

Response Surface Modelling of Adiabatic Flame Temperature in Aluminum–Potassium Perchlorate Pyrotechnics

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ABSTRACT

This study applies Design of Experiments and Response Surface Methodology (RSM) to the ternary Al/KClO₄/binder system, using the adiabatic flame temperature as the target response. A three factor Box–Behnken design was constructed in the Al content (26–38 wt.%), binder content (2–10 wt.%) and initial temperature of the reactants (298–398 K), and the flame temperature of each of the fifteen resulting formulations was computed from a fully transparent Hess law energy balance based on tabulated NIST–JANAF data, rather than from a proprietary equilibrium code. The thermochemical calculation yielded a reaction enthalpy of $-10.6 \text{ kJ}\cdot\text{g}^{-1}$. The effective dissociation coefficient was calibrated so that the stoichiometric flame temperature fell within the literature range of 2900–3200 K; this agreement therefore represents consistency with the calibration target rather than an independent validation of the model. A full quadratic response surface model fitted the computed data with a coefficient of determination of 0.9990 and a maximum relative error below 0.13%, and passed all residual adequacy checks. The temperature was governed primarily by the quadratic effect of the aluminum content and the linear cooling effect of the binder, whereas the initial temperature showed a comparatively weak contribution within the investigated range, acting primarily additively and independently of composition. Numerical optimization located a maximum adiabatic temperature of about 3089 K at 32.7 wt.% aluminum and the lowest binder loading.

Abbreviations

BBD	Box–Behnken design
DoE	Design of experiments
RSM	Response surface methodology
RMSE	Root-mean-square error

1. Introduction

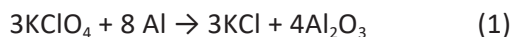
Pyrotechnic compositions are intimate mixtures of a metallic or non metallic fuel and a solid oxidizer that, once ignited, sustain a self propagating exothermic reaction. They are used across a wide range of applications – illuminating and signal flares, delay and ignition trains, gas generators, incendiaries

and heat producing devices, and the performance of each application is governed by a small number of characteristic outputs such as the adiabatic flame temperature, the burning rate, the volume and composition of gaseous products, and the luminous or thermal output [1–3]. Among these, the adiabatic flame temperature is one of the most fundamental thermodynamic parameters because it defines the theoretical upper limit of the energy released during combustion and strongly affects ignition behavior, luminosity, and the phase composition of combustion products [4, 5].

Aluminum is one of the most important metallic fuels in energetic materials because of its high heat of oxidation and low cost, whereas potassium per-

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chlorate remains one of the most widely used oxidizers owing to its high oxygen content and favorable storage and handling characteristics [6-8]. In the aluminum / potassium perchlorate system the energy is released through the reduction of the perchlorate by the metal, which can be written in stoichiometric form as Eq. (1):



This reaction is strongly exothermic, and it drives the flame temperature into the region of 2900-3200 K reported for this class of thermite type compositions [9, 10]. In practical formulations, an organic binder is added to allow the mixture to be pressed or cast. In the present simplified model, the binder is represented by an empirical CH_2O surrogate and acts predominantly as a thermal diluent because its energetic contribution is small relative to the Al/KClO_4 reaction.

The combustion of pyrotechnic mixtures is difficult to predict from first principles. Reactions may occur in both condensed and gaseous phases and proceed through a complex sequence of heating, decomposition, oxidation, melting, evaporation and secondary gas-phase reactions [11-13]. As a consequence, there is no single closed form relationship that links composition to combustion output across a broad range, and formulation has traditionally relied on extensive trial and error experimentation. This makes the field a natural candidate for systematic, model based approaches that can extract the maximum amount of information from a minimum number of trials.

Design of Experiments (DoE) combined with Response Surface Methodology (RSM) provides exactly such a framework. These methods are well established in propellant manufacture and in adjacent areas of energetic materials processing, and a small number of studies have begun to apply them to pyrotechnic formulation [14, 15]. Recent work has, for example, used central composite designs and RSM together with thermochemical simulation to screen and optimize pyrotechnic compositions, demonstrating that response surfaces can reproduce simulated combustion parameters with useful accuracy [16-18].

Despite this progress, the application of DoE and RSM to pyrotechnic systems remains limited. A further methodological challenge is that thermochemical response data are often reported without complete access to the calculation workflow, including software versions, thermodynamic databases, species selections and equilibrium assumptions.

This incomplete reporting can make independent verification and reproduction of simulation-derived response surfaces difficult [19-21]. Furthermore, published response-surface models have primarily focused on compositional factors, whereas process conditions are less frequently incorporated as independent variables. This omission may be significant because the initial reactant temperature affects the enthalpy balance and, consequently, the attainable adiabatic reaction temperature [22]. The role of the initial temperature is of particular interest, because it determines whether preconditioning of a charge can be used as an additional handle on performance, or whether its effect is simply additive and independent of composition.

The present work addresses these gaps for the specific case of the mentioned system. Its novelty lies in three elements taken together. The combustion response – the adiabatic flame temperature – is obtained not from a black box code but from a fully transparent Hess law energy balance built entirely on tabulated NIST–JANAF thermochemical data, so that every computed value is traceable within the stated modelling assumptions. A three factor Box–Behnken design is used to study not only the aluminum and binder contents but also the initial temperature of the reactants as an explicit, independent factor, allowing its relative contribution and its interaction with composition to be quantified rather than assumed. Besides, the entire workflow is implemented with open, general purpose scientific software, providing a compact and fully reproducible template for the statistical modelling of pyrotechnic combustion.

