

# Hydrogen Based Compounds as Energetic Catalysts for Liquid Rocket Engines: Implications and Applications

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**Abstract** - In the current scenario of space propulsion, liquid propellants have significantly proved useful in the upper stage rocket engines. Over the past couple decades, the world had inclined positively towards cryogenic fuel(s) viz., liquid oxygen and liquid hydrogen due to their high specific impulse. A higher specific impulse implies lower duration to achieve design cruise velocity for a given rocket initial and instantaneous mass. Liquid hydrogen and liquid oxygen as fuel and oxidizer can generate one of the highest enthalpy release in combustion, producing a specific impulse of up to 450 seconds at an effective exhaust velocity of 4.4 kilometres per second. Whereas, selected disadvantages are encountered in the form of storage and production. This indicates overdependence on cryogenic propellants and has necessitated the active research effort for better alternatives. As an interesting alternative, the combination of Dinitrogen Tetroxide ( $N_2O_4$ ) and Monomethyl Hydrazine (MMH) have been used for many space applications owing to an extreme storage stability and hypergolic nature. Present study aims to express the effect of hydrogen-based compounds on the rocket performance. Four distinctive compounds from two groups of hydrogen-based compounds are tested with the varying oxidizer and fuel proportions to obtain a new, cost-effective and user-friendly composition that can be prepared at room temperature. The investigation attempt and explains the effect of hydrogen based energetic propellants using  $N_2O_4$  and MMH as the base composition for upper stage performance. The work is motivated by the need of efficient space operations with attractive propulsive alternatives to minimize overdependence on cryogenics, which will ultimately result in cost effectiveness. Various energetic materials were tested with the base composition by using standard NASA-CEA complex chemical equilibrium model. The performance was evaluated in terms of variation in specific impulse and characteristic velocity both of which are significant parameters. To, validate the practical utility, the role of chamber pressure, supersonic area ratio and optimal Oxidizer to fuel ratio (O/F) was determined. The work led to two interesting findings, a composition of beryllium hydride with base composition for high performance of rockets and the negative impact of hydrogen on liquid propellants.

**Keywords:** Hydrogen Based Compounds, Energetic Materials, Thrust, Specific Impulse, Characteristic Velocity

## Nomenclature

C\* : Characteristic Velocity  
Isp : Specific Impulse  
O/F : Oxidizer to Fuel Ratio  
 $N_2O_4$  : Dinitrogen Tetroxide  
MMH : Monomethyl Hydrazine  
(L) : Liquid Form

## I. INTRODUCTION

Rockets are multi-utility propulsive frameworks in which thrust from engine pushes it or drives it forward. Since the invention of gunpowder in China, humans have sent cylinders soaring into the skies with the help of controlled explosions. These craft and their engines, called rockets, have taken on many roles as fireworks, signal flares, and weapons of war (refer figure 1). But in the last seven decades, rockets also have let us send robots, animals, and people into orbit around Earth and even beyond. Maintaining Newton's third law of movement, they create tremendous energy from a small volume, in brief time frame to get away from the draw of gravity (figure 2).

In the modern-day world, rockets are required for a wide scope of uses, like ballistic missiles, launch vehicles, earth orbiting satellites, upper stages, ejection seats, human space flight and space investigation. Most rockets are arranged to acquire an additional kick of push to defeat its weight. Rockets are the most un-proficient frameworks and require enormous energy, which they consume off from the fuels that might be solid, fluid, or crossover. Likewise, they require immense capital venture, which implies that rocket testing and crashes as consequence (refer figure3) are at no expense passable and in this manner the interest for reusable and reasonable rockets has been expanding.



(a)  
Fig. 1 Rocket used as weapon (\*google.com).

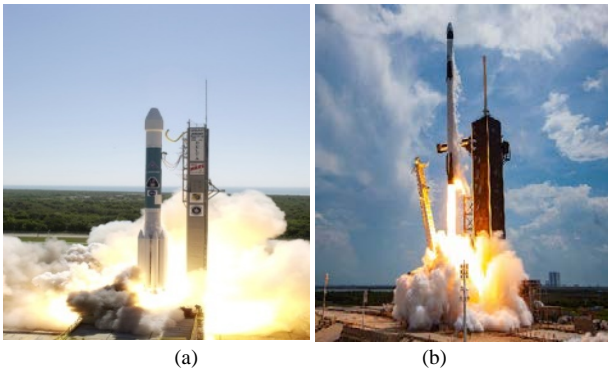


Fig. 2 (a &amp; b) Rocket during launch (\*google.com)

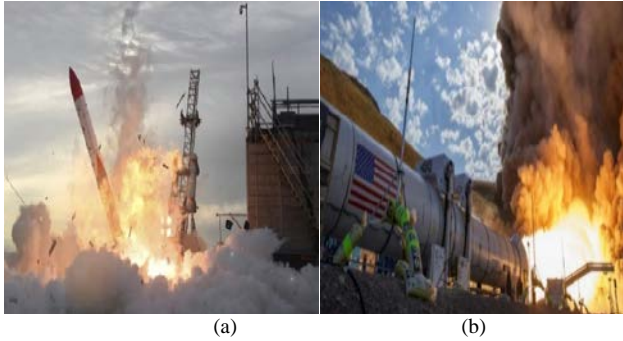


Fig. 3 (a &amp; b) Rocket during crash and testing (\*google.com)

As widely known, upper stages utilize liquid propellants, which are appealing a direct result of their high explicit motivation and control. A cryogenic engine furnishes more power with every kilogram of cryogenic propellant it utilized. However, there are a few hindrances identified with its utilization. Cryogenic fuels are put away in high-pressure force tanks that require more grounded amalgams and thicker dividers, which make the vehicle tanks heavier, accordingly lessening reasonableness and execution. Whenever released, the liquid can bubble into an exceptionally thick, cool gas and when breathed in, could be deadly. Fluid fuels can be an effective elective when certain energetic materials are added to them, without compromising the presentation of the rockets. They are financially reasonable and can be put away without any problem. Liquid Hydrogen is most widely used as cryogenic fuel because of its low molecular weight and high energy output when burned alongside liquid oxygen.

Hydrogen also provides low-density liquid fuel for navigation thrusters in orbit. The study aims to investigate the effects of hydrogen and hydrogen-based compounds onto a conventional liquid propellant base composition to obtain hybrid propellant compositions. The two key parameters, which are used for analyzing the performance of these propellants, are the Specific Impulse ( $I_{sp}$ ) and the Characteristic velocity ( $C^*$ ). The specific impulse is a method for portraying and assessing the thermodynamic properties and propellant performance. At the point when the thrust and the flow rate stay consistent all through the consuming of the fuel, the specific impulse is the ideal opportunity for which the rocket engine gives a push

equivalent to the weight of the propellant consumed (equation 1).

$$I_{sp} = F/q * g_o \quad (1)$$

where,

' $F$ ' is thrust, ' $q$ ' is the rate of mass flow, and ' $g_o$ ' is standard gravitational acceleration ( $9.80665 \text{ m/s}^2$ ).

