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# Screening of metal additives in ABS polymer fuel for enhanced performance in hybrid rocket motors: A computational analysis using CEA

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## ABSTRACT

This study investigates the potential of metal additives in acrylonitrile butadiene styrene (ABS) polymer fuel to enhance hybrid rocket motor (HRM) performance through computational analysis, Chemical Equilibrium with Applications (CEA), software. ABS was selected as the base fuel due to its thermoplastic nature, which allows for the creation of complex fuel geometries through 3D printing, offering significant flexibility in fuel design. Hybrid rockets, which combine a solid fuel with a liquid oxidiser, offer advantages in terms of operational simplicity and safety. However, conventional polymer fuels often exhibit low regression rates and suboptimal combustion efficiencies. In this research, we evaluated a range of metal additives—aluminium (Al), boron (B), nickel (Ni), copper (Cu), and iron (Fe)—at chamber pressures ranging from 1 to 30 bar and oxidiser-to-fuel (O/F) ratios between 1.1 and 12, resulting in 1800 unique test conditions. The main performance parameters used to assess each formulation were characteristic velocity ($C^*$) and adiabatic flame temperature. The results revealed that each test produced a different optimum O/F ratio, with most ratios falling between 4 and 6. The highest performance was achieved at a chamber pressure of 30 bar across all formulations. Among the additives, Al and B demonstrated significant potential for improved combustion performance with increasing metal loadings. In contrast, Fe, Cu, and Ni reached optimal performance at a minimum loading of 1%. Future work includes investigating B-Al metal composites as additives into the ABS base polymer fuel, and doing experimental validation tests where the metallised ABS polymer fuel is 3D printed.

## 1. Introduction

Hybrid rocket motors (HRMs) are an innovative approach to aerospace propulsion, integrating the advantages of solid fuels and liquid oxidizers to generate thrust [1]. Due to the distinct physical states of the fuel and oxidiser, hybrid rockets are relatively safe and are less expensive to fabricate [2]. It is because of these advantages that hybrid rockets are the obvious choice for suborbital flight missions [3]. The large-scale application of hybrid rockets are inhibited because of the low regression rates due to the boundary layer combustion mechanism [4]. Research to overcome this issue has been reported in literature where the HRM fuels are fabricated into sophisticated port geometries with the aim of increasing the surface area of contact with the gaseous oxidiser [5].

The operational principle of HRMs involves the injection of a liquid oxidizer into a combustion chamber, where it interacts with the solid fuel, facilitating combustion and enabling precise control over thrust levels by adjusting the oxidizer flow rate. This versatility, combined with their mechanical simplicity, enhances safety and reliability compared to traditional solid and liquid rocket systems.

Despite their advantages, HRMs face challenges primarily related to the choice of solid fuel. Hydroxyl-Terminated Polybutadiene (HTPB) has been widely used in hybrid systems due to its favourable mechanical properties; however, its thermosetting nature limits its reprocessing capabilities, making it unsuitable for

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advanced manufacturing techniques like 3D printing [6]. In contrast, Acrylonitrile Butadiene Styrene (ABS), presents a compelling polymer fuel alternative as a thermoplastic material that allows for the creation of complex geometries through 3D printing [7]. This property not only enhances design flexibility but also enables optimization of fuel formulations to improve performance characteristics. The performance of rocket motors is typically evaluated using key parameters such as characteristic velocity ($C$*) and specific impulse ($I_{sp}$) [5]. $C$* measures how effectively the propulsion system converts propellant energy into thrust, and is defined as [8]:

$$C^* = \frac{P_c A_t}{\dot{m} R T_c} \tag{1}$$

where $P_c$ is the chamber pressure, $A_t$ is the throat area, $\dot{m}$ is the mass flow rate of the propellant, $R$ is the specific gas constant, and $T_c$ is the chamber temperature. $I_{sp}$ is a crucial performance metric in rocket propulsion, defined as the thrust produced per unit weight flow rate of the propellant. It is typically expressed in seconds and indicates how effectively a rocket uses its propellant to generate thrust. A higher $I_{sp}$ signifies a more efficient propulsion system, as it reflects the ability to produce greater thrust from a given amount of propellant [9]. Mathematically, $I_{sp}$ can be expressed as [8]:

$$I_{sp} = \frac{C^*}{g_0} \tag{2}$$

where $g_0$ is the acceleration due to gravity. This relationship implies that improvements in $C^*$ directly enhance $I_{sp}$ which justifies why in this work, $C^*$ was the main performance parameter that was investigated on the National Aeronautics and Space Administration (NASA) Chemical Equilibrium with Applications (CEA) software, as an increase $C^*$ in typically indicates enhanced combustion efficiency, which can lead to higher fuel consumption rates and thus a greater regression rate. The CEA software is a tool used for analysing combustion processes in rocket propulsion systems by calculating the thermodynamic properties of combustion products based on chemical equilibrium principles. It allows engineers and scientists to simulate various fuel compositions, oxidizer types, and operating conditions to predict performance metrics [10].

