(RESEARCH ARTICLE)

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# Modelling of the formulated solid rocket propellant characteristics

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## Abstract

This study is a mathematical model to obtain the characteristics performance of magnesium metal (powder) and carbon on a potassium nitrate-sucrose (KNSU) solid propellant formulation. Characterization of propellant is, as a general rule, important to determine its performance before it can be suitable for use for a rocket flight or any mission. Method of ballistic load cell evaluation was used to validate results and a mathematical model using the combustion exhaust products was solved to obtain the characteristics performance parameters of the propellant.  The carbon constituent which acts as an opacifier and coolant was kept constant at 2% in order to arrest some of the heat during the combustion process and helped to lower the combustion temperature, because high combustion temperature could lead to combustion chamber rupture or failure. The effect of addition of magnesium which was optimized for 3% in the formulation contributed significantly in improving the overall performance of the propellant. The utilization of magnesium in KNSU propellant provided higher values parameters and better performance compared to when not included. This was confirmed with the model equations. The propellant combustion products equation was used to model and obtain the characteristics performance parameters. This gave propellant specific impulse (122.9s), combustion temperature (1821K), heat ratio (1.1592), molecular weight (36.89g/mole), propellant density (1912.5kg/m3) and characteristics velocity (1000m/s) result while maintaining the same chamber pressure.

## 1. Introduction

All Solid Rocket Motors have the same form of principle but there is universal design method to utilize for design of various subsystems of Solid Rocket Motors such as the propellant. For example, approach to propellant to be formulated may vary with mission scenario, background experience and class of application.

For applications of rocket either for unguided military mission for upper atmosphere or any launch vehicle for space missions, the optimum Solid Rocket Motors design has to satisfy optimum total impulse, an optimum thrust-time profile, an optimum nozzle configuration an optimum chamber pressure and a preferred solid propellant grain configuration [1,2]

Classification of propellants in respect of the physical state of the fuel and oxidizer constituents of the propellant are solid propellants, liquid propellants and hybrid propellants [3]. Solid propellants have been the commonly used due to reliability, cost effective and simple to design [4,5]. Different formulations of various combinations of chemical constituents would give propellants of different physical and chemical properties, as well as combustion characteristics and performance [4,5].

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The preferable use of Solid Chemical propellant (SCP) by many designers and manufacturers in different forms of rockets are due mainly to the advantageous area over the others chemical propellants with respect to simplicity of production, cost effectiveness, and dependable in terms of storage time and performance chemical potential energy [6].

The selection of propellant is usually carried out at the early stage of Solid Rocket Motors design based on the performance of the rocket and the available knowledge of the designer and manufacturer. It is therefore important to explore propellants of better performance characteristics with less mass (weight) to hit higher attitudes.[2,7,8]

The specific impulse, burning rate, temperature sensitivity, density and specific heat ratio are propellant properties that represent independent design variables [9]

Researchers have been working extensively to obtain the optimal design for a rocket vehicle that would achieve the safety, operability, reliability, performance and cost objectives of a rocket [10]

One of the main objectives in many rocket optimisation is minimizing the gross lift off mass/weight [11,12,13,14,15,16]

Traditionally the total vehicle mass (inert mass and propellant mass) are seen as a primary driver towards the final vehicle cost, as cost is always an essential factor developing the rocket based vehicle [1]

Many researchers have been working over the years to improve and develop new propellant formulations significantly to meet the need of the type reaching targets and missions with less weight [4,5] and propellant mass fraction can be sometimes be up to 70-90% of the rocket total mass, then improving and developing new propellant formulations to meet this need is therefore very significant)[12,14,17]

The aim of this work is to improve the performance of a KNSU rocket propellant fuel using magnesium metal and carbon. As KNSU has some shortcomings of brittleness, hygroscopic nature and caramelization amongst others [6,18]. The objectives are to: model the thermodynamics characterization and ballistic properties of the propellant . Validate the predicted propellant properties such as pressure and thrust generated by the propellant to characterize the fuel. These are to achieve: higher specific impulse, less smoke or reduced smoke, more flame, less hygroscopic propellant, less brittle, thus it can withstand more stress during handling without breaking, lower propellant mass to reach higher altitude.

