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Combustion and Propulsion Characteristics of Composite Solid Propellants under Elevated Conditions

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Abstract;- **Research efforts in Composite solid propellants are mostly carried out at standard operating static conditions and hence majority of the studies have taken place by considering lower values of supersonic area ratio and chamber pressure. The work addresses evaluation of the combustion and propulsion characteristics under elevated conditions. Composite solid propellant [AP/HTPB/Al] is selected and systematic parametric studies are carried out using NASA-CEA. The simulations were carried out for elevated chamber pressure, supersonic area ratio conditions along with varying fuel concentration and O/F ratio. The performance was analyzed in terms of change in specific impulse and characteristic velocity. The study comprises of investigating the optimized composition criterion under varying conditions. The simulation predictions were duly verified and validated with the benchmark experimental and theoretical works. The results were compared with the preceding static testing of the composite propellant under normal conditions. Results show that high values of controlling parameters and high energy materials do affect the composite propellant performance. Based on the results, an effort is made to reason out the trends obtained under elevated operating conditions for the necessary effects. Additionally, useful information regarding the inclinations of energetic materials under elevated conditions is explicated..**

Keywords;- **Solid composite propellants, Al/HTPB/AP, Specific Impulse, Characteristic velocity, Supersonic area ratio, Chamber Pressure, Oxidizer to Fuel ratio.**

I. INTRODUCTION

Rockets have revolutionized the space technology and human endeavor in space. The magnitude of the space operations relies heavily on the chemical rockets and thus draws immense emphasis on propellants and testing. Typically, the solid propellants are tested under standard prefixed conditions primarily carried out with a scaled model. The utility of propellants depends heavily on the state of testing standards. These propellants are widely tested with large scale or lab scale static motors under controlled conditions with chamber pressure varying from 10 to 70 bars and supersonic area ratio in the range of 10 to 100. The necessity of physical insight in to the phenomenon is detailed using set of design and performance parameters. The chamber pressure and supersonic area ratio are important design and control parameters to yield physical insight about the performance. The controlling parameters are known to have significant influence on the propellants under diverse conditions. The performance is analyzed in

terms of change in specific impulse and related independent parameters. The work is driven by the prevailing issues in composite solid propellants as experimental research is only being carried out by considering relatively lower values of controlling parameters like the nozzle area ratio, chamber pressure and oxidizer to fuel ratio rather than analyzing the controlling parameters under elevated conditions. The solid propellants are treated under standard conditions with a scaled model under statically controlled conditions to avoid uncontrollable combustion. Trends of composite solid propellants at elevated conditions of nozzle area ratio, chamber pressure and oxidizer to fuel ratio are not experimentally validated. Practically, the rockets using propellants operate under varying conditions and thus it is mandatory to understand the nature of characteristic parametric changes under varying conditions.

The processes inside the combustion chamber of solid propellant rockets can be explained for an ideal situation by different relationships. The key parameters include physical, chemical and mechanical properties of propellant, combustion gas conditions, and rocket operating conditions. Three important factors namely, the specific impulse (I_{sp}), characteristic velocity (C*) and thrust coefficient (C_F) are of paramount importance in rocket propulsion. Theoretically, the nozzle expansion ratio or supersonic area ratio (A_e/A^* or ε) can be expressed in terms of specific heat ratio of combustion gases (ɣ) and pressure ratio (P_e/P_c) as:

$$\varepsilon = \frac{\sqrt{\left(\frac{\gamma-1}{2}\right)\left(\frac{2}{(\gamma+1)}\right)^{\frac{(\gamma+1)}{(\gamma-1)}}}}{\left(\frac{P_e}{P_c}\right)^{\frac{1}{\gamma}}\sqrt{\left\{1-\left(\frac{P_e}{P_c}\right)^{\frac{(\gamma-1)}{\gamma}}\right\}}} \quad (1)$$

Where,
P_e = Exit Pressure
P_c = Chamber Pressure
γ = Specific heat of combustion gases

Equation (1) dictates that the supersonic area ratio (A_e/A^*) is a strong function of specific heat ratio of combustion gases (γ) and pressure ratio (P_e/P_c) i.e. change in chamber pressure will lead to change in the supersonic area ratio.