This study has explored the effect of adding metal additives in varying concentrations to the ABS polymer fuel on the rocket performance. In hybrid rocket systems, metal additives can significantly improve thermal efficiency and combustion characteristics [11]. Each of the five metal additives evaluated—aluminium (Al), boron (B), nickel (Ni), copper (Cu), and iron (Fe)—has unique properties that contribute to enhanced performance. Al is known for its high energy content and exothermic reaction during combustion, studies have shown that incorporating Al can improve specific impulse by enhancing the oxidation process and reducing unburned residues in the exhaust [11,12]. B is another high-energy additive that can significantly increase combustion efficiency. Its combustion produces boron oxide, which contributes additional energy to the reaction. Boron's ability to burn at high temperatures allows for better thermal management within the combustion chamber [11,13–15]. Ni acts as a catalyst in certain combustion reactions, promoting more complete oxidation of fuel components. This catalytic effect can enhance thermal efficiency by reducing the activation energy required for combustion reactions [16,17]. Cu can improve thermal conductivity within the propellant matrix, leading to better heat distribution during combustion. This property helps maintain optimal combustion temperatures and enhances overall combustion efficiency [18,19]. Fe serves primarily as a fuel enhancer by facilitating more efficient oxidation reactions during combustion. Its presence can lead to higher flame temperatures and improved regression rates of solid fuels [20,21].

The aim of this study is to evaluate the effects of these five metal additives—Al, B, Ni, Cu, and Fe—on the performance of ABS polymer fuel in hybrid rocket motors. By systematically analysing how these additives influence combustion efficiency and specific impulse, the research seeks to identify optimal formulations that enhance the overall performance of ABS-based fuels. This investigation is particularly relevant given the need for improved combustion characteristics in hybrid rocket systems, which often struggle with low regression rates and suboptimal efficiencies.

Through computational analysis using the NASA CEA software, the study will assess a range of chamber pressures and oxidizer-to-fuel ratios to determine how each metal additive affects key performance metrics, particularly, $C$*. The comprehensive evaluation across 1800 unique test conditions aims to establish a clear understanding of how varying concentrations of these additives can lead to enhanced combustion performance. This knowledge is essential for optimizing fuel formulations that maximize thrust and efficiency in hybrid propulsion systems.

**Table 1**
Benchmark fuel candidate NASA CEA optimum performance parameters (at 30 bar and 5 O/F).

| Fuel Parameter | HTPB/$N_2O$ | ABS/$N_2O$ |
|---|---|---|
| Characteristic Velocity/($m \cdot s^{-1}$) | 1628.3 | 1606.4 |
| Temperature/K | 3144.1 | 2963.6 |

## 2. Methodology

### 2.1. Materials and preparation of ABS polymer fuel

ABS is a terpolymer synthesized through the polymerization of acrylonitrile, styrene, and polybutadiene, represented by the chemical formula:

$$(C_8H_8)_x(C_4H_6)_y(C_3H_3N)_z \tag{3}$$

where $x$, $y$, and $z$ denote the molar fractions of each ABS constituent. For this study, ABS was sourced from Advanced Polymers, featuring a specific molar composition of 0.355623 for acrylonitrile, 0.434954 for styrene, and 0.209423 for butadiene [22]. The reduced formula utilized in the NASA CEA software was calculated as follows:

$$\begin{aligned} &0.355623(C_3H_3N) + 0.434954(C_8H_8) + 0.209423(C_4H_6) \\ &= C_{5.3842}H_{5.803}N_{0.3556} \end{aligned} \tag{4}$$

Similarly, using the group addition method and applying these specific molar compositions, the enthalpy of formation for the ABS polymer was determined to be 68.7648 kJ/(g·mol).

### 2.2. Metal additives and fuel composition

The study investigated five metal additives: Al, B, Ni, Cu, and Fe. Each metal was analyzed at varying loadings of 1.00%, 2.50%, 5.00%, 10.0%, and 20.0% by weight relative to the ABS polymer fuel, ensuring that the total composition of the fuel remained at 100%. The oxidiser used was nitrous oxide ($N_2O$), which was maintained as the only constituent of the oxidiser (100%) throughout all tests.

### 2.3. CEA tests setup and results recording

The experimental design included varying the oxidizer-to-fuel (O/F) ratios at values of 1.1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, and 12 for

