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Numerical and Thermochemical Analysis of Hybrid Rocket Fuels with Metallic Additives

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***Abstract*— A theoretical assessment of various fuels and additives which aid in increasing the performance parameters of rocket engines was completed. It is focused mainly on hybrid rocket engines and their behavior when operating on different fuels. By making a comparative study, the fuels to oxidizer combinations are analyzed in detail. One of the main studies of this project was to analyze the vaccum specific impulse production in a hybrid rocket engine. A detailed parametric study was made to ascertain which fuel-oxidizer combination gave better performance. Conclusions were made as to optimized fuel/oxidizer (O/F) combinations. Then, fuel oxidizer combinations were again studied, now by considering additives, which are meant to improve its performance. The additive considered for this study is Aluminum and it constitutes about five percent of the fuel. Aluminum is chosen as it gives very high performance and is easily available and reasonable in cost. It shows an improvement in the vaccum specific impulse. Also, the oxidizer to fuel ratio was a major parameter to determine the performance. The performance parameters are studied at different O/F ratios. Obtaining a high performance at a low O/F ratio proves that the fuel-oxidizer with an additive is a better choice. The major choice of fuels used here are HTPB hydroxyl-terminated polybutadiene) and Paraffin. Liquid oxygen and gaseous oxygen are used as oxidizers. The NASA-CEA analysis is used to obtain the output performance parameters and the plots are made. An intensive study on the numerical approach for simulation of the combustion process in the hybrid rocket and its various characteristics are done. More emphasis is given to the computational fluid dynamics aspect and certain recent methodologies developed are studied. The nozzle erosion characteristic, which is one among the ongoing research in hybrid rocket development, is reviewed here. The performance of paraffin-based fuels and their future applications is studied and shown that validation is one of the major processes for a methodology to be adopted for the upcoming purposes.**

Keywords—hybrid rocket; Paraffin; Vacuum specific impulse; combustion chamber

I. INTRODUCTION

Though liquid propellant rockets are highly efficient and give higher performance and are also re-start able in comparison to solid rocket motors, their construction is quite a complex structure. This problem is overcome by solid rocket motors where the fuel and oxidizer are combined in a similar solid phase and combustion takes place at ignition temperature of the fuel. But the uncontrollable nature and explosive dangers mark a huge disadvantage. In hybrid rockets, there is good operational flexibility and non-explosive nature, thereby making it a better choice than both solid and liquid rockets engines. The configuration in a hybrid rocket can either be fuel in solid-state and oxidizer in the liquid state or vice versa. The first developments of hybrid rockets consisted of coal as fuel and nitrous oxide as the oxidizer. Also, graphite and liquid oxygen were considered as a combination. But these tests were not successful due to less burn rate and high rate of sublimation. In the later stages, there was a significant improvement in hybrid rocket technology, where hydrogen peroxide and polyethylene were introduced as a combination. Better results were obtained showing a uniform burn rate and less impact due to cracks. Much theoretical research about the fuel selections led to various combinations of fuels and oxidizers, and certain binders which enhance the performance. This led to the development of some of the largest hybrid rockets, where a thrust of 300 kN was achieved using an HTPB(Hydroxyl-terminated Polybutadiene) and liquid oxygen combination.[1] With significant improvements, the thrust value raised to almost one Mega Newton. The later stages introduced a fuel that had the regression rate higher than any other fuel, which is Paraffin. The rate at which the solid fuel surface recedes along the burn is the regression rate. It mainly depends on the dimensions of a combustion chamber. The study of regression rate has been a challenging aspect for hybrid rockets. Due to the ablative fuel, a convective heat transfer is caused on the surface of the fuel which in turn creates a blocking mechanism; the main reason for the low regression rate [2]. To rectify this, the introduction to multi-port grains was established. But this, in turn, created complexity in the system concerning injection and casting and other operational parameters. Further developments included ways to improve the single port-type geometry, addition of energetic particles, and different methods of fuel injection systems [2].

One of the efforts put forth by Karabeyoglu [2] was the introduction of liquefying fuels. It is generally based on the idea of paraffin wax, where the fuel melts on the surface creating a liquid layer that is thin and has a low value of viscosity. The droplets of this fuel are then entrained by the gas. With the mass transfer, a high regression rate is achieved in paraffin fuel. This paved the way for efficient single port-type geometry in hybrid rockets. Paraffin fuels are often said to have low melting temperature and cannot be used for high-temperature range with long burning times [2].

This issue has been proven experimentally by Ernico [3] that paraffin fuels can burn for longer periods. For the experimental purposes, a motor of 1kN thrust with high test peroxide and paraffin was used and was tested up until 80 seconds(fuel-rich burn condition).[3] It is also proven that the heat does not penetrate the grain during the process of burn, which is the theory put forth by Karabeyoglu. (Paraffin liquid layer theory) [2], [4], [5]. This is proven by using thermocouples in the fuel grain. It was noted that the grain remained at room temperature unless it was not exposed to port flow. The process of entrainment is used to increase the fuel-burning area and thus to decrease the blocking effect. This can be used as an appreciable application of space missions and is a perfect entrant for the launch systems.

The process of entrainment is described in Fig. 1

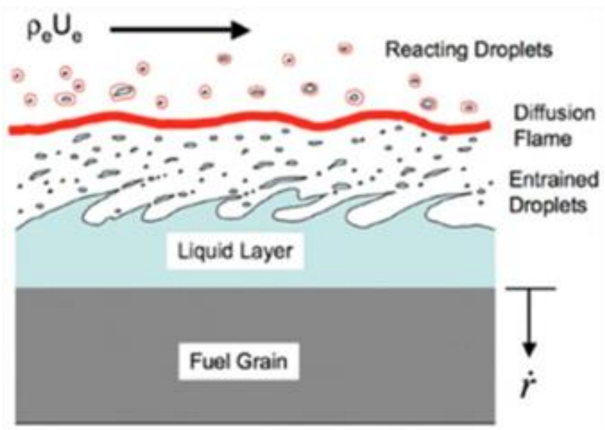

Fig. 1.Liquid layer theory demonstration

An optical investigation of this phenomenon is shown in [4] where an exponential relation is observed involving the viscosity layer and the regression rate value.

A. Applications of hybrid rockets

For the upcoming space era, hybrid rockets are a promising future. It includes microsatellites, planetary landers, and orbital vehicles. The development of hybrid rocket motors has been for several decades and is being widely studied in recent times. The main aim is to develop a safe, controllable, and less expensive vehicle that will help with the development of the future of rocket propulsion.

This created a new era in space technology development. Studies have been made at Stanford University for using hybrid rockets as a medium for planetary missions. A concept called in-situ propellant production was developed. It is based on the concept of producing propellants instead of carrying them, which thereby reduces the cost and mass during take-off. Such concepts can be done with vehicles like hybrid rockets. This idea helped in a 40% increase in efficiency. There is also an advanced version of the reusable nozzles, which can be highly applied to future propulsion systems. It can also help in reducing pollution in the environment, with high reliability and operations.

Fig. 2 shows a basic outline of some of the important parts of a hybrid rocket engine and Fig. 3 shows a more detailed illustration of the engine design.

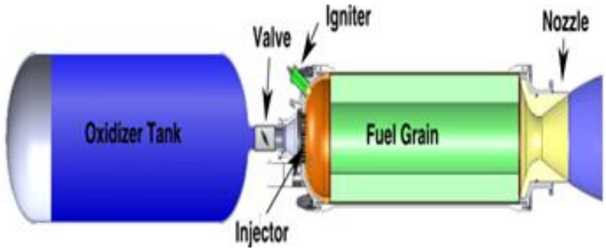

Fig. 2 Engine principle

One of the great challenges faced in hybrid rocket vehicles if nozzle erosion. Though the concept of ablative cooling can be applied to hybrid rockets (as is applied to solid rockets), the range at which the hybrid rockets thermal materials behave is different from that of solid rockets. The reason for this erosion is the presence of very high oxygen concentrations in the products of combustion. Therefore, numerical simulations must be used to analyze the nozzle erosions. This project is focused upon hybrid rocket fuel selections and the performance comparison with and without the addition of metallic additives. A thermochemical analysis is performed using chemical equilibrium analysis software. This gives us various performance parameters of the engine and gives a better insight into the selection of metallic additives.