The adjoining rocket performance parameters includes specific impulse (I_{sp}), characteristic velocity (C*) and thrust coefficient (C_F). The theoretical framework for abovementioned performance parameters can be refereed as:

$$CF = F/Pc.At \quad (2)$$

$$C_F = \Gamma\sqrt{\left(\frac{2}{(\gamma-1)}\right)\left\{1-\left(\frac{P_e}{P_c}\right)^{\frac{(\gamma-1)}{\gamma}}\right\}} + \frac{(P_e-P_a).\,\varepsilon}{P_c} \quad (3)$$

Where,

$$\Gamma = \sqrt{\gamma\left(\frac{2}{(\gamma+1)}\right)^{\frac{(\gamma+1)}{(\gamma-1)}}}$$

F = Thrust produced by rocket
A_t = Area of nozzle at throat
P_a = Ambient pressure

Thrust coefficient 'C_F' is a figure of merit of the nozzle and signifies nozzle effectiveness. Equations 2-3 states that the meanwhile, 'C_F' is a function of specific heat of combustion gases γ, supersonic area ratio (A_e/A^*), pressure ratio (P_e/P_c), it is independent of the chamber temperature(T_c) and the mean molecular weight of the exhaust products. Except for 'γ', thrust is completely free from the choice of propellant and depends only on the operating pressure. The optimum value of thrust coefficient is obtained if the rocket is operating in a vacuum and Pa = 0, whereas, for high value of 'C_F', low value of 'γ' and high value of nozzle expansion ratio (A_e/A^*) are preferred. The dependence of 'C_F' on (A_e/A^*) vanishes, if pressure thrust is 0, however, the trend remains unaltered. The characteristic velocity (C*) depends mainly on the conditions in the combustion chamber. It depends on 'T_c', 'M' and 'γ', with 'P_c' influencing it indirectly through 'T_c'.

$$C^* = \gamma\, Pc.At/\dot{m} \quad (4)$$

$$C^* = \sqrt{\frac{g.R.T_c}{M}} \times \frac{1}{\Gamma} \quad (5)$$

Where,

T_c = Chamber temperature
M = Molecular mass of the combustion gases
$\dot{m}$ = Net mass flow rate of the gases through the nozzle

Equation 5 states that, C* is independent of the downstream conditions beyond that of the nozzle. A higher value of C* is always desirable through a high chamber temperature and a low mean molecular weight of exhaust products.

From Equation (4) we can say that C* is a function which converts mass-flow '$\dot{m}$' into chamber pressure 'P_c' i.e. C* is not a nozzle parameter and is a transfer function of $\dot{m}$ and P_c. C* is sensitive to the combustion process and is a true measure of propellant performance thus, essential for merit of the chamber. The specific impulse (I_{sp}) is detailed as:

$$Isp = C_F\, C^*/g \quad (6)$$

$$I_{sp} = \sqrt{\frac{2\gamma}{(\gamma-1)}\,\frac{R.T_c}{M.g}\left\{1-\left(\frac{P_e}{P_c}\right)^{\frac{(\gamma-1)}{\gamma}}\right\}} \quad (7)$$

'I_{sp}' is a product of the pressure generating capacity in the rocket (C*) and velocity generating property (C_F which is a chamber parameter). Like 'C*', it needs a higher chamber temperature and a low mean molecular weight of exhaust products. 'I_{sp}' value depends on the nozzle expansion ratio (A_e/A^*). Low value of 'γ' is desirable for a high value of 'I_{sp}' and when γ=1, it becomes infinite. It is important to note that the mean performance parameters are a strong function of controlling parameters viz, chamber pressure and area expansion ratio. Thus, to fundamentally understand the operations under elevated conditions, it is necessary to adjust the understanding of inter-relation between the operating parameters.

Appreciable work had been done in the past and reviews can be found in [1-17] which provide an excellent assessment of the advancement till the end of the century and in recently. Present work emphases on the importance of operating condition, testing the controlling parameters and their role in relation to the performance. A base composite propellant [AP/HTPB/Al] is selected and extensive testing is being carried out to fundamentally understand the role of operating chamber pressure, supersonic area ratio and varying fuel concentration on the performance. The cases of standard testing and testing under elevated conditions of pressure and supersonic area ratio are undertaken to evaluate the performance change. In addition to establishing relationship between the controlling parameters, determining their roles and effects on the rocket performance parameters and quantitatively as well as qualitatively verifying the trends of specific impulse and characteristic velocity w.r.t. controlling parameters, the work also emphasizes on incorporating the use of energetic materials like Iron in the base propellant composition of to get an enhanced propellant performance. A comparison of the trend obtained by adding Iron to the base composition at standard conditions is made with that at elevated conditions. A quantitative analysis is done of the variation in trends obtained. The evaluation of combustion and propulsion features of propellants under varying conditions is an aspect yet to be comprehensively explored. Present work attempts to investigate the combustion and propulsion features of the composite propellant under elevated condition. The specific objectives of the work are:

a) To understand the importance of operating conditions, testing the controlling parameters and their role in relation to the performance.