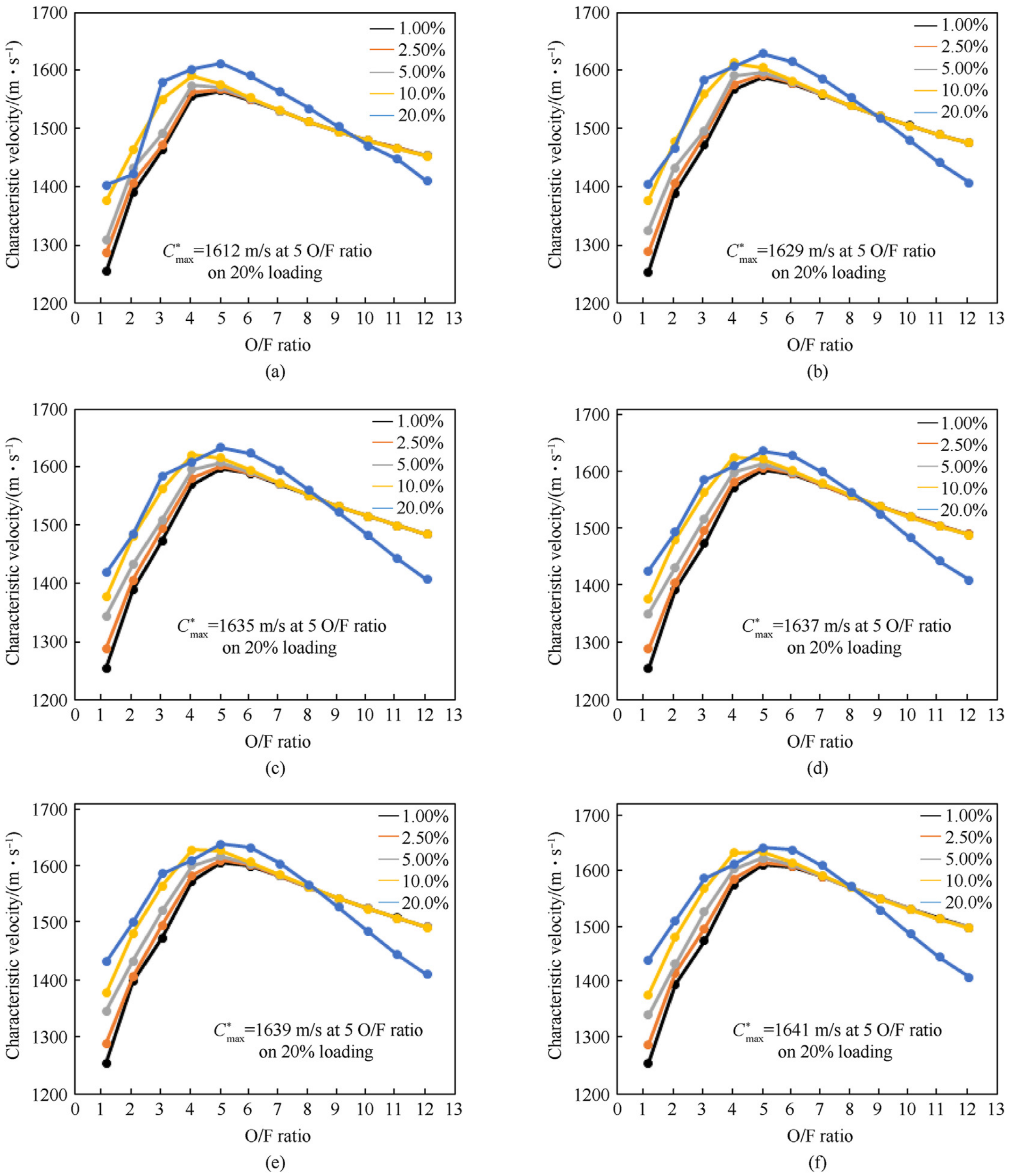


**Fig. 1.** The effect of O/F ratio on the characteristic velocity for different aluminium loading on the ABS base polymer fuel with varying chamber pressures: (a) 1 bar; (b) 5 bar; (c) 10 bar; (d) 15 bar; (e) 20 bar; (f) 30 bar.

each fuel composition while conducting tests at chamber pressures of 1, 5, 10, 15, 20, and 30 bar under each O/F ratio. This comprehensive approach resulted in a total of 1800 unique test cases, focusing specifically on investigating $C^*$ as a performance metric in each scenario. The $C^*$ recorded was of the equilibrium output and not the frozen conditions.

## 3. Results

The NASA Chemical Equilibrium with Applications (CEA) results provide valuable insights into the thermodynamic performance of rocket propellants by simulating combustion processes under various conditions. Observing how the characteristic velocity ($C^*$) responds to different chemical formulations and operating conditions is particularly relevant because it serves as a key indicator of the propellant's combustion efficiency and overall effectiveness in converting chemical energy into thrust. $C^*$ reflects the maximum achievable velocity of exhaust gases exiting the combustion chamber, which directly correlates to the thrust produced by the rocket engine. The peak $C^*$ benchmark for this study is pure HTPB $C^*$ studied at same conditions in NASA CEA, 1628 m/s which agrees with 1625 m/s reported in literature [8]. NASA CEA computed peak $C^*$ value for pure ABS, 1607 m/s, became the starting value that all the metal additives were meant to improve in order to match and possibly supersede the HTPB $C^*$. The benchmark fuels candidates, which are frequently referenced in this results section are summarised in Table 1. These results are obtained at optimum conditions studied, i.e. at 30 bar and O/F ratio of approximately 5.

The analysis of the $C^*$ data obtained in this study reveals that for the metallised-propellants, the curves exhibit a consistent shape across different metal loadings (1%, 2.5%, 5%, 10%, and 20%) at pressures ranging from 1 bar to 30 bar. All curves demonstrate an

