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OPTIMISATION OF THE FORMULATION OF A DOUBLE – BASED SOLID PROPELLANT

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ABSTRACT
The study investigated the optimization of the formulation of a double – based solid propellant using Sorbitol as fuel and Potassium nitrate as oxidizer. This research provides an insight into a way of preventing the negative effect of poor propellant formulation on the predetermined rocket mission. The design is based on the fact that specific impulse, temperature, density and thrust of the product are functionally related to specific propellant formulation and these are fitted to multiple regression equations describing responses to optimal formulation using response surface methodology (RSM). From the model equations developed, the potassium nitrate ratio had a positive linear and negative quadratic effect on specific impulse and density and a strong positive linear and strong negative quadratic effect on temperature and thrust. The model fitness value (F- value) of 972.07, 29072.37, 32434.66 and 969.43 implies that the model is significant since there is only a 0.01% chance that an F- value that is large could occur due to noise. The coefficients of determination (R^2) values gotten are 0.9999, 0.9974, 0.9999 and 0.9974 and the adjusted coefficients of determination (adjusted R^2) values are 0.9964, 0.9999, 0.9999 and 0.9964 which further validates the model. The optimum performance values obtained are 90.2119 s, 1643.84 K, 1843.02 Kg/m^3 and 950.854 N for specific impulse, temperature, density and thrust respectively. These values were in good agreement with the experimental results. An optimum double base propellant formulation of 34.18% sorbitol and 65.82% potassium nitrate can be used in launching rockets and missile systems because of its high specific impulse and thrust.

Keywords: Optimum, response surface method, sorbitol, potassium nitrate, solid propellant.

I. INRTODUCTION
Propellants are mixtures of chemical compounds that produce large volume of gas at controlled and predetermined rates. Their major applications are in launching projectiles from guns, rockets, and missile systems (Jacqueline, 1998). Double based solid propellant is a type of solid propellant of composition of a single fuel and single oxidizer only. For example a propellant of composition of sorbitol as fuel and potassium nitrate as oxidizer respectively. Chemical propellants provide a simple and effective way of creating propulsion for flight (Krishnan *et al*., 1998).

Optimization is greatly required to formulate a solid propellant of a good performance for effective and efficient propulsion to check such occurrence. The solid propellant, which is the rocket fuel, is developed when the rocket missions are known (Arnon *et al*., 2010).

The Response surface methodology is a reliable and powerful tool for optimization of solid propellant formulation and more efficient for maximizing propellant efficiency and performance (Ogunleye, *et al*., 2015). Adhering to proven optimal techniques will result in a high quality propellant. Successful optimization studies for solid propellants brought a propellant of a good performance for effective and efficient propulsion (Raphael and Zafer, 1996; Sevda, 2010).

However, despite the tractable mathematics involved in formulating a good propellant, limited treatment of the subject appears in the literature (Amir and Wan, 2011). In this work, an optimization studies in which a double based solid propellant of optimal formulation for propellant of a good performance were carried out. This work is to design a double based solid propellant with optimal formulation for a propellant of good properties, through

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developing a mathematical model for some propellant properties in terms of the propellant formulation, formulating and solving the optimisation problem that maximises the solid propellant performance and validating the model developed.
The study was restricted to the analysis of the effect of varying the double based solid propellant ingredients on propellant properties. An emphasis was laid on the propellant of composition of sorbitol and potassium nitrate as fuel and oxidizer respectively. Also, the grain geometries considered for the design was hollow bates grains.

II. RESEARCH METHODOLOGY

A methodology for design and optimization studies of double based solid propellant where a propellant formulation of optimal properties for a good propellant performance was considered. The set out objectives for this study were executed in the following four phases: Model Development, Optimization, and Validation.
The models were developed using a Response Surface Methodology (RSM). Basically, RSM relates product properties by using regression equations that describe interrelations between input parameters and product properties (Jouhaud *et al.*, 2007). The preliminary task is the identification of input parameters and output variables involved in propellant design.

Propellant design was considered for the purpose of identifying the design inputs and output parameters. The input variables identified were the quantities of ingredients while the output variables identified were the propellant properties at the exit of the rocket motor after propellant combustion.