## 2. Material and methods

This method involves performance parameters measurements mathematical model development and model validation of the propellant. The propellant constituents used are oxidizer (potassium nitrate), fuel or binder (sucrose), fuel (magnesium) and opacifier (carbon). The propellant characteristics performance parameters of interest in this work are the specific impulse, density, combustion temperature, characteristic velocity, molecular weight and heat ratio of the propellant.
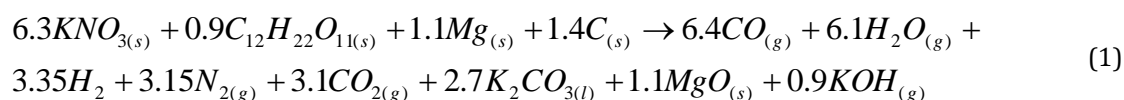
### 2.1. Mathematical Modeling of the Propellant Characterization

Mathematical modeling of the propellant performance parameters using the propellant combustion equation was used to relate the propellant formulation and to characterize it.

*2.1.1. Combustion temperature modeling*

A rocket motor operates on the basic principle of converting heat energy, from chemical reactions, to kinetic energy. Thus it is essential to know the temperature delivered by the propellant to the combustion chamber; analytically we can calculate the adiabatic flame temperature gotten from, as a result of our balanced chemical equation.

Using the propellant combustion products balance equation (assuming no changes in kinetic energy and potential energy)

$$6.3KNO_{3(s)} + 0.9C_{12}H_{22}O_{11(s)} + 1.1Mg_{(s)} + 1.4C_{(s)} \rightarrow 6.4CO_{(g)} + 6.1H_2O_{(g)} +$$
$$3.35H_2 + 3.15N_{2(g)} + 3.1CO_{2(g)} + 2.7K_2CO_{3(l)} + 1.1MgO_{(s)} + 0.9KOH_{(g)}$$

(1)

Enthalpy of reactants = Enthalpy of products.

$$H_R = H_P \qquad (2)$$

$$\sum_R n_i \, [\bar{h}_f^o + \Delta\bar{h}] = \sum_p ne \, [\bar{h}_f^o + \Delta\bar{h}]_o \qquad (3)$$

The enthalpies of formation values are now applied to equation (1) as shown in Table 1

**Table 1** Enthalpies of Formation of Elements and Compounds Used at 298.15K (Source: NIST chemistry web book).

| Constituents | States | $\bar{h}_f^o$ (KJ/mol) |
|---|---|---|
| $KNO_3$ | Solid | -494.63 |
| $C_{12}H_{22}O_{11}$ | Solid | -2226.1 |
| Mg | Solid | 0 |
| C | Solid | 0 |
| CO | Gas | -110.53 |
| $H_2O$ | Gas | -241.83 |
| $H_2$ | Gas | 0 |
| $N_2$ | Gas | 0 |
| $CO_2$ | Gas | -393.52 |
| $K_2CO_3$ | Liquid | -1150.18 |
| MgO | Solid | -601.8 |
| KOH | Gas | -424.72 |

The enthalpies of formation can be gotten from CRC hand book of chemistry and physics [19] or thermo-chemical tables NIST chemistry web book. [20]

Using the above equation and substituting in the values for $h_f$ , $n_i$ and $n_e$ gives;

$$6.3(-494.63+0)+0.9(-2226.1+0)+1.1(0)+1.4(0)=6.4(-110.53+CO)+6.1(-241.83+H_2O)+$$
$$3.35(0+H_2)+3.15(0+N_2)+3.1(-393.52+CO_2)+2.7(-1150.18+K_2CO_3)+1.1(-601.8+MgO)$$
$$+0.9(-424.72+KOH)$$
$$-5119.66=(-707.2+6.4CO)+(-1475.16+6.1H_2O)+(0+3.35H_2)+(0+3.15N_2)+$$
$$(-1219.92+3.1CO_2)+(-3052.65+2.7K_2CO_3)+(-661.98+1.1MgO)+(-208.935+0.9KOH)$$

