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Estimation of Ideal Specific Impulse of Paraffin Wax-Fueled Lab-Scale Hybrid Rocket Motor Using Chebyshev Method

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Abstract
This paper primarily aims on the theoretical specific impulse characterization of a lab scale paraffin wax-powered hybrid rocket motors, focusing on area ratios ranging from 2.0 to 5.0 The study follows the balanced stoichiometric chemical reactions of pure paraffin wax combustion with gaseous oxygen as the oxidizer and determines the exhaust mixture's specific heat ratio . A transcendental non-linear function related to exit Mach number and area ratio was derived, allowing for calculations using numerical methods including Bisection, Newton-Raphson and Chebyshev. The methods were assessed for zero convergence of the function with minimal iterations, which is essential for computation of theoretical or ideal specific impulse. Furthermore, a theoretical estimation study was conducted to predict the specific impulse for four pure paraffin wax fuels which include n-docosane ($C_{22}H_{46}$),n-hexacosane ($C_{26}H_{54}$),n-triacontane($C_{30}H_{62}$) and also n-hexatriacontane($C_{36}H_{74}$), under an averaged chamber temperature of 3400^0K and maintaining chamber pressure of 1.0 MPa with an assumption of fully expanded nozzle condition in static bed test to analyze their ideal performance. The findings highlight the specific impulse estimation, creating valuable approach on basic performance of the hybrid rocket propulsion system and providing optimization insights for selection of pure paraffin wax-based fuels with better operational performance.

Keywords: exit mach number, area ratio, specific impulse numerical methods, paraffin wax.

1. Introduction

The current space industry is in thirst of advanced optimized technologies to achieve the larger deep space missions at most economical way, apart from the conventional rocket systems like solid or liquid the hybrid rocket motors encompass a uncommon propulsion unit that integrate elements of conventional solid based and liquid rocket engines [1-4]. Hybrid rockets utilize a solid fuel grain, typically made from elastomeric compounds or even soft solids which has good a good affinity towards combustion, accompanied by liquid or gaseous oxidizer, such as liquid or gaseous oxygen or other oxidizers. This combination allows for a controlled combustion process, where the fuel ignites upon contact with the oxidizer, produce high temperature expulsion of jet gases through the nozzle to generate the propulsive force[1]. Hybrid rocket propulsion provides several advantages over conventional rocket systems, including better safety, simplicity, and better controllability [1]. The studies performed by Sutton, et.,al (2001) depicts that for a typical hybrid motor propulsion system, both fuel composition and oxidizer are kept separate until combustion; this reduces the risk of unwanted ignition, and thrust regulation can be made much more accurate [2]. For conventional design of a hybrid rocket motor especially on the lab-scale aspect it is vital to follow the isentropic and other fundamental mathematical relations in designing the flow geometry and performing the performance computations based on the operational standpoints [3].

1.1 Working Operation of a typical Hybrid Rocket Unit

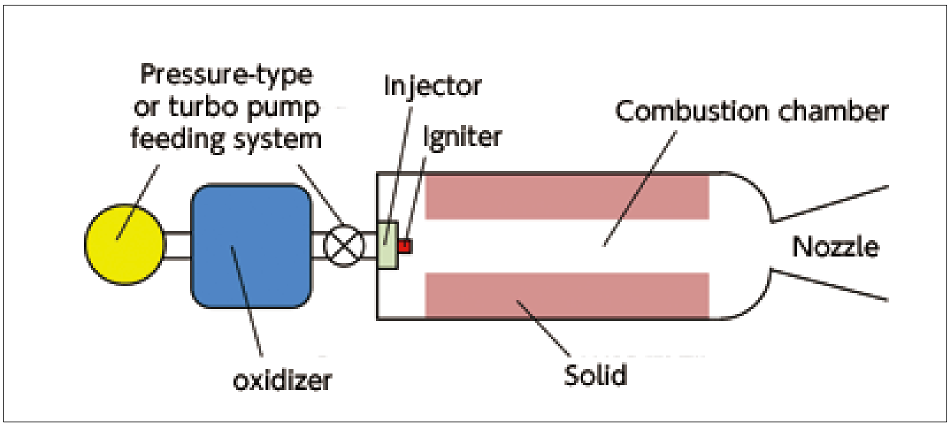
In this motor unit both solid fuel composition and a liquid or gaseous oxidiser are combined in a typical hybrid rocket motor and stored apart until they are burned. The following are some of the essential elements: [1],[2],[4]. Figure.1 presents the functional structure of a hybrid rocket.