Characteristic velocity ( $C^*$ ) give a measure of the energy available from the combustion process (equation2).

$$C^* = P_c A_t / q \quad (2)$$

where,

' $P_c$ ' is the combustion chamber pressure and ' $A_t$ ' is the area of the nozzle throat. It is important to note that the characteristic velocity complements the specific impulse values and is used to verify the simulations. The energy released in the form of heat when a compound undergoes complete combustion with oxygen under standard conditions is known as the heat of combustion ( $\Delta H_c^0$ ). It can also be formulated as the difference between heat of formation ( $\Delta H_f^0$ ) of the products and reactants. The heat of reaction ( $\Delta H_r$ ) is given by the equation (3).

$$\Delta H_r(T) = \Delta H_f(T)_p - \Delta H_f(T)_R \quad (3)$$

An expansion in enthalpy discharge brings about an increment in Specific Impulse, which is needed. The enthalpy discharge appears as dynamic energy of the exhaust stream. A prerequisite of adequate oxygen considers most extreme energy discharge. This is conceivable when the particles contain connections between first line components i.e., C-N, N-C, N=O, N=N, N-F and -ON in fuel definitions. More oxygen balance is procured when more bonds are available. Furthermore, the density of propellant should be just about as high as conceivable to store however much energy per volume as could reasonably be expected. Various research endeavours are being placed has/had been transcendently helpful for different rocket propulsion system, missiles and power generation systems throughout the long term.

Appreciable scientific work and reviews can be found in [1-10]. Moore and Berman [1] presented a self-igniting hybrid rocket propellant system employing 90 per cent hydrogen peroxide as the oxidizer and polyethylene as the fuel. Tormey [2] extended the practical utility with understanding that there is a limit-set up by natural and inexorable laws of chemistry and physics. Ross [3] discussed the high specific impulse ( $I_{sp}$ ) potentialities of nuclear propulsive devices for space-vehicle application.

The work highlighted the obstacle as offset by the relatively massive equipment requirement. A single measure for rating any propulsive system, based on its dynamic effectiveness and including this mass effect, was derived as a system specific impulse. Sollott *et al.*, [4] carried out a study in the

field of modern high-energy materials with special emphasis on homoleptic polynitrogen compounds. The work highlighted the nature of energetic materials and their use in propellant systems.

Borman [5] reviewed the global development of oxidizers, plasticizers, binders, high energy density materials and their insensitive forms. Zandbergen [6] provided a starting point for both practical liquid rocket engine selection and engineering. Muhalim and Krishnan [7] detailed the design procedure for a reaction control rocket engine using  $N_2O_4$  and MMH as the principal propellant constituents. The operating conditions like the supersonic area ratio, O/F value and so on were provided for optimum conditions in the simulations. Liu *et al.*, [8] extended the simulations to study the reactive nature of hypergolic mixture of Monomethyl hydrazine (MMH) and Dinitrogen Tetroxide ( $N_2O_4$ ). The work provided a detailed account on the chemical nature of the base composition, which is necessary to understand how it can behave on the addition of energetic materials. Gajjar and Malhotra [9] investigated the base energetic propellants comprising of Monomethyl hydrazine (MMH) and Dinitrogen Tetroxide ( $N_2O_4$ ) for hybridization.

Simulations were directed for hybrid chemical propellant composition(s) to enhance performance of upper stage liquid rocket engines and significantly reducing the overdependence on cryogenics. In recently, Ray and Malhotra [10], extended the study further with focus on suitable energetic materials among all the elements for wide range of significant specific impulse variation. The work entailed distinct chemical composition(s) from base Monomethyl hydrazine (MMH) and Dinitrogen Tetroxide ( $N_2O_4$ ) which can be effectively utilized for Thrust augmentation and termination with collateral impact on special impulse. Over the last decade, the specific research efforts have been directed to the utilization of Hydrogen and Hydrogen based compounds as potential rocket propellants.

As widely known, Liquid hydrogen has/had proven to be a tremendous rocket propellant even beyond cryogenics. However, the collective hydrogen utilization has led to the search for attractive alternatives with hydrogen for chemical propellant requirement.

Present work attempts to investigate the nature of hydrogen-based compounds as energetic catalysts for futuristic liquid propellant engines. The work is inspired by the necessity to reduce the over dependence on cryogenics, which demands high system and operational maintenance alongside providing information about practicable efficient alternatives of liquid hydrogen-based compounds which can be used under standard conditions for enhanced performance with minimal capital venture.

The specific objectives of the work are

1. To investigate the nature of hydrogen-based compounds as high energy catalysts for upper stage liquid rocket propellant(s).

2. To explore possibility of a high-performance propellant composition as a low cost, practical alternative to the cryogenic propellants to reduce capital venture and mission cost.
3. To investigate the role of key controlling parameters.

## II. SIMULATIONS AND SOLUTION METHODOLOGY

Current work examines the change in  $I_{sp}$  when hydrogen-based compounds were added in various proportions with the base fuel and oxidiser. The simulations were systematically carried out in NASA CEA and the importance of simulations was to find active hydrogen based energetic materials, which could result insignificant variation the  $I_{sp}$  of the rocket.

Moreover, the simulations could be used to understand how hydrogen and different hydrogen constructed compounds affect the thrust produced. The performance was investigated in terms of ' $I_{sp}$ ' and validated with characteristic velocity ' $C^*$ ' as the design parameter of the rocket. The numerical model followed the chemical equilibrium with the input conditions as:

1. The base composition is taken as MMH/ $N_2O_4$  (30/70).
2. Chamber pressure (1-25bar/ 5 bar increment).
3. Supersonic area ratio (375).
4. Addition of energetic hydrogen-based materials in the fuel and oxidiser composition(s).

It is important to note that the data presented represents the repeatability and reproducibility of the third order.

## III. RESULTS AND DISCUSSIONS

Simulations were carried out with the base composition (MMH/ $N_2O_4$ ) by adding energetic materials in the fuel, and oxidizer of the propellant to understand the change and the nature of change in  $I_{sp}$  and  $C^*$  values of the propellant. In order to understand the effect of various energetic hydrogen-based materials, the simulations were carried out as

1. Changing the fuel components for every 5% and keeping oxidiser intact.
2. Changing the oxidiser components for every 5% keeping fuel intact.

Observations were made with variety of specific impulse and characteristic velocity against the grouping of every component with fuel and oxidizer. Before the primary recreations, deliberate investigations were done to validate the software predictions. The composition introduced in the underneath tables were tested and it was established that the preceding simulation readings coordinated reasonably well (refer table I).

TABLE I REPRESENTS THE VERIFICATION AND THE VALIDATION OF SOFTWARE PREDICTIONS ([10]).