We collect like terms and thus:

$$-5119.66+7325.8=6.4CO+6.1H_2O+3.35H_2+3.15N_2+3.1CO_2+2.7K_2CO_3+1.1MgO+0.9KOH$$

$$2206.184=6.4CO+6.1H_2O+3.35H_2+3.15N_2+3.1CO_2+2.7K_2CO_3+1.1MgO+0.9KOH$$

The solution of the equation is obtained by simply substituting in values for at a certain temperature. This temperature is equal to the adiabatic flame temperature (AFT) when the right hand side of the equation is equal to the left hand side (=2206.184K).

After much iteration it was found out that AFT lies between say 1800K – 1900K. From Joint Army-Navy-NASA-Air Force (JANNAF) tables, [21] the values are as shown in Table 2.

**Table 2** Enthalpy of Formation of Product Species at 1800K and 1900K.

| Species | Values @1900K (KJ/mole) | Values @1800K(KJ/mole) |
|---------|--------------------------|-------------------------|
| CO | 53.126 | 49.526 |
| H2O | 67.706 | 62.693 |
| H2 | 49.541 | 46.169 |
| N2 | 52.548 | 48.978 |
| CO2 | 85.419 | 79.431 |
| K2CO3 | 302.542 | 281.622 |
| MgO | 81.065 | 75.558 |
| KOH | 88.052 | 82.216 |

Iterating at 1900K and substituting,

$$2206.184 = 6.4(53.126) + 6.1(67.706) + 3.35(49.541) + 3.15(52.548) + 3.1(85.419) +$$
$$2.7(302.542) + 1.1(81.065) + 0.9(88.052)$$
$$= 2334.584 KJ / mol$$

Iterating at 1800K and substituting,

$$2206.184 = 6.4(49.526) + 6.1(62.693) + 3.35(46.169) + 3.15(48.978) + 3.1(79.431) +$$
$$2.7(281.622) + 1.1(75.558) + 0.9(82.216)$$
$$= 2172.064 KJ / mol$$

From here, we can see that the adiabatic flame temperature for the reaction lies between 1800K and 1900K. Therefore we interpolate to locate the particular temperature as follows:

$$= 2334.584 KJ / mol \qquad 1900K$$

$$= 2206..184 KJ / mol \qquad AFT (xK)$$

$$= 2172.064 KJ / mol \qquad 1800K$$

$$\frac{1900 - 1800}{1900 - x^0 K} = \frac{2334.584 - 2172.064}{2334.584 - 2206.184}$$

$$\frac{100}{1900 - xK} = \frac{162.520}{128.400} = 1.2657$$

$$x(AFT) = 1821 K$$

Thus the theoretical adiabatic flame temperature of the propellant is $1821 K$

Specific heats ratio, k

The specific heat ratio of a mixture is defined by [4] the equation

$$k = \frac{C_{p_{mix}}}{C_v} \qquad (4)$$

$$k = \frac{C_{p_{mix}}}{C_{p_{mix}} - R} \qquad (5)$$

$$k = \frac{1}{1 - \dfrac{R}{C_{pmix}}} \qquad (6)$$

Where $C_{p_{mix}} = \dfrac{1}{n_T}\left[\sum\left(n_i C_{pi}\right) + \left(n_s C_{ps}\right)\right] \qquad (7)$

$n_T$ = total number of gas moles

$n_i$ = number of moles of gas component i

$C_{pi}$ = specific heat capacity of gas component i

$n_s$ = number of moles of condensed phase product

$C_{ps}$ = specific heat capacity of condensed phase product

Specific heat determination

$$C_{P_{mix}} = \frac{1}{n_T}\left( \begin{array}{l} n_{CO}C_{P_{co}} + n_{H_2O}C_{P_{H_2O}} + n_{H_2}C_{P_{H_2}} + n_{N_2}C_{P_{N_2}} + n_{CO_2}C_{P_{CO_2}} + n_{K_2CO_3}C_{P_{K_2CO_3}} + \\ n_{MgO}C_{P_{MgO}} + n_{KOH}C_{P_{KOH}} \end{array} \right)$$

The specific heat ($C_p$) of species values at 1800k and 1900K as shown in Table 3.

