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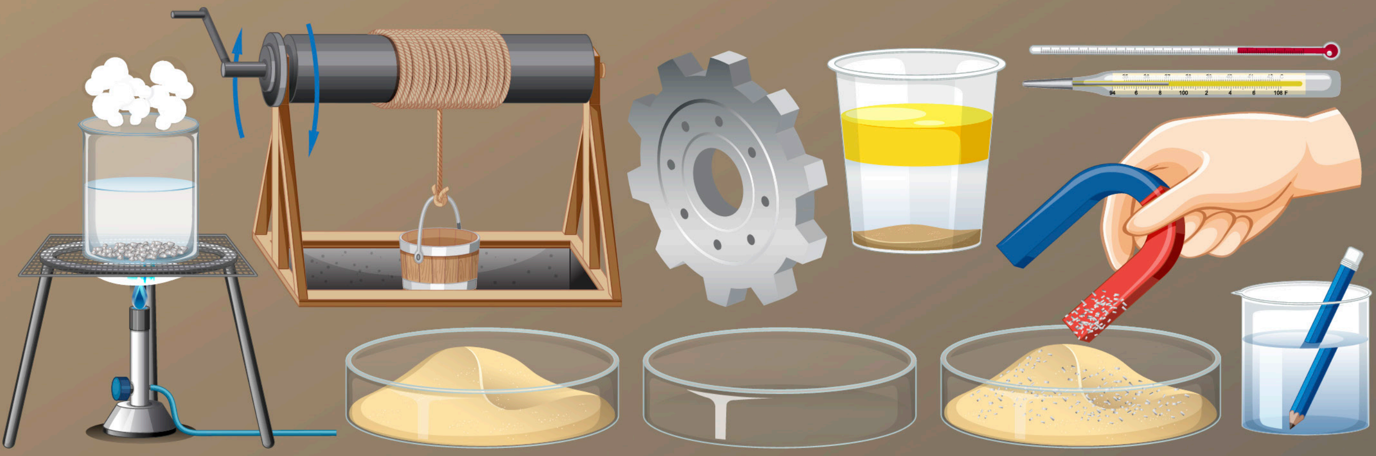

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# Advanced Predictive Modelling for the Optimization of Graphite Crucible Pots from Kaolin Clay and Functional Additives

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## ABSTRACT

This research investigates the optimization of graphite crucible pots made from kaolin clay and functional additives. The study demonstrates that kaolin clay enhances mechanical strength through ceramic bonding while preserving high thermal conductivity from the graphite matrix. Various additives were evaluated to customize the crucible properties, including silicon carbide, granite, borosilicate glass powder, and sodium silicate binder. Predictive models were developed alongside Response Surface Methodology (RSM) optimisation to formulate graphite crucible compositions with optimal mechanical strength and thermal shock resistance. Furthermore, Finite Element Analysis (FEA) was used to simulate thermal and mechanical stresses experienced by the crucibles during operation. The results reveal a strong correlation between experimental and predicted values for optimization, highlighted by high regression coefficient ($R^2$) values. The optimal composition was determined to be 43.5721% kaolin clay, 3.31722% granite, and 7.05904% borosilicate glass, yielding a crucible with a hardness of 55.78, compressive strength of 25.02 MPa, thermal conductivity of 3.32 W/mK, thermal expansion of 2.3760E-5 per °C, and a density of 2.35424 g/cm³. FEA demonstrated that this optimized crucible can withstand temperatures exceeding 2000 degrees Celsius. Comparative analysis showed that the optimized graphite composite crucible significantly outperformed the commercial EQ-CB-G001015-LD graphite crucible, exhibiting higher density and superior temperature resistance, thereby reflecting enhanced material properties. The findings provide valuable insights into the formulation and design of composite crucibles with improved performance, presenting promising advancements for industrial applications.