- Combustion Chamber Unit: The basic combustion process takes place in this section. It contains the solid fuel grain and creates a regulated burning environment.
- Fuel Grain: The solid fuel, often made from rubber or plastic-based compounds, is designed to burn steadily, releasing energy in a controlled manner.
- Oxidizer Injection System: The oxidizer, contained in a high-pressure container, with a suitable injection into the combustion chamber to allow ignition to occur. This can be a liquid or gaseous substance, such as nitrous oxide. The injection is performed by a controlled pressure feed or a turbo feed flow control mechanism.
- Ignition: When the oxidizer gets inducted to the fuel grain, combustion begins, producing hot gases.
- Thrust Generation: Through the designed nozzle, the expelled high temperature gases are released, producing forward propulsive force for rocket.

1.2 Paraffin wax based solid fuel and oxidizer as gaseous oxygen (Gox)

Based on experimental studies performed by Siva et al., (2018) it is evident that for a mini scale or a lab scale testing purpose the common fuel deployed in hybrid rocket motor is paraffin wax and which has got more accessibility in comparison with other fuels. Paraffin wax is often combined with an oxidizer either gaseous or liquid in nature to create a hybrid propellant system. This combination allows for effective controlled combustion and performance in hybrid rocket applications [5]. The advanced numerical analysis performed by Migliorino, et al.,(2019) reveals that by using the gaseous oxidizer the combustion chamber was attained at a temperature of 3450^0K with ratio of oxidizer and fuel (O/F) to be found as 1.17 to 1.38[6],[18],[19]. The lab scale area ratio was maintained about 2.45 and similar kind of lab tests and studies carried out by Shanks, et al., (2000) for typical area ratios[7]. In this study, the area ratio has been fixed between 2.0 and 5.0 based on real-time availability of components, operational requirements, and insights drawn from similar past literature. This range is selected to optimize the analysis of propulsion dynamics and advanced fuel performance while ensuring practical feasibility for both research and educational purposes. The area ratio, a crucial parameter in nozzle design, influences the flow behavior and the efficiency of the rocket system.

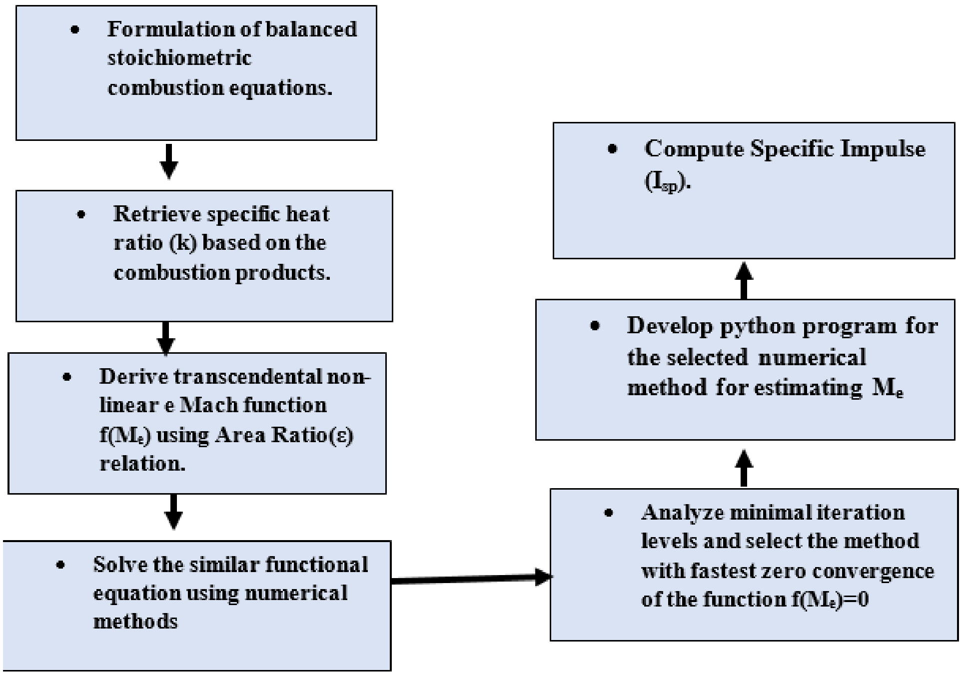
Figure 1: Schematics of Hybrid Rocket Unit