Also, an extensive literature survey is done based on various aspects of numerical simulations on hybrid rockets, focusing on several design and methodologies proposed by researchers to give better values of specific impulse and fuel regression rates, with different combinations of fuels and oxidizers, and also a study on paraffin-based fuels and its development and challenges faced due to nozzle erosion due to the use of graphite as a material is focused in this project.

II. Literature Review

A. Previous research on the selection of fuels

Research based on solid fuel ramjets and hybrid rockets by adding metallic additives indicates a significant increase in the performance parameters. The increase in density impulse and specific impulse with the addition of metallic additives is a key factor is the performance of the engine. This research paper focuses mainly on the selection and ranking of the metallic additives selected. It gives a method to develop a good balance between the material cost and the gain from the performance.

As an example, considering a low energy oxidizer such as nitrous oxide, aluminum can be a good additive and is also readily available. Paraffin is ranked as the best selection accounting for fuels as it provides a hydrophobic nature, high regression rate, and is considered in terms of the low cost. Boron has significantly shown low results when it comes to performance parameters and less generation on the benefits of cost. [6] Among the additives considered for this study, aluminum hydride provides the best performance parameters.

A major conclusion from this study relies upon how the selections of fuels are useful to the engine's performance. The fuels selected do not account much in terms of the regression rate, but rather tends to increase the specific impulse of the engine. The selection of these fuels is beneficial in terms of the performance parameters but does not give many advantages over the cost performance.

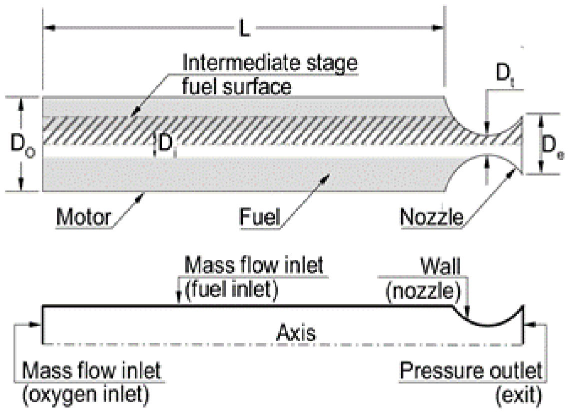

Fig. 3.Illustration of a hybrid rocket engine

B. The use of computational models

The design models of hybrid rocket engines can be analyzed thoroughly using tools to compute the two main characteristics of hybrid rockets, the preliminary design and its model, and motor performance. To develop computational models, a hybrid rocket performance code helps in analyzing the designs. The code involves the use of performance parameters as its input values. These performance parameters are calculated using various thermodynamic properties. To calculate the thermodynamic properties of the fuels, a NASA Lewis code, called the Chemical equilibrium analysis is performed. This tells about the combustion and theoretical performance of the rocket. The input parameters include the oxidizer to fuel ratio, the nozzle expansion ratio, and the chamber pressure. Thus, an input file is created, and the NASA-CEA (Chemical Equilibrium Applications) application runs this file to save the output data calculated. The outputs from these calculations help to solve the governing ordinary differential equations. Therefore, different fuel and oxidizer mixtures can be analyzed using the CEA analysis software. These propellant combinations help to analyze motor performance. The design and performance parameters were studied for a model of a Phoenix -1A hybrid rocket motor. The design model included the grain size and the nozzle dimensions, and the performance parameters were computed using numerical methods. These two codes use the chemical equilibrium analysis software to input the thermodynamic properties. This computational tool was a predictive model for the development of the Phoenix- 1A rocket. The hybrid rocket performance simulation tool was developed, and the tools used in this now help in the progression of the development of the Phoenix-1B rocket motor. Therefore, this gives an idea of how to approach to calculate the thermochemical properties of a given mixture. The data sheets of the CEA software also help us to perform a comparison between the fuels and analyze better fuel-oxidizer combinations.

C. The use of metalized formulations

The use of metallic formulations in solid and hybrid rockets enhances performance rates. The metallic additives were experimentally analyzed by adding the same compositions of the various selected fuels [7]. Comparing the results with that of the conventionally used aluminum propellants, it was shown that the addition of micro and nanostructures helped in enhancing the performance of the rocket engines. It showed a high increase in ballistic performances, which includes a higher specific impulse in solid rockets. In hybrid rockets, the use of metalized additives improves the regression rates, specific impulse, and reduces throat erosion. Hydroxyl-terminated polybutadiene (HTPB) is a polymer widely used in propulsion both for solid propellants and hybrid fuels. With HTPB as a solid fuel, additives like aluminum hydride and lithium aluminum hydride are found to be suitable in terms of gravimetric specific impulse. It helps in improving the solid fuel regression rates and in hybrid rockets, helps in reducing the nozzle erosion. Though experiments have found large advantages in the use of nano-sized metallic additives, it has challenges like soot formation and its behavior in stratospheric ozone layers [8], [9] Therefore, the dual metal formulation is a technique followed which helps in optimizing the performance and also helps in increasing the mechanical behavior. When comparing the theoretical and experimental results, it should also be accounted for losses, as the maximum thrust or any other parameter may not account for the predicted value. These may be due to combustion losses which include instability, heat transfer, and friction losses.

Yash Paul [10] performed a thermal decomposition of paraffin fuels. With adding additives, the radiant heat transfer and high exothermic reaction temperatures increased the efficiency of the combustion process. It is shown that not the metallic oxides formed, but rather the heat produced from various metalized formulations (such as boron and aluminum) is the main mechanism [10]. The application of boron as an additive is limited due to its issues associated with complete combustion. They are applied to short ignition times with HTPB and are proved theoretically and experimentally in several literature surveys. The addition of additives to a pure paraffin fuel must be taken under serious considerations as it has many chances for developing a combustion instability condition and the formation of oxide layers in the combustion chamber which in turn affects the regression rate conditions. An illustration of applications of Paraffin fuel is shown in Fig. 4 Other additives like lithium, beryllium, and magnesium can also be applied and are usually meant to improve the energy characteristic of the given solid propellant. Aluminum and boron have typical features that have high gravimetric and volumetric heat release [10]. The entrainment process can be further enhanced using nano-sized particles. It helps in developing fuel-rich conditions and the regression rate when blended with paraffin fuels. This concept was proved by Seongjoo [11] where the fuel was blended with nano and micro-sized particles and electron microscopy tests were done to evaluate the homogeneity. Nanomaterials showed a high value of viscosity; therefore, the addition of microparticles produced a higher regression rate value. Hence, characteristic velocity, for the overall selected range for the oxidizer to fuel ratio for the micro fuel is greater than that of the nano-particle fuel.

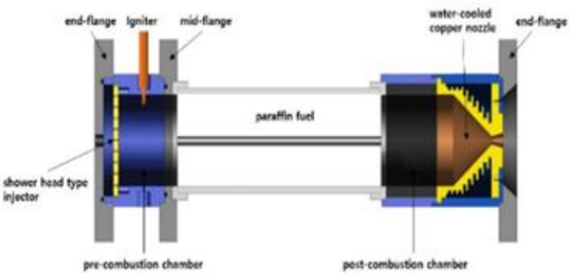

Fig. 4.An example of the application of Paraffin fuel with Aluminum additive, experimental setup

III. METHODOLOGY

A. *Fuel selection*

For analyzing the output of hybrid engines, two fuels are being taken into consideration.