**Table 3** Specific Heat (Cp) of Product Species at 1800K and 1900K

| Species | Values @ 1900K (J/kmol) | Values @ 1800K(J/kmol) |
|---------|--------------------------|-------------------------|
| CO | 36.091 | 35.911 |
| $H_2O$ | 50.496 | 49.749 |
| $H_2$ | 33.917 | 33.537 |
| $N_2$ | 35.796 | 35.6 |
| $CO_2$ | 85.419 | 59.701 |
| $K_2CO_3$ | 209.2 | 209.2 |
| MgO | 55.278 | 54.204 |
| KOH | 58.504 | 58.204 |

By extrapolation, $C_p$ @$1821K$ , we have

**Table 4** Extrapolated Specific Heat (Cp) of Product Species at 1821K (AFT)

| Species | State | Values @ $1821K$ (J/kmol) |
|---------|-------|---------------------------|
| CO | Gas | 35.949 |
| H2O | Gas | 49.906 |
| H2 | Gas | 33.617 |
| N2 | Gas | 35.6 |
| CO2 | Gas | 59.701 |
| K2CO3 | Liquid | 209.2 |
| MgO | Solid | 54.978 |
| KOH | Gas | 58.267 |

n$_{Tgas}$ = total number of gas moles

n$_{Ti}$ = total number of moles in mixture

$$n_{T_{gas}} = n_{CO} + n_{H_2O} + n_{H_2} + n_{N_2} + n_{CO_2} + n_{KOH}$$

$$n_{T_{gas}} = 6.4 + 6.1 + 3.35 + 3.15 + 3.1 + 0.9 = 23 \text{ moles}$$

$$n_{Ti} = n_{CO} + n_{H_2O} + n_{H_2} + n_{N_2} + n_{CO_2} + n_{K_2CO_3} + n_{MgO} + n_{KOH}$$

$$n_{Ti} = n_{Tmix} = 6.4 + 6.1 + 3.35 + 3.15 + 3.1 + 2.7 + 1.1 + 0.9 = 26.8 \text{ moles}$$

$$C_{P_{gas}} = \frac{1}{23}\left( \begin{array}{l} (6.4 \times 35.949) + (6.1 \times 49.906) + (3.35 \times 33.617) + (3.15 \times 35.641) + (3.1 \times 59.774) + \\ (0.9 \times 58.267) \end{array} \right)$$

$$C_{P_{gas}} = 43.70268 (JK^{-1}mol^{-1})$$

$$C_{P_{mix}} = \frac{1}{26.8}\left( \begin{array}{l} (6.4 \times 35.949) + (6.1 \times 49.906) + (3.35 \times 33.617) + (3.15 \times 35.641) + (3.1 \times 59.774) + \\ (2.7 \times 209.2) + (1.1 \times 54.978) + (0.9 \times 58.267) \end{array} \right)$$

$$C_{P_{mix}} = 60.53887 (JK^{-1}mol^{-1})$$

Where R= universal gas constant, $R = 8.314(J/molK)$

$C_v$ = specific heat at constant volume

$$C_V = 60.53887 - 8.314 = 52.22487$$

$$k_{mix} = \frac{C_P}{C_V} = \frac{60.53887}{52.22487} = 1.1591$$

$$k_{mix} = 1.1591$$

Effective molecular weight of the mix calculation:

Using the combustion equation,

**Table 5** Moles and Mass of the product species of the combustion equation

| Product species | Moles, n | Mass of Products species, mp (g) |
|---|---|---|
| CO2 | 3.1 | 136.4295 |
| CO | 6.4 | 179.2646 |
| H2O | 6.1 | 109.8932 |
| H2 | 3.35 | 6.7532 |
| N2 | 3.15 | 88.2422 |
| K2CO3 | 2.7 | 373.1549 |
| KOH | 0.9 | 50.4951 |
| MgO | 1.1 | 44.3348 |
| | | |