2. Methodology for Theoretical Computation and Data Analysis

The below process chart fig. 2 presents the methodology carried out for this theoretical study work with suitable numerical methods and mini python-based program. Before proceeding to the actual process, it is important to understand and study about paraffin wax fuel and its variants and their critical operating temperature and pressure values.

Figure 2: Process Methodology



Paraffin wax-based fuels are commonly applied as a cost-effective fuel for lab-scaled hybrid rocket syetems based on their easily availability and optimal reactivity. Based on the thermal energy analysis performed by Valez, et al.,(2015) and Sari, et al.,(2015) the variants of paraffin wax are selected and their thermal properties were studied especially for alkane based wax variants like n-docosane , n-hexacosane , n- triacontane and n-hexatriacontane [8],[9],[15]. Before proceeding to the methodology, it is important to have an overview of some basic properties of the mentioned paraffin wax types.

Table. 1 shows the properties of following paraffin wax variants under specified operating conditions [10-13].

Table 1: Properties of different Paraffin wax variants

Paraffin wax Type	Chemical Formula	Approx.Melting Point (T_p) in(^{0}K)	Critical Temperature T_{cr} in (^{0}K)	Critical Pressure P_{cr} in (MPa)
n-docosane	$C_{22}H_{46}$	317	800	1.116
n-hexacosane	$C_{26}H_{54}$	327	828.3	1.002
n-Triacontane	$C_{30}H_{62}$	330	844	0.994
n-hexatriacontane	$C_{36}H_{74}$	342	849	0.986

The mentioned attributes creates an insightful overview of the reaction of fuels when its reacted with gaseous oxygen.

2.1 Formation of balanced stoichiometric combustion equations

The general combustion equation of alkane when it reacts with oxygen in its gaseous form is given by the below equation [6-15].

$$C_nH_{2n+2\,(s)} + \frac{3n+1}{2} O_{2(g)} \text{---->} (n+1)\, H_2O_{(g)} + nCO_{2(g)} + \qquad (1)$$

It is observed that value of carbon chain number 'n' should be taken as the input in the above equation (1) to balance the carbon, hydrogen and oxygen atoms on both sides of the above chemical reaction. From table.1 we can observe that the 'n' value will be from 22 to 36 based on the no of samples taken. Accordingly, the balanced chemical equations are presented in table 2.for the fuel variants.