Paraffin- Reason for selection

•Good to operate at extreme temperatures.

•It has a general formula of CnH2n+2 with a structure consisting of straight-chain (sometimes also branched). It is hydrophobic, unlike other performance additives which are sensitive to air.

•It is of low cost compared to other binders.

•They have a high regression rate which is 3-4 times greater than classic binders.

•It is non-toxic and has a very high lifetime.

HTPB- Reason for selection –An elastomeric polymer, HTPB is classic hybrid rocket fuel. It is readily available, and its properties are well-known.

•It is promising hybrid rocket fuel in propulsion systems.

•It has a very high production of combustion heat when mixed with oxidizers and is primarily is taken from solid rocket background.

B. *Oxidizer Selection*

•The performance of the engine is studied by considering Lox (liquid oxygen) and Gox (gaseous oxygen) as oxidizers.

• Liquid oxygen is widely used by the space industry due to its high performance and safety. Combining with the respective fuels, a comparative study is made.

•Studies have shown that additives and binders help to increase the specific impulse and regression rate of fuels.

•Other oxidizers include nitrous oxide, which produces high levels of chemical energy and is non-toxic.

•Hydrogen peroxide is another oxidizer that can produce very high ignition temperatures.

C. *Selection of input values used in CEA analysis*

The chemical equilibrium analysis is performed to get the output parameters of the fuel combinations as follows. Below listed are the parameters considered to study the combinations. Through this output, the vaccum specific impulse is taken into major consideration to analyze.

D. *Input Parameters*

CEA data

1. Problem type- Rocket
2. Pressure considered- 2 MPa (this is a chosen value to study the output at that pressure value)
3. Fuel selection- Paraffin and HTPB from the charts (additive is also added if needed)
4. Oxidizer selection- O2 and O2 (L)
5. Oxidizer to fuel ratio- Low value -1, High value -8, Interval-0.5
6. Chamber to exit pressure ratio- 20 MPa
7. Temperature- 298 K
8. Infinite area combustor is assumed

9. Conditions – equilibrium, trace value of 10-5. Products in mass fractions, no transport properties or ionized species, Heat in SI units.

10. Output file length- Long

E. Metallic additive

Apart from comparing the fuel and oxidizer mixture, adding an additive to the fuel, and comparing the results is also performed.

Aluminum- Reason for selection

•Addition of aluminum to the fuel in a small percentage helps in improving the specific impulse. It has good combustion properties, when burnt; a huge amount of energy is released in the combustion chamber leading to the expansion of gases.

•As this is in a fixed volume, the pressure rises, and the gases expand through the nozzle at a very high velocity. This leads to a higher specific impulse.

•The reason for choosing aluminum though there are other compounds such as beryllium is because of its non-toxic nature and is an inexpensive fuel.

Various plots are generated between the O/F ratio of the fuels and oxidizers and the vaccum specific impulse at the exit.

Combinations

•Paraffin-Lox, Paraffin with Al –Lox

•Paraffin-Gox, Paraffin with Al –Gox

•HTPB-Lox, HTPB with Al-Lox

•HTPB-Gox, HTPB with Al-Gox

From Fig. 5 to Fig. 8 it is found that Paraffin with gaseous oxygen combination and HTPB with Gox combination, including 5% aluminum can produce an increase in its vacuum specific impulse. Also, a high value of Ivac (vacuum specific impulse) can be achieved in a lower O/F ratio when considering the addition of a metallic additive. This shows us that the metallic additive gives a significant increase in performance.

F. Plot Description

The following plots are obtaining by taking the range of O/F (Oxidizer to Fuel) ratios to the vaccum specific impulse.

•Four graphs are plotted from which it can be analyzed which fuel oxidizer combination gives us higher performance.

•It is also important to note which fuels would give a better performance at a low mixture ratio. Then, a comparison is made by adding aluminum to the fuels.

•Though fuels without aluminum produces a high Ivac as the O/F ratio increases, it is important to note that fuels with aluminum produce Ivac at a higher value at a particular low O/F ratio and then decreases as the O/F ratio increases.

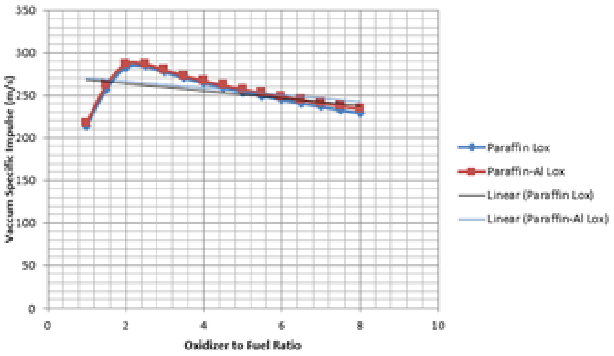

Fig. 5Paraffin-Lox, with and without additive

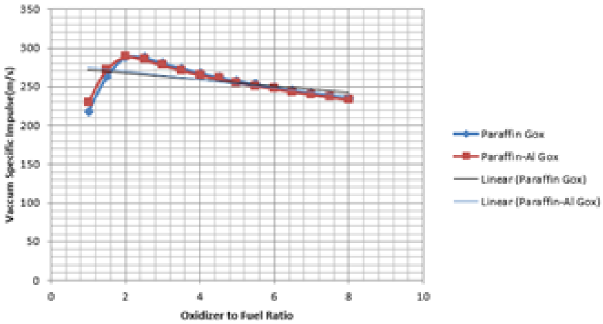

Fig. 6 Paraffin-Lox, with and without additive

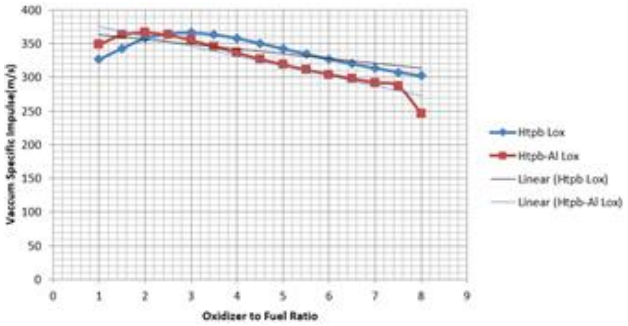

Fig. 7 HTPB-Lox, with and without additive

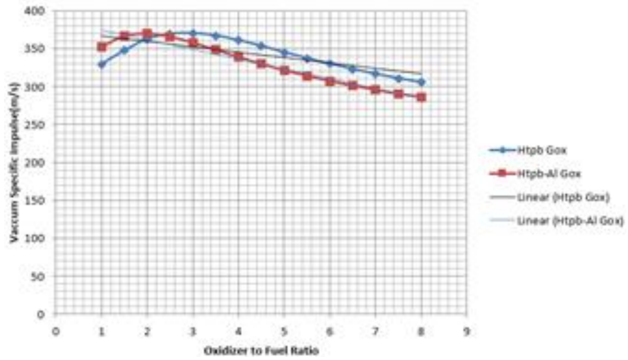

Fig. 8 HTPB-Gox, with and without additive

IV. OBSERVATIONS

It can be inferred from the following plots that a high value of the impulse can be achieved at a lower O/F ratio when Aluminum is added and also helps in increasing the vaccum specific impulse.

•Paraffin and Gox combination with Aluminum as additive produce a vaccum specific impulse value of about 288.2 ms, which is higher compared to Paraffin-Lox combination with Aluminum.

•Similarly, HTPB and Gox combination with Aluminum produces a vaccum specific impulse of about 370.3 ms, which is higher than when the fuel is mixed with Lox.

•From these observations, it is seen that a fuel mixed with Gox helps in improvising the performance compared to Lox.

•Reasons- Gox tends to have higher efficiency and thus gives higher specific impulse.

•Gaseous oxygen helps in making use of the entire propellant and will enhance the process of mixing in the chamber. This is the reason it gives higher efficiency.