Therefore, the molecular weight given as:

$$MW = \frac{\sum mp}{\sum n_i}$$

$$= \frac{988.567}{26.8} = 36.8868 \text{ g/mol}$$

## 2.2. Other Characteristics Performance Parameters

The other mathematical calculation evaluation of the propellant performance parameters such as the propellant specific impulse, propellant density and molecular weight were computed using MATHCAD tool.

*2.2.1. Propellant Specific impulse (Isp) calculation*

Acceleration due to gravity: $g_{acc}$ = 9.81 m/s$^2$

Nozzle exit pressure: $P_e$ = 14.7psi

Chamber combustion pressure: $P_o$ = 112 psi

Propellant specific impulse, Isp

$$I_{SP} = \frac{1}{g_{acc}} \left[ \left[ 2T_C \frac{R_u}{M} \left( \frac{k}{k-1} \right) \right] \left[ 1 - \left( \frac{P_e}{P_o} \right)^{\frac{k-1}{k}} \right] \right]^{\frac{1}{2}}$$

$I_{SP}$ = 122.9 S

*2.2.2. Characteristics Velocity, C-star*

Temperature: $T_c$ = 1821 K

The universal gas constant: $R_u$ = 831 J/kgmol K

The Molecular Weight of the propellant: M = 36.8868 g/ mol

The Propellant Gas Constant: $R_g = \dfrac{R_u}{M}$ = 225.392 J/kgK

The specific heat ratio: k = 1.15919

Characteristic velocity, c-star

$$C_{star} = \left[ \left( \frac{R_g T_c}{k} \right) \left( \frac{k+1}{2} \right)^{\left( \frac{k+1}{k-1} \right)} \right]^{\frac{1}{2}}$$

$$C_{star} = 1000.264 \text{ m/s}$$

*2.2.3. Ideal Density of the Mix Calculation for KNSUMgC Propellant*

% composition of oxidizer: $F_{KNO_3}$ = 0.65

% composition of sucrose fuel: $F_{SU}$ = 0.30

% composition of magnesium fuel: $F_{Mg}$ = 0.03

% composition of opacifier carbon: $F_C$ = 0.02

$$F_{total} = F_{KNO_3} + F_{SU} + F_{Mg} + F_C =$$

*2.2.4. Ideal Density*

Density of KNO3 oxidizer: $\rho_{KNO_3}$ = 2110 kg/m³

Density of Sucrose fuel: $\rho_{SU}$ = 1590 kg/m³

Density of Magnesium fuel: $\rho_{Mg}$ = 1740 kg/m³

Density of opacifier carbon: $\rho_C$ = 2250 kg/m³

$$Density_{mix} = \frac{1}{\left(\dfrac{F_{KNO_3}}{\rho_{KNO_3}}\right) + \left(\dfrac{F_{SU}}{\rho_{SU}}\right) + \left(\dfrac{F_{Mg}}{\rho_{Mg}}\right) + \left(\dfrac{F_C}{\rho_C}\right)} \quad kg/m^3$$

$$Density_{mix} = 1912.534 \ kg/m^3$$

## 3. Results and discussion

The experimental results from the load cell, software results and mathematical calculations carried out are presented in Tables 6 to 8 and Figures 1 to 3.