Table 2 Balanced stoichiometric equations

Paraffin wax Type	Chemical Formula	Chemical reaction
n-docosane	$C_{22}H_{46}$	$C_{22}H_{46(s)} + \frac{67}{2}O_{2(g)}$---->$22CO_{2(g)} + 23\, H_2O_{(g)}$
n-hexacosane	$C_{26}H_{54}$	$C_{26}H_{54(s)} + 39.5O_{2(g)}$ ------> $26\, CO_{2(g)} + 27H_2O_{(g)}$
n-triacontane	$C_{30}H_{62}$	$C_{30}H_{62(s)} + 45.5O_{2(g)}$ ------> $30\, CO_{2(g)} + 31H_2O_{(g)}$
n-hexatriacontane	$C_{36}H_{74}$	$C_{36}H_{74(s)} + 55O_{2(g)}$ ------> $36\, CO_{2(g)} + 37H_2O_{(g)}$

The combustion results in energy release and combustible products in terms of water vapor and carbon dioxide mixture. The gaseous mixture composition is taken for calculating the magnitude of isentropic specific heat ratio (k) and value of gas constant (R) .

2.2 Deduce the values of k of the combustion products

Specific heat ratio pertained to combustible gases contributes a primary role in the assessing the thermodynamic efficiency of the fuel. It is found that the significant standard value of measurement as per the computational analysis performed by Migliorino, et al.,(2019) is found to be the range from 800-

1000^0K [6]. Accordingly in this study the theroretical calculation for specific heat value for constant pressure is taken for CO_2 and H_2O vapor at the exit [10-13].

2.2.1 Equations used for calculation of specific heat ratio

The following assumptions are made while before performing the theoretical calculations

- The flow is isentropic and the effects of heat transfer and boundary layers are not taken into consideration for ideal calculation.
- The standard temperature is maintained at the exit for 1000^0K, assumimg the material is able to withstand the mentioned operating temperature.
- The multiphase effects of the products not taken into account to minimize the complexity of the calculations; however, the balanced stoichiometric calculations are clearly undertaken to impart accuracy for the work.

The relationship between k and C_p which is specific heat at constant pressure is mentioned as [14], [17-20].

$$C_{p_{mix}} = \frac{k_{mix} R_{mix}}{k_{mix} - 1} \quad ; \text{where } R_{mix} = \frac{8314}{M_{mix}} \text{ J/kg-K} \qquad (2)$$

The above equation represents the thermodynamic constants in terms of exhaust combustion mixture of the paraffin wax products. Where $C_{p_{mix}}$ is the C_p of the mixture (J/kg-K),
k_{mix} is the specific heat ratio and R_{mix} is the gas constant of the mixture (J/kg-K) which is dependent on molar mass of the mixture M_{mix} (g/mol).It is important to note that the expressions can be only be used once the chemical equations are balanced properly on the reactant and product side. [15].
The $C_{p_{mix}}$ is also calculated based on the mole fraction y_i of the combustible products and individual k value for products C_{p_i} performed by Yaws (2014) given as [16].

$$C_{p_{mix}} = \sum_i y_i \, C_{p_i} \qquad (3)$$

on equating (2) and (3) the k_{mix} values can be obtained.

2.3 Transcendental equation in terms of Mach Number using Area Ratio (ε) relation

In nozzle design and performance analysis of rockets, the area ratio plays an important role in assessing the thrust and exit parameters. One such parameter is the exit design Mach number M_e based on the below mathematical expression [2],[17-18],[20]. The suffix 'e' stands for exit in a nozzle.

$$\varepsilon = \frac{1.0}{M_e}\left[\left(\frac{2.0}{k+1}\right) 1 + \frac{{M_e}^2}{2}(k-1)\right]^{\frac{k+1}{2(k-1)}} \qquad (4)$$

From (4) a transcendental non-linear equation can be derived in terms of exit Mach number 'M_e'

$$f(M_e) = \frac{k+1}{k-1}(\varepsilon M_e)^{\frac{2(k-1)}{k+1}} - \left(\frac{2}{k-1}\right) - {M_e}^2 = 0 \qquad (5)$$

The value of k is taken based on the gaseous combustion mixture of the products, there has to be a value for M_e for which it must satisfy the above equation to give $f(M_e) = 0$. The ordinary mathematical techniques will not yield the required solutions, instead numerical methods has been used to solve the non-linear equation with suitable method with minimal iterations.