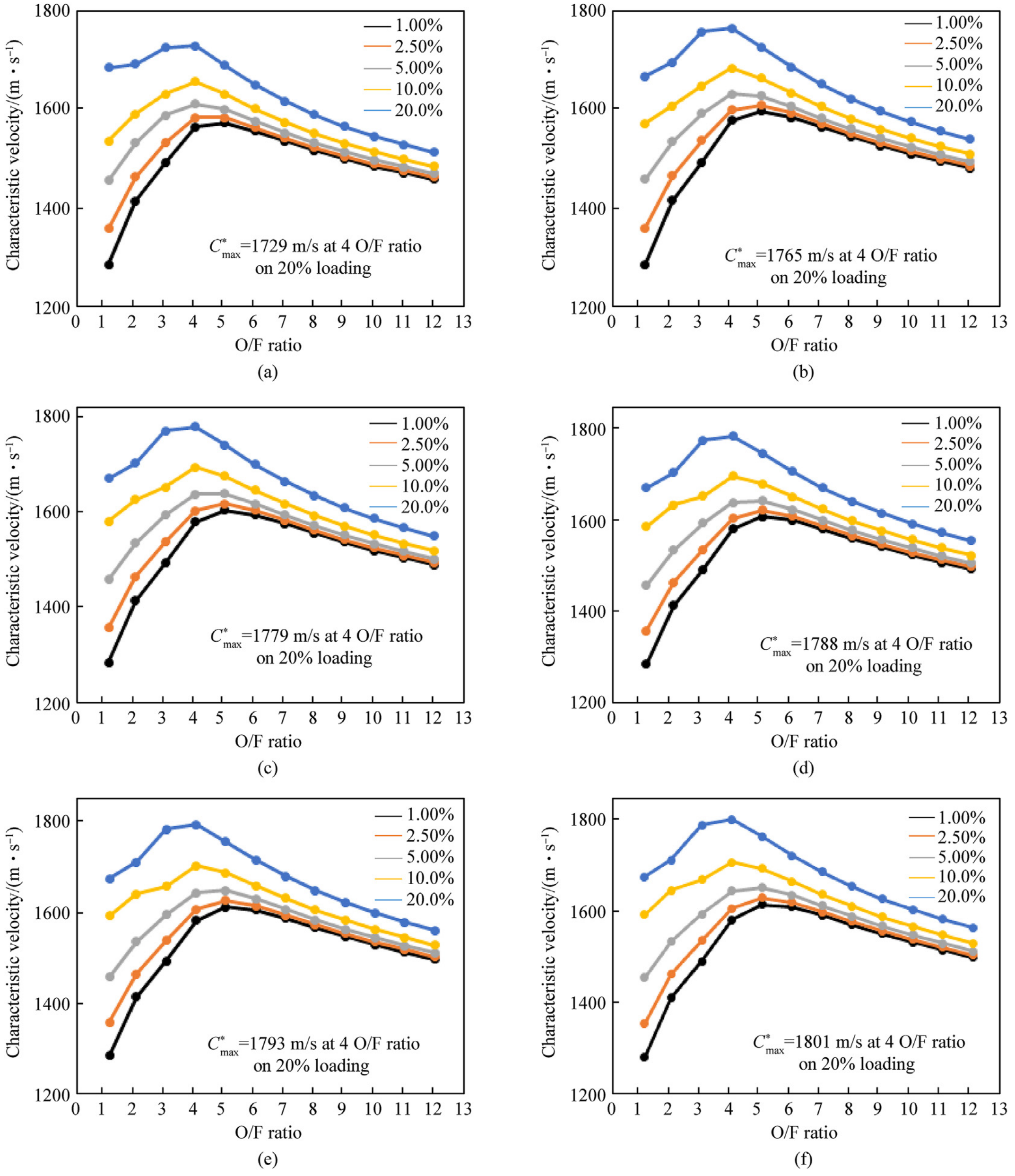


**Fig. 2.** The effect of O/F ratio on the characteristic velocity for different boron loading on the ABS base polymer fuel with varying chamber pressures: (a) 1 bar; (b) 5 bar; (c) 10 bar; (d) 15 bar; (e) 20 bar; (f) 30 bar.

initial increase in $C$* from the starting O/F ratio of 1.1 to a peak at between 4 and 6, after which a decline is observed.

The analysis of the NASA CEA results for aluminium-loaded ABS polymer fuels (Fig. 1) reveals significant insights into their combustion characteristics. The relationship between the oxidizer-to-fuel (O/F) ratio and characteristic velocity ($C$*) indicates that peak performance occurs at an O/F ratio of 5 for 20% aluminium loading, while lower loadings reach their peak at O/F ratio of either 4 or 5 with no clear trend observed across the studied pressures. Characteristic velocities across the examined pressures range from 1612 m/s to 1641 m/s, surpassing the non-metallised ABS $C$* of 1607 m/s and aligning closely with HTPB's $C$* of 1628 m/s. This suggests that the addition of aluminium enhances the combustion efficiency of ABS, making it a competitive option compared to traditional propellants like HTPB.

The analysis of the NASA CEA results for boron-loaded ABS polymer fuels (Fig. 2) reveals that optimum performance occurs at an O/F ratio of 4 for boron loadings of 5%, 10%, and 20%, while a peak is reached at an O/F ratio of 5 for lower loadings of 1% and 2.5%. Notably, the highest $C$* is consistently achieved at the 20% loading across all pressure groups, with values ranging from 1729 m/s to 1801 m/s. These results indicate that the incorporation of boron significantly enhances the combustion efficiency of ABS, providing superior performance compared to non-metallised ABS, which has a $C$* of 1607 m/s and that of the traditional propellant, HTPB, which has a $C$* of 1628 m/s.

The relationship between the oxidizer-to-fuel (O/F) ratio and characteristic velocity ($C$*) for iron (Fig. 3) indicates that peak performance occurs at an O/F ratio of 5 for loadings of 1%–10%, while a peak is reached at an O/F ratio of 4 for the 20% loading. Notably, the highest characteristic velocities are consistently achieved at the 1% loading across all pressure groups, with values