b) To study behavior/trends and role of energetic materials in base propellants for increasing performance at elevated conditions

II. SIMULATIONS AND SOLUTION METHODOLOGY

The work involves utilization of specialized chemical propulsion software NASA CEA (Chemical Equilibrium with Applications). The software tool calculates chemical equilibrium compositions and properties of complex mixtures from any set of reactants and determines thermodynamic and transport properties for the product mixture. Applications include assigned thermodynamic states, theoretical rocket performance, Chapman-Jouguet detonations, and shock-tube parameters for incident and reflected shocks. The composition of the oxidizers and fuels are varied stepwise and the theoretical rocket performance parameters like Specific Impulse, Characteristic Velocity are noted down and parametric analysis is done based on the software predictions. The present study is carried out by comparing results by varying the controlling parameters like chamber pressure, supersonic area ratio and oxidizer to fuel ratio (O/F) from lower to elevated conditions. The species present in the composite solid propellant composition are chosen either directly by choosing the solid propellant option or if new options are to be investigated then the atoms of the fuel to be chosen are selected from the periodic table.

III. RESULTS

The operating conditions are varied w.r.t. the base propellant composition of Ammonium Perchlorate as the oxidizer (70%), HTPB (Hydroxyl Terminated Polybutadiene) (15%) as the binder and Aluminum (15%). Addition of energetic material in the base composition in the form of Iron is also made at standard and elevated conditions. Prior to the main results, the software predictions were validated with existing experimental and theoretical data (please see Table 1). Analyzing the data, one can clearly note that the software predictions match reasonably well with the preceding experimental and theoretical work. Hence, it is likely to give good physical insight into understanding the effect of the controlling parameters in composite solid propellants. The first part of the study is devoted to evaluating the optimum composite propellant composition. This is done to compare this result with increment/ decrement in performance parameters associated with elevated operating conditions. First, the base composition AP/HTPB/Al [70/15/15] is validated for extensive utilization. Figure 1 shows the variation of performance parameter specific impulse with aluminium concentration.

Table 1: Validation of simulation predictions with preceding experimental and theoretical work.

Composition	*Exp./ Theo. (sec)*	*Simltn. (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 *et. al.*,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 [68/14/18] at (Pc=6.89MPa) ***www.lr.tudelft.nl***	266	264.02
AP/PBAN/Al [70/12/16] at (Pc=6.89MPa) ***www.lr.tudelft.nl***	267	263.97

It is important to note that, aluminium is used in crystalline form. Looking at the plot one can note that the 'Al' gives the maximum 'I_{sp}' at 15%(weight). The optimum composition is determined by increasing the mass fraction of Al in steps of 1 %, ranging from no Al to 45 % of 'Al' by total mass. The results are shown in Figure 1. A non-monotonic trend is seen that peaks around 15 % of 'Al' by mass. The corresponding 'Isp' is around 265s. The high I_{sp} values seen are largely explained on basis of the flame temperature of 'Al' which is around 3700 K, which is significantly higher than the adiabatic flame temperature for hydrocarbon fuels.

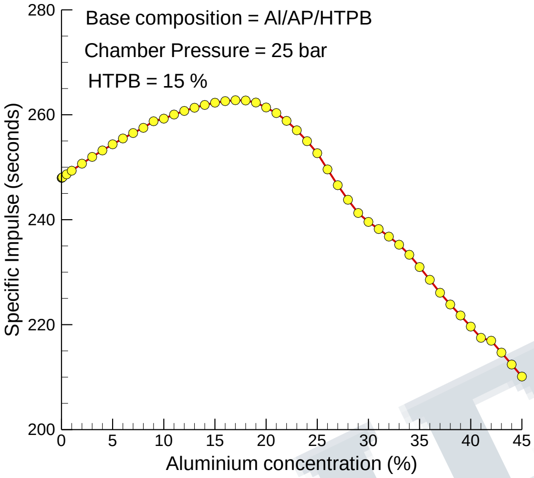

Figure 1: Variation of specific impulse with Aluminium concentration.