## INTRODUCTION

Crucibles have been a vital instrument for melting metals and other materials for thousands of years (Ubani & Onyenanu, 2024). Crucibles were used in metalworking activities requiring melting and casting processes as early as 6000 BC in Eastern Europe and Iran (Feuerbach, 2002; Ubani & Onyenanu, 2024). Crucibles serve as holding vessels that enable the heating of metals and other substances to their melting points without losing control or coming into direct contact with the heat source (Krishnamurthy, 2022). Typically, crucibles are made of refractory materials like clay, graphite, silicon carbide, and others that can withstand high temperatures (Taiwo *et al.,* 2023; Ubani & Onyenanu, 2024). Crucibles are ceramic containers used in high-temperature applications; they serve as stationary reaction vessels in which high-temperature transformations take place without the crucible coming into direct contact with the heating source (Adeoti *et al.,* 2019a; Adeoti *et al.,* 2019b; Ubani & Onyenanu, 2024). Because graphite has some beneficial qualities, it is most frequently employed in crucibles to melt non-ferrous metals like copper, zinc, aluminum, and alloys (Ubani & Onyenanu, 2024). Thermal shock resistance, a self-lubricating inner surface, chemical inertness against common slags and corrosive environments, a very high melting point surpassing 3500°C, and very little reactivity with ferrous and non-ferrous melts are some of these characteristics (Adeoti *et al.,* 2019b). The efficiency and effectiveness of these crucible pots hinge on these properties. Traditionally, graphite crucible pots are manufactured by compressing and baking graphite powder. However, this conventional method often results in products that are fragile and susceptible to cracking under the stress of extreme heating and cooling cycles, which can lead to significant melt losses and contamination (Jhavar *et al.,* 2013).

Researchers have investigated the creation of ceramic-graphite composite materials as a solution to these issues. By enhancing the mechanical strength and resilience of the crucibles to heat shock, these composites enable improved performance in demanding environments. Combining kaolin clay with graphite has shown great promise as a ceramic addition that can improve crucible pots' mechanical qualities without sacrificing their heat conductivity (Madukasi *et al.,* 2025). According to studies, kaolin clay reduces thermal expansion and increases resistance to thermal shock (Abubakar *et al.,* 2021). Also, it has been demonstrated that additional functional additives, including silicon carbide (SiC), improve high-temperature stability and wear resistance (Liu, 2013).

In light of these developments, predictive modelling such as Response Surface Methodology (Idogho *et al.,* 2025; Onyenanu *et al.,* 2024) offers a useful tool for improving the material properties of graphite crucible

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pots. Response Surface Methodology (RSM) allows researchers to evaluate the effects of multiple variables and their interactions on specific responses, facilitating the identification of optimal conditions for desired properties (Madukasi *et al.,* 2025; Offodum *et al.,* 2025). The interactions between various components, such as kaolin clay and other additives, can be assessed and improved by scientists using this advanced predictive modelling technique, leading to tailored material qualities that meet specific operating requirements. To provide improved performance, greater durability, and fewer failures during high-temperature operations, this study optimises graphite crucible pots using predictive modelling. Thus, the primary objective of this study is to optimize (Ezechukwu *et al.,* 2025) graphite crucible pots from kaolin clay and additives using predictive modeling, focusing on thermal stability, mechanical strength, and cost efficiency for high-temperature industrial applications.

## LITERATURE REVIEW

This review examines relevant studies focused on optimizing graphite crucibles to enhance their mechanical strength, thermal resistance, and chemical durability, as well as on applying predictive modelling techniques.

### Optimization of Crucible Pots

Soemowidagdo (2019) researched to optimize the performance of compact crucible furnaces by adjusting the positioning of the crucible pot. The study involved a crucible pot with a diameter of 170 mm and a height of 250 mm, with the supporting height varied at increments of 20, 40, 60, 80, and 100 mm. The performance of the furnace was evaluated based on the rate of temperature rise required to melt 3 kg of aluminium, with temperature changes monitored using an infrared thermometer. The findings indicated that a pot support height of 60 mm resulted in optimal performance, achieving a temperature of 600 °C in just 35 minutes.