2. Materials and Methods

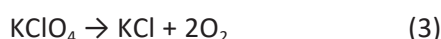
2.1. Pyrotechnic system

The system studied in this work is the ternary formulation $\text{Al}/\text{KClO}_4/\text{organic binder}$. Aluminum was chosen as the metallic fuel and potassium perchlorate as the oxidizer; these are among the most widely used components of modern energetic compositions, offering a high heat of reaction combined with a relatively well characterized thermochemistry. An organic binder was included as the third component, both to reflect real cast or pressed formulations and to provide an independent compositional factor for the statistical design. All compositions are expressed as mass fractions (Eq. 2), and the three components always sum to 100 %:

$$w_{\text{Al}} + w_{\text{KClO}_4} + w_{\text{binder}} = 100\% \quad (2)$$

2.2. Combustion model

The combustion of the mixture was represented by the decomposition of the perchlorate followed by the aluminothermic reduction of the liberated oxygen. The stoichiometric core reaction is as described in Eq. (1), which is balanced in all four elements and corresponds to a stoichiometric aluminum content of 34.2 wt.% for the binary Al/KClO₄ pair. Away from stoichiometry the model treats the excess reagent as an inert, heat absorbing diluent: in fuel rich mixtures the excess aluminum is carried through as condensed metal, whereas in fuel lean mixtures the excess perchlorate decomposes according to Eq. (3):



with the released oxygen acting as a gaseous dilu-

$$-\Delta H_r^0(298) + \sum_{i \in \text{react}} n_i \int_{298}^{T_0} C_{p,i} dT = \sum_{j \in \text{prod}} n_j \int_{298}^{T_{ad}} C_{p,j} dT + \sum_k n_k \Delta H_{\text{phase},k} \quad (4)$$

The sensible-enthalpy contributions of the gaseous products O₂, CO₂, and H₂O were included in the product-side enthalpy balance using the NIST Shomate thermodynamic functions. For O₂ and CO₂, the temperature-dependent C_p(T) expressions were integrated piecewise over the applicable temperature

$$H^o(T) - H_{298.15}^0 = At + \frac{Bt^2}{2} + \frac{Ct^3}{3} + \frac{Dt^4}{4} - \frac{E}{t} + F - H, \quad t = \frac{T}{1000} \quad (5)$$

The standard reaction enthalpy was evaluated from the tabulated enthalpies of formation of the species involved (eq. 6),

$$-\Delta H_r^0(298) = \sum_{\text{prod}} n_j \Delta H_{f,j}^0 - \sum_{\text{react}} n_j \Delta H_{f,j}^0 \quad (6)$$

giving $-\Delta H_r^0 = -6714$ kJ per three moles of oxidiser, i.e. -10.6 kJ·g⁻¹ of stoichiometric mixture. All standard enthalpies of formation, molar heat capacities and phase transition data (melting of KCl and Al₂O₃, and the associated latent heats) were taken from the NIST–JANAF thermochemical tables and the CRC Handbook; the principal values used are collected in Table 1.

The temperature-dependent heat-capacity correlations used for the gaseous products are summarized in Table 2.

Because the temperature of interest exceeds the melting points of the condensed products, the sensible enthalpy term of each product was evaluated piecewise, adding the solid heat capacity up to the melting point T_m, the enthalpy of fusion ΔH_m, and the

ent. For simplicity, the binder was approximated by an empirical CH₂O surrogate, with one mole of CH₂O corresponding to about 4.5 wt.% binder relative to the stoichiometric Al/KClO₄ mixture. Its simplified oxidation contribution was included through the formation of CO₂ and H₂O.

2.3. Adiabatic temperature calculation

The constant pressure adiabatic flame temperature T_{ad} was computed from a Hess-law energy balance at 1 atm (101.325 kPa). The enthalpy released by the reaction at the reference temperature (298.15 K), augmented by the sensible enthalpy of the pre heated reactants, is set equal to the enthalpy required to raise all combustion products from the reference temperature to T_{ad}, including any phase change contributions (Eq. 4):

ranges. For H₂O(g), whose reported gas-phase C_p(T) correlation starts at 500 K, the sensible-enthalpy increment relative to 298.15 K was evaluated directly from the NIST Shomate enthalpy expression (Eq. 5), thereby avoiding extrapolation of the C_p(T) correlation below its stated validity range.

liquid heat capacity above T_m (Eq. 7):

$$\int_{298}^T C_p dT = C_p^s(T_m - 298) + \Delta H_m + C_p^l(T - T_m), \quad T > T_m \quad (7)$$

At the high temperatures reached by this system the endothermic dissociation of the products (principally Al₂O₃ and KCl) becomes an important heat sink and is the physical mechanism that limits the real flame temperature. Rather than solving the full dissociation equilibrium, this effect was represented by an effective heat sink term that switches on above 2500 K and grows with temperature in proportion to the total number of product moles n_{tot} (Eq. 8):

$$H_{\text{diss}} = k_d n_{\text{tot}} (T - 2500)^2, \quad T > 2500 \text{ K} \quad (8)$$

The effective dissociation coefficient k_d was calibrated once using the stoichiometric binary Al/KClO₄ composition by requiring the calculated adiabatic temperature to be approximately 3140 K, consistent with the literature range of 2900–3200 K for this system. This calibration gives k_d ~ 1.37 J·mol⁻¹·K⁻². The

Table 1. Principal thermodynamic data used in the adiabatic-temperature calculation