2.1 Experimental design

In this study, Design Expert (6.0.8) software was used to design the experiment with the aim of optimizing the response of the propellant parameter involved in the experiment using response surface methodology (RSM). This requires having a 'good' fitting model that provides an adequate representation of the mean response because such a model is to be utilized to determine the value of the optimum condition (Khuri, 1996).

This methodology is a collection of statistical techniques and mathematical techniques that uses quantitative data from the appropriate experiment to determine regression and model equations and operating condition which was useful for developing, improving and optimizing processes (Montgomery, 2009).

The design was based on the fact that specific impulse, temperature, density and thrust of the product are functionally related to specific propellant formulation and attempts were made to fit multiple regression equations describing responses to optimal formulation.

2.2 Model assumptions

The following assumptions were made about the propellant combustion process.
(i) A double base propellant is considered. Here fuel and oxidizer are contained within the same molecule which decomposes during combustion.
(ii) Propellants are at room temperature (298 K).
(iii) There is no appreciable friction and all boundary layer effects are neglected.
(iv) Combustion gas properties throughout the motor are constant.
(v) A solid rocket motor of De Laval nozzle was used for the firing test.

2.3 Response equations for propellant properties

The resulting weights for each ingredient in different propellant formulation were generated. A central composite rotatable design was adopted (Cocharan and Cox, 1957). In this design, experiments were randomized in order to minimize the effects of unexplained variability in any responses due to extraneous factors. In order to analyse the experimental design by response surface methodology, it was assumed that there existed n mathematical functions, $f_h(h=1,2,....,n)$, for each response variable, Y_h in term of m independent ballistic variable $X_i(i=1,2,....,m)$.

$$Y_h = f_h(X_1, X_2,...., X_m). \quad (1)$$

In this experiment, n = 4 and m = 1. In order to approximate this function, a second order polynomial equation was assumed.

$$Y_h = b_{h_o} + \sum_{i=1}^{m} b_{h_i} X_i + \sum_{i=1}^{m} b_{h_{ii}} X^2{}_i + \sum_{i \neq j=1}^{m} b_{h_{ij}} X_i X_j \qquad (2)$$

Where b_{h_o} is the value of fitted response at the centre point of the design, i.e. $(0,0)$, and b_{h_i} , $b_{h_{ii}}$ and b_{ij} are linear, quadratic and cross product regression term respectively.

2.4 Optimisation model of propellant formulation

A multi objective optimisation problem was formulated to maximise specific impulse, density and thrust while minimizing temperature subject to mission requirement as given below:

$$\begin{aligned} &\text{Maximise } Y_1 = f(X_1), \\ &\text{Maximise } Y_3 = f(X_1), \\ &\text{Maximise } Y_4 = f(X_1), \\ &\text{Minimise } Y_2 = f(X_1). \\ &\text{Subject to:} \\ &\quad -1 \le X_1 \le 1. \end{aligned} \qquad (3)$$

Where X_1 is coded ratio values for independent propellant variables and Y_1, Y_2, Y_3 and Y_4 are response variables of propellant formulation.

III. RESULTS AND DISCUSSION

3.1 Validation of double based propellant formulation

The results of the rocket motor firing tests optimized using RSM were verified experimentally to validate the model.

This observation is corroborated by the Richard Nakka's study on solid rocket propellant design. The scientist worked on sorbitol and potassium nitrate and observed that as sorbitol increases, specific impulse decreases while as potassium nitrate increases, specific impulse increases also (Nakka, 2013).

3.2 Development of the Performance Models for Propellant Formulation

In developing the mathematical models for the performance properties of the solid propellant, regression analyses were conducted in obtaining the models. All main effects, linear and quadratic, and interaction were calculated for each model. The regression coefficients as well as the correlation coefficient obtained for each model are shown in Table 1. Correlation analysis was used as tools for assessment of the effects of two or more independent factors on the dependent variables (Boonmee *et al.*, 2010). The correlation coefficients for the responses such as specific impulse, temperature, density and thrust (R^2 = 0.9974, 0.9999, 0.9999 and 0.9974, respectively) are quite high for response surfaces, and indicated that the fitted quadratic models accounted for more than 99 % of the variance in the experimental data. These were found to be highly significant. Based on t-statistics, the regression coefficients that are not significant at 95 % were discarded while only those that are significant were selected for developing the model equations (4) to (11).