In another study, Adeoti (2019) optimized a clay-bonded graphite crucible by combining clay, graphite, and selected additives (MgO and SiC) using D-optimal design methodology within the Design-Expert software (version 6.08). The samples were air-dried for two weeks, followed by oven drying at 100 °C and firing in a muffle furnace at 1100 °C. Mechanical tests were conducted to assess bulk density, linear firing shrinkage, and apparent porosity. The results indicated that Run 7, comprising 80% clay, 10% graphite, and 10% MgO and SiC, yielded the lowest bulk density of 1.80. Conversely, run 9 achieved the lowest apparent porosity with a composition of 70% clay and 30% additives. Notably, run 13, with 80% clay, 10% graphite, and 5% each of MgO and SiC, exhibited the highest bulk density (2.91), the lowest linear shrinkage (2.15), and an apparent porosity of 28.20. These results were consistent with literature values, confirming that Run 13 represented the optimal composition based on computer analysis and mechanical testing.

### Predictive Modelling

Ndirika (2006) developed a mathematical model to predict the output capacity of a threshing process in a throw-in-feed system using Buckingham's Pi Theorem for dimensional analysis. The model was validated against experimental data from a stationary mechanical millet thresher, demonstrating a strong correlation with an R-squared value of 0.99. Additionally, the statistical analysis indicated no significant difference between the predicted and measured output capacities at a 5% significance level, confirming the model's reliability.

Similarly, Nkakini, Ekemube, and Igoni (2019) created a predictive model for fuel consumption during harrowing operations, also employing dimensional analysis with Buckingham's Pi Theorem. The study was conducted on loamy sand soil in Rivers State Agricultural Development Program Farm and utilized a Factorial Randomized Complete Block Design (RCBD) for experimentation. Key parameters, including draught, harrowing speed, depth, moisture content, cone index, and cut width, were meticulously measured. The validated fuel consumption model showed strong agreement between predicted and actual results, with a low root mean square error (RMSE) and t-test results indicating no significant difference at both 95% and 99% confidence levels. This suggests the model's applicability for predicting fuel consumption in similar agricultural operations.

## MATERIALS AND METHODS

### Materials

The major material utilised for this investigation is kaolin clay, while other functional additives used are listed as follows: graphite powder, granite powder, borosilicate glass powder, silicon carbide powder, and sodium silicate binder.

**Table 1:** Materials Characterization and Processing Details

| Material | Source | Processing Method | Particle Size (μm) | Compliance/Quality Notes |
|---|---|---|---|---|
| Kaolin Clay | Alkaleri mine site, Nigeria | Sedimentation, levigation, milling, and sieving | 75–150 | Purified to API specifications |
| Graphite Powder | Capital Ceramics Nigeria Limited | Milling and sieving of as-received powder (90% ≤145 μm) | 75–150 | High-purity, uniform particle distribution |
| Granite Powder | Local sources (Nigeria) | Crushing, milling, and sieving | 75–150 | Off-white color, consistent particle size |

| | | | | |
|---|---|---|---|---|
| Borosilicate Glass Powder | Commercial supplier | None (pre-processed) | <150 | Industry-standard purity, ready for use |
| Silicon Carbide Powder | Commercial supplier | None (as-received) | <150 | Meets specifications, no further processing needed |
| Sodium Silicate Binder | Commercial-grade solution | Characterized by viscosity and pH | Liquid solution | Complies with organic binder requirements |

### Experimental Design

For this study, the thermal and mechanical performance of the composite material was investigated to fine-tune five product attributes, which are measured as responses from a design experiment.

Response 1: Hardness value BHN
Response 2: Compressive Strength N/mm2
Response 3: Thermal Conductivity (C) W.M-1. K-1
Response 4: Thermal expansion µm/mm/$^0$C
Response 5: Density g/cm$^3$

Again, the three primary material mixture factors that affect the performance of the insulating composite vary as shown:

$40\% \leq C$ (Kaolin Clay) $\leq 48$
$2\% \leq B$ (Granite) $\leq 10\%$
$7\% \leq C$ (Borosilicate Glass) $\leq 8$

### Production Process

The production process developed involves specific unit operations to transform the raw materials into functional graphite crucibles. The overall process flow involves raw material preparation and characterization, formulation of crucible compositions, shaping of green bodies, densification through sintering, and rigorous characterization and testing of the sintered samples.