Species	ΔH_f^0 (298 K), kJ·mol ⁻¹	M, g·mol ⁻¹	C_p (solid), J·mol ⁻¹ ·K ⁻¹	C_p (liquid), J·mol ⁻¹ ·K ⁻¹	T_m , K	ΔH_m , kJ·mol ⁻¹
Al	0.0	26.98	28.3	31.8	933	10.7
KClO ₄	-432.75	138.55	–	–	–	–
KCl	-436.5	74.55	50.0	73.6	1044	26.3
Al ₂ O ₃	-1675.7	101.96	130.0	192.5	2327	111.1

Table 2. Temperature-dependent heat capacities of gaseous products used in the enthalpy balance

Gaseous species	Temperature dependence of $C_p(T)$, J·mol ⁻¹ ·K ⁻¹
O ₂ (g)	100-700 K: $C_p(T) = 31.32234 - 0.02023531T + 5.786644 \times 10^{-5}T^2 - 3.650624 \times 10^{-8}T^3 - 7374/T^2$
	700-2000 K: $C_p(T) = 30.03235 + 0.008772972T - 3.988133 \times 10^{-6}T^2 + 7.88313 \times 10^{-10}T^3 - 741599/T^2$
	2000-6000 K: $C_p(T) = 20.91111 + 0.01072071T - 2.020498 \times 10^{-6}T^2 + 1.46449 \times 10^{-10}T^3 + 9245722/T^2$
CO ₂ (g)	298-1200 K: $C_p(T) = 24.99735 + 0.05518696T - 3.369137 \times 10^{-5}T^2 + 7.948387 \times 10^{-9}T^3 - 136638/T^2$
	1200-6000 K: $C_p(T) = 58.16639 + 0.002720074T - 4.92289 \times 10^{-7}T^2 + 3.8844 \times 10^{-11}T^3 - 6447293/T^2$
H ₂ O(g)	500-1700 K: $C_p(T) = 30.09200 + 0.006832514T + 6.793435 \times 10^{-6}T^2 - 2.534480 \times 10^{-19}T^3 + 82139/T^2$
	1700-6000 K: $C_p(T) = 41.96426 + 0.008622053T - 1.499780 \times 10^{-6}T^2 + 9.8119 \times 10^{-11}T^3 - 11157640/T^2$

Note: The appropriate $C_p(T)$ correlation was applied within its stated temperature range. For H₂O(g), the sensible enthalpy relative to 298.15 K was evaluated directly using the corresponding NIST Shomate enthalpy function; therefore, the 500-1700 K $C_p(T)$ correlation was not extrapolated below 500 K. Source: NIST Chemistry WebBook (Chase, 1998).

same coefficient was subsequently kept fixed for all compositions and all Box–Behnken design points and was not adjusted individually for any formulation. Thus, the term represents an empirical approximation of the aggregate high-temperature dissociation heat sink rather than a full chemical-equilibrium treatment. The energy balance was solved for T_b by bisection to a tolerance below 1 K. The reaction enthalpy of -10.6 kJ·g⁻¹ obtained with this scheme is in good agreement with values reported for thermite type systems, confirming that the underlying thermodynamics are physically sound.

2.4. Design of experiments

A three factor Box–Behnken design (BBD) was used to plan the calculations and to build the response surface. The three independent factors were the aluminum content (A), the binder content (B) and the initial temperature of the reactants (C); the potassium perchlorate content was taken as the

balance and was therefore not an independent variable. Each factor was studied at three coded levels (-1, 0, +1), which were mapped onto the real factor ranges given in Table 3: 26-38 wt.% for aluminum, 2-10 wt.% for the binder and 298-398 K for the initial temperature.

The coded and natural variables are related by Eq. 9:

$$x_i = \frac{X_i - X_{i,0}}{\Delta X_i} \quad (9)$$

where: X_i is the natural value of factor i , $X_{i,0}$ its value at the center level and ΔX_i the step to the ± 1 level.

The BBD places the design points at the mid points of the edges of the cube defined by the three factors, together with replicated points at the center; the corners of the cube are not sampled. For three factors this yields twelve edge points plus center replicates, giving fifteen runs in total when the centre point is replicated three times.

Table 3. Independent factors of the Box–Behnken design and their coded levels

Factor	Symbol	Low (−1)	Centre (0)	High (+1)
Al content, wt.%	A	26	32	38
Binder content, wt.%	B	2	6	10
Initial temperature T°,K	C	298	348	398

2.5. Response surface model and statistical analysis

The adiabatic temperatures computed for the fifteen design points were fitted with a full second order (quadratic) response surface model of the form Eq. 10):

$$\hat{y} = \beta_0 + \sum_{i=1}^3 \beta_{ii} x_i^2 + \sum_{i < j} \beta_{ij} x_i x_j \quad (10)$$

in which $\hat{y}$ is the predicted adiabatic temperature, β_0 the intercept, β_i the linear coefficients, β_{ii} the quadratic coefficients and β_{ij} the two factor interaction coefficients. The coefficients were estimated by ordinary least squares. The quality of the fit was assessed using the coefficient of determination and its adjusted value, together with the regression F-statistic, t-statistics, and associated p-values of the individual polynomial terms. Since the response values were generated deterministically by the thermochemical model, the replicated centre points contain no experimental pure error. Therefore, the F- and t-statistics and the associated p-values are interpreted here as indicators of the relative contribution of the polynomial terms to the quadratic approximation rather than as tests of significance against experimental random noise. Because the estimated pure error is zero, a conventional lack-of-fit F-test based on the ratio of lack-of-fit variance to pure-error variance is not applicable to the present deterministic dataset. The relative importance of the terms was visualized using a Pareto chart of the standardized effects. Model adequacy was assessed primarily from R^2 , adjusted R^2 , RMSE, maximum relative deviation, and residual diagnostics.