2.4 Solving the transcendental equation using numerical methods

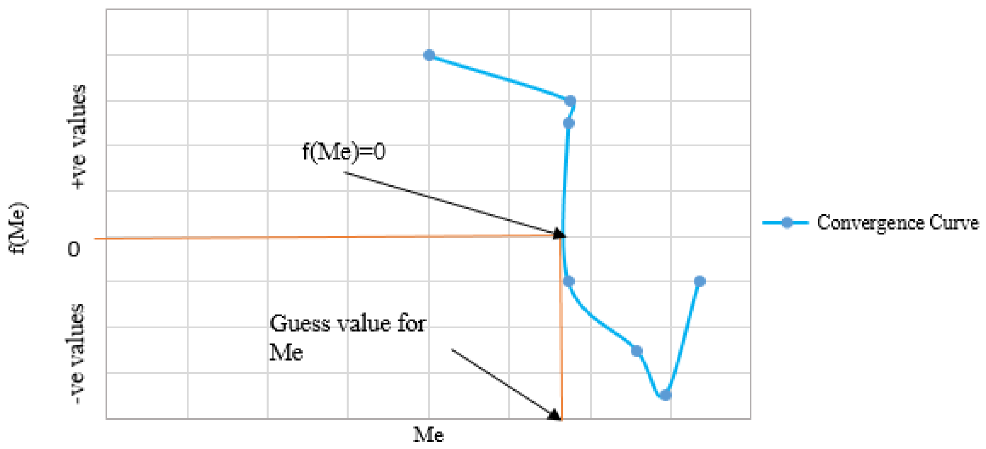
This section mainly focus on the critical concepts of convergence of the function $f(M_e) = 0$ based on the minimal iteration levels . As per published work by Sankara Rao (2021) the methods and explanation has conveniently depicted in his book on 'Numerical Methods for Scientists and Engineers''[21]. In this method the work focus is mainly on the convergence rate of the function within a tolerance of 10^{-12} to have better accuracy for the typical values of M_e.

2.4.1 General Approach of Numerical Methods:

The methods like Bisection, Newton -Raphson and Chebyshev Method has common procedure with different algorithms to solve the function [21]. The common procedures include the following:

- Start with initial guess value with an interval for the root is chosen based on the function's behaviour
- The root is approximated iteratively using specific algorithms based on method used.
- The iteration process continues till the result satisfies a pre-defined convergence criterion say, $|f(M_e)|<$ tolerance (eg :- 10^{-12} to 10^{-9}) or may approaches to '0' as shown in fig. 3.
- The method say $f(M_e)$ assumes function is continuous, differentiable for Newton Raphson and Chebyshev method
- The rate of convergence and efficiency vary among methods depending upon the functions.

Figure 3: A typical convergence curve for f(Me)=0



In this work Chebyshev method is used as the iteration levels are minimum with faster convergence of the function which approaches to a required tolerance value based on the specified initial guess interval $[M_{ea}, M_{eb}]$. Where M_{ea} is the first value and M_{eb} is the second value. Either M_{ea} or M_{eb} is chosen based on the possibility of faster convergence which can yield the required tolerance value for $f(M_e)$. The formula or algorithm for chebyshev method is given below [21].

$$M_{e_{N+1}} = M_{e_N} - \frac{f(M_e)_N}{f'(M_{e\,N})}\left[1 + \frac{f(M_e)_N \;\; f''(M_e)_N}{2[f'(M_e)_N]^2}\right] \qquad (6)$$

Where

- M_{e_N} : Current approximation of the root
- $M_{e_{N+1}}$: Next approximation
- $f(M_e)_N$: Value of the function at M_{e_N}
- $f'(M_e)_N$: First derivative of function at M_{e_N}
- $f'(M_e)_N$: First derivative of function at M_{e_N}

The estimated iteration levels for the mentioned type of similar transcendental function is shown in fig 4. which implies that Chebyshev method is the most suitable method to proceed for the calculation of M_e. This test is performed by taken a sample equation of the following form