Specific impulse $(Y_1) = -18.22105 + 93.99968X_1 - 19.82647X_1{}^2$ (4)

$$R^2 = 0.9974 \qquad (5)$$

Temperature $(Y_2) = 642.27763 + 695.41863X_1 - 95.96242X_1{}^2$ (6)

$$R^2 = 0.9999 \qquad (7)$$

Density $(Y_3) = 1725.63219 + 73.52010X_1 - 7.21867X_1{}^2$ (8)

$$R^2 = 0.9999 \qquad (9)$$

Thrust $(Y_4) = -2319.09260 + 2834.716181X_1 - 597.90733X_1{}^2$ (10)

$$R^2 = 0.9974 \qquad (11)$$

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Table 1: Estimated Coefficients of the Response Equation for Propellant Properties

Ballistics Properties	**Model Factors**	**Coefficients**	**t-values**	**p-values**
Specific Impulse (Y_1)	Constant	-18.22105	88.03	0.0001*
	X_1	93.99968	7.49	0.0001*
	X_1^2	-19.82647	-2.71	0.0002*
		R^2 = 0.9974		
Temperature (Y_2)	Constant	642.27763	1603.76	0.0001*
	X_1	695.41863	125.22	0.0001*
	X_1^2	-95.96242	-13.14	0.0001*
		R^2 = 0.9999		
Density (Y_3)	Constant	1725.63219	1837.41	0.0001*
	X_1	73.52010	17.27	0.0001*
	X_1^2	-7.21867	-0.99	0.0003*
		R^2 = 0.9999		
Thrust (Y_4)	Constant	-2319.09260	884.96	0.0001*
	X_1	2834.71618	225.89	0.0001*
	X_1^2	-597.90733	-81.85	0.0002*
		R^2 = 0.9974		

*Significant at p value < 0.05 at 95 % confidence interval

The potassium nitrate ratio had a positive linear and negative quadratic effect on specific impulse and density. Also, the potassium nitrate ratio had a strong positive linear and strong negative quadratic effect on temperature and thrust. Similarly, the sorbitol nitrate ratio had a strong positive linear and strong negative quadratic effect on specific impulse and density. Also, the sorbitol ratio had a positive linear and negative quadratic effect on temperature and thrust. The interaction of sorbitol and potassium nitrate ratio had no statistical significant effect on the properties in consideration.

3.3 Adequacy Test of the Models for Propellant Properties

The fitted models were tested for adequacy and consistency by analysis of variance, ANOVA for all the propellant performance model responses and presented in Table 2. The analysis of variance was calculated to assess how well the model represents the design data. The results from the statistical analysis of variance reveal that the F-values for specific impulse, temperature, density and thrust (972.07, 29072.37, 32434.66 and 969.43 respectively) were significant at the 95 % level. On this basis, it can be concluded that the selected performance models adequately represent the data for specific impulse, temperature, density and thrust. There were no outliers to the regressions. The model F- value of 972.07, 29072.37, 32434.66 and 969.43 implies the model is significant. There is only a 0.01% chance that a model F- value this large could occur due to noise. If the value of probability is less than 0.5, it indicates the model terms are significant. In this case, regression values of 264.24, 70837.78, 1343.18 and 240300 are significant model term as compared with the residual which include the lack of fit of 0.64, 6.09, 0.10 and 619.66 respectively. This shows there is an insignificant lack of fit. The lack of fit value is an indication of the failure of the model representing the experimental data, at which points not included in the regression or variations in the models cannot be accounted for by random errors. It therefore implies that if there is a significant lack of fit, the model should be discarded.