Composition	Experiments/ Theoretical (sec)	NASA-CEA Simulations (sec)
AP (80%)/Al (20%) (by volume). K. S. Williams, PhD thesis, Texas, A & M University, 2012.	246	242.59
AP/HTPB/Al [70/10/20] (mass). K. S. Williams, 2012	258	247.08
AP/HTPB/Al [70/15/15]. P. Kuentzmann, 2002.	265	260
AP/HTPB/Al [64/14/18]. Venkatachalam <i>et al.</i> , 2002	265	263.37
AP/HTPB/Al [(50-10)/(35-75/15]. Nevada Aerospace science associate (nassarocketry.com)	(238-175)	(230-170)
AP/HTPB/Al [64/14/18] at (PC=6.89 Mpa) www.lr.tudelft.nl	266	264.02
AP/HTPB/Al [70/12/16] at (PC=6.89 Mpa) www.lr.tudelft.nl	267	263.97

To begin with, the base composition (MMH/N<sub>2</sub>O<sub>4</sub>) was tested in the ratio of 30:70 respectively. The resultant specific impulse of 38.85 sec and characteristic velocity of 1711.3 m/sec were noted with selected concentration (refer figure 4) to denote a comprehensible understanding of the comparison made with the hybrid compositions. For energetic catalysts first, liquid hydrogen (figure 5) was added to the fuel (figure 6 (a & b)) and oxidiser in varying proportion ((figure 7 (a & b))). The result clearly shows predictable monotonic trend.

Furthermore, to find alternatives of liquid hydrogen, two hydrogen-based compound groups viz., hydrocarbons and hydrides were taken into consideration. Four compounds from each group were chosen and systematic numerical experiments were conducted by adding each compound to the base propellant in varying concentration to understand the impact of hydrogen on specific impulse. As observed (refer figure 6(a)), when liquid hydrogen was added to monomethyl hydrazine, keeping dinitrogen tetroxide constant, the specific impulse boosted up to 7.4% from the base  $I_{sp}$  (358.85 sec) resulting in a 385.34 sec at H<sub>2</sub>/MMH/N<sub>2</sub>O<sub>4</sub> = 25.5/4.5/70. Characteristic Velocity showed a similar trend with a maximum value of 2053.1 m/sec. This is due to its most defining characteristics as lowest molecular weight and the capability to burn with extreme intensity which makes it a powerful rocket propellant.

Noticeable fluctuations were shown when Liquid hydrogen was added to the oxidiser in varying proportions, keeping the fuel intact. Slight increase in  $I_{sp}$  by 0.4% at 15% H<sub>2</sub> (L)

with an  $I_{sp}$  of 360.26 sec was noted. But the  $I_{sp}$  fell gradually with increasing concentration of liquid hydrogen. The thrust dropped by 18.03% at 95% hydrogen with an  $I_{sp}$  of 294.16 sec. Metals exposed to the extreme cold of liquid hydrogen become brittle. Hence any fuel burning in presence of liquid hydrogen takes a much longer during resulting in decreased  $I_{sp}$ .

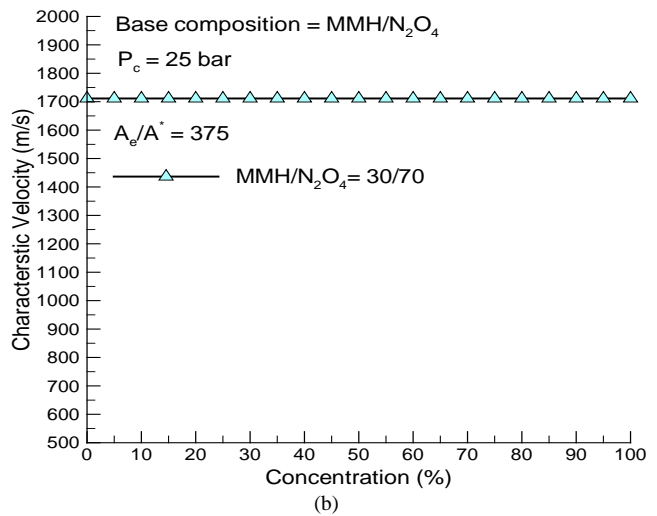
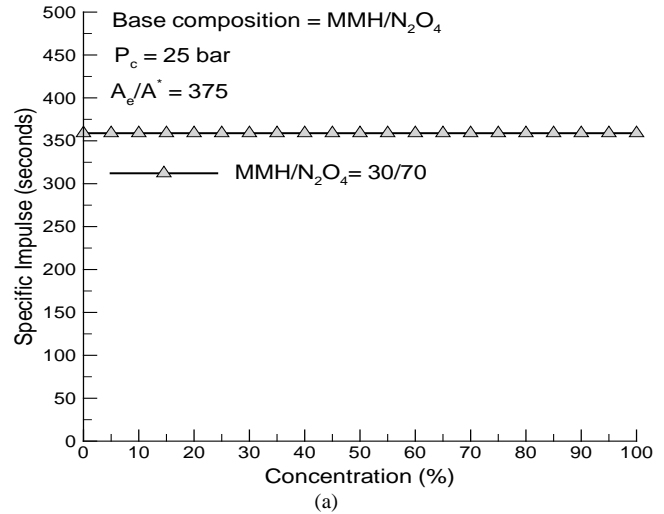


Fig. 4 (a) Specific Impulse and (b) Characteristic Velocity of the base composition



Fig. 5 Liquid Hydrogen (\*google.com)



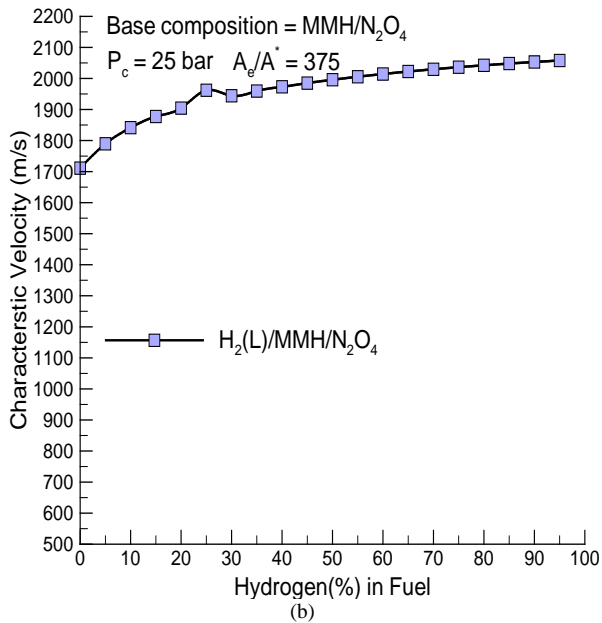
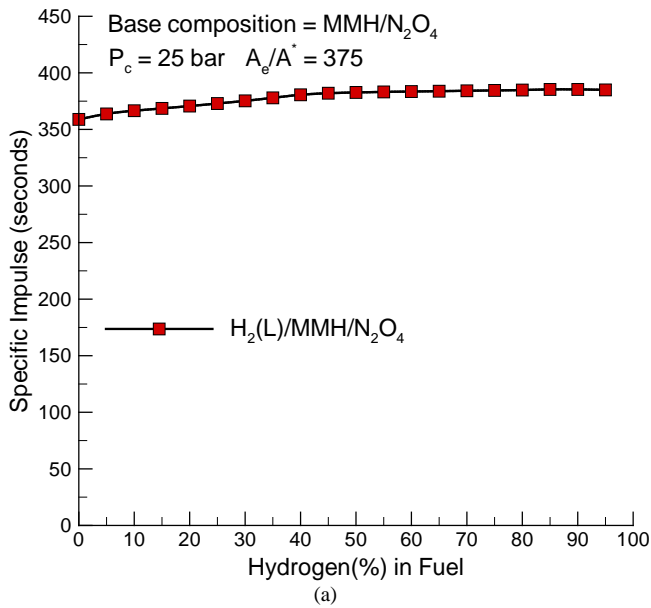