•Flame temperature is high when compared to liquid oxygen. Lox in the combustion process mainly relies on atomization.

•The injector should provide optimum performance for higher efficiency. Gox also has the advantage of easy availability in pressurized cylinders while Lox is not.

•Thermally insulated containers are required for the transport of Lox, (also should be stored at low temperature), while Gox can be stored as transported easily.

•The valve systems used for Lox in rockets are complex. The only disadvantage of Gox when compared to Lox is its density.

• Lox has a density that is almost 1000 times higher, therefore, a small tank volume would be sufficient for Lox, while needs a larger volume.

•For a design of a small hybrid rocket, gaseous oxygen would be an option.

•When it comes to fuel selection, the recent improvement in technologies are highly based on paraffin fuels. The reason behind this is the high regression rate of paraffin fuels.

•During its combustion, a layer with a less viscosity parameter and low surface tension is formed over the fuel surface. When the oxidant gas can flow, it causes the fuel droplets to pass into the gaseous stream, thereby causing instability.

•Therefore, the rate of mass transfer of paraffin fuel becomes higher which in turn gives a very high value of regression rate.

A. *Comparison of HTPB, Paraffin and Polymethyl Methacrylate Fuels*

A comparison of Paraffin, HTPB, and PMMA (Polymethyl Methacrylate) is shown in [12] These fuels are mixed with various oxidizers to do a comparative study among the following combinations. Thus, a total of nine fuel-oxidizer combinations are studied here [12]. The reason for choosing PMMA is because it is non-toxic. However, it has a low regression rate compared to other fuels.[13] The reactions associated with PMMA and HTPB are fast and take place in a gaseous phase. The performance parameters for this analysis include the adiabatic flame temperature, specific impulse, and characteristic velocity. A range from 1 to 8.5 is chosen for the oxidizer to fuel ratio with a pressure of 10 bar [12]. The chamber temperature is assumed to be 2800 K. Characteristic velocity tells about the efficiency of the process of combustion and the propellants chosen. It is given by the following equation [12]:

$$C^* = \frac{\frac{\sqrt{KRT}}{\sqrt{M}}}{\sqrt{\frac{2}{k+1} * \frac{k+1}{k-1}}} \quad (1)$$

Where k is the specific heat and T is the temperature in the combustion chamber. The various plots obtained for these nine combinations to analyze the characteristic velocity can be seen in [12]. It can be inferred that liquid oxygen with any combination of fuel provides a high value of C*. Therefore, Lox when combined with Paraffin or HTPB shows almost a similar value with a difference in the O/F ratio. PMMA is shown to have the least value among the selected fuels. Nitrous oxide with any fuel combination shows a lesser performance. It can be said the nitrogen does not contribute to the oxidation of fuels and there is no heat released from it, and therefore, there is a reduced effective molecular mass [14]. Better engine performance is provided when there is less consumption of the propellant, which in turn shows a high value of specific impulse. Liquid oxygen with HTPB and Paraffin shows such as performance. This is because liquid oxygen has a very high potential in the oxidation process. This method of comparison of fuels is considered a vital process for a conventional hybrid rocket. The chemical energy is converted to heat during the process of combustion inside the chamber. This heat can be lost to the surroundings or can be used to increase the temperature inside the chamber [15], [16]. When the heat is not passed to the surroundings, there exists a maximum temperature inside the combustion chamber of the products. This is the adiabatic flame temperature. Therefore, it mainly depends on the reactants and when there is a complete combustion process, which means that the amount of air used must in an appropriate stoichiometric value. In real applications, this exact value of high temperatures is difficult to achieve as there is a loss of heat to the surroundings. This parameter is very important for the combustor and nozzle performances and design. When the heat energy of the combination used is higher, there is a high amount of kinetic energy transfer to the process. This should be the main motive of the oxidizer selected. Paraffin and Lox show this type of process and thus exhibits a very high temperature of above 3000 K, thereby being the peak values for adiabatic flame temperature, specific impulse, and characteristic velocity. However, hydrogen peroxide and nitrous oxide provide a huge advantage in their density, storage capabilities, and also facilitate the reduction of the size of the chamber [17]. The addition of metallic additives to the solid fuels and using cryogenic oxidizers (liquid) will increase the performance.

B. Observations and Comparisons

The selections of propellant pairs are considered important for theoretical research. Regression rate, mass flow mainly depends on the geometry of the fuel grain such as its diameter and width. HTPB has very little compatibility with greatly energetic components. Therefore, it does not have a high application for future purposes. Though PMMA has a transparent property where the burning can be observed, it produces a comparatively low value of the regression rate. The present time is much focused on paraffin-based fuels due to better performances and as it is easy to gain. Considering oxidizers, as gaseous oxygen is easily available, it is a reliable choice for many laboratory purposes. Nitrous oxide is a self-pressurizing oxidant with high chemical energy. Also, hydrogen peroxide gives a good performance and is easy to store which adds a huge advantage. Therefore, it can be said that not only the regression rate can determine the performance of a propellant pair, but several parameters should be considered. So, a trade-off is to be performed based on the mission requirements and its purpose.

C. Regression rate analysis of HTPB with oxidizers

The improvement of the regression rate in hybrid rockets is done using several methodologies developed by researchers. One such method is inducing a swirl in the flow. Xingliang [18] perform a comparative study with HTPB as a fuel along with a selection of certain oxidizers. The results are computed through numerical simulations and the validation of the methodologies developed is done using experimental results. Combinations such as HTPB/Gox, HTPB/N2O HTPB with metallic additive/N20, HTPB/98HP, and HTPB/90HP are analyzed. [18], [19] A global reaction model for the combustion process is developed in ANSYS. An illustration of the hybrid rocket motor used for the experimental data is shown in Fig. 9.

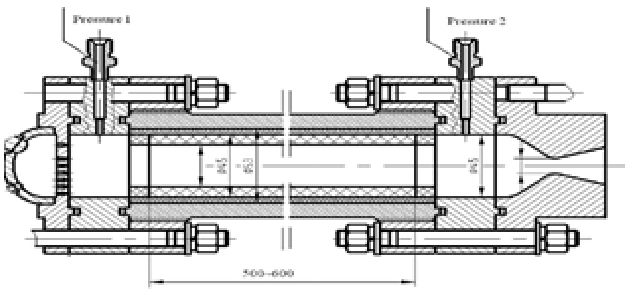

Fig. 9Hybrid rocket motor for an experimental test

A two-dimensional axisymmetric domain is used for the computation. Based on the test motor used, the length and diameter of the grain, the expansion ratio in the nozzle are designed. For the mesh design, a quad, structured mesh is utilized. Inlet size is considered equal to the grain port and the oxidizer is injected from the inlet port. At the surface of the grain, the solid and gas coupling reactions occur. The chemical reactions taking place here are governed by the Navier-Stokes equations. Lower Reynolds number effects are computed using the RNG turbulence model. The main product in the pyrolysis of HTPB is the 1,3 Butadiene. It can be expressed as follows

$$R = A\, e^{\frac{E_a}{RT}} \quad \text{.......................................(2)}$$

Where A is the pressure coefficient, R is the Universal gas constant, T is the temperature and E_a is the activation energy

The temperature profile and the concentration of the species are mainly focused on the following computation (using a global reaction rate model). A region of diffusive flame occurs on the surface of the grain as the oxidizer is injected from the inlet. Heat transfer passes on to the surface of the grain and thus pyrolysis takes place. Through the process of diffusion and convection, the fuel vapor of transported to the flame zone. With turbulent diffusion in the chamber, it gets mixed with the gaseous oxygen. The total energy transfer in this process mainly determines the value of the regression rate. In this study, the radiation heat flux is assumed to be zero. Through this simulation, the error is around 13% between the numerical and experimental results, showing a nominal and appreciable agreement between the results. Thus, it is important to validate the methodology adopted. From the results, it is shown that HTPB/Gox shows a high value of characteristic velocity. The performance in terms of energy output is the lowest for the HTPB/N2O combination as it has the smallest value of characteristic velocity. It is also shown that metal particles like Aluminum and magnesium in small quantities with HTPB can increase the characteristic velocity. Also, HTPB/Gox shows the highest value in its specific impulse. The combination HTPB/98HP has a high-density property and therefore also shows a higher density specific impulse value. HTPB/N2O has the lowest value of specific impulse, as it exhibits a low energy property. But this is used in the hybrid rocket application as it helps in the simplification of the construct of the oxidant feed system [18] as it can self-pressurize with its high value of vapor pressure.