The suitability of the model was also tested using the coefficient of determination (R^2). This is the proportion of variation in the response that is attributed to the model. For a good model, R^2 should not be less than 80%. R^2 values that are close to unity signify the suitability of the empirical model to the actual value. From the result, the R^2 values are 0.9999, 0.9974, 0.9999 and 0.9974. A large value of R^2 does not always imply the adequacy of the model. Thus, the adjusted R^2 of over 90% is more appropriate to evaluate the model adequacy (Li *et al.*, 2011). The adjusted R^2 values from the table are 0.9964, 0.9999, 0.9999 and 0.9964 which further validates the model.

Table 2: Analysis of Variance for Propellant Performance Models

Ballistic Properties	Source of Variation	Sum of Squares	d.f.	Mean Squares	p-values	Adjusted R^2	F-values
Specific Impulse	Regression	264.24	2	132.12	0.0001*	0.9964	972.07
	Residual	0.68	5	0.14			
	Total	264.92	7				
Temperature	Regression	70837.78	2	35418.89	0.0001*	0.9999	29072.37
	Residual	6.09	5	1.22			
	Total	70843.88	7				
Density	Regression	1343.18	2	671.59	0.0001*	0.9999	32434.66
	Residual	0.10	5	0.021			
	Total	1343.28	7				
Thrust	Regression	2.403E+005	2	1.201E+005	0.0001*	0.9964	969.43
	Residual	619.66	5	123.93			
	Total	2.409E+005	7				

*Significant level at $p < 0.05$

3.4 Optimal formulation for solid Propellants

The Response surface methodology was used for the optimization of solid propellant formulation for the understanding of the factors affecting propellant formulation. The models (Y_1, Y_2, Y_3 and Y_4) were useful for indicating the direction in which to change variables in order to maximise specific impulse, density and thrust while minimising temperature. The regression equations were solved for maximum specific impulse, density and thrust and minimum temperature. The optimum performance values obtained are 90.2119 s, 1643.84 K, 1843.02 Kg/m^3 and 950.854 N for specific Impulse, density, temperature and thrust, respectively. The optimum ingredients ratio (coded) predicted for each corresponding response and actual compositions or mass fractions for optimum response are presented in Table 3.

As shown on Table 3, the coded level lies within the experimental range and this indicated the validity of the selection of the variables range. The actual compositions or mass fractions obtained for optimum responses as shown on Table 3 are 0.3418sorbitol and 0.6582potassium nitrate.

Table 3: Optimal Formulation for Solid Propellants

Coded ratio	Ingredient ratio	
X_1	A	B
0.33	0.6582	0.3418

The response surfaces were plotted for the relationship between the independent and dependent variables for selected model equations which gave the optimum responses. The relationship of specific Impulse with solid propellant formulation indicates that as the potassium nitrate ratio increases so also there is an increase in specific impulse, whereas, when moving in the direction of sorbitol ratio, an increase in the ratio brings a decrease in specific impulse until an optimum specific impulse is achieved. For the relationship of temperature with propellant formulation, the unit positive change in potassium nitrate ratio gives an increase in temperature, but a positive change in sorbitol ratio brings a decrease in temperature until an optimum temperature is achieved. The relationship of density with propellant formulation shows that the increase in sorbitol ratio yields a decrease in density whereas an increase in potassium nitrate ratio resulted into an increase in density until an optimum density is achieved. Also, the relationship of thrust with propellant formulation indicates that the increase in sorbitol ratio yields a decrease in thrust whereas an increase in potassium nitrate ratio resulted into an increase in thrust. The behaviour of specific impulse and thrust with the propellant formulation are very similar which implies that the two responses could be related. The behaviour of density and temperature with the propellant formulation are very similar. This suggested that the two responses are much related. The desirability plot to determine the point of optimality for optimum formulation is shown in Figure 1 and Figure 2. The optimum propellant properties were obtained where the coded and actual values are 0.33 and 1.98 respectively.