The non-monotonic trend seen is also a result of the variation of the adiabatic flame temperature with the fuel concentration. Lower and higher concentration of fuels lead to lower flame temperatures and hence have lower 'I_{sp}'. The results are cross-checked with secondary parameter viz., characteristic velocity 'C*' (Figure 2).

The 'C*' variation indicates trend like the 'I_{sp}' that on increasing the 'Al' concentration from 0 to 15% the characteristic velocity increases till 15% and then decreases drastically. The above-mentioned result certifies usage of 15% Aluminium in the base composition. One of the important attribute of 'Al' is generation of high temperatures generated (4100 K) as increase in pressure results increasing effective velocity and hence increased thrust. Aluminium agglomerates in the liquid state help to dampen combustion instabilities.

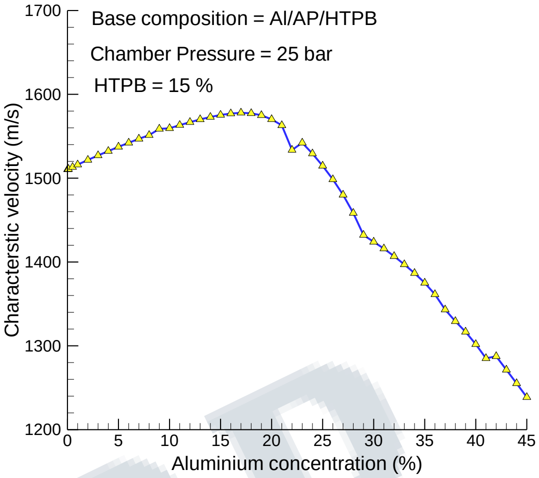

Figure 2: Variation of characteristic velocity with Aluminium concentration.

Figure 3 shows that the base composition taken into consideration was Al/HTPB/AP in the ratio 15/15/70 with a minimal supersonic area ratio 10 and chamber pressure 25 bar for which the corresponding Isp was noted to be 262.3 s. Figure 4 signifies the value of the characteristic velocity 'Cstar' which was noted to be 1575.4 m/s w.r.t. the same base compositon of Al/HTPB/AP and at the same base conditions as above. Firstly, the dependence of I_{sp} with varying supersonic area ratio for different values of constant chamber pressure was taken into consideration.

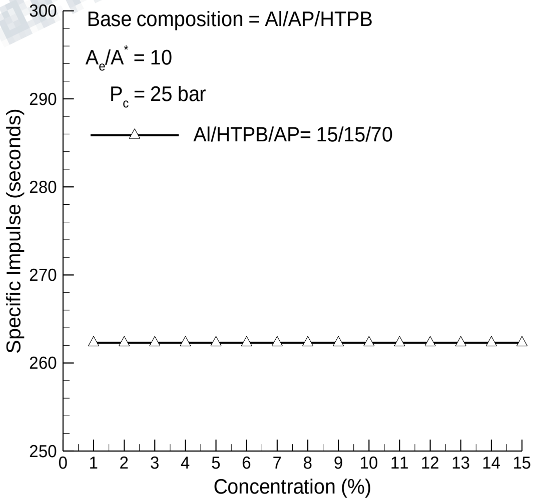

Figure 3: Variation of specific impulse with base composition.

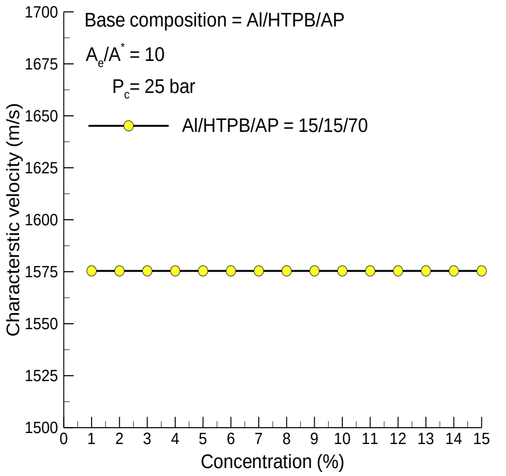

Figure 4: Variation of characteristic velocity with base composition.