Fig. 6 Variation of (a) Specific Impulse and (b) Characteristic Velocity with varying Liquid Hydrogen proportion in fuel

The first hydrocarbon tested was Methane (CH<sub>4</sub>) (figure 8). When added to either fuel or oxidiser, Methane followed a similar downward trend (refer figure 9). The only visible difference was that, the slope was steeper when added to the oxidiser. The maximum decrease observed was of 16.87% when tested with fuel at 95% Methane with an I<sub>sp</sub> of 298.32 sec.

Whereas, when tested with the oxidiser, methane showed enhanced decrement of 54.84 % at 95% concentration by weight with a resulting I<sub>sp</sub> of 162.05 sec.

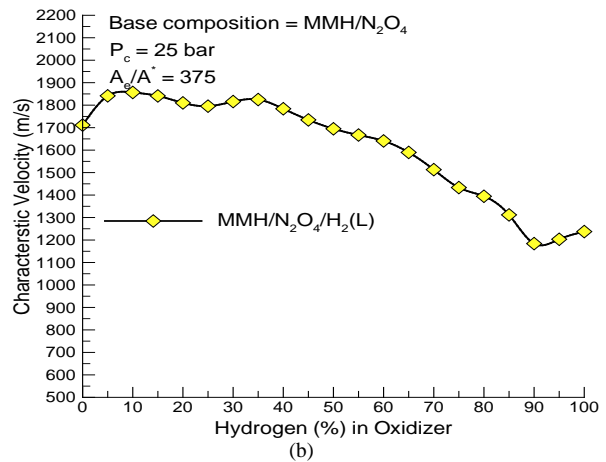
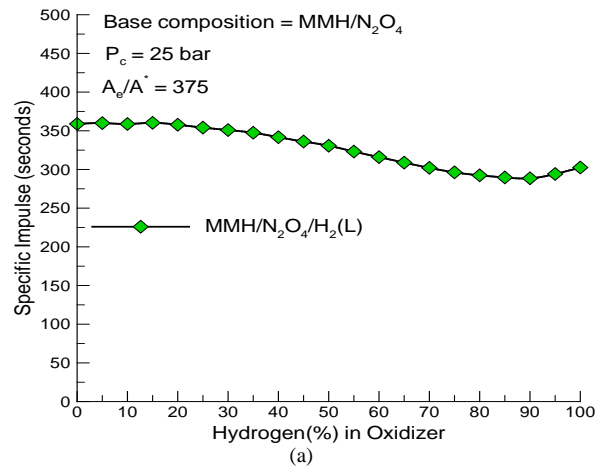


Fig. 7 Represents variation of (a) Specific Impulse and (b) Characteristic Velocity with varying Liquid Hydrogen proportion in oxidizer

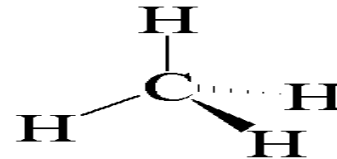
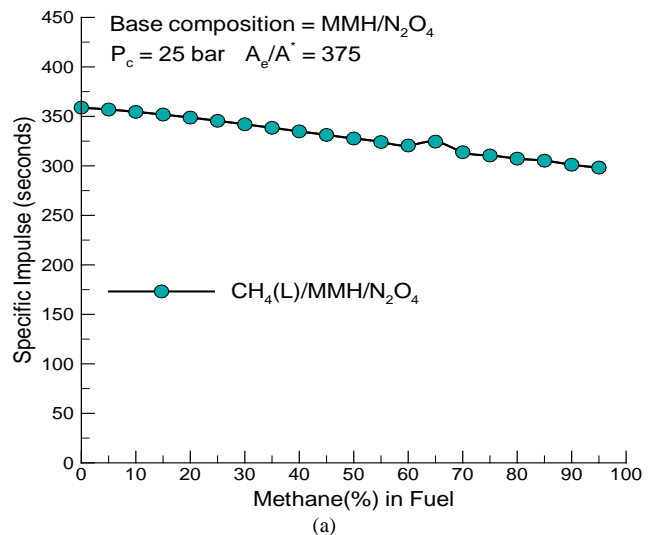
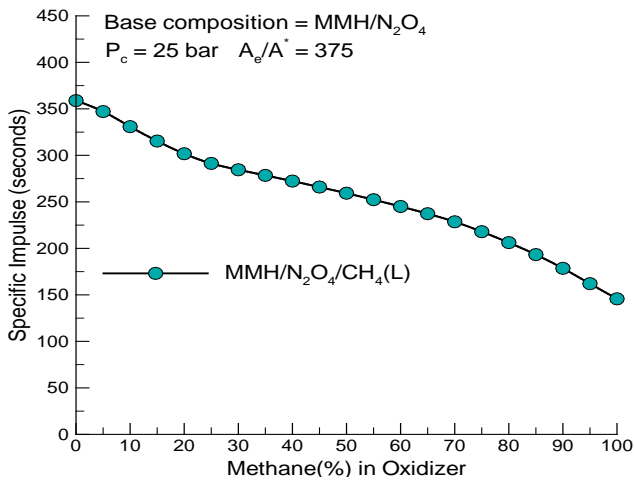


Fig. 8 Molecular structure of Methane (CH<sub>4</sub>) (\*google.com)





(b)  
Fig. 9 Variation of I<sub>sp</sub> with varying Methane proportion in (a) fuel and (b) oxidiser

Moving on to one of the conventional hydrogen-based rocket fuels, Jet-A (L) (figure 10) was tested with fuel and oxidiser respectively. As observed, Jet-A caused a fall in I<sub>sp</sub> by 16.87% upto 298.32 sec at 95% concentration (refer figure 11(a)) and a fall of 36.24% to an I<sub>sp</sub> of 223.82 sec at 95% Jet A (L) for oxidizer (refer figure 11(b)).