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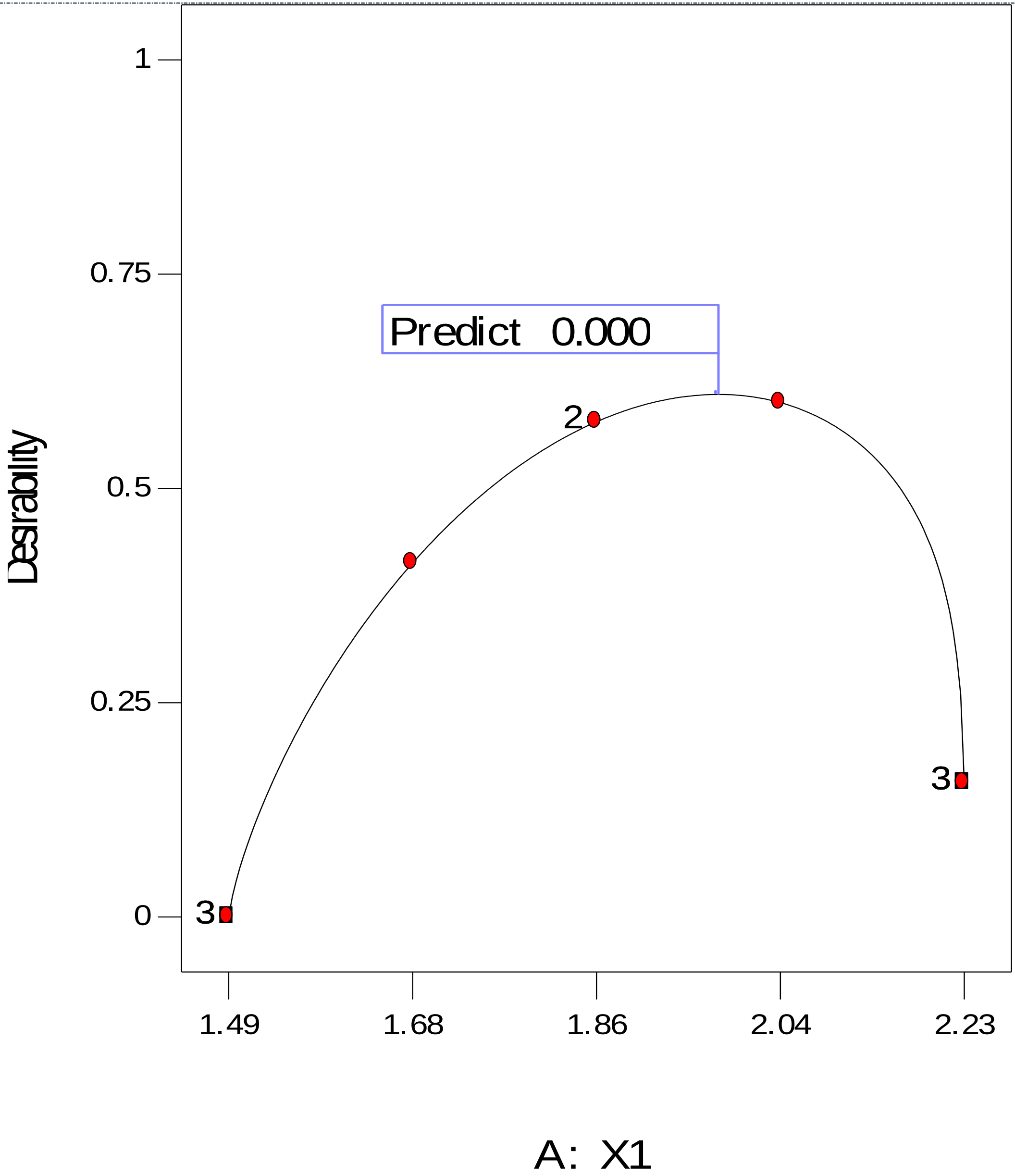