The predictive accuracy of the fitted model (Eq. 11) was quantified by the relative deviation between the model prediction and the thermochemical computed value at each design point,

$$\varepsilon = \frac{\hat{y} - y}{y} \cdot 100\% \quad (11)$$

and summarized by the root mean square error. Model adequacy was checked through residual analysis, comprising a plot of the residuals against the fitted

values and a normal probability plot of the residuals. Finally, the fitted surface was numerically maximized over the experimental region to locate the composition of maximum adiabatic temperature.

2.6. Software

All calculations were performed in Python 3.11. The thermochemical energy balance was implemented as a stand alone routine using only the tabulated data described above, so that every computed temperature is fully traceable. The response surface regression and the analysis of variance were carried out with the statsmodels 0.14, numerical optimization of the fitted surface with SciPy 1.13, and all figures were produced with Matplotlib 3.8. No proprietary equilibrium or design of experiments software was required.

3. Results and Discussion

3.1. Experimental design and thermochemical dataset

To evaluate the combustion behavior of the ternary Al/KClO₄/binder system, a three factor Box–Behnken design (BBD) was constructed. The three independent factors were the aluminum content (A), the binder content (B) and the initial temperature of the reactants (C); the potassium perchlorate content (Eq. 12) was treated as the dependent balance, so that the mass fractions always summed to 100%:

$$w_{\text{KClO}_4} = 100 - w_{\text{Al}} - w_{\text{binder}} \quad (12)$$

Each factor was varied over three coded levels (−1, 0, +1). Aluminum was studied between 26 and 38 wt.%, the binder between 2 and 10 wt.%, and the initial temperature between 298 and 398 K. The resulting design, illustrated in Fig. 1, places the experimental points at the mid points of the edges of the factor cube together with a replicated center point; the corners of the cube are deliberately left unpopulated, which is the distinguishing feature of the BBD relative to a full factorial design and which avoids the extreme (and often physically unattainable) combinations of all three factors simultaneously.

The adiabatic flame temperature of each of the fifteen formulations was obtained from a transparent thermochemical calculation rather than from a proprietary equilibrium code. The combustion chemistry was represented by the aluminothermic

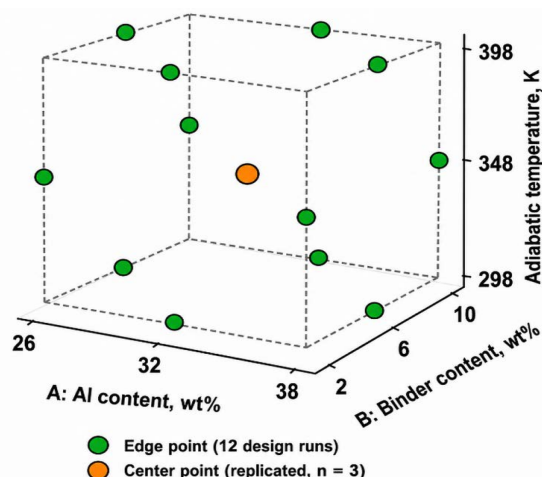


Fig. 1. Three-factor Box–Behnken design. Green markers are the twelve edge-point runs; the orange marker is the replicated center point ($n = 3$). Cube corners are intentionally not sampled. Factors: A = Al content, B = binder content, C = initial temperature T_0 .

reduction of potassium perchlorate (Eq. 1), for which the standard reaction enthalpy (Eq. 13), evaluated from tabulated enthalpies of formation, is

$$\Delta H_r^0(298\text{K}) = (3\Delta H_f^0[\text{KCl}] + 4\Delta H_f^0[\text{Al}_2\text{O}_3]) - 3\Delta H_f^0[\text{KClO}_4] = -6714\text{kJ} \quad (13)$$

per three moles of oxidizer, equivalent to $-10.6\text{ kJ}\cdot\text{g}^{-1}$ of stoichiometric mixture – a value fully consistent with the strongly exothermic character reported for this class of thermite type compositions. The stoichiometric fuel fraction of the binary Al/KClO_4 pair is 34.2 wt.% Al.

The adiabatic (constant pressure) flame temperature T_{ad} (Eq. 14) was found by solving the enthalpy balance in which the heat released by the reaction, corrected for the sensible enthalpy of the preheated reactants, is entirely absorbed by the combustion products as they are raised from the reference temperature to T_{ad} :

$$-\Delta H_r^0 + \sum_{\text{reactants}} n_i \int_{298}^{T_0} C_{p,i} dT = \sum_{\text{products}} n_i \int_{298}^{T_{\text{ad}}} C_{p,i} dT + \sum_k n_k \Delta H_{\text{phase},k} \quad (14)$$

The heat-capacity integrals and phase-transition enthalpies (fusion of KCl and Al_2O_3) were based on tabulated NIST–JANAF data, whereas the effective high-temperature dissociation term was introduced empirically as described in Section 2.3. With this model, the stoichiometric binary composition reaches $\approx 3140\text{ K}$, within the literature range of 2900–3200 K reported for Al/KClO_4 . Since this temperature range was used to calibrate the effective dissociation coefficient, the agreement should be interpreted as consistency with the calibration target rather than as an independent validation of the model.

The complete design and the computed responses are summarized in Table 4.