### Raw Material Preparation and Characterization

The key raw materials utilized are graphite powder, kaolin clay, granite powder, borosilicate glass powder, and silicon carbide powder. These are locally sourced within Nigeria to promote sustainable indigenous production. The materials are crushed and finely ground using a ball mill to obtain homogeneous powder batches below 75 microns in size. This fine powder state enhances mixing and densification during sintering. The raw materials then undergo multi-fold characterization analyses to gain critical insight into their properties. Elemental characterization is carried out using X-ray fluorescence spectroscopy (XRF) to quantify major and minor elemental constituents in weight percentages. Phase analysis employs X-ray diffraction (XRD) to identify crystalline compounds present. Additional analyses, such as particle size distribution, specific surface area, and chemical reactivity tests, provide a comprehensive material profile. This characterization data forms the baseline to design optimized crucible compositions tailored for high performance.

### Formulation of Crucible Compositions

Based on the input from the raw material characterization, several crucible compositions are developed throughout the design space. The weight percentages of each raw material are changed in methodical combinations under the direction of theoretical density modelling and preliminary testing. As the major structural phase, graphite weight is kept between 30 and 40%, with additions of silicon carbide, kaolin, granite, and borosilicate glass ranging between 5 and 15% each. Based on their qualities as measured during characterization, additives are selected to give the graphite matrix qualities including strength, refractoriness, resistance to thermal shock, and

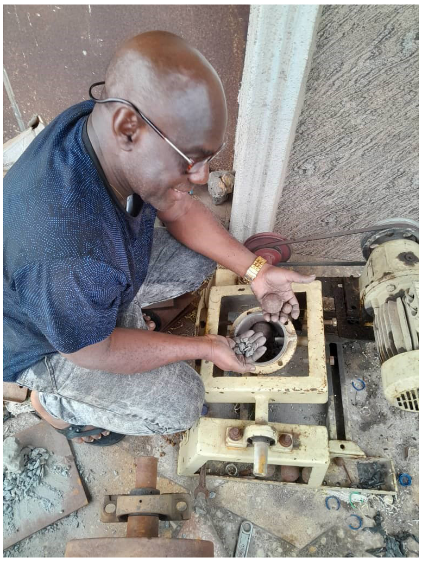


**Figure 1:** Crushing the raw materials using a locally-made ball mill

**Figure 2:** Prepared Graphite Crucible Test Samples with Varying Compositions

immunity to corrosion. Fifteen crucible compositions are completed for experimental assessment.

### Raw Material Mixing and Binder Addition

For experimental testing, bulk quantities of formulations with preset compositions are made. Zirconia milling media is used to properly dry-mix weighed amounts of raw material powders according to each recipe for two hours in stainless steel containers. To prevent inhomogeneity during the green body fabrication and sintering stages, the moisture level is tracked and kept below 1%. To create consistent plastic slurry mixtures, a 5-7% aqueous solution of sodium silicate binder is gradually added while being continuously mixed after the liquid has been blended uniformly. Before shaping, these are soaked overnight for maximum workability and plasticity.

### Green Body Formation

The freshly manufactured plastic slurries are uniaxially pressed into pre-lubricated graphite die moulds of conical crucible forms with a hydraulic press under 20 MPa pressure to form 'green' compacts that keep their geometry. The pressing parameters are optimised to remove defects while maintaining net dimensions. Formed compacts are gently ejected and air-dried at room temperature for two days to provide adequate strength before the binder is removed via thermal disintegration in the next stage.

**Figure 3:** Pressed green crucible bodies formed via uniaxial compaction using hydraulic pressing

### Densification via Sintering

In order to create a porous ceramic structure, dried green compacts are heated gradually from ambient temperature to 500°C over the course of eight hours in a muffle furnace, which breaks down the organic binder phase. A final high-temperature sintering treatment is then applied for two hours at 1200°C in a programmable box furnace to accomplish complete densification through shrinkage, microstructural development, and particle bonding. To reduce thermal strains, heating and cooling rates are gradually maintained at 5°C/min.