**Table 6** Results of Software, Validation Test and Mathematical Model

| Parameter | Notation | PROPEP | VALIDATION TEST | MODEL | Unit |
|---|---|---|---|---|---|
| Specific impulse | Isp | 118.5 | 117.9 | 122.9 | s |
| Combustion Temperature | Tc | 1873 | 1818 | 1821 | K |
| Molecular Weight | MW | 37.34 | 38.88 | 36.89 | g/mole |
| Isentropic heat ratio | K | 1.1317 | 1.1508 | 1.1592 | - |
| Propellant Density | $\rho_p$ | 1910 | 1874.6 | 1912.5 | kg/m³ |
| Characteristic velocity | c-star | 950 | 997.2 | 1000 | m/s |

**Table 7** Ballistic Load Cell Results of Propellant Samples

| Propellant Samples | %Mg Composition | Exit Temperature Te (K) | Thrust F(N) | Burn time tb(s) |
|---|---|---|---|---|
| Control | 0 | 113 | 1017 | 3.93 |
| 1 | 0 | 1108 | 1013 | 3.9 |
| 2 | 1 | 1191 | 1018 | 4.0 |
| 3 | 2 | 1222 | 1022 | 3.88 |
| 4 | 3 | 1301 | 1027 | 4.0 |
| 5 | 4 | 1297 | 987 | 4.12 |
| 6 | 5 | 1278 | 934 | 4.26 |
| 7 | 6 | 1267 | 894 | 4.31 |
| 8 | 7 | 1214 | 887 | 4.33 |
| 9 | 8 | 1056 | 827 | 4.4 |
| 10 | 9 | 1034 | 805 | 4.51 |
| 11 | 10 | 1013 | 782 | 4.6 |

**Table 8** Result of Propellant Characteristics Performance Parameters

| Propellant Samples | Specific impulse, Isp (s) | Heat ratio, K | Chamber Temp., Tc (K) | Characteristic velocity, C-star (m/s) | Propellant density, $\rho_p$ (kg/m³) | Molecular weight Mw (g/mole) |
|---|---|---|---|---|---|---|
| Control | 114.8 | 1.1512 | 1576 | 973.2 | 1899 | 36.59 |
| 1 | 113.4 | 1.1547 | 1568 | 963.3 | 1904 | 36.86 |
| 2 | 116.9 | 1.1524 | 1677 | 989.4 | 1906 | 37.09 |
| 3 | 113.9 | 1.1511 | 1716 | 966.5 | 1908 | 37.24 |
| 4 | 118.0 | 1.1508 | 1826 | 997.2 | 1910 | 37.33 |
| 5 | 116.8 | 1.1497 | 1816 | 988.3 | 1912 | 37.36 |
| 6 | 114.3 | 1.1487 | 1786 | 969.4 | 1914 | 37.34 |
| 7 | 110.6 | 1.1468 | 1764 | 942.3 | 1916 | 37.28 |
| 8 | 110.3 | 1.1456 | 1686 | 939.6 | 1918 | 37.18 |
| 9 | 104.5 | 1.1444 | 1463 | 896.1 | 1920 | 37.06 |
| 10 | 104.2 | 1.1432 | 1429 | 894.3 | 1922 | 36.9 |
| 11 | 103.3 | 1.1425 | 1398 | 887.1 | 1924 | 36.74 |
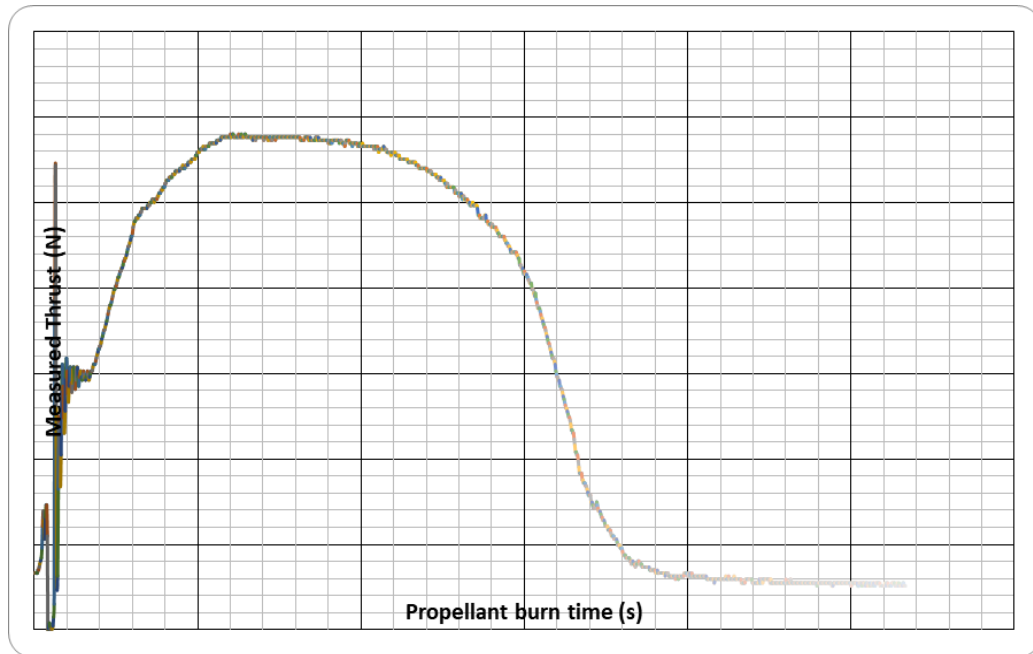