V. Numerical Analysis

The basic mechanism that works in a hybrid rocket engine is the boundary layer combustion. For a basic design of a hybrid engine, it becomes challenging to compute the heat transfer and conduction process. From Fig. 10 Flow complexity in a hybrid rocket combustion chamber for a basic description. To study how the combustion takes place in the combustion chamber, it is important to design a preliminary model to analyze the performance.

A. Basic concepts of flow

To create a basic design to analyze the performance, assume an inviscid, compressible, and one-dimensional flow. The flow parameters vary as a smooth curve across the cross-section. The continuity equation, energy, and momentum conservation laws can be applied. The k–e turbulence model is used to study turbulence in the flow. Since the geometry is studied in a one-dimensional approach in the computation, the flow can be modeled using a 1-d Euler's equation. A combustion chamber, post-combustion chamber, combustion port, injector, and nozzle are the major parts of the geometry. The fuel grain is an embedded part of the combustion chamber. From Fig. 11 Preliminary design with the wall, inlet, outlet, and grain is shown. The regression rate constants a and n are dependent upon the fuel being used [8].

The regression rate on the fuel is given by

$r = aG^n$……………………………………………...(3)

Where G is the oxidizer mass flux rate, r is the regression rate coefficient, a is the regression rate coefficient, and n the exponential factor.

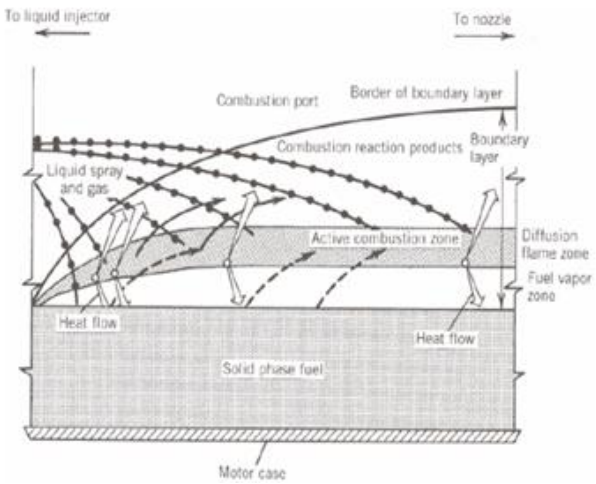

Fig. 10 Flow complexity in a hybrid rocket combustion chamber

The results obtained which are thermodynamic variables, temperature, and chamber pressure, and so on are calculated through the one-dimensional compressible flows and the fuel regression rates. Now with these assumptions, the simulation can be d.

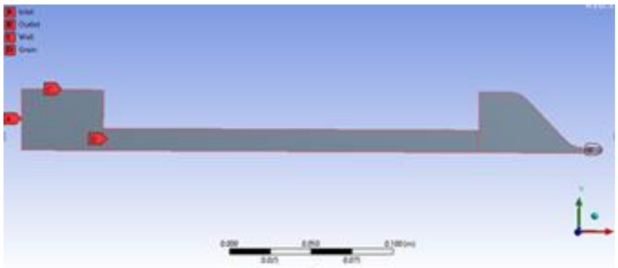

Fig. 11 Preliminary design with the wall, inlet, outlet, and grain

B. Methodology

The following settings are set to study the flow properties, a density-based solver with the inviscid flow, as a density-based solver is used to solve the governing equations with species transport. With a six degree of freedom present in flow solver, choosing a dynamic mesh will help in analyzing the path of the moving object in the flow field. A second-order implicit formulation is used to provide more accuracy. The selected time step is about 10^{-7} seconds [8]. For the mesh, both triangular and quadrilateral elements are used. This simulation uses HTPB as the fuel and the oxidizer as nitrous oxide.

Reason for selection- Nitrous oxide can be considered as a better substitute for hydrazine. It is also considered popular among hybrid rocket applications. It can be stored under pressure at room temperature and is much less toxic compared to hydrazine. Nitrous oxide has a low boiling point. When treated with a catalyst, it can form into a mixture of oxygen and nitrogen. From the obtained results, the occurrence of shock waves can be analyzed and it is noted how high the temperature and pressure increases during the process of combustion and the velocity of the flow through the nozzle. This is a major parameter that determines the overall performance of a specific fuel oxidizer combination. Table 1 shows the difference between the experimental model, the axisymmetric model, and the one-dimensional model.[8].

TABLE I. REPRESENTATION OF SPECIFIC IMPULSE IN VARIOUS MODELS

Impulse	Experimental result	1-D model	Axi-symmetric model
Specific Impulse (s)	145.4	149	147.4

Therefore, using the numerical simulation insight into nature of the three-dimensional flow in the chamber is given. Any simulation is considered convincing when it is validated. Therefore, when compared with the experimental results, the results are in good agreement.

C. *Analysis of numerical simulation results in a Paraffin based hybrid rocket*

The practical applications of hybrid rocket engines are still a challenging aspect due to the fuel regression rates which are low. Several modifications have been made such as adding metallic additives, modifying fuel injection methods, the use of grains with multi ports, and so on. But these increase the complexity of the system.

Recent applications include the use of paraffin fuels. It can be noted that, during the burn of the paraffin fuel, the melted fuel has a low viscosity which increases the regression rate. The reason behind this is the entrainment phenomenon which occurs in the combustion process. The entrainment of the fuel droplets into the gas stream gives a result of an increased regression rate.

D. *Propellant grain*

For the design of the propellant grain[8], a paraffin grain with an initial grain port diameter of 15 mm was used. Along with the grain, a blackening additive is added to improve the thermal radiation. This increases the specific impulse. This propellant grain when used in experiments yields good performance results. The increase in the regression rate of fuels has one of its reasons for increasing the port diameter with a constant oxidizer mass flux. It results in high regression rates both in numerical and experimental results. The regression rate of the fuel is a function of chamber pressure and oxidizer mass flux.

E. *Computational Fluid Dynamics Simulations*

The numerical simulations are performed to study the design of a 1 kN hybrid rocket engine [20] A mesh refinement feature allows refining or coarsening the mesh according to the geometry. Different refinement levels were considered and the number of elements in the fine, coarse, and medium levels was computed. For the mass flow, both paraffin fuel and oxygen were used. A pressure-based solver is used in this simulation. In a pressure-based solver, both the mass conservation and momentum equations are used, and as they are coupled together and are non-linear, the governing equations are solved repeatedly by an iteration process until the solution converges. A simple algorithm is adopted to perform the simulations. The concepts of the kinetic theory of species and the ideal gas equation play a major role. The specific heat capacities are chosen when there is more than one species included. The database contains the heat capacity values for pure species. A shear stress transport k- e model is chosen to give an accurate formulation in the near-wall regions. Neglecting the entrainment effect, the Eddy Dissipation Model is used, in which the reaction rates are controlled by turbulence. Equations of Arrhenius chemical kinetics can be avoided in this model. The following equation is applied which is obtained from CEA kinetics.

$$247\ C2H4 + 261\ O2 + 9\ H2 \rightarrow 489\ CO + 5\ CO2 + 8\ H + 476\ H2 + 23\ H2O \quad \ldots\ldots\ldots (4)$$

Fig. 10 shows the basic design for the current analysis. This design can be modeled to three different kinds of mesh, fine, medium, and coarse. Based on the type of mesh, a variation in the temperature throughout the combustion chamber can be noticed.