**Figure 4:** The samples undergoing Densification via Sintering

### Testing Methods (Thermal and Mechanical Properties Investigation)

Various tests were conducted on the crucible material samples that had been developed. These tests were done to verify the mechanical properties of the sample. The summary of the test parameters, applicable standards, equipment used, sample descriptions, test conditions, and output metrics is presented in Table 2 below.

**Table 2:** Summary of Test Parameters, Standards, Equipment, and Output Metrics for Characterizing Graphite Crucible Samples

| Test Parameter | Method/ Standard | Equipment Used | Sample Details | Test Conditions | Output Parameters |
|---|---|---|---|---|---|
| Hardness | Vickers hardness (ASTM C1327) | Leco LM-700AT Vickers hardness indenter | Polished cross-sections | Load: 100g, Dwell time: 15s, 20 random indentations per sample | Hardness value (HV) |
| Compressive Strength | Diametral compression (ASTM D1621) | Shimadzu AG-X universal tester | Cuboidal samples (10×10×15 mm) | Crosshead rate: 0.5 mm/min until fracture; 5 replicates | Maximum load at failure, compressive strength (MPa) |
| Density & Porosity | Archimedes' principle | Sartorius balance | Sintered specimens (5 replicates) | Fluid medium: Deionized water | Bulk density (ϱ<sub>b</sub>), theoretical density (ϱ<sub>t</sub>), porosity (%) |
| Thermal Analysis | TGA/DTA (Simultaneous) | PerkinElmer STA 6000 | Raw material powders | Temperature range: 30–1300°C, Heating rate: 10°C/min, Air atmosphere | Weight loss (TGA), endothermic/ exothermic peaks (DTA) |
| Dilatometry | Thermal expansion analysis | NETZSCH DIL 402C dilatometer | Cylindrical samples (Ø5 mm × 10 mm) | Temperature profile: 30–1300°C, Sintered at 1200°C | Dimensional changes, coefficient of thermal expansion (CTE) |

## Predictive Modelling Techniques

### Finite Element Analysis (FEA)

FEA simulations using SolidWorks were used to model the thermal and mechanical stresses experienced by the crucible during operation. This was done by simulating the optimal values of the material properties generated with a specified crucible geometry.

### Thermal Modelling using SolidWorks

Computational simulation offers significant advantages over traditional experimentation by enabling virtual prototyping and parametric analysis of products and processes without needing multiple physical iterations. This study used thermal modelling to gain insights into temperature distributions and optimize crucible compositions and geometries through virtual testing before fabrication.

### Geometry Creation

Models with 50 mm, 70.5 mm, and 100 mm wall thicknesses were created through solid extrusion of 2D sketches. Hollow cylinder shapes of an inner diameter of 105.70 mm, outer diameter of 209.58 mm, and height of 250 mm were also designed to emulate crucible pot forms. All models were

**Figure 5:** Designed/ Fabricated Crucible Pot

constructed with reference planes, axes, and dimensions defined to ensure consistency and repeatability. Fillets and rounds were added to replicate sample edge features observed through microscopy. Geometries were kept as simplified uniform blocks for the preliminary analysis, but could be refined further with CAD tools as required.

### Mesh Generation

Automatic meshing was employed to discretize the geometry into finite elements for solving the heat transfer partial differential equations. Tetrahedral elements were preferred for higher geometric flexibility to conform to arbitrary shapes. Mesh sensitivity analysis was conducted by varying element densities and examining outputs such as maximum temperature and CPU times until grid independence was reached. Maximum element size was reduced from the initial 6 mm to the final 2 mm through successive simulations. Element counts were monitored and stabilized by nearly 50,000 elements found to provide acceptable accuracy within reasonable computational costs. An adaptive mesh was applied near geometric features like edges to better capture boundary effects. Mesh quality parameters ensured model accuracy and solver stability.

### Boundary Conditions

For all external surfaces, insulating conditions were established by setting the surface heat flux to zero. During early heating cycles, convection was thought to have a small impact in comparison to conduction. To simulate contact with a heating element, a temperature-dependent heat transfer coefficient profile was applied to the lower base surface. The boundary condition curve throughout the intended dwell period was constructed using temperature-time data from actual cylindrical furnace calibrations. For the model domain, the starting temperature was set at a consistent room temperature of 25°C. Both steady-state and transient analyses were configured using variable time steps managed by solver algorithms. To lower the percent error below 1%, convergence tolerances were increased.