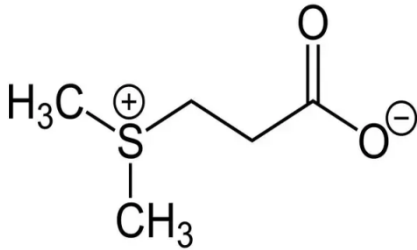
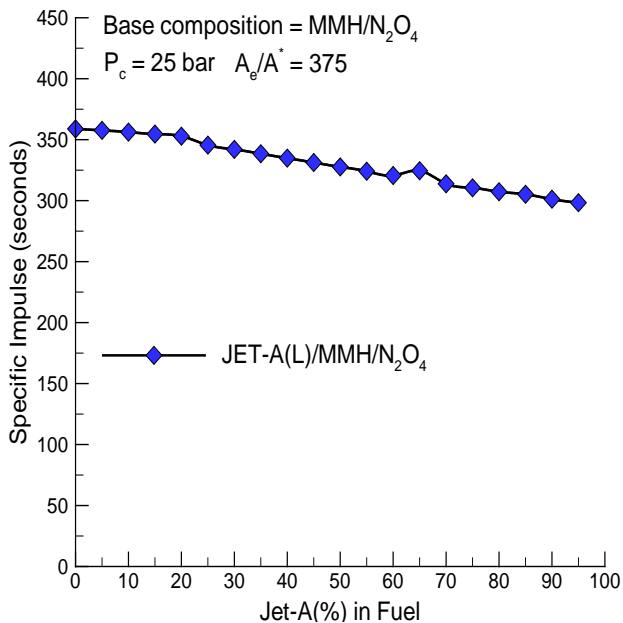


Fig. 10 Molecular structure of Jet-A(L) (\*google.com)



(a)

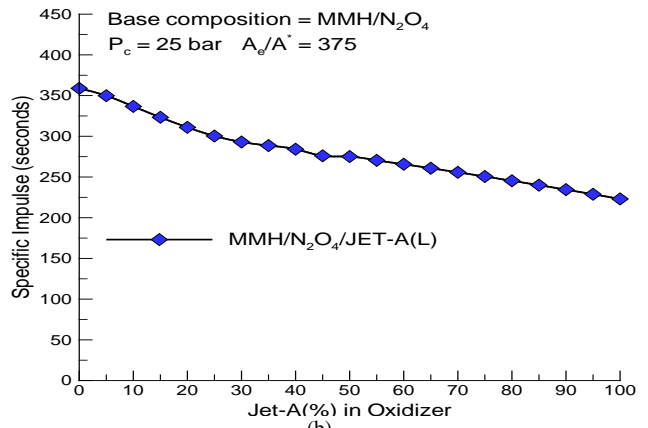


Fig. 11 Variation of I<sub>sp</sub> with varying Jet-A (L) proportion in (a) fuel and (b) oxidizer

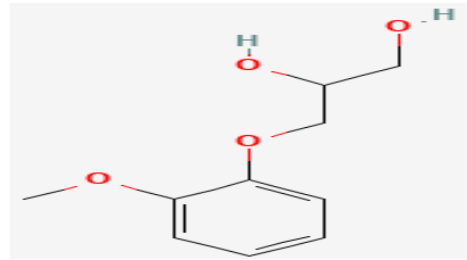


Fig. 12 Molecular Structure of RP-1 (Dimethyl 4-cyclohexene-1, 2-dicarboxylate) (\*google.com)

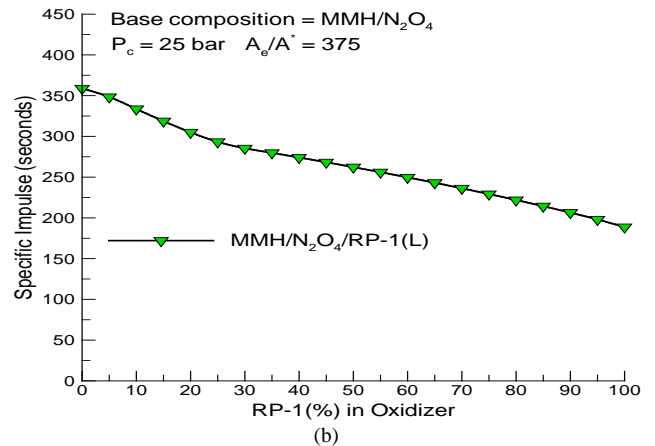
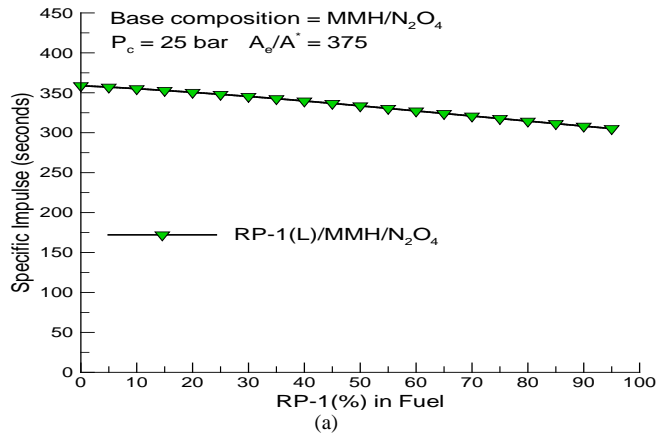


Fig.13 Variation of I<sub>sp</sub> with varying RP-1 proportion in (a) fuel and (b) oxidiser

When RP-1 (figure 12) was tested with the base propellant with changing concentrations, persistent decrement of  $I_{sp}$  was noticed (figure 13). A decrease of 14.97 % of  $I_{sp}$  at 95% concentration of RP-1 in fuel was noted in comparison to a decrement of 44.81% of  $I_{sp}$  at 95% concentration of RP-1 in oxidiser.