A sudden increase in temperature can be seen near the exit of the injector, and as the combustion proceeds, the grain surface begins to burn, and a very high temperature is noted at the post-chamber. Predictable temperatures in the regions of the post chamber and the nozzle are gained with the fine mesh design. The reaction zone lies in close proximity to the grain. An illustration of the design and a model of a fine mesh are shown in Fig. 10 and Fig. 11 respectively. In a fine mesh, an increase in temperature occurs linearly and a high temperature in the range of 1500 K-1900 K can be found (post-combustion chamber and the beginning of the nozzle). Considering the chamber, solid grain, and the outlet, a fine mesh is created as in Fig. 12.

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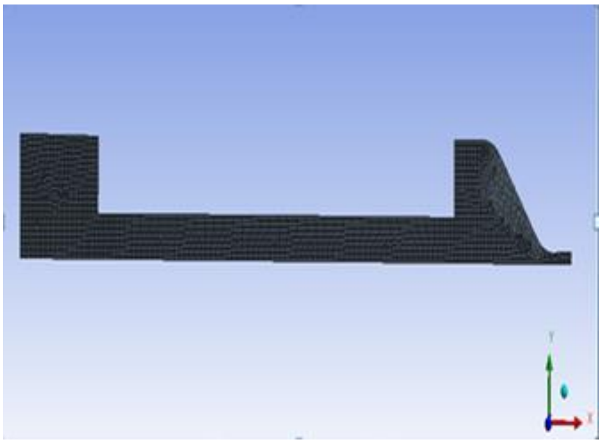

Fig. 12 Creation of a fine mesh

This helps create the boundary conditions for various sections (wall, inlet, outlet, grain) and a standard solution initialization is performed. The temperature and velocity across the entire model can be analyzed. This helps in understanding the nature of flow across the chamber.

By extracting the temperature profiles and comparing the values from the three mesh types, as shown in Fig 13, it can be found that the medium and fine mesh levels obtain values very close to each other. Also, when compared to experimental and CEA analysis values of both temperature and pressure, medium and fine meshes are in good agreement and showed a very low error of less than 3.5%.

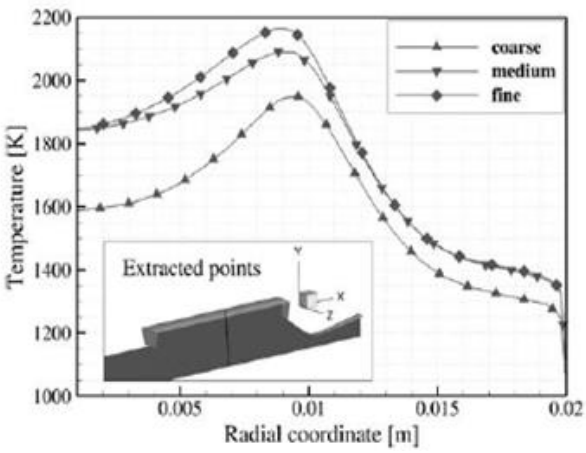

Fig 13 Variations in temperature with the mesh types

Reference [21] shows a design of a 1kN breadboard manufactured by CIRA. The main aim of this design is to produce the ability of re-ignition, produce maximum burn time, and better throttling abilities. A design code is implemented with input values of paraffin regression rates and the regression rates at the nozzle throat regions (sources taken from various literature reviews) and the injector system design(with an injector plate that can be replaced) is also given by the code based on the chosen oxidizer. Detailed designs and material selection about this can be found in [20].

This design is then analyzed using CFD to study the heat flux across the design. The pressure and temperature conditions for the inlet mass flow rate are given. For paraffin and oxygen, the inlet temperature is given to be about 300 K and the mixture ratio is 1.6 [20]. For the mesh design here, an unstructured mesh is used. This type of mesh usually uses a tetrahedron element in three dimensions. The elements are arranged in their manner in the domain. A study between the fine and coarse mesh is done here and a comparison is made between the temperature and pressure distribution.

The nozzle was designed using graphite and its properties were tabulated at 300 K. The performed thermal analysis on the design gives a better understanding of the circulation of heat flux in the chamber. It is found that the highest temperature is at the throat of the nozzle with temperatures reaching near 1700 K [20]. Similar methods can be adopted for designs with 200kN or 1000 N breadboards and tested. Therefore, this design methodology paves a new way for the development of hybrid rockets with an enhanced fuel regression rate. It is to be noted that, before performing the analysis, the selection of fuel is a major aspect and thorough research should be done before proceeding with the experimental analysis. Validation of numerical analysis is very important which gives an insight into how accurate the methodology is adopted.

The simulations that include the gas surface interactions are currently being largely focused on different methodologies. Global reaction mechanisms with chemical kinetics approach are used to model and obtain the reactions in the gaseous phase and the formation of species is to a very high extent. Thus, a two-step global reaction-mechanism is adopted [22]. It is given as follows.

$C_4H_6+3O_2 \rightarrow 4CO+ 2H_2O +H_2$……………………. (5)

$CO+0.5O_2 \leftrightarrow CO_2$………………………………… (6)

The reaction with C4H6 (pyrolysis product of HTPB) in the first global reaction is an irreversible process and is assumed as a first-order reaction. The latter reaction results in the formation of CO2, which is a reversible process.

One of the CFD approaches is explained in [7]. To determine the internal ballistics and the gas surface modeling, Reynolds averaged Navier Stokes equation (RANS) with transport properties are applied. Equations of mass and energy conservation are used to couple the gas-phase equations and phase of solid fuels. This helps in determining the surface temperature and the regression rate of fuels. It is to be noted that non-uniformity in the flow field helps in the regression rate enhancement. Two types of injection methods are introduced [7]. Given the injection area, oxygen is introduced uniformly throughout the cross-section of the pre-chamber.

This determines the axial distribution of fuel regression. It is seen from the numerical simulations that a recirculation zone at the end of the motor is developed which encourage the propellant mixing parameters. This gives a higher heat transfer to the walls. Thus, a higher regression rate is seen. As the fuel grain is regressed, the recirculation zone grows larger and the regression rate is induced further. To further increase the recirculation zone, a larger port diameter can be introduced which is higher than the diameter of the jet, which in turn helps in increasing the mixing process, causing a high regression rate. If the modeling is accompanied by a radiative heat transfer term, a better understanding and agreement with the experimental results can be achieved.

F. Analyzing nozzle erosion characters in a Paraffin based hybrid rocket

One of the major challenges faced in a hybrid rocket is the nozzle surface erosion. (shown in Fig. 14). This is typically higher than in solid propellant motors. Numerical simulations show that nozzle erosion is a strong function of mixture ratio and chamber pressure. The layer protecting the surface of the nozzle, the design, selection of material, and the interaction between the gases and the protection layer are some of the major parameters for modeling. Therefore, highly complex physical and chemical reactions occur in the design and analysis procedures and calibration with the current experimental data is considered important [9]. As ablative materials (carbon-based) are used, the interaction between this and high-temperature chemical reactors are considered for the numerical simulations. The approach used in [7] consists of a thermochemical ablation model with a Navier Stokes flow solver. This helps in analyzing the heterogeneous reactions taking place on the surface. The solver also encompasses a model for the interaction of the boundary layer with the gas. In a paraffin-based hybrid rocket, this interaction can be analyzed involving the grain and the chamber wall. A code for the radiative heat transfer is used to analyze the thermal radiation [7].

