2O_2 and N_2O present a quite similar trend for O/F larger than 3 with peak values under 3000K. Taking into account the reactions of PMMA with H_2O_2 and N_2O, the optimum O/F lies around 6.5 and 8, respectively.

Summarizing, all the performance parameters investigated, i.e. characteristic velocity, specific impulse and adiabatic flame temperature, show the highest values for the Paraffin/LOX hybrid rocket propellant pair. HTPB/LOX performance parameters are slightly lower, however, following the same trend of LOX/Paraffin. PMMA/LOX presents the lowest values of the performance parameters, however, while c* and Isp follow the same trend of the other fuels reacting with LOX, the adiabatic flame temperature decreases with a higher slope. The performance parameters of the storable oxidizers, H_2O_2 and N_2O, displays higher values over a wider range of O/F when reacting with HTPB and paraffin wax, however, the peak of the performance parameters of PMMA are quite close to that of the other fuels.

When only the specific impulse and characteristic velocity are taken into account, LOX is shown as the best oxidizer alternative. However, according to the literature [1,3,6] the storable oxidizers, H_2O_2 and N_2O, present significant advantages in bulk density, providing competitive or superior amounts of impulse on a per unit volume basis when compared to LOX. In addition, storable oxidizers tend to optimize at a high O/F ratio, which implies on a minimization of the size of the combustion chamber containing the solid fuel, thus reducing the overall mass of the rocket [1].

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The Isp values of the best performing hybrid rocket propellant pairs, LOX/HTPB and LOX/Paraffin, resembles the liquid propellant LOX/Kerosene, which is largely used in boosters and core engines. Fuels based on paraffin wax or PB polymerers allow additives in their composition, which collaborates with the enhancement of the motor performance. When light metal additives are used in solid fuels, combined with cryogenic liquid oxidizers, the hybrid pair can deliver results comparable to some liquid propellants or even better.

4. Design of a test bench and propulsive system preliminary study

Aiming at the design of a low-cost test bench to be installed at the University facilities, the ideas for the design are mainly defined by a theoretical approach and the analysis of the propellant pairs, but also taking into account the use of materials easily found in the market and characteristics allowing safety handling.

The design aspects of a test bench require a prior establishment of the propulsive parameters, in order to define dimensions and boundary conditions. The calculation of the combustion chamber and the geometry of the propellant grain are strongly related to parameters such as regression rate, fuel mass flow, which is inversely proportional to the specific impulse, and oxidant mass flow, which depends on the O/F ratio. As shown in Eq. 2, dimensions such as diameter and height of the propellant grain are directly influenced by the choice of propellant pair propulsive parameters defined and studied, which makes it important to choose carefully bearing in mind the conditions allowed at the environment of operation. Therefore, the realization of the theoretical analysis is shown as an extremely important step.

$$h_f = \frac{\dot{m}_f}{\pi D_i \dot{r} \rho_f} \tag{2}$$

Where $\dot{m}_f$ is the fuel mass flux, D_i is the diameter of the grain, $\dot{r}$ is the regression rate of the fuel and ρ_f is the density of the fuel.

Despite being the oxidant with the best performance parameters, liquid oxygen is clearly not adequate for the purposes of this work because of its cryogenic nature. On the other end, considering the readiness of gaseous oxygen, GOX, and the same performance parameters of LOX, it can be a reliable choice for the laboratory test bench. Combining the hydrogen peroxide performance values with its ease of handling and storage presents another great alternative, considering application in real rockets. Due to its advantages, such as high chemical energy, safety and low cost, as well as its self-pressurizing nature, nitrous oxide is a great option for oxidant .

The choice of fuel not only depends on its regression rate or density but rely on its availability and purpose of the test bench. Despite the great performance parameters, the difficulty to obtain HTPB can be an obstacle for the project. The performance parameters of PMMA are much lower when compared to the other fuels, however, its transparent property allows the burning to be observed and can be very interesting for didactic purposes. Paraffin presents a great performance and high regression rates, easy to obtain and is the focus of many studies in the current time. Therefore, it looks as the best choice for research purpose.

5. Conclusions

The current work presented a detailed study of several hybrid propellant pairs propulsive parameters using the chemical equilibrium software CEA-NASA. Three fuels, paraffin wax, HTPB and PMMA, reacting with three oxidizer, LOX, H_2O_2 and N_2O, have been simulated considering equilibrium condition during the expansion in the nozzle. Comparisons with data from the literature were carried out and the propulsive parameters obtained in this project proved to be in reasonable agreement.

The specific impulse, characteristic velocity and adiabatic flame temperature over a range of O/F from 1 to 8.5, for a chamber pressure of 10 bar, have been obtained and analyzed. In the following the most relevant results are summarized:

- The Paraffin/LOX pair presents the highest values for all the propulsive parameters here considered;
- HTPB/LOX pair shows slightly lower performance parameters value, however, following the same trend of LOX/Paraffin;
- PMMA/LOX pair presents the lowest values of the performance parameters;

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- The performance parameters of the storable oxidizers, H_2O_2 and N_2O, displays higher values over a wider range of O/F when reacting with HTPB and paraffin wax;
- LOX is shown as the best oxidizer alternative in this research;

However, according to the literature [1,3,6], H_2O_2 and N_2O present significant advantages in bulk density, providing competitive or superior amounts of impulse on a per unit volume basis when compared to LOX. Therefore, one of the next steps of the research aims to investigate the impulse density of the hybrid pairs.

The great performance showed by the Paraffin-LOX combination instigates future research and promising results as paraffin presents regression rates about three times higher than conventional hybrid fuels. Therefore, it looks the best choice for research purpose the design of a test bench using GOX/paraffin, to be installed in the Propulsion Laboratory at Federal University of ABC.

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