### Simulation

Steady-state simulations were run to establish initial thermal gradients through the crucible systems and confirm expected one-dimensional conduction profiles. Transient analyses were then performed using a time increment of 10 seconds up to a target of 2000°C. Temperature contours, spatial gradients, time histories, and energy balance plots were monitored at intervals from the Results pane.

### Data Collection and Analysis

Experimental testing and predictive modelling were used in the data collection process. Standardised techniques were used to assess mechanical and thermal characteristics, including density, porosity, compressive strength, hardness, expansion, and thermal conductivity (e.g., ASTM C1327, D1621). For reliability, averages with standard deviations were calculated for each test, which was run on several replicates. Crucible compositions were statistically optimised with the use of Design-Expert software and Response Surface Methodology (RSM). A central composite design (CCD) examined how the five main responses were affected by borosilicate glass, granite, and kaolin clay. The significance of each variable and interaction was ascertained using regression models and ANOVA. Optimized crucibles' mechanical and thermal behaviour under operating conditions was verified using SolidWorks Finite Element Analysis (FEA) simulations. For high-temperature applications, this two-pronged strategy of empirical and computational data analysis guaranteed solid optimization and accurate crucible performance prediction.

## RESULTS AND DISCUSSION

### Experimental Results

A preliminary study on crucible material formulation was done by investigating the components that are used for its development. Six (6) excipients were chosen for the crucible material formulation based on their function. Two of them and Kaolin clay were used as variables in D-Optimal custom design, as they may affect the responses. The ranges of variables were also studied by using a D-optimal mixture in Design Expert software. Table 4 shows the summary data table of the actual design after the experiment.

**Table 3:** Presentation of key findings from physical tests

| Run | Factor 1 | Factor 2 | Factor 3 | Response 1 | Response 2 | Response 3 | Response 4 | Response 5 |
|---|---|---|---|---|---|---|---|---|
| | A: Kaolin Clay (Wt.%) | B: Granite (Wt.%) | C: Borosilicate Glass (Wt.%) | Hardness (BHN) | Compressive Strength (N/mm$^2$) | Thermal Conductivity (W.M $^{-1}$K $^{-1}$) | Thermal Expansion (µm/mm/$^0$C) | Density (g/cm$^3$) |
| 1 | 48 | 2 | 7 | 75.1 | 24.7 | 4.26 | 1.36575E-05 | 2.48 |
| 2 | 46 | 10 | 8 | 96.1 | 24.73 | 4.98 | 3.70826E-05 | 2.42 |
| 3 | 44 | 8 | 7.5 | 61.3 | 20.2 | 3.56 | 2.1312E-05 | 2.29 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 4 | 44 | 2 | 7.5 | 53.8 | 18.59 | 3.36 | 3.27472E-05 | 2.324 |
| 5 | 42 | 8 | 8 | 62.7 | 20.6 | 3.76 | 3.43927E-05 | 2.33 |
| 6 | 48 | 6 | 7 | 111.3 | 29.8 | 5.35 | 1.61129E-05 | 2.445 |
| 7 | 40 | 8 | 7 | 74.2 | 22.7 | 3.82 | 5.16796E-05 | 2.19 |
| 8 | 44 | 2 | 7.5 | 53.8 | 18.59 | 3.36 | 3.27472E-05 | 2.324 |
| 9 | 48 | 2 | 8 | 75.006 | 28.53 | 4.12 | 8.67911E-05 | 2.485 |
| 10 | 48 | 6 | 7.5 | 114.006 | 30.62 | 6.12 | 1.57398E-05 | 2.477 |
| 11 | 40 | 10 | 7.5 | 70.8 | 25.6 | 3.66 | 1.95184E-05 | 2.31 |
| 12 | 40 | 10 | 7.5 | 70.8 | 25.6 | 3.66 | 1.95184E-05 | 2.31 |
| 13 | 40 | 4 | 8 | 91.605 | 21.82 | 5.29 | 3.00008E-05 | 2.308 |
| 14 | 44 | 6 | 7 | 76.2 | 35.8 | 4.37 | 3.30657E-05 | 2.4 |
| 15 | 44 | 6 | 7 | 76.2 | 35.8 | 4.26 | 1.36575E-05 | 2.4 |
| 16 | 48 | 10 | 7 | 107.338 | 28.53 | 7.1 | 4.09594E-05 | 2.468 |
| 17 | 40 | 4 | 7.5 | 85.84 | 20.18 | 4.44 | 2.0158E-05 | 2.323 |
| 18 | 40 | 2 | 7 | 41.987 | 15.22 | 3.14 | 1.13594E-05 | 2.319 |
| 19 | 44 | 8 | 7.5 | 83.623 | 33.8 | 4.5 | 8.22735E-05 | 2.44 |
| 20 | 48 | 6 | 7.5 | 114.006 | 30.62 | 6.12 | 1.57398E-05 | 2.477 |