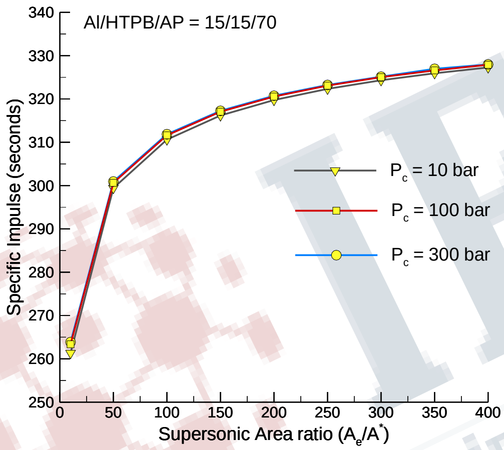

Figure 5: Variation of specific impulse with varying supersonic area ratio (Ae/A).*

Figure 5 shows the trend of increment in I_{sp} with varying supersonic area ratio from 10 to 400 for different values of constant chamber pressure which are 10 bar, 100 bar and 300 bar respectively. The base composition of Al/HTPB/AP in the ratio 15/15/70 was considered. It is to be noted that for respective values of constant chamber pressure, the variation in I_{sp} is less than 1% corresponding to each supersonic area ratio value. Also, the increment of I_{sp} w.r.t. varying supersonic area ratio followed the same trend for low, intermediate and high chamber pressure values of 10bar, 100bar and 300bar respectively. The approximate increment in I_{sp} from nozzle area ratio 10 to 50 is 15%, from 50 to 100 is 4%, from 100 to 150 is 2%, from 150 to 200 is 1%, from 200 to 250 is **0.8%**, from 250 to 300 is 0.6%, from 300 to 350 is **0.4%** and from 350 to 400 is **0.4%**. It can be noted that the rate of increment decreases monotonically as the area ratio increases. The increment in Isp w.r.t the supersonic area ratio can be reasoned out since Isp is a function of the thrust coefficient C_F which is a direct function of the supersonic area ratio. Figure 6 verifies the result seen in figure 5 with the variation of I_{sp} with varying chamber pressure from 10 bar to 300 bar for three different values of supersonic area ratio.
The values considered are 10, 100 and 300 to signify low, intermediate and high supersonic area ratio respectively. It can be noted that the increment in Isp values from supersonic area ratio 10 to 100 is approximately **18-19%** and from supersonic area ratio 100 to 300 is approximately **4%** i.e. the increment in I_{sp} is substantial initially when supersonic area ratio is small but as the supersonic area ratio gets larger, the increment in Isp is not substantial. Hence for subsequent very high supersonic area ratio values, the Isp values get relatively invariant and redundant with the supersonic area ratio.

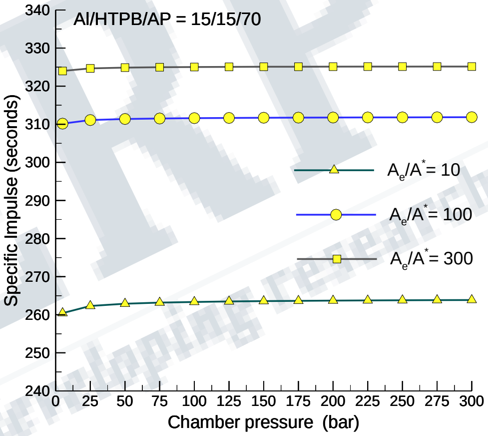

Figure 6: Variation of specific impulse with varying chamber pressure

The plots in figure 5 and 6 show that supersonic area ratio is the more dominating controlling parameter of I_{sp} because it is directly proportional to the supersonic area ratio.

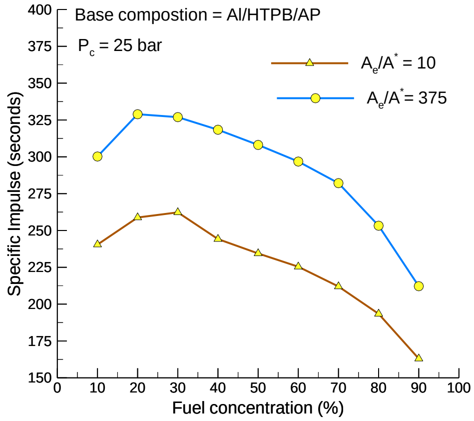

Figure 7: Variation of specific impulse with fuel concentration (%).