G. Numerical simulation approach

The given paraffin-based hybrid rocket is analyzed using a solver called RANS, Reynold's Averaged Navier Stokes. It is used to analyze time-dependent flows in the chamber. This solver is applied for a three-dimensional flow and turbulent flow. To solve the meshes, the Riemann solver approximation is used. It is based on a numerical scheme called the Gudonov scheme which solves the partial differential equations in fluid dynamics, linearising the equation, thereby solving the problem faster. Also, a second order Runge-Kutta scheme is used. The use of the Prandtl number and Schmidt number helps in computing the turbulent viscosity, thermal conductivity, and mass diffusivity [7]. This solver is used to analyze the surface gas interactions in the nozzle (made of graphite) and the combustion chamber (paraffin grain). Graphite is a widely used material for nozzle designs [7]. The nozzle can be affected due to high temperatures and pressures. It can be seen that there is a high rise in temperature on its surface due to internal heat transfer processes. Radiative heat transfer is one of the major causes which can cause temperature rise above 2000 K.

Other reasons include the various heterogeneous reactions occurring with carbon. These reactions also get coupled with each other and thus an increase in the erosion rate can be seen here. The model used in [7] is used to analyze the thermo-chemical processes in the combustion taking into account the diffusion of particles, the role of ablative materials, changes in the boundary layer along with the chemical reactions in the nozzle, and its surface. The following are the surface reactions taking place with carbon. These heterogeneous reactions are modeled using a reaction mechanism called graphite oxidation kinetics [7].

$$\mathrm{C + H20 \rightarrow CO + H2}$$
(7)

$$\mathrm{C + CO2 \rightarrow 2CO}$$
(8)

$$\mathrm{C + O \rightarrow CO}$$
(9)

$$C+1/2O2 \rightarrow CO$$
(10)

To determine the erosion, the following equations are used.

$$M = k_j p_i^n{}_i$$
(11)

Where i is the different species in the reactions, p is the partial pressure, k is the specific heat constant, n is the order of the reaction.

The Arrhenius equation is used to describe the specific rate constant [7].

$$K_j = AT_w^{b_j} e^{\frac{E_j}{RT_w}} \qquad (12)$$

Where, A, b_j, are the temperature exponents, Tw is the temperature at the wall and E_j is the activation energy.

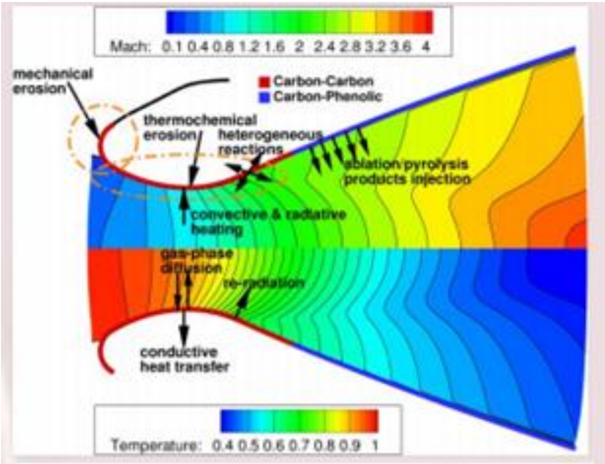

Fig. 14 An illustration of the erosion process in a nozzle

Due to these reactions on the surface, the complete erosion rate is specified as the sum of the mass flow rates of individual species [7]. The first three reactions are characterized by the absorption of energy while the reactions with oxygen and monoatomic oxygen are accompanied by the release of heat energy. Therefore, the oxygen present in the exhaust gas can range up to significantly higher values with oxygen-rich conditions, and this is found to be higher than in solid rocket motors. The interaction of the gas with the wall is analyzed using boundary conditions that are integrated with the solver [7]. Re-radiation occurs from the graphite surface as the surface absorbs gases from the combustion process.

A numerical setup consisting of an appropriate boundary condition is to be set up to find the interaction between the fuel and the surface. The entrainment process is to be considered in the case of modeling paraffin combustion. Paraffin, which is a normal alkane, has carbon numbers between 25 to 45, has its critical pressure lying below the chamber pressure in the case of hybrid rockets [7]. The melted paraffin is assumed to be in a supercritical pressure level, where there are no boundary conditions existing for the liquid droplets [7].

To compute the time dependent flow, The RANS approach is used and the entrainment process is included in the turbulent flow mixing. In the surface energy equation, the radiation from the grain is neglected as paraffin has a low value of melting temperature. A difference between the entrainment process in supercritical and subcritical regions is shown in Fig. 15. It can be seen that there exists no boundary layer for the supercritical regime.

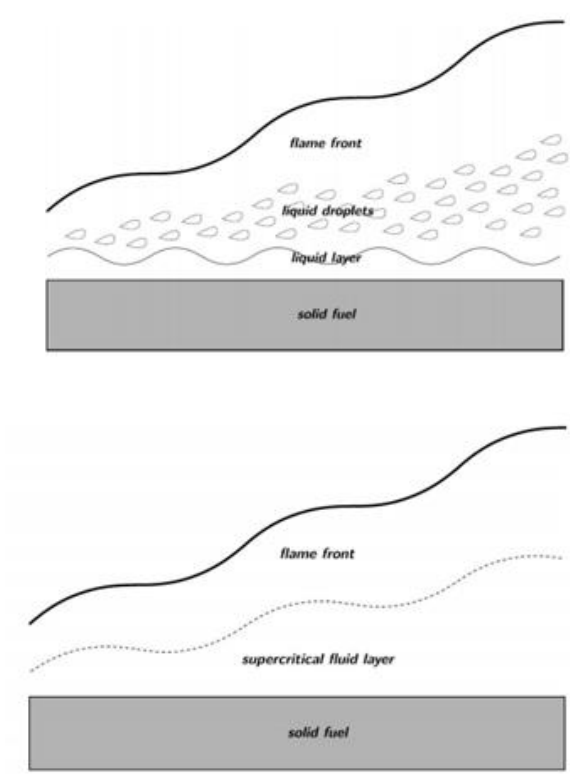

Fig. 15 Entrainment in a subcritical and a supercritical regime

The temperature at the wall is therefore assumed to be the same as that of the grain temperature. To measure the radiative heat flux, for the nozzle and the grain, a separate thermal radiation model is to be computed. The effects due to soot and the radiation from it are yet to be studied for future purposes. The integration of the radiative heat transfer equation gives an idea of the total radiation intensity near the wall. The kinetic modeling is done using $C_{32}H_{66}$ as the paraffin wax, whose specific heat value and thermal conductivity are considered to be constant. The properties of paraffin wax can be referred to from [7].

The injection of the melted fuel and the process of transforming this fuel into gas species are the two main processes to be considered for modeling for the thermochemical analysis. In a thermally perfect gas model, the properties of paraffin are considered to be at a liquid state as below the value of critical temperature, this fluid tends to proceed as a liquid. Here, the global reaction consists of ten species for the combustion process of paraffin wax and gaseous oxygen. The global reaction is specified as follows. The forward rate coefficients for the reactions are obtained using the Arrhenius function [7]. The backward rate coefficients are obtained by the equilibrium constants. The value of constants A and n are mentioned in [7].

$$C_{32}H_{66} \rightarrow 16\ C_2H_4 + H2 \quad (13)$$

$$C_2H_4 + O_2 \rightarrow 2CO + 2\ H_2 \quad (14)$$

$C_2H_4 + 2H_2O \rightarrow 2CO + 4H_2$ (15)

$CO + H_2O \leftrightarrow CO_2 + H_2$ (16)

$H_2 + ½ O_2 \leftrightarrow H_2O$ (17)

$O_2 \leftrightarrow 2O$ (18)

The CFD model for the combustion process of paraffin wax and gaseous oxygen has a high advantage as it couples the processes and interactions between the complex reactions and can be evaluated qualitatively.

The radially acting flow field (non-uniform) is one of the major reasons for nozzle ablation which is due to the regression of the paraffin wax. A comparison of the mass flux of wall ablation in the nozzle and the complete engine is shown here in Fig. 16.