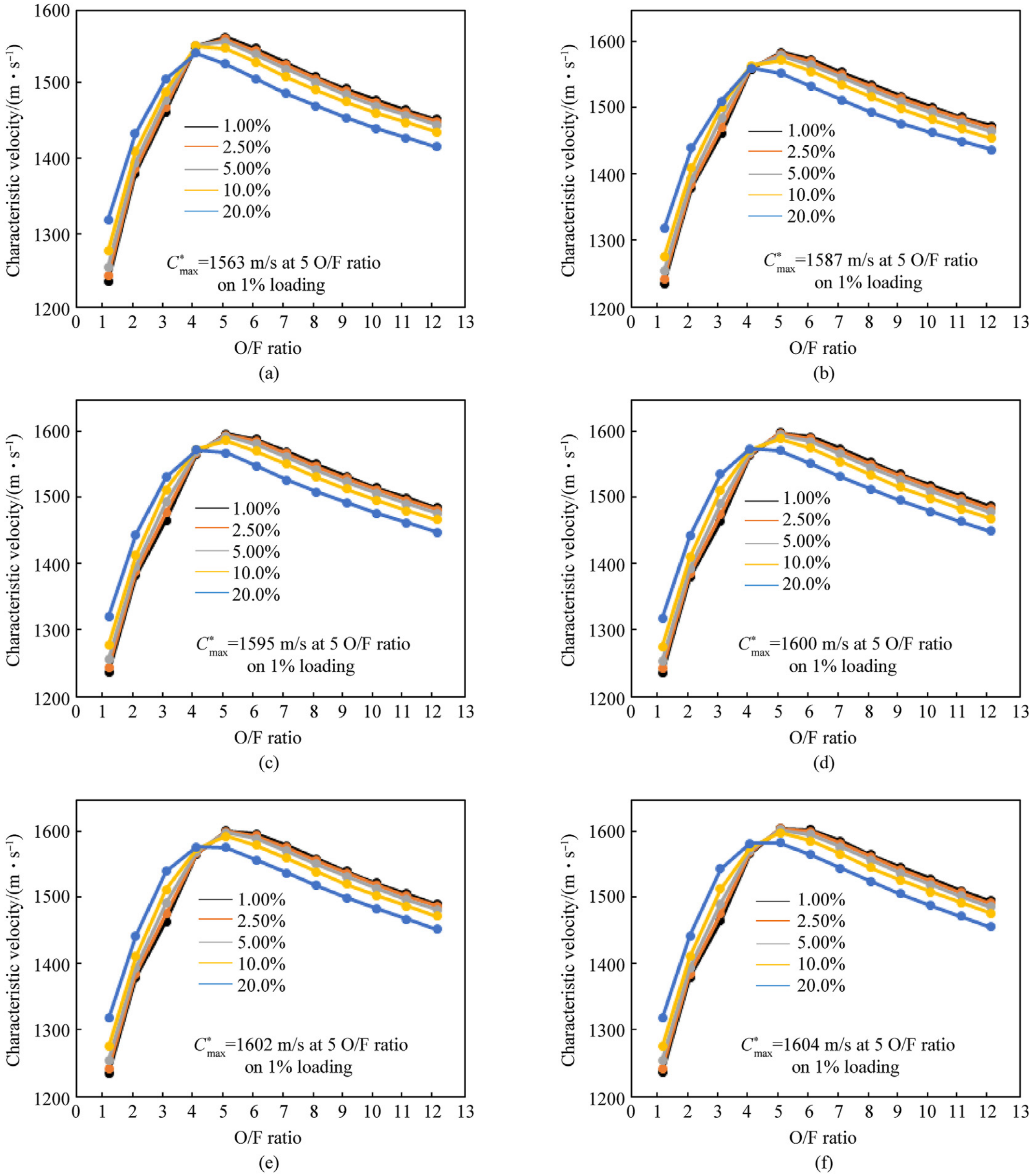


**Fig. 3.** The effect of O/F ratio on the characteristic velocity for different iron loading on the ABS base polymer fuel with varying chamber pressures: (a) 1 bar; (b) 5 bar; (c) 10 bar; (d) 15 bar; (e) 20 bar; (f) 30 bar.

ranging from 1563 m/s to 1604 m/s. This suggests that the addition of iron does not yield a desirable improvement in combustion performance, as the ABS polymer fuel without any iron loading achieves a peak *C** of 1607 m/s, which is inferior compared to that of HTPB, which has a *C** of 1628 m/s.

Similar to Iron, the relationship between the oxidizer-to-fuel (O/F) ratio and characteristic velocity (*C**) for Copper (Fig. 4) indicates that peak performance occurs at an O/F ratio of 5 for loadings of 1%–10%, while a peak is reached at an O/F ratio of 4 for the 20% loading. Notably, the highest characteristic velocities are consistently achieved at the 1% loading across all pressure groups, with values ranging from 1563 m/s to 1604 m/s. This suggests that the addition of copper also seems to not have a desirable output on the combustion performance because at no iron loading the ABS polymer fuel has a peak *C** of 1607 m/s which is inferior compared to that of HTPB, 1628 m/s.

Similar to Iron and Copper, the relationship between the oxidizer-to-fuel (O/F) ratio and characteristic velocity (*C**) for Nickel (Fig. 5) indicates that peak performance occurs at an O/F ratio of 5 for loadings of 1%–10%, while a peak is reached at an O/F ratio of 4 for the 20% loading. Notably, the highest characteristic velocities are consistently achieved at the 1% loading across all pressure groups, with values ranging from 1563 m/s to 1604 m/s. This suggests that the addition of copper also seems to not have a desirable output on the combustion performance because at no iron loading the ABS polymer fuel has a peak *C** of 1607 m/s which is inferior compared to that of HTPB, 1628 m/s.