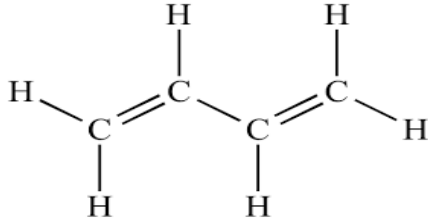


Fig. 14 Molecular structure of Butadiene (\*google.com)

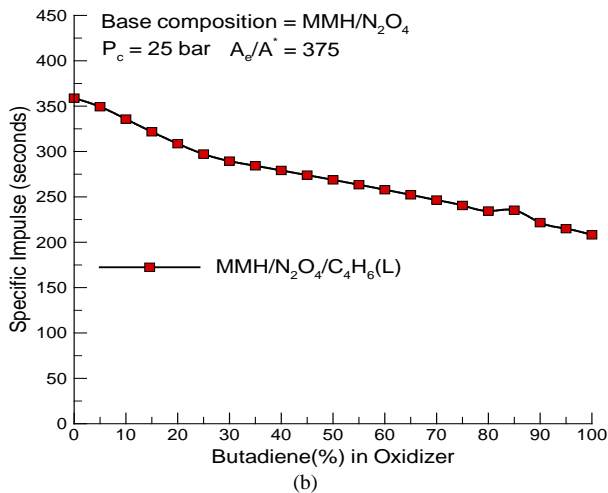
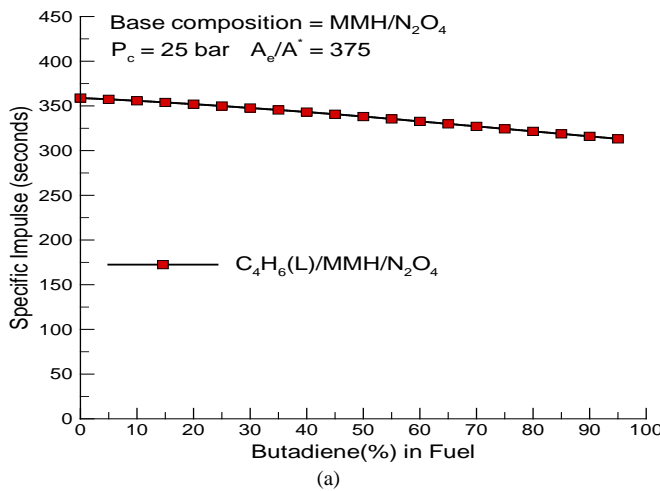


Fig. 15 Variation of  $I_{sp}$  with varying Butadiene proportion in (a) fuel and (b) oxidizer

Lastly, from the group of hydrocarbons, Butadiene (figure 14) was tested. As deduced, similar to other hydrocarbons, it followed a downward trend with a mild slope, when added to the fuel compared to when added to the oxidizer which resulted to drastic fall of  $I_{sp}$  (figure 15). Specific impulse drop of 12.73% at 95% butadiene was spotted in fuel followed by a fall of 40.91% at 95% butadiene in

oxidiser. This monotonic trend by Butadiene can be attributed to the alkane molecules as being non-polar, they are insoluble in water, which is a polar solvent, but are soluble in non-polar and slightly polar solvents.

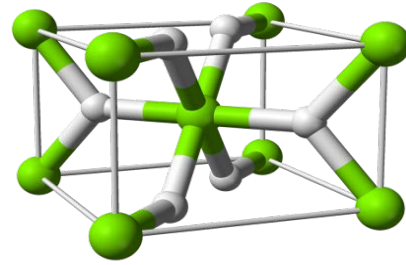


Fig. 16 Molecular structure of Magnesium Hydride (\*google.com)

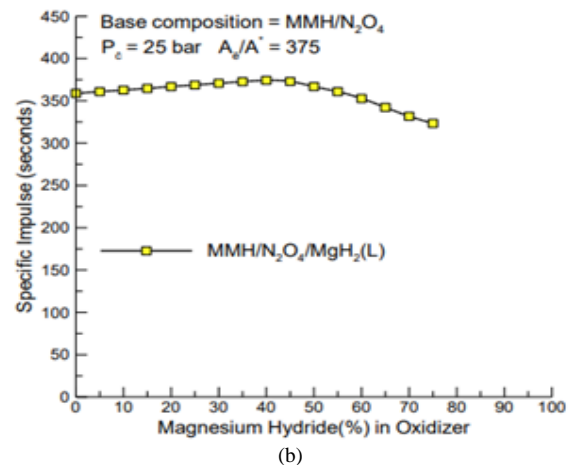
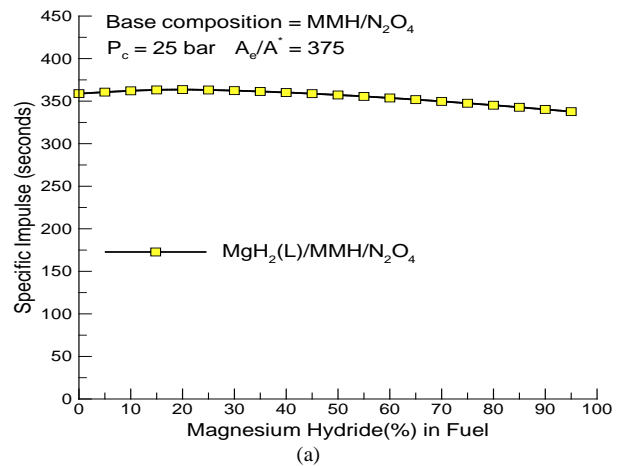


Fig. 17 Variation of  $I_{sp}$  with varying Magnesium Hydride proportion in (a) fuel and (b) oxidizer

Next, the second group of hydrogen-based compounds viz., Hydrides were tested. Starting with the addition of Magnesium Hydride (figure 16) with fuel and oxidizer, the following observations were drawn. When added to the fuel, a slight rise of  $I_{sp}$  occurred but stopped at 20%  $MgH_2(L)$  by weight with an increase of 1.32% resulting in  $I_{sp}$  value of 363.57 sec (figure 17(a)). The trend then started changing its course ensuing into a fall of 5.9 % at 95%  $MgH_2(L)$  with an  $I_{sp}$  of 337.66 sec.

When Magnesium Hydride was added to the oxidizer (figure 17(b)), a rise of 4.28% was noticed at 40%  $MgH_2(L)$  ( $I_{sp} = 374.22$ ). After this peak point, the  $I_{sp}$  fell by 9.9% at 75%  $MgH_2$  ending up at 323.31 sec.

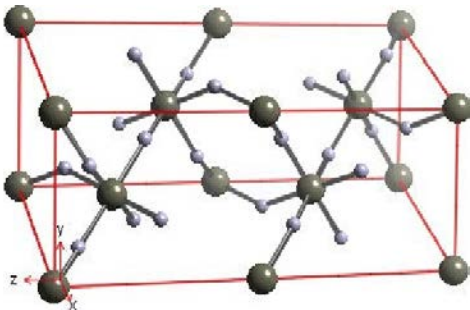


Fig. 18 Molecular structure of Aluminium Hydride (\*google.com)