Sample equation, $AM_e^j - C - BM_e^2$ (7)

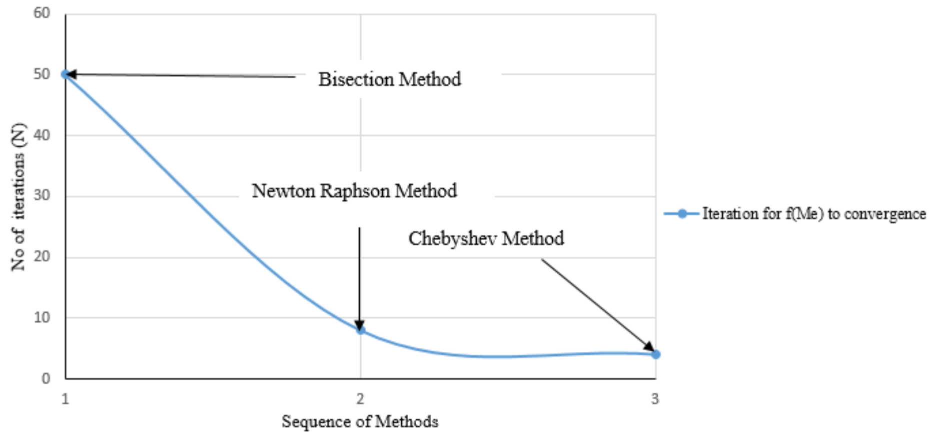
Where A and B are coefficients of M_e; C is a constant based on k value for a typical sample of paraffinwax and j is an exponent which yields a fractional power to M_e as presented in table. 3

Table. 3 Numerical values of coefficients and variables in (7)

A	B	C	j
-1.197	-0.13	-1	0.023

The expression (6) which resembles that of (5), and accordingly the minimal iteration levels are performed using M.s Excel .v2010 spreadsheet to avoid the complexity of manual calculations.

Figure 4: A typical iteration curve for f(Mₑ) sample equation



2.5 Computation of Specific Impulse

As mentioned in section1. Specific impulse is a major attribute in validation and performance assessment of any rocket propulsion unit. It quantifies how effectively a rocket converts propellant into thrust. By definition specific impulse is mathematically expressed as [2],[17],[20].

$$I_{sp} = \frac{C}{g_0} , \quad (8)$$

where C is the effective exhaust gas velocity which is equal to ideal exit velocity (V_e) under $p_e=p_a$ condition. Taking g value as 9.81 m/s^2 . But in practical this value may slightly change depending upon the location of testing and other parameters.

Based on the retrieved Mach values M_e from (6) I_{sp} can be computed as

$$I_{sp} = \frac{\sqrt{kRT_e}}{g_0} \times M_e \qquad (9)$$

The values of k and R are taken for the mixture values of the exhaust burnt products of paraffin wax fuel variants individually.

The exit temperature is calculated based on the initial fix value of chamber temperature $T_c=3400^oK$