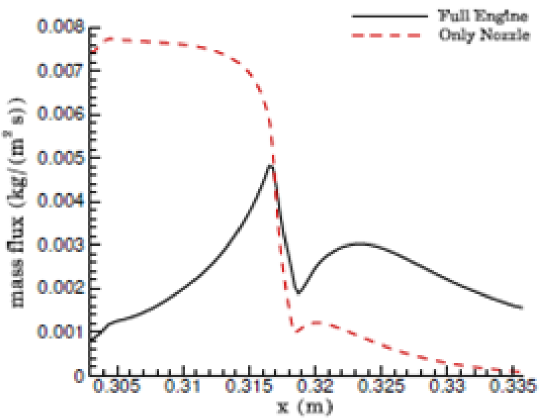

Fig. 16 Mass flux distribution due to wall ablation

The non-uniformity in temperature, velocity, and the mass fractions of the species significantly affects the ablation of the nozzle. The converged section of the nozzle shows the highest ablation compared to the full engine section, and the diverged section shows a relatively low value. Refer to Fig. 16 to Fig 18 for an idea of the effects of wall ablations

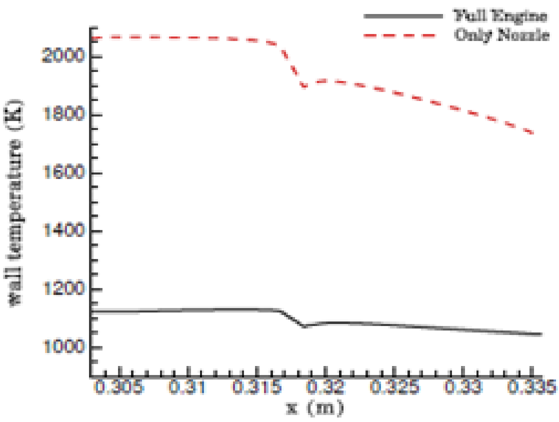

Fig. 17 Temperature distribution due to wall ablation

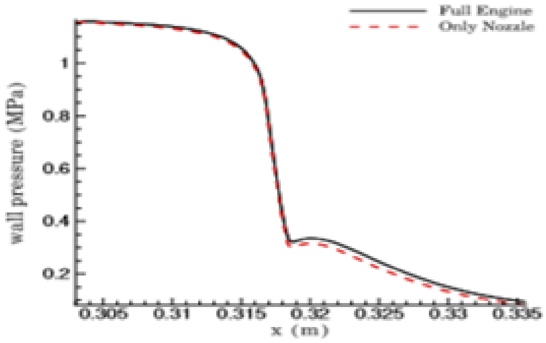

Fig 18 Pressure distribution due to wall ablation

The wall pressure distributions are noted to be the same for both the full engine and the nozzle only analysis. But there is a significant difference in the temperature distribution. This high values in the temperature of the nozzle section are due to the complex chemical species interactions with the wall causing non-uniformity and also due to its interaction with the ablative materials.

VI. Summary and Discussions

Several solutions have been adopted to mitigate the drawbacks of hybrid rockets. The idea of vortex injection, understanding swirl intensities have been some of the major areas of focus. One of the studies included the use of hydrogen peroxide and polyethylene for vortex injections, with the use of a cylindrical port grain. Numerical simulations were focused on the post chamber length reduction and the method of swirl injection provided better motor efficiencies. A linear relation between the regression rate value and the swirl intensity is obtained [22] which can be used for future design missions for a hybrid rocket operation.

This relation is obtained by a test matrix where several types of the combustion chamber, varying in the post chamber length and the type of injection systems. The diameter of the grain port also plays a major role. CFD and experimental tests were used to obtain a linear relation. The swirl numbers occurred between the geometric values of 2 and 3.5[22]. Also, another advantage of using a short length post chamber is that the erosion rate in the internal side is significantly reduced. They are exposed to a lower influence due to hot combustion gas; therefore, they have less influence on the O/F ratio. It does not affect the efficiency of the motor and swirl injection is found to be a validating solution for this application.

A review on the various types of propellants and their applications was put forward by Pradhan [21] which focuses on solid, liquid, and hybrid rocket propellants. Some of the major characteristics of propellant of any type are the regression rate, thrust and impulse, combustion burning techniques, injection methods, propellant grain structure, density, and temperature. Additives like carbon nanotubes, graphene, and aluminum energize the process in the chamber. To obtain thrust in the desired direction, it is important to note that there is an equal distribution of grain [21]. The use of aluminum can affect the thermal insulator due to the formation of Aluminum oxide slag [22]. This should be reduced by some size enhancement techniques. HTPB with Aluminum powder and ammonium perchlorate is considered an efficient combination for mitigating this issue and is considered one of the major leaps forward in the fuel enhancement techniques. Liquid hydrogen is one of the major ones as it is an ecofriendly propellant and is widely used in liquid propellant rockets. However, it faces issues with storage capabilities. In the case of gaseous propellants, which are stored in a compressed form, nitrous oxide, carbon dioxide, hydrogen, and oxygen, hydrocarbons are some of the notable choices. These are mainly applied in industrial fields and electronic industries and applications. Long-range missions with very high specific impulse applications make use of liquid hydrogen. The use of gaseous propellants comes with challenging aspects due to their low density, explosion characteristics, fewer storage capabilities, and volatility.

The main reason for hybrid rockets that can be used for future applications is that it paves a way for an application of green propellants, which helps develop an eco-friendly technology by reducing pollution and emissions. They are high energy liquid propellants that are less toxic than conventional fuels. They are under research for replacing the chemical propellants for future purposes of a spacecraft propulsion system. The high risk with the storage and transport of propellants can be reduced significantly and is also reliable in case of human exposure factors. They also tend to have lesser values of a freezing point compared to a hydrazine fuel, therefore maintaining the temperature in the spacecraft consumes less power than that of conventional rockets. High test peroxide is one of the promising fuels. It can be decomposed through a catalyst and can emit hot gases, which in turn ignites the solid fuel.

Also, it is a storable oxidizer [22]. It accounts for gaseous injection and allows for start, restarts, and stop capabilities for the engine. This improves the atomization process and the application of vortex injection further increases the performance. The oxidizer is passed into the combustion chamber with a tangential velocity, developing further the heat flux and the combination of chemicals and the turbulence factor. The component of the swirl is determined by the swirl number. An illustration of swirl injection effects can be seen in Fig. 19

It is given by the ratio of the axial fluxes between the swirling momentum and the axial momentum [22]. It gives information about the rotational flow and its variation along the length of the chamber. Modifying the injector designs are now the major field of research in hybrid rocket technology.

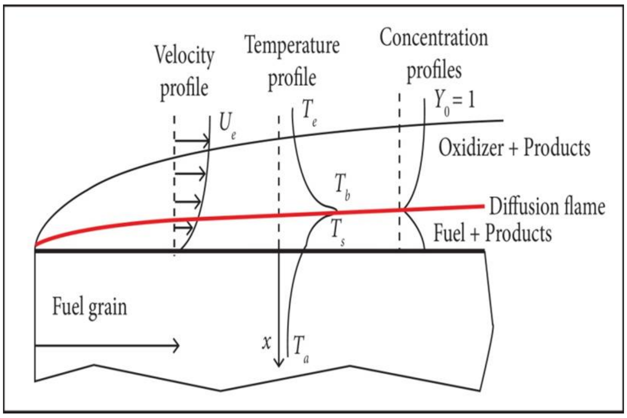

Fig. 19 Swirl injection effects

The future hybrid rockets are to be developed according to the mission requirements. The Mars missions also have hybrid rockets as part of the application. Therefore, this is a huge development for several years and is expected to be the highest achievement in the propulsion systems, which paves way or new methods of launch capabilities.

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