The adiabatic temperature spans 2862.5–3080.0 K across the design space. The three replicated center points (runs 13–15) return identical values of 3051.6

K; because the response is generated deterministically, the pure error is effectively zero, and the small residual scatter discussed below arises solely from lack of fit of the polynomial surface.

3.2. Response surface model

The thermochemical dataset was fitted with a full second order (quadratic) response surface model in the three coded factors x_1 (Al), x_2 (binder) and x_3 (initial temperature) (Eq. 15):

$$T_{\text{ad}} = \beta_0 + \sum_{i=1}^3 \beta_i x_i + \sum_{i=1}^3 \beta_{ii} x_i^2 + \sum_{i < j} \beta_{ij} x_i x_j \quad (15)$$

Ordinary least squares regression yielded the fitted equation (Eq. 16)

$$\hat{T}_{\text{ad}} = 3051.6 - 2.84x_1 - 44.92x_2 + 2.39x_3 - 108.07x_1^2 - 9.26x_2^2 - 12.23x_3^2 - 27.62x_1x_2 \quad (16)$$

Table 4. Box–Behnken design and computed adiabatic temperature for the Al/KClO₄/inder system

Run	A	B	C	Al, wt.%	Binder, wt%	KClO ₄ , wt.%	T ₀ , K	T _{ad} , K
1	-1	-1	+0	26.0	2.0	72.0	348.15	2950.8
2	+1	-1	+0	38.0	2.0	60.0	348.15	3002.2
3	-1	+1	+0	26.0	10.0	64.0	348.15	2921.6
4	+1	+1	+0	38.0	10.0	52.0	348.15	2862.5
5	-1	+0	-1	26.0	6.0	68.0	298.15	2932.5
6	+1	+0	-1	38.0	6.0	56.0	298.15	2925.0
7	-1	+0	+1	26.0	6.0	68.0	398.15	2937.5
8	+1	+0	+1	38.0	6.0	56.0	398.15	2930.0
9	+0	-1	-1	32.0	2.0	66.0	298.15	3075.4
10	+0	+1	-1	32.0	10.0	58.0	298.15	2980.2
11	+0	-1	+1	32.0	2.0	66.0	398.15	3080.0
12	+0	+1	+1	32.0	10.0	58.0	398.15	2984.8
13	+0	+0	+0	32.0	6.0	62.0	348.15	3051.6
14	+0	+0	+0	32.0	6.0	62.0	348.15	3051.6
15	+0	+0	+0	32.0	6.0	62.0	348.15	3051.6

Note: A = Al content, B = binder content, C = initial temperature T₀; KClO₄ is the balance

with the two remaining interaction terms (x_1x_3 and x_2x_3) being negligible.

The quadratic model provides an excellent approximation of the deterministic thermochemical response, with a coefficient of determination of $R^2 = 0.9990$. The overall regression F-value is 534 ($p < 10^{-6}$); in the present deterministic dataset, this statistic reflects the strength of the quadratic approximation relative to the residual approximation error rather than significance against experimental random variability.

The corresponding response surface is shown in Fig. 2 as a function of aluminum and binder content at the central initial temperature. The surface is a smooth dome: the temperature rises towards the stoichiometric aluminum content and falls on both the fuel lean and fuel rich sides, while increasing binder content lowers the temperature monotonically. The design points, projected onto the surface, lie close to it, reflecting the excellent fit.

Figure 3 presents the same response as a two dimensional contour map, which locates the optimum more precisely.

Numerical maximization of the fitted model over the experimental region places the temperature optimum at 32.7 wt.% Al and 2.0 wt.% binder (with the initial temperature near its center value), predicting a maximum adiabatic temperature of 3089 K. The optimum binder content coincides with the lower bound of the factor, which is physically reasonable.

dominant aluminum and binder terms. Therefore, the overall influence of the initial temperature is described here as comparatively weak rather than statistically insignificant.

In contrast, the linear aluminum effect ($p = 0.076$), the linear initial-temperature effect ($p = 0.119$), and both interactions involving initial temperature showed comparatively weak contributions to the fitted quadratic model. The negligible linear aluminum term is a direct consequence of the design being centred close to the temperature maximum, where the first derivative of the response

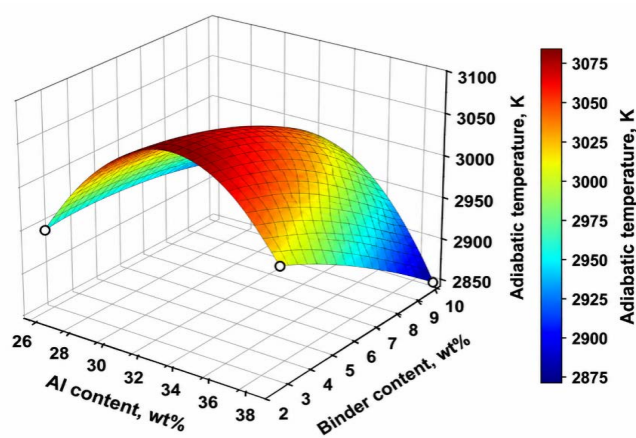


Fig. 2. Response surface of the adiabatic temperature as a function of aluminum and binder content, at the central initial temperature. White markers show the design points projected onto the fitted surface.