With the following relation

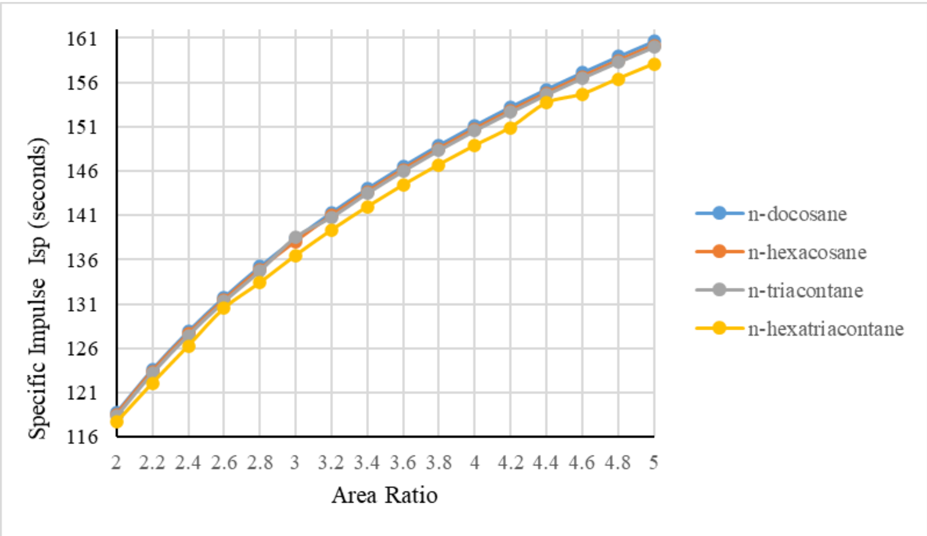
$$T_e = T_c \left(\frac{P_e}{P_c}\right)^{\frac{k-1}{k}}, \qquad (10)$$

where the ratio of $\frac{P_e}{p_c}$ is taken as approx. 0.010132 based on chamber pressure P_c=1.0MPa

3. Results and Discussion

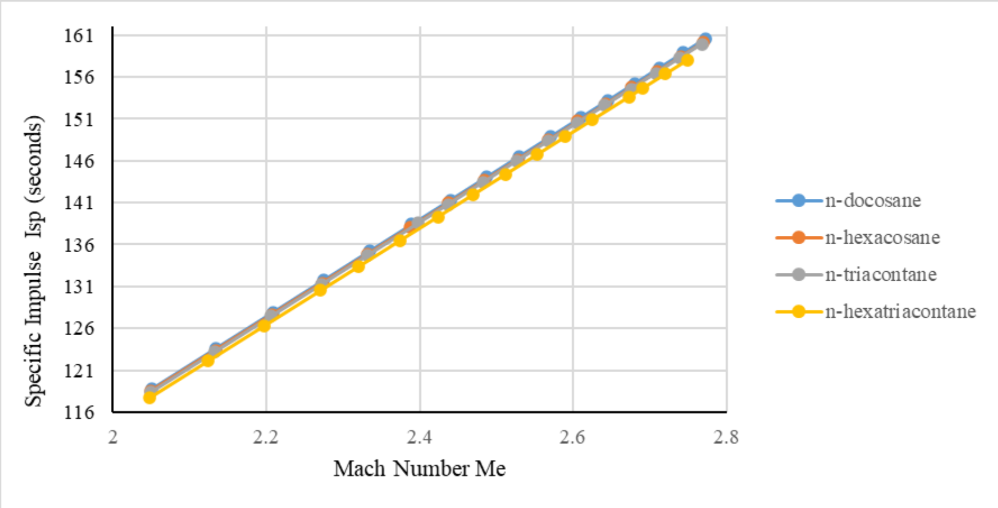
The theoretical computation study reveals that the effect of area ratio plays a major role in increasing the Isp value to a larger extent based on the choice of selection of propellant. The variation is plotted for all the mentioned paraffin waxed fuels as shown in fig.5

Figure 5: Variation of I_{sp} with Area Ratio



The study reveals that the theoretical variation of I_{sp} for M_e under ideal condition for various fuels which is an additionally insight to review the impact of Mach on Specific impulse of the rocket system as shown in fig.6. This is validating the expression (9) theoretically. The increase in Mach number based on the increase in area ratio as shown in fig. 6 which is in accordance with (4) which validates the isentropic flow equation based on area ratio [18],[19].