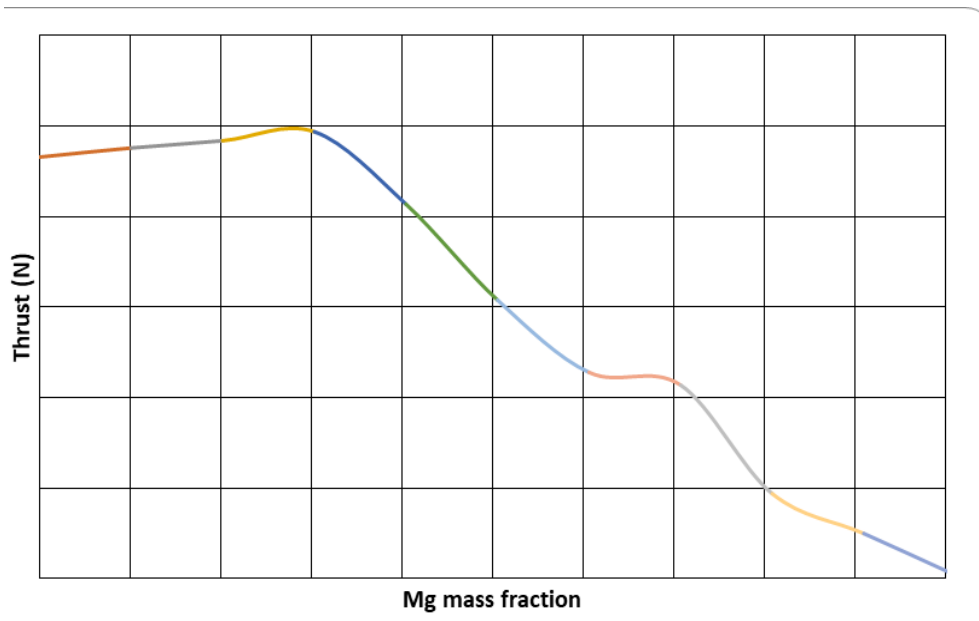**Figure 1** Measured Thrust and Burn Time Curve