A hypothesis can be posited that the enhanced performance of boron, followed by aluminium, in ABS fuel is primarily due to their respective energy contributions and combustion characteristics. In contrast, copper, nickel, and iron demonstrate comparable behaviours owing to their lower reactivity and minimal influence on overall energy output during combustion. Previous studies have corroborated these findings, indicating that certain metal additives

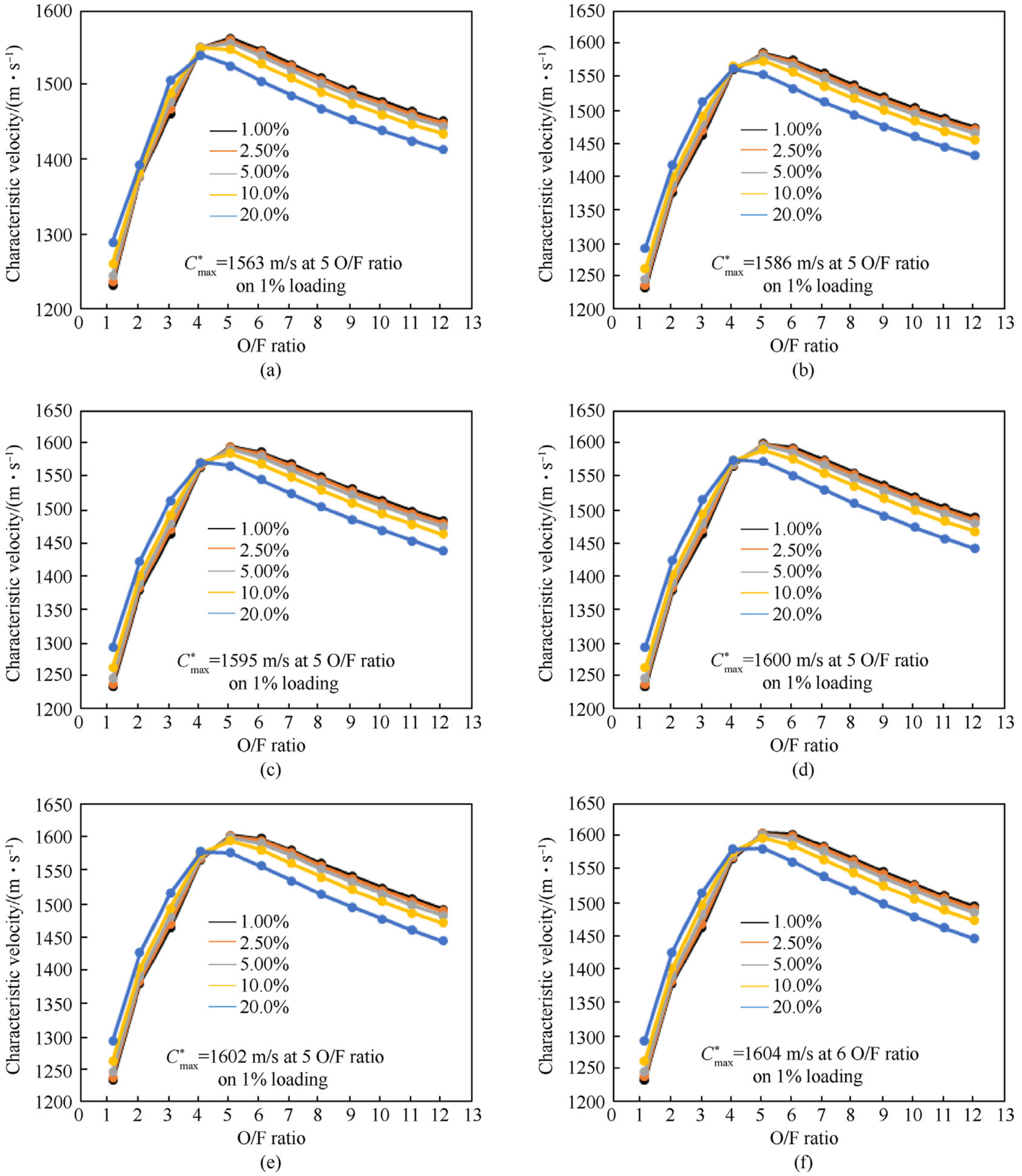


**Fig. 4.** The effect of O/F ratio on the characteristic velocity for different copper loading on the ABS base polymer fuel with varying chamber pressures: (a) 1 bar; (b) 5 bar; (c) 10 bar; (d) 15 bar; (e) 20 bar; (f) 30 bar.

do not yield significant improvements in fuel performance [23]. This analysis remains theoretical, necessitating further research to fully understand these behaviours.

Fig. 6 presents a bar graph comparing the average characteristic velocity ($C$*) of various metal-loaded ABS formulations at three pressure levels: 1 bar, 15 bar, and 30 bar, with calculations based on O/F ratios of 4, 5, and 6. The data indicate that $C$* consistently increases with rising pressure across all formulations, highlighting the influence of pressure on combustion performance. Notably, nickel, copper, and iron exhibit similar performance characteristics at both high and low metal loadings; however, all three metals perform inferiorly compared to non-metal-loaded ABS.

In contrast, the inclusion of aluminum at lower loadings significantly enhances performance, bringing $C$* values closer to those of HTPB. Boron, even at the lowest studied loading, emerges as the most effective metal additive. At 20% loading, nickel, copper, and iron show worsened combustion performance, while aluminum slightly surpasses HTPB, and boron demonstrates significantly improved performance compared to HTPB. This suggests that further enhancements could be achieved by optimizing the concentrations of aluminum and boron within the ABS matrix.

However, it is crucial to consider the rheological properties of the thermoplastic during this optimization process. As metal loading increases, maintaining the printability of ABS becomes essential to prevent brittleness and ensure successful 3D printing applications. Balancing performance gains with processing characteristics will be key in developing high-efficiency metal-loaded ABS fuels suitable for advanced propulsion systems.