Figure 1: Desirability Plot for Optimum Formulation in Actual value

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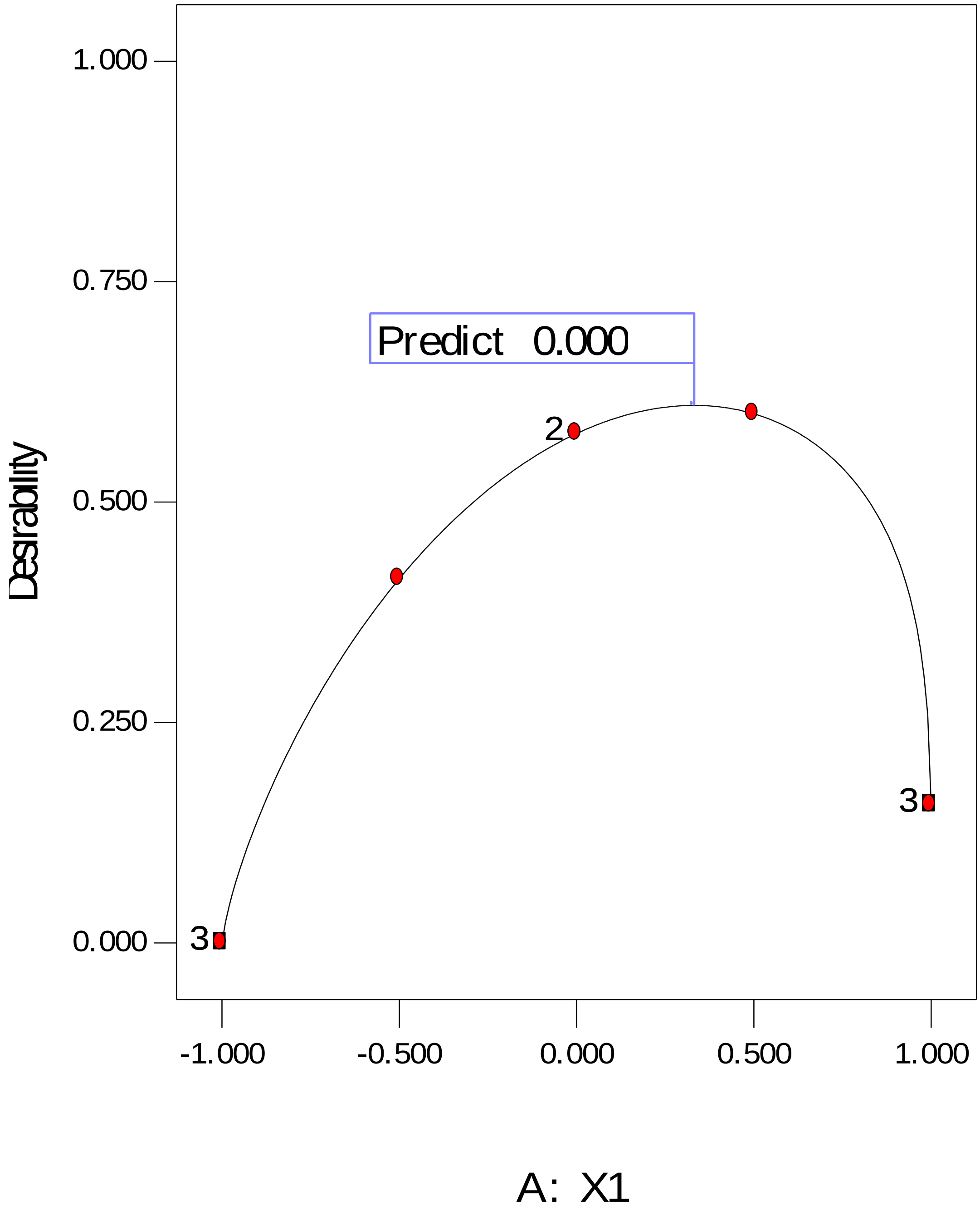

Figure 2: Desirability Plot for Optimum Formulation in Coded value

3.5 Validation of the optimal propellant formulation

The optimum condition was verified experimentally. The results obtained were 89.78, 1643.80, 1896.99 and 890.550 for specific impulse, temperature, density and thrust respectively. These experimental values at the optimum propellant formulations were in good agreement with the simulated results. This shows the efficiency and effectiveness of Response surface methodology adopted for the design. The validation on the basis of specific impulse which is the measure of propellant efficiency and performance is shown in Table 4. This confirmed that the optimum formulation is very good for solid propellant design.