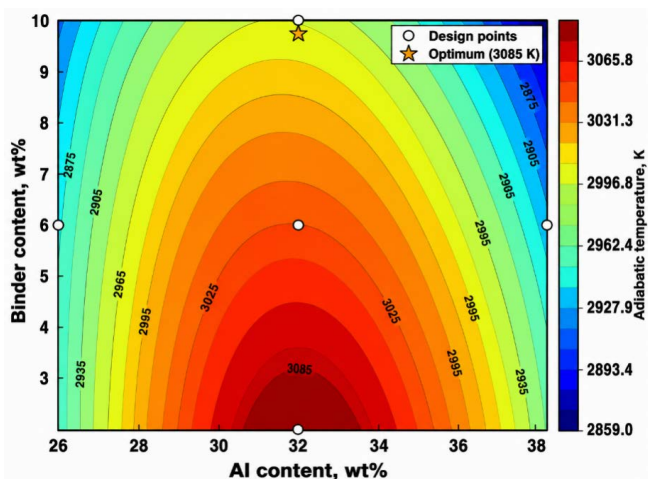


Fig. 3. Contour map of the adiabatic temperature over aluminum and binder content. White circles are the design points; the star marks the predicted optimum (3089 K at 32.7 wt.% Al, 2.0 wt.% binder).

The organic binder acts predominantly as a thermal diluent, so the temperature is maximized at the lowest binder loading. The optimum aluminum content lies essentially at the center of the studied range, consistent with the strong curvature of the surface in the x_1 direction.

3.3. Relative importance of the model terms

The relative importance of the model terms is visualized as a Pareto chart of the standardized effects (absolute t values) in Fig. 4.

The standardized effects indicate that five terms make the largest contributions to the fitted quadratic response surface. The dominant contribution is the quadratic aluminum term (A^2 ; $|t| = 57.6$), whose large negative coefficient produces the pronounced temperature maximum and reflects the transition from fuel-lean to fuel-rich compositions. This behavior is physically consistent with the thermochemistry of the Al/KClO₄ system: the adiabatic temperature reaches a maximum close to the stoichiometric fuel–oxidizer ratio, whereas excess oxidizer on the fuel-lean side and excess unreacted aluminum on the fuel-rich side act as heat-absorbing components. The second strongest contribution is the linear binder term (B ; $|t| = 35.2$), consistent with the role of the binder as a thermal diluent, followed by the Al $\times$ binder interaction ($|t| = 15.3$). The quadratic binder and initial-temperature terms make smaller contributions to the polynomial approximation. Although the quadratic initial-temperature term C^2 exceeds the conventional regression threshold, its standardized effect is substantially smaller than those of the

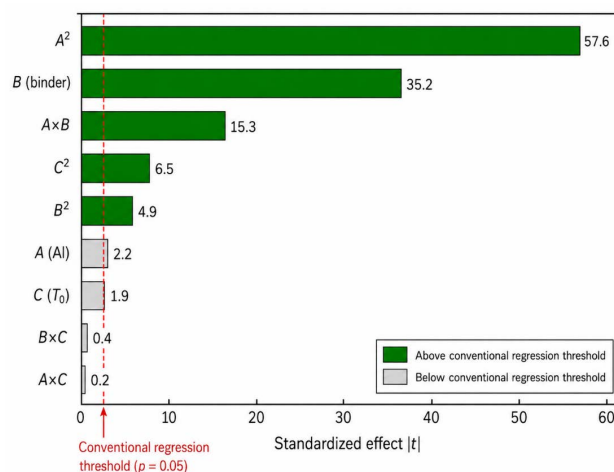


Fig. 4. Pareto chart of the standardized effects ($|t|$) of the model terms. The dashed line corresponds to the conventional $p = 0.05$ regression threshold; for the present deterministic dataset, the standardized effects are used to compare the relative contributions of the polynomial terms.

vanishes. The comparatively weak contribution of the terms involving the initial temperature indicates that preheating acts primarily as an additive sensible-enthalpy contribution and has little interaction with composition within the investigated range.

3.4. Model validation and adequacy

The predictive quality of the fitted model was assessed by comparing the RSM predictions with the thermochemical computed temperatures for all fifteen runs. The parity plot in Fig. 5 shows the predicted values plotted against the computed values together with the line of perfect agreement.

All points lie essentially on this line: the root mean square error is only 2.1 K and the maximum relative deviation (Eq. 17), evaluated as

$$\varepsilon = \frac{\hat{T}_{ad} - T_{ad}}{T_{ad}} \cdot 100\% \quad (17)$$

does not exceed 0.13% over the entire design space. This confirms that the quadratic surrogate reproduces the underlying thermochemistry to well within any practically relevant tolerance and can therefore replace the full calculation for rapid interpolation and optimization.

Model adequacy was further examined through residual diagnostics, shown in Fig. 6.

In the plot of residuals against fitted values (Fig. 6a) the residuals scatter randomly about zero within a narrow band of ± 3.6 K, with no funnel shape or systematic trend, indicating that the variance is homogeneous and that no important term has been

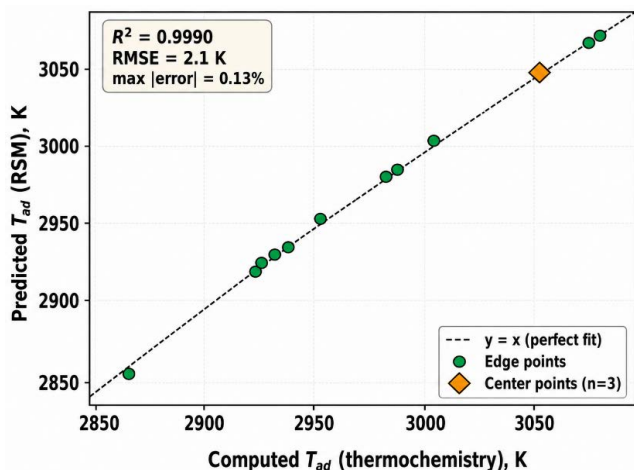


Fig. 5. Parity plot of RSM-predicted versus thermochemical computed adiabatic temperature for all fifteen runs. The dashed line is the line of perfect agreement ($R^2 = 0.9990$, RMSE = 2.1 K, maximum error 0.13%).

omitted from the model. The normal probability plot of the residuals (Fig. 6b) is close to linear, with a correlation coefficient of 0.99, so the normality assumption underlying the regression is satisfied. Taken together with the high R^2 and the low prediction error, these diagnostics confirm that the second-order model provides an adequate representation of the deterministic response surface.