Fig. 7 illustrates the adiabatic flame temperatures for various metal additives at a 1% loading across different pressure groups. The results indicate that the flame temperatures are relatively comparable for all metals examined and remain below the

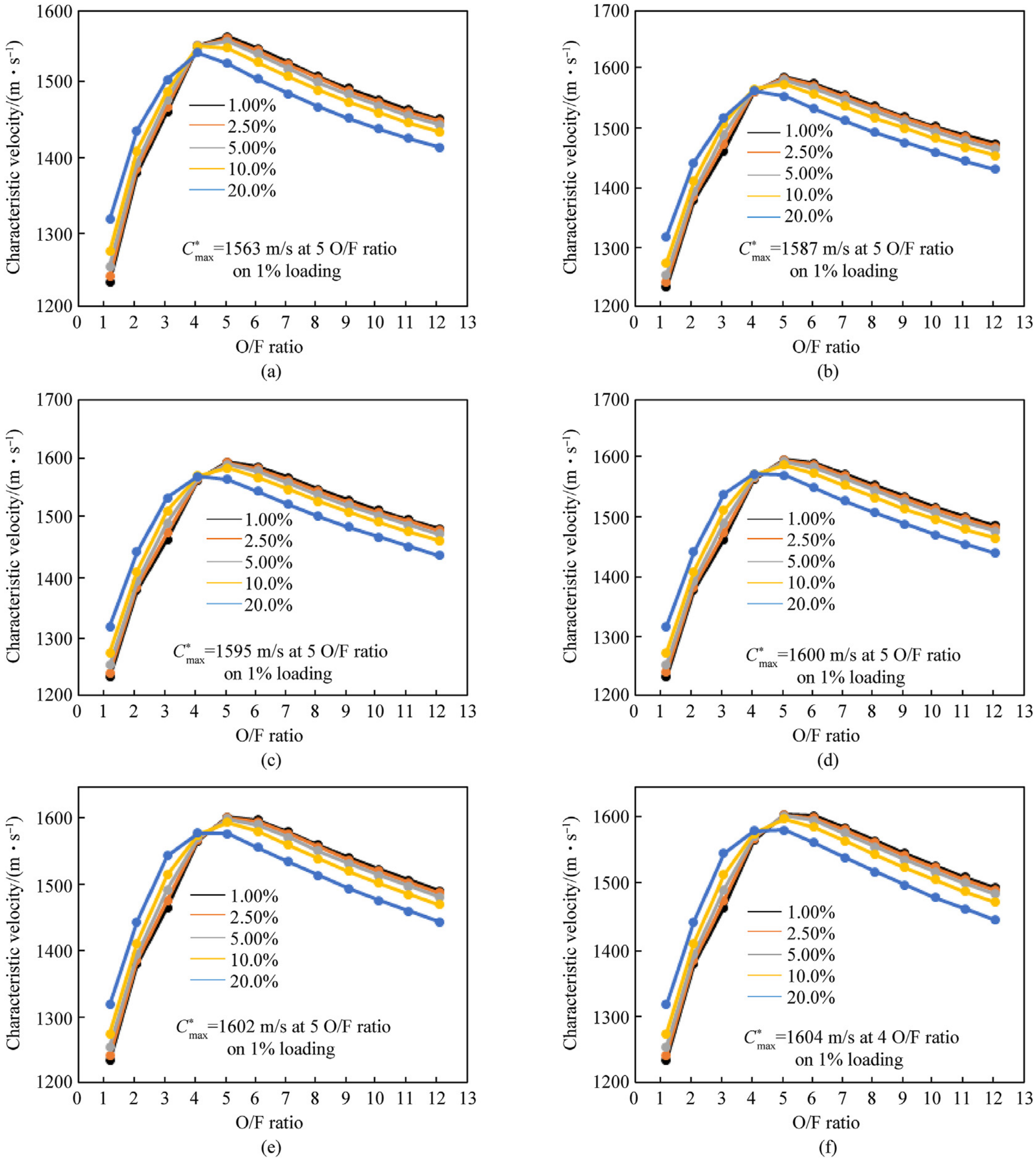


**Fig. 5.** The effect of O/F ratio on the characteristic velocity for different nickel loading on the ABS base polymer fuel with varying chamber pressures: (a) 1 bar; (b) 5 bar; (c) 10 bar; (d) 15 bar; (e) 20 bar; (f) 30 bar.

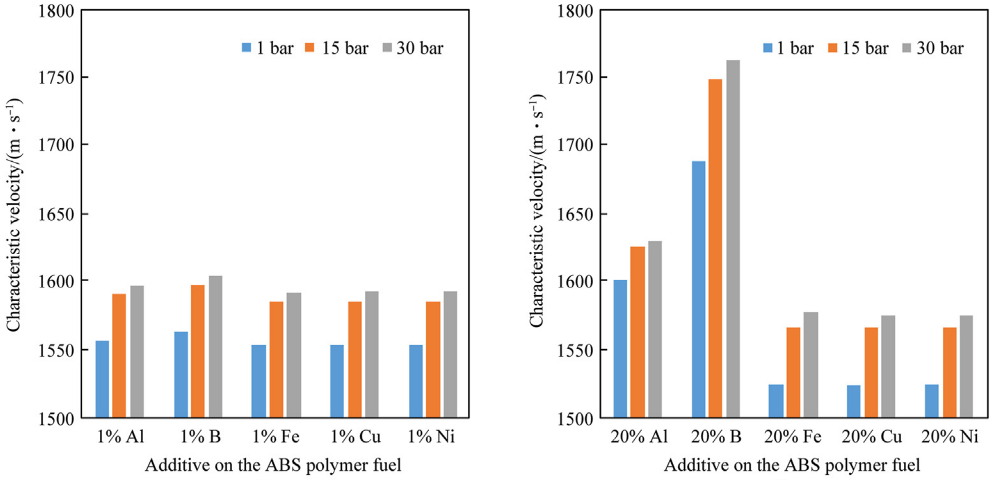
recommended operating temperature of hybrid rocket motors, which is approximately 3300 K. This observation underscores the importance of investigating and controlling thermal effects within hybrid rocket motors to ensure that the materials used can withstand the high temperatures generated during combustion.