Table 4: Results of the Validation Experiments

Ballistic properties	RSM	Experimental Result
Specific Impulse(s)	90.2119	89.78
Temperature(K)	I643.84	1643.80
Density(Kg/m^3)	1843.02	1896.99
Thrust(N)	950.798	890.550

IV. CONCLUSION

The propellant ingredients and their proportions determine the solid propellant performance. This informed the trend of the behaviours of propellant samples considered in this study.

The (Response surface method) RSM was successfully applied to the determination of the optimum formulation for double based solid propellants since the model F- value of 972.07, 29072.37, 32434.66 and 969.43 implies the model is significant and there is only a 0.01% chance that an F- value this large could occur due to noise. The R^2 values gotten are 0.9999, 0.9974, 0.9999 and 0.9974 and the adjusted R^2 values are 0.9964, 0.9999, 0.9999 and 0.9964 which further validates the model. The optimum performance values obtained are 90.2119 s, 1643.84 K, 1843.02 Kg/m^3 and 950.854 N and these values were verified experimentally and the results obtained were 89.78s, 1643.80K, 1896.99Kg/m^3 and 890.550N for specific impulse, temperature, density and thrust respectively. The experimental values at the optimum propellant formulations were in good agreement with the simulated results. This shows the efficiency and effectiveness of response surface methodology adopted for the design. The developed performance model is an effective tool for determining optimal condition for double based solid propellant formulation.

Also, the mathematical models developed establish the relationship between the double based solid propellant ingredient and its properties.

REFERENCES

[1] Amir, A. and Wan Khairuddin, W. (2011). The Study of Burning Characteristics of AP/HTPB/AL Basic Components of a Composite Propellant, Journal of Aerospace Engineering and Technology, 1, 1, 21-26.
[2] Arnon, L., Francois, B. and Rudolf, S. (2010). Solid Propellant Grain Geometry design, a model for the evolution of Star shaped interfaces, A Bachelor Project, Amsterdam University, Omvang 12EC, 185-200.
[3] Boonmee, K., Chuntranuluck, S., Punsuvon, V. and Silayoi, P. (2010). Optimization of biodiesel Production from Jatropha (Jatropha Curcas L.), using Response surface methodology, Kasetsart Journal of Natural Science, 44, 290-299.
[4] Cocharan, W. G. and Cox, G. M. (1957). Experimental Designs (edited by R.A. Bradley, D. G. Kendall, J. S. Hunter and G. S. Watson), John Wiley and sons, New York, 6, 335–375.
[5] Jacqueline, A. (1998). The Chemistry of Explosives, the Royal Society of Chemistry, Cambridge, United Kingdom, 9, 55 - 60.
[6] Krishnan, S., Chakravarthy, S. R. and Athithan, S. K. (1998). Propellants and Explosives Technology, Allied Publishers Limited, India, 7, 47 – 76.
[7] Li, Y., Jiang, L., Sui, X and Wang, S (2011). Optimization of the aqueous enzymatic extraction of palm kernel oil by response surface methodology. Procedia Engineering, Vol 15, 2011, pp 4641 and 4642.
[8] Montgomery, D. C. (2009). Water Treatment Principles and Design, Wiley Interscience, New York, 1, 175 - 180.
[9] Ogunleye, O. O., Hamed, J. O. and Alagbe, S. O. (2015). Optimization of Potassium Nitrate Based Solid Propellant Grains Design Using Response Surface Methodology, Advances in Science and Technology Research Journal, 9, No. 27, 123 – 134.
[10] Raphael, T. H. and Zafer, G. (1996). Elements of Structural Optimization third revised and expanded edition, Kluwer Academic Publishers, 5, 356 - 360.
[11]. Richard Nakka (2013) Solid propellant burn rate, Richard Nakka's Experimental Rocketry web.
[12] Sevda, A. (2010). Internal Ballistic Design Optimization of a Solid Rocket Motor, M. Sc. thesis submitted to the Graduate School of Natural and Applied Sciences of Middle East Technical University, 114-124.

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