Figure 7 shows the variation of Isp with varying fuel concentration (%) for the base composition of Al/HTPB/AP at chamber pressure 25 bar. For a lower supersonic area ratio of 10, the max I_{sp} of 262.3s was noted at 30% fuel concentration i.e. the optimum O/F ratio for lower supersonic area ratio appeared to be 2.33. But for higher supersonic area ratio of 375, the maximum I_{sp} of 328.9s is noted at **20%** fuel concentration i.e. the optimum O/F ratio for higher supersonic area ratio appeared to be 4.

The % increase in I_{sp} was found to be **27%** at fuel concentration 30% for both area ratio values of 10 and 375. From this, it is inferred that O/F ratio is a function of supersonic area ratio.

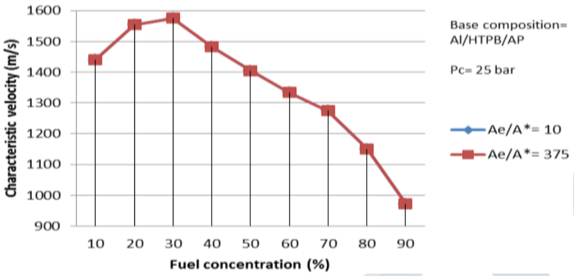

Figure 8: Variation of characteristic velocity with fuel concentration (%) under varying area ratio.

The results in Figure 8 were cross-checked with secondary parameter characteristic velocity ‘Cstar’ but the ‘Cstar’ variation indicated that it’s not a function of supersonic area ratio as the maximum ‘Cstar’ value was obtained at fuel concentration of 30% and was noted to be 1575.4 m/s irrespective of the supersonic area ratio. Irrespective of the area ratio values, ‘Cstar’ follows the same trend with the same values for variation with fuel concentration (%). This behaviour can be justified as C* is not a nozzle parameter and hence is not dependent of the supersonic area ratio.

It is a function of and figure of merit of the chamber pressure according to equation 6.

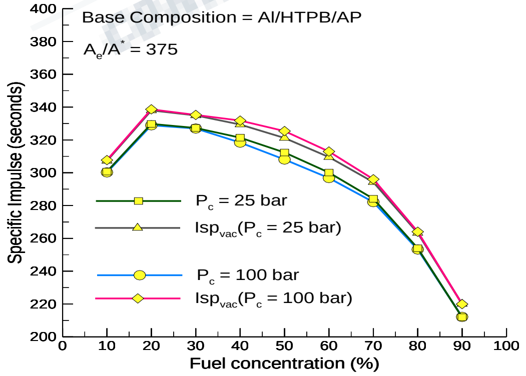

Figure 9: Variation of specific impulse at sea level and specific impulse at vaccuum with variation in fuel concentration (%)

Figure 9 shows the variation of I_{sp} at sea level and vaccuum with variation in fuel concentration for the base composition Al/HTPB/AP at supersonic area ratio 375 and for constant chamber pressure values of 25 bar and 100 bar respectively. It can be noted that the I_{sp} values in vaccuum are always higher than the corresponding I_{sp} values at sea level for each increment in fuel concentration. This is because in vacuum Pa=0 so C_F would be maximum and hence I_{sp} since its directly propeortional to C_F according to equation 6.

The maximum variation between I_{sp} at vacuum and at sea level was noted to be approximately **4%** at 60% fuel concentration when chamber pressure is taken as 25 bar and approximately **4%** at 50% fuel concentration when chamber pressure is taken to be 100 bar. The plot again signifies that the trend followed by I_{sp} at various chamber pressures is the same and that out of chamber pressure and area ratio, the dominant controlling parameter of I_{sp} is the area ratio as increasing chamber pressure from 25 bar to 100 bar doesn’t show a significant increase in the I_{sp} value. Figure 10 gives the relationship between I_{sp} and Al concentration in the Al/HTPB/AP mixture at chamber pressure 25 bar.