Figure 6: Variation of I_{sp} with M_e



From fig.5 and fig. 6 it is a quite evident that based on the molecular composition of hydrocarbons the performance values are also varying based upon the selection. The hydrocarbons like n-docosane to n-triacontane having carbon chain numbers 22 upto 30 shows higher performance value lying on the same curve with $C_{22}H_{46}$, whereas higher composition like n-hexatriacontane having ‘n’ value 36 yield slightly lesser value because the combustion requires more heat as for longer chains, the increasing molecular weight and physical limitations start to offset the benefits, leading to slightly lower performance values. Also, the increase in molecular mass or molar mass also significantly affects the values of specific heat ratio ‘k’ as shown in fig.7. The drop in the specific heat ratio for heavier fuels is rooted in the fundamental molecular properties of the combustion products and the way energy is distributed among their degrees of freedom which validates the studies performed by McAllister et al.,(2011) [14].

Figure 7: Variation of k with Molar mass of exhaust Products

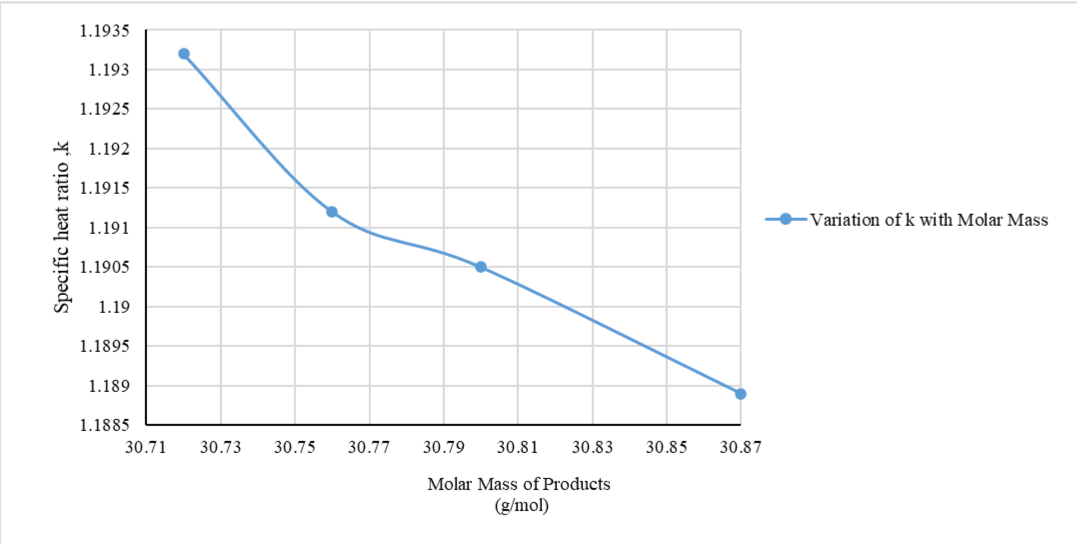


Table 4: Values of computed ideal Isp range for paraffin fuel types

Paraffin wax fuel	Area ratio (ε) range	Isp (seconds)
n-docosane	2.0 to 5.0	118.76 to 160.76
n-hexacosane	2.0 to 5.0	118.56 to 160.14
n-triacontane	2.0 to 5.0	118.3 to 160.01
n-hexatriacontane	2.0 to 5.0	117.7 to 158.04

Based on the theoretical computation the ideal Specific impulse range values are obtained as is depicted in table.4. The data highlights the relationship between the Specific impulse (Isp) and the paraffin wax fuel type across an area ratio of 2.0 to 5.0. The decrease in Isp with increasing molecular mass is due to the heavier molecular structure of the fuels.

4. Conclusion

This theoretical analysis highlights the suitability and selection of of pure paraffin wax fuels for hybrid rockets, with shorter-chain hydrocarbons like n-docosane ($C_{22}H_{46}$) showing higher specific impulse. When specific impulse needs to be maximized for any application, higher-volatility and shorter-chain-carbon-number fuels are superior. These characteristics make them particularly attractive for hybrid rocket propulsion systems when high performance is desired. Practical values may vary due to fuel density, oxidizer-to-fuel ratio, and environmental conditions. In real time experimental validation is essential to refine these insights for real-world applications

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