At a 20% metal loading, significant differences emerge in the adiabatic flame temperatures among the additives. Nickel, copper, and iron demonstrate minimal increases in flame temperature, suggesting that their incorporation at this higher loading does not substantially enhance combustion efficiency. In contrast, both boron and aluminium exhibit significant increases in adiabatic flame temperatures, indicating their superior performance as metal additives. This enhancement in thermal output correlates with improved combustion characteristics and overall performance.

However, it is crucial to recognize that while increasing metal loading can enhance performance, it may also lead to structural compromises within the motor. Higher temperatures can exacerbate thermal stresses and potentially exceed the yield strength of the fuel grain, which could result in material failure during operation. Therefore, a careful balance must be maintained between optimizing metal loading for performance gains and ensuring the structural integrity of the hybrid rocket motor. Continuous monitoring of these parameters is essential to develop safe and efficient propulsion systems that maximize performance without compromising reliability.

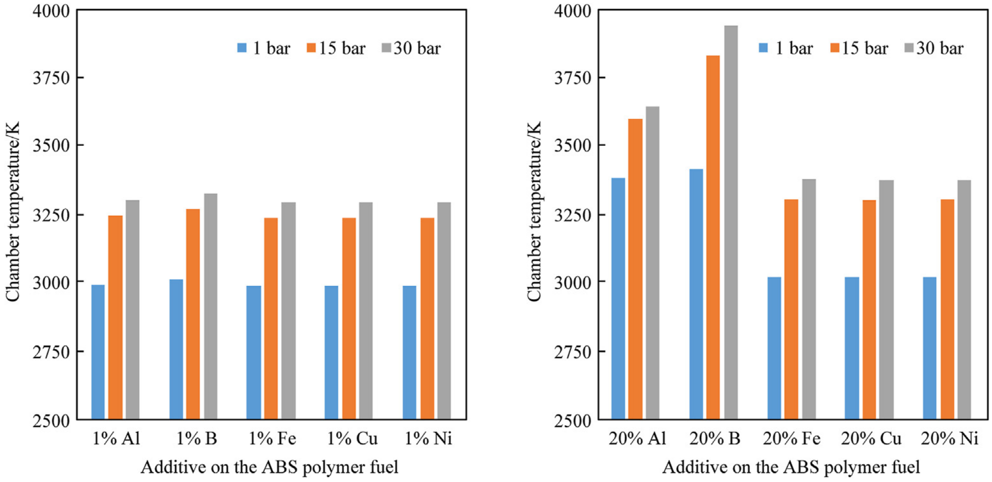
## 4. Conclusions

In conclusion, this study has significantly narrowed the scope of new material formulations for hybrid rocket fuels by theoretically analysing 1800 different combinations. This comprehensive approach allowed us to identify promising candidates for novel fuel development, with each formulation exhibiting an optimal oxidizer-to-fuel (O/F) ratio typically falling between 4 and 6, with 5



(a) (b)

**Fig. 6.** Characteristic velocity ($C$*) of the different fuel formulations (a) at 1% metal loading; (b) at 20% metal loading at 1 bar, 15 bar, and 30 bar.



(a) (b)

**Fig. 7.** Chamber Temperatures of the different fuel formulations (a) at 1% metal loading; (b) at 20% metal loading at 1 bar, 15 bar, and 30 bar.

being the most prevalent. The results indicate that increasing pressure consistently leads to enhanced characteristic velocity ($C$*), underscoring the importance of pressure in improving combustion performance. However, it is crucial to consider structural integrity when operating at high pressures, as this can introduce significant mechanical stresses on the rocket motor.

Moreover, while higher metal loading generally improved performance, careful attention must be paid to the printability of the thermoplastic material to avoid print failures during manufacturing. The increase in metal loading also resulted in elevated combustion temperatures, particularly with boron and aluminium, which, while beneficial for performance, raises concerns about compromising the structural integrity of the motor. This necessitates design complexities such as enhanced cooling systems and reinforcements to ensure safe operation.

As this work is part of an ongoing study, computational fluid dynamics (CFD) simulations are being employed to theoretically validate these findings and to explore effect of various port geometries on the combustion of these fuels aimed at further improving performance. The CFD analysis will provide valuable insights into the behaviour of Fe, Ni, and Cu, which appear to have minimal to no contribution to the combustion performance of ABS fuel, in contrast to Al and B. These findings will be further validated through laboratory experiments and live firing tests conducted on a hybrid rocket motor test stand. To address mechanical concerns associated with increased temperatures and mechanical stresses exerted by the solid fuel on the rocket motor, graphene will be incorporated into the polymer matrix for added reinforcement. Additionally, investigating these metal additives at the nanoscale with the hope of using less solids loading for an improved combustion performance will be explored in the live rocket motor test to further validate and refine our results. This multifaceted approach aims not only to enhance propulsion efficiency but also to ensure the safety and reliability of advanced hybrid rocket systems.

## CRediT authorship contribution statement

**Gail Ndlovu:** Writing – review & editing, Writing – original draft, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Bilainu Oboirien:** Supervision. **Patrick Ndungu:** Supervision.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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