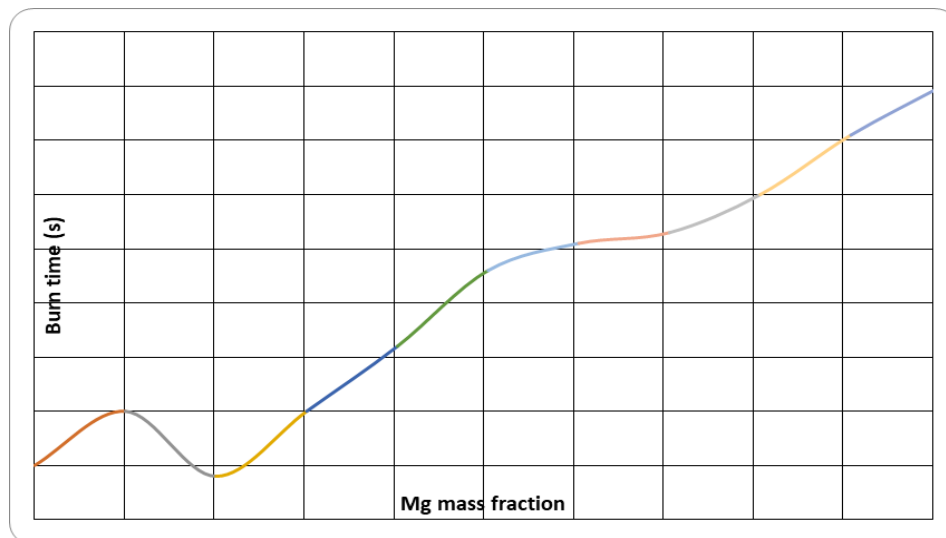**Figure 2** Thrust vs. Magnesium Mass Fraction Curve



**Figure 3** Propellant burn time vs. Magnesium Mass Fraction Curve

## 4. Discussion

The load cell instrumentation was helpful in determining the thrust generated by the propellant and the duration of the burn, usually referred to as the burn time. The propellant combustion products equation (1) was used to model and obtain the characteristics performance parameters. This gave propellant specific impulse (122.9s), combustion temperature (1821K), heat ratio (1.1592), molecular weight (36.89g/mole), propellant density (1912.5kg/m$^3$) and characteristics velocity (1000m/s) result while maintaining the same chamber pressure.

It was observed that utilization of a propellant evaluation program (software) to compare the propellant formulation with that of the , mathematical model showed that their results were close to the result obtained indicating, that basic assumptions made in the mathematical solutions were valid.

Table 8 is the test results (samples 1-11) that showed the effect of addition of magnesium to the propellant formulation and revealed that parameters such as specific impulse, chamber temperature, characteristics velocity, heat ratio were

greatly improved as compare to when magnesium was not present in the formulation. Figure 3 showed the result of magnesium on the propellant burn time. Magnesium was found to be increasing the propellant burn time and forced the sucrose from burning so spontaneously and aggressively resulting in shorter burn time.

It was observed that addition of magnesium to the formulation really justified by the amount of improvement brought upon the propellant performance. The need to necessarily select and use a propellant of higher composition of magnesium of average cost for  parameters such as specific impulse, thrust, characteristic velocity, chamber temperature, thrust coefficient and heat ratio are  raised to desired points  is  justified(22).

The utilization of 2% carbon which acted as an opacifier and/or coolant helped to contain some of the heat during the combustion process from directly hitting the walls of the motor thereby limiting or reducing high combustion temperature that could lead to the rocket motor rupture or failure. In this case, when increased beyond this percentage, the propellant was excessively smoky. Smoky fuel is the presence of high magnesium oxide (MgO) and other solids in the combustion products which result in air pollution, and can be harmful to human lives and the environment. A Smoky fuel is usually avoided especially in military application. (22) Also, carbon helped in aiding the curing of the propellant, improve the physical and mechanical properties such as plasticity (rubbery-like) textures.

## 5. Conclusion

The mathematical modeling of the combustion exhaust products was employed to characterize the propellant and results well agreed with experimental ballistic test results as well as the software result-PROPEP, which is a software program designed for the characterization of solid rocket motor propellants. This also confirmed the experimental results that inclusion of magnesium in the propellant formulation significantly improved the overall performance parameters of the propellant. The higher the values of these parameters, the better the performance of the propellant.

The use of magnesium adequately reduces the challenge of a smoky propellant that the KNSU propellant produces, improved the specific impulse and thrust generated.

This work has therefore solved the challenge of hygroscopicity of sugar propellants and improved the characteristics performance parameters of such propellants.

Rocket-grade chemical ingredients are recommended to be used to get characteristics performance results close to that of the software performance results.

## Compliance with ethical standards

*Acknowledgments*

*Disclosure of conflict of interest*

There are no conflicts of interest

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