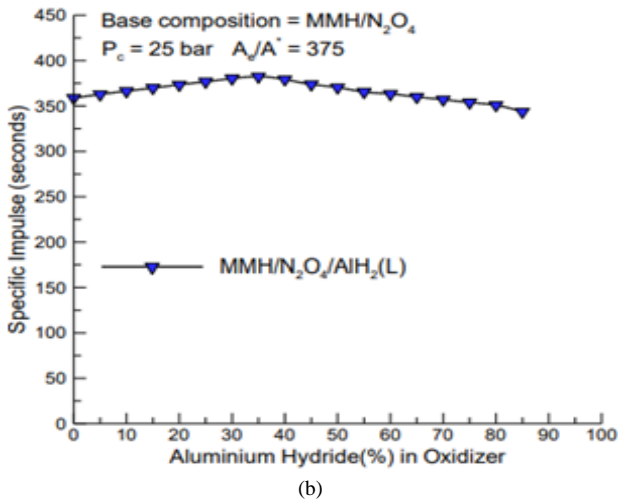
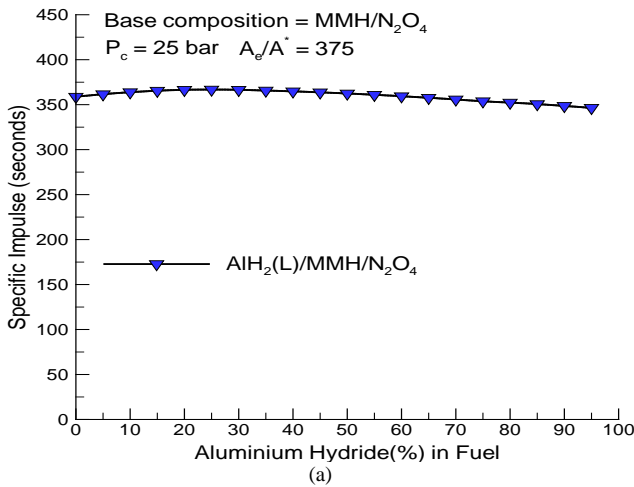


Fig. 19 Variation of  $I_{sp}$  with varying Aluminium Hydride proportion in (a) fuel and (b) oxidizer

The second compound tested was Aluminium Hydride (figure 18). When  $AlH_2$  was added to the fuel and oxidizer, effect followed a similar trend of initial rise continuing to mild fall (Figure 19). When added to fuel, rise of 2.21% at 25 %  $AlH_2(L)$  ( $I_{sp} = 366.8$  sec) was noted. But value of  $I_{sp}$  had fallen by 3.46% at 95%  $AlH_2(L)$  to 246.44 sec. Furthermore, when  $AlH_2(L)$  was added to the oxidizer, the

$I_{sp}$  increased to 382.37 sec showing rise of 6.55% at 35%  $AlH_2(L)$  followed by a fall of 4.23 % to 343.61 sec at 85%  $AlH_2(L)$ .

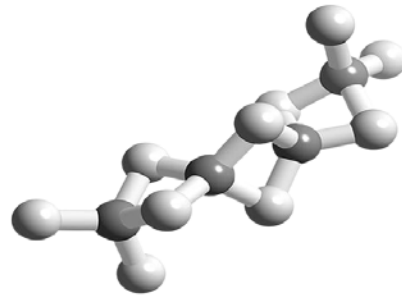


Fig. 20 Molecular structure of Beryllium Hydride (\*google.com)

For Beryllium Hydride (figure 20), result highlighted some interesting and promising fluctuations. When  $BeH_2(L)$  was added to the fuel (figure 21(a)), it exhibited a gradual increase in  $I_{sp}$  from the very beginning at a rise of 18.95% with an  $I_{sp}$  of 426.84 sec at 95%  $BeH_2(L)$  by concentration. When added to the oxidizer (figure 21(b)), higher  $I_{sp}$  value were obtained as at 30%  $BeH_2(L)$ ,  $I_{sp}$  rose by 20.29% to a value of 431.65 sec. This value stayed almost constant till 70% of the concentration in the propellant mixture and fell drastically further to a specific impulse of 362.99 sec at 70%  $BeH_2(L)$ .

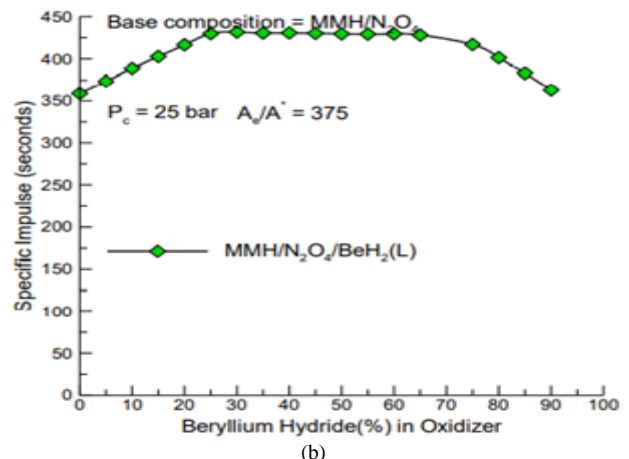
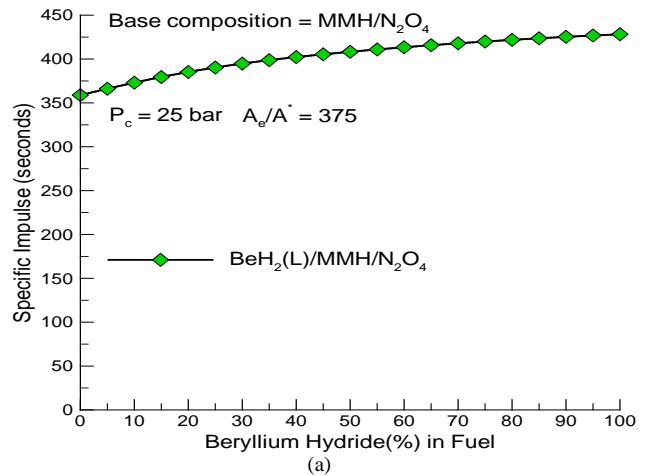


Fig. 21 Variation of  $I_{sp}$  with varying Beryllium Hydride proportion in (a) fuel and (b) oxidizer



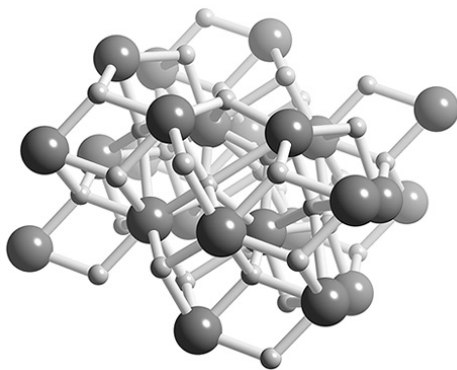


Fig. 22 Molecular structure of Calcium Hydride (\*google.com)