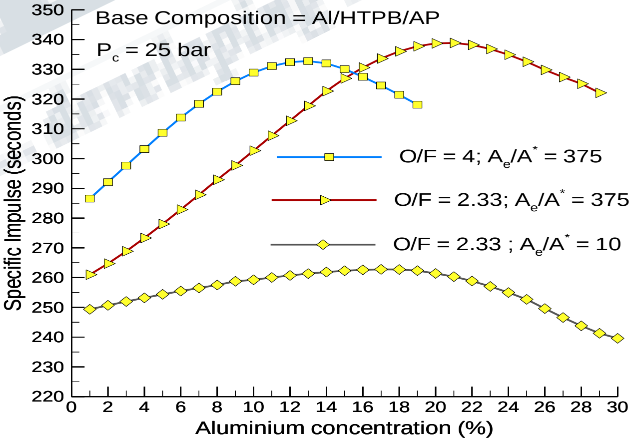

Figure 10: Variation of Specific Impulse with Aluminum concentration (%)

At O/F ratio 2.33 and area ratio 10, the maximum I_{sp} of 262s was obtained at approximately 16% ‘Al’ concentration which validates the optimum concentration of Al at low supersonic area ratio to be 15%.

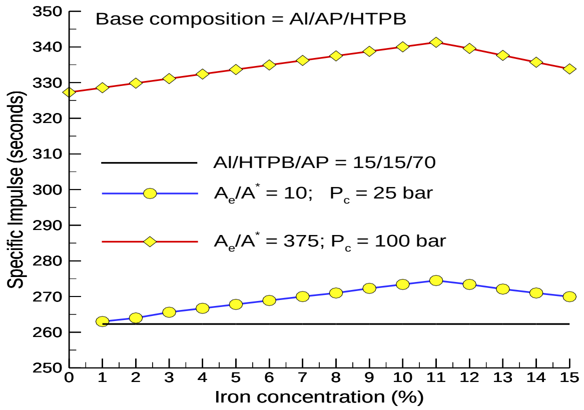

Figure 11: Variation of Specific Impulse with Iron cooncentration (%)

In contrast, at O/F ratio 2.33 and at elevated supersonic area ratio of 375, the maximum I_{sp} of 338s was obtained at 21% Al concentration. Also, at O/F ratio 4 and supersonic area ratio 375, the maximum I_{sp} of 332s was obtained at 13% 'Al' concentration. It is thus shown that optimum 'Al' concentration for obtaining maximum I_{sp} is a function of supersonic area ratio. Figure 11 shows the variation of I_{sp} with Iron concentration in the base composition of Al/HTPB/AP which taken in the ratio of 15/15/70. It can be noted from the plot that addition of Fe to the fuel acts as a catalyst. The trend increases until 11% iron concentratin and decreses thereafter is identical for both values of supersonic area ratio (375 and 10) at chamber pressures 100 bar and 25 bar respectively. For both cases the maximum 'Isp' is obtained at 11% iron concentration. Fe gives approximately **4.65%** rise in I_{sp} to the base composition of Al/HTPB/AP at supersonic area ratio 10 and chamber pressure 25 bar. For elevated conditions of supersoinc area ratio 375 and chamber pressure 100 bar, Fe approximately gives a rise of **4.28%** to the base compostion of Al/HTPB/AP.

IV. SUMMARY

Out of supersonic area ratio and chamber pressure, supersonic area ratio is the more dominant controlling parameter because changing it showed substantial changes in Isp till a particular limit under elevated conditions but changing chamber pressure didn't show substantial changes in the Isp even under elevated conditions. Also when operating under elevated condition of supersonic area ratio 375, it was noted that the optimum fuel concentration shifted from 30% (which was the case for lower values of supersonic area ratio) to 20%. But characteristic velocity remained unchanged or was indifferent to the changes made in supersonic area ratio which signified that characteristic velocity was not a function of the supersonic area ratio. It was also noted that under elevated conditions of high supersonic area ratio and high chamber pressure, the trend followed by Isp at sea level and in vacuum was the same with approximately only 4% variation in the values. The reason behind the use of Aluminum at 15% concentration in the base composition under lower values of supersonic area ratio & chamber pressure was established. It was also noted that the optimum Al concentration for obtaining maximum Isp is a function of the supersonic area ratio. 11% Iron is required to be added to cause increment of 4% in Specific Impulse at O/F greater than 1 at lower values of controlling parameters. The same was also verified by adding Iron under elevated conditions of supersonic area ratio and chamber pressure.

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