The results demonstrate that a compact Box–Behnken design combined with response surface methodology captures the combustion behavior of the Al/KClO₄/binder system with high fidelity, using only fifteen formulations and a transparent thermochemical model in place of a proprietary equilibrium solver. The fitted surface reproduces the two governing physical trends – a composition of maximum temperature near the stoichiometric aluminum con-

tent, and a monotonic cooling effect of the binder acting predominantly as a thermal diluent – and quantifies their interaction. The dominance of the quadratic aluminum term and of the linear binder term, together with the comparatively weak influence of the initial temperature, provides a clear and physically interpretable ranking of the factors that would be difficult to obtain from a one factor at a time study.

A limitation of the present study is the absence of direct experimental validation of the calculated adiabatic flame temperatures. The present results are entirely model-based; therefore, the absolute temperature values should be regarded as engineering estimates rather than experimentally validated predictions. In addition, the thermochemical model assumes complete reaction, treats dissociation through a single effective term, and does not resolve the condensed/gaseous partitioning of the alumina product in detail. Nevertheless, because the same model underlies every design point, the relative trends and the fitted response surface are robust, and the methodology is directly transferable to experimentally measured responses such as burning rate or luminous output. Extending the design to a genuinely multi response formulation, and validating the predictions against experimental firings, are the natural next steps of this work.

4. Conclusion

A three factor Box–Behnken design combined with Response Surface Methodology was used to model the adiabatic flame temperature of the aluminum/potassium perchlorate/binder system. Using only fifteen formulations, the temperature

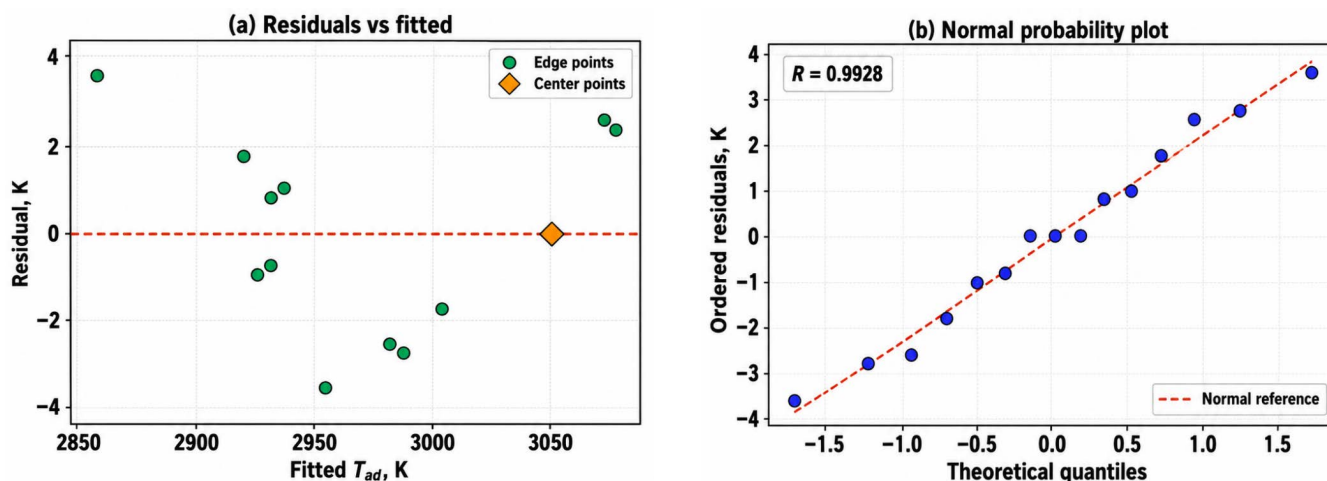


Fig. 6. Residual diagnostics for the fitted model: (a) residuals versus fitted values; (b) normal probability plot of the residuals.

was mapped over the ranges 26–38 wt.% Al, 2–10 wt.% binder and 298–398 K initial temperature. The temperature of each formulation was obtained from a fully transparent Hess law energy balance based on tabulated NIST–JANAF data rather than a proprietary equilibrium code, so that every computed value is traceable. The model reproduced the reaction enthalpy of $-10.6 \text{ kJ}\cdot\text{g}^{-1}$, while the effective dissociation coefficient was calibrated to yield a stoichiometric flame temperature within the literature range of 2900–3200 K. The latter agreement therefore represents consistency with the calibration target rather than an independent validation of the model.

A full quadratic response surface model fitted the fifteen computed points with $R^2 = 0.9990$ and a maximum relative error below 0.13%, so that the polynomial surrogate reproduces the thermochemical calculation to well within any practical tolerance. Residual diagnostics confirmed the adequacy of the fit: the residuals scattered randomly about zero within $\pm 3.6 \text{ K}$ and followed a normal distribution.