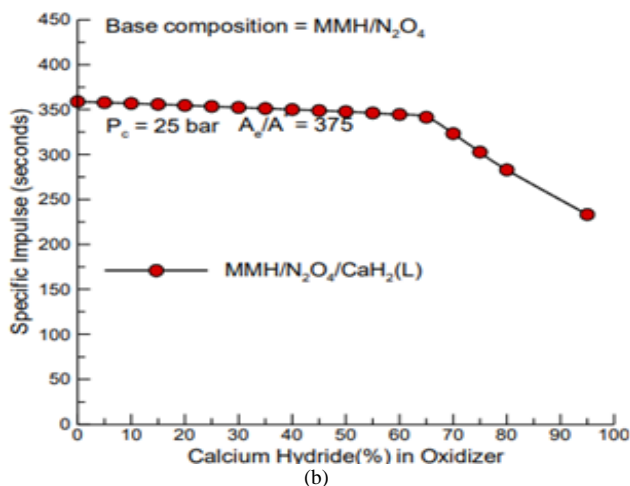
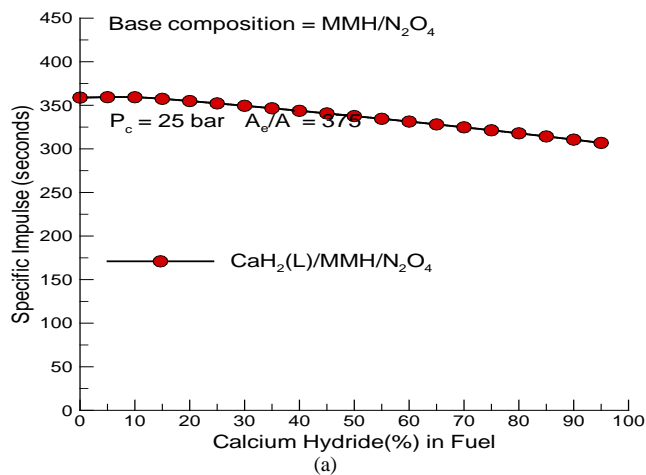


Fig. 23 Variation of  $I_{sp}$  with varying Calcium Hydride proportion in (a) fuel and (b) oxidizer

Calcium Hydride (figure 22) was the last compound tested from the group of hydrides. It starts off with a menial increase of 0.13% at 5%  $CaH_2$  (L) concentration with an  $I_{sp}$  value of 359.33 sec. But the trend shifts towards a gradual downfall by 1% at every concentration till a drop of 14.49% at 95%  $CaH_2$  (L),  $I_{sp}$ =306.87 sec (figure 23). When added to the oxidizer,  $I_{sp}$  falls with increasing concentration of  $CaH_2$  (L) in the mixture till 70 %  $CaH_2$  (L), from where  $I_{sp}$  drastically drops by 35 % to 233.19 sec.

**Stratified Thrust Termination:** Thrust termination is a phenomenon that implements controlled missions. Stratified thrust termination is an effective technique for hybridization and reusability. A simple injection of a catalyst to the base propellant at the desired time in the necessary proportion instigates chemical propulsion for thrust optimization. This can also be broadly used for damage control during failed missions. It is classified into three different categories depending on the various conditions for various missions. Instantaneous, Intermittent and Stunted are the various ways of controlling the thrust. Instantaneous thrust termination reduces the specific impulse of the missile to extreme low within a very short span of time. Intermittent has similar features but comparatively the drop is less. Stunted thrust termination gives more of a gradual decrease in specific impulse over a noticeable amount of period. With concurrent technological advancement, the missile system necessitates active research efforts to upgrade it for national security. An example of instantaneous thrust termination would be adding 95% methane concentration by weight to nitrogen tetroxide which reduces the  $I_{sp}$  by 54%, more than half (refer figure 9(b)). Addition RP-1 to nitrogen tetroxide at 95% gives an  $I_{sp}$  reduction by 44% and is most suitable for Intermittent thrust termination. Stunted thrust termination can be best portrayed by the addition of Butadiene to monomethyl hydrazine (refer figure 15(a)) which gives a gradual decrease in  $I_{sp}$ , with increasing compound composition.

From the above series of simulations that had been carried out, it was observed that the presence of hydrogen-based compounds as energetic catalysts for upper stage propulsion depicts singular unified behavior. The notable changes were thoroughly observed to fundamentally understand the operative reaction principle for enhanced understanding and utility. As Liquid Hydrogen inflicted a positive impact on the specific impulse when added to the base composition. This is because when liquid hydrogen is burned in presence of pure liquid oxygen, complete combustion occurs, which results in release of extreme energy which boosts up the specific impulse of the rocket. Due to the scarcity of liquid hydrogen in the atmosphere, hydrogen-based compounds had been tested as alternatives. The results were more adverse. Due to a higher bond energy of the products than the reactants there is negative heat release which results in decreasing  $I_{sp}$ . But this trend was not in complete accordance with certain hydrogen-based compounds, such as beryllium hydride at a certain concentration elevated the specific impulse value. The reason for the significant heterogeneous changes owing to the different hydrogen-based energetic catalyst addition in the base composition can be attributed to the alteration of the existing reaction mechanism by induced interference which directly results in the modified performance (here,  $I_{sp}$ ). The change and the rate of change for any particular catalyst in the base composition depend upon the internal molecular arrangements to facilitate the energy transfer with and the product compositions.

#### IV. CONCLUSION

From the systematic simulations carried out and thorough data analysis, several noticeable conclusions can be drawn:

1. Hydrogen based composition(s) were expected to have similar results as liquid hydrogen. This assumption was proved incorrect.
2. Simulation carried out with a semi-cryogenic catalyst viz., liquid hydrogen with the base propellant which results in an average higher Isp compared to when added to the oxidizer.
3. Hydrocarbons principally do not affect the specific impulse. But, in selected cases there were several alterations. Hydrocarbons showed a greater and steeper fall in Isp when added to oxidizer than the fuel.
4. Hydrides gave a higher rise in Specific Impulse than Hydrocarbons. They resulted in higher rise in Isp when added to oxidizer as compared to their addition in fuel. Hydrides tend to act better as thrust activators whereas hydrocarbons can be classified as thrust terminators.
5. Beryllium hydride in oxidizer had an attractive series of results. The composition,  $\text{MMH/BeH}_2/\text{N}_2\text{O}_4 = 30/14/56$ , gives an Isp of 431.65 sec. This is an appealing alternative to the cryogenic propellant in upper stage rocket propulsion engine and advanced high-performance missiles. This composition has high Isp and can be made in standard conditions resulting in sufficient reduction of the expenditure focusing production and storage.
6. Methane, RP-1 and Butadiene had proved to be useful during the need for thrust termination due to their instant drops in Specific Impulse.
7. *Potential applications of the present study:* Results from the above compositions can be used in missile systems,

re-entry vehicles, launch systems, space shuttles, power generation and many more. The work conveys wide scope of utilizations including simple dealing with, stability, cost viability and could be broadly utilized in Surface to Surface, Surface to Air, Anti-Tank, Multi Target, IRBM (Intermediate Range Ballistic Missile), Guided and Supersonic rockets under shifting conditions.

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