The fitted model gave a clear and physically interpretable ranking of the factors. The temperature was governed primarily by the quadratic effect of the aluminum content, which produces a well defined maximum near the stoichiometric composition, and the linear thermal-dilution effect of the binder, together with their interaction. In contrast, the initial temperature and its interactions with composition made comparatively weak contributions to the fitted response surface within the investigated range. From a thermochemical perspective, this indicates that pre-heating primarily contributes additional sensible enthalpy to the reactants, whereas the attainable adiabatic temperature is governed predominantly by the fuel–oxidizer ratio and the thermal-dilution effect of the binder. Numerical optimization of the surface located a maximum adiabatic temperature of about 3089 K at 32.7 wt.% aluminum and the lowest binder loading, consistent with the diluent role of the binder.

The absolute temperatures should be regarded as engineering estimates, since the model assumes complete reaction and represents high temperature dissociation through a single effective term; because the same model underlies every design point, however, the relative trends and the fitted surface remain robust.

Author Contributions

Dinara Muktaly – Conceptualization, Methodology, Supervision, Project Administration and Writing – Review & Editing. **Olesya Tyumentseva** – Validation, Supervision, Writing – Review & Editing. **Oksana Chervyakova** – Validation, Writing – Review & Editing. **Aigerim Imash** – Validation, Visualization. **Bagdatgul Milikhat** – Validation, Visualization. **Aslan Akberliyev** – Validation, Data Curation, Writing – Original Draft. **Lyazzat Mussapyrova** – Validation, Visualization, Writing – Original Draft.

Conflict of Interest

The authors declare that they have no conflict of interest.

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Моделирование поверхности отклика адиабатической температуры пламени пиротехнических составов Al/KClO₄

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АННОТАЦИЯ

В настоящем исследовании методы планирования эксперимента и методология поверхности отклика (RSM) применены к трехкомпонентной системе Al/KClO₄/связующее, при этом в качестве целевого отклика выбрана адиабатическая температура пламени. Для содержания алюминия (26–38 мас.%), связующего (2–10 мас.%) и начальной температуры реагентов (298–398 К) был построен трехфакторный план Бокса–Бенкена, а температура пламени для каждого из пятнадцати полученных составов рассчитана на основе полностью прозрачного энергетического баланса по закону Гесса с использованием табличных данных NIST–JANAF, без применения закрытого программного обеспечения для равновесных термохимических расчетов. Модель воспроизвела как энтальпию реакции, равную -10,6 кДж·г⁻¹, так и приводимый в литературе для данной системы диапазон температур пламени 2900–3200 К. Полная квадратичная модель поверхности отклика описала расчетные данные с коэффициентом детерминации 0,9990 и максимальной относительной погрешностью менее 0,13%, а анализ остатков подтвердил адекватность модели. Наибольший вклад в изменение температуры вносили квадратичный эффект содержания алюминия и линейный охлаждающий эффект связующего, тогда как начальная температура в исследованном диапазоне оказывала сравнительно слабое влияние, действуя преимущественно аддитивно и практически независимо от состава. Численная оптимизация показала, что максимальная адиабатическая температура около 3089 К достигается при содержании алюминия 32,7 мас.% и минимальном содержании связующего.

Ключевые слова: пиротехнические составы, алюминий/перхлорат калия, адиабатическая температура пламени, планирование эксперимента, методология поверхности отклика, план Бокса–Бенкена

Al/KClO₄ пиротехникалық құрамдарындағы жалынның адиабаталық температурасын жауап беті арқылы модельдеу

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АҢДАТПА

Бұл зерттеуде тәжірибені жоспарлау әдісі және жауап бетінің әдіснамасы (RSM) Al/KClO₄/байланыстырғыш үшкомпонентті жүйесіне қолданылып, мақсатты жауап ретінде жалынның адиабаталық температурасы таңдалды. Алюминий мөлшері (26-38 масс.%), байланыстырғыш мөлшері (2-10 масс.%) және реагенттердің бастапқы температурасы (298-398 K) бойынша үш факторлы Бокс–Бенкен жоспары құрылды. Алынған он бес құрамның әрқайсысы үшін жалын температурасы жабық тепе-теңдік бағдарламасын қолданбай, NIST–JANAF кестелік деректеріне негізделген Гесс заңы бойынша толық қадағаланатын энергетикалық баланс арқылы есептелді. Модель осы жүйе үшін реакция энтальпиясының -10,6 кДж·г⁻¹ мәнін де, әдебиетте келтірілген 2900-3200 K жалын температурасы аралығын да қайта өндірді. Толық квадраттық жауап беті моделі есептік деректерді детерминация коэффициенті 0,9990 және ең үлкен салыстырмалы қателігі 0,13%-дан төмен мәнмен сипаттап, қалдықтар бойынша модель адекваттылығын бағалаудың барлық тексерулерінен өтті. Температураға негізінен алюминий мөлшерінің квадраттық әсері және байланыстырғыштың сызықтық салқындату әсері ықпал етті, ал бастапқы температура зерттелген аралықта салыстырмалы түрде әлсіз үлес көрсетіп, негізінен аддитивті түрде және құрамнан тәуелсіз әсер етті. Сандық оңтайландыру алюминий мөлшері 32,7 масс.% және байланыстырғыштың ең төмен мөлшері кезінде жалынның адиабаталық температурасының шамамен 3089 K максимал мәнін анықтады.

Түйін сөздер: пиротехникалық құрамдар, алюминий/калий перхлораты, жалынның адиабаталық температурасы, тәжірибені жоспарлау, жауап бетінің әдіснамасы, Бокс–Бенкен жоспары