## Predictive Model Outcomes

### ANOVA and Models Generated

The presented table concisely summarizes the final regression equations for Hardness, Compressive Strength, Thermal Conductivity, Thermal Expansion, and Density in both coded and actual factor forms, providing a clear comparison between the two representations. The coded factor equations (with factors A, B, and C scaled between -1 and +1) facilitate the assessment of relative factor significance by comparing coefficient magnitudes, while the actual factor equations (expressed in original units) allow for direct predictions in practical applications. Each response variable's equation includes linear, interaction, and quadratic terms, highlighting the complex relationships between the input factors (Kaolin Clay, Granite, and Borosilicate Glass) and the measured properties.

**Table 4:** Final regression equations in terms of coded factors for each response variable.

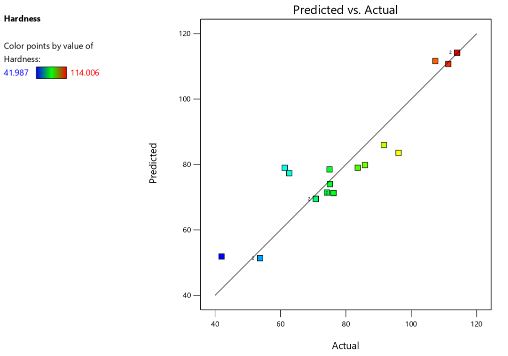
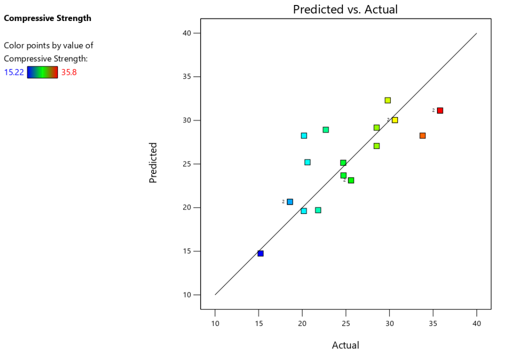
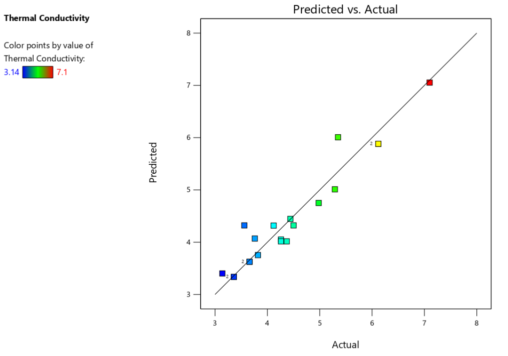
| **Response Variable** | **Equation in Terms of Coded Factors** |
|---|---|
| Hardness | Hardness=+78.75+14.41A+9.45B+4.29C+7.38AB−4.02AC−1.98BC+21.02A2−17.93B2−3.16C2Hardness=+78.75+14.41A+9.45B+4.29C+7.38AB−4.02AC−1.98BC+21.02A2−17.93B2−3.16C2 |
| Compressive Strength | Compressive Strength=+2.83+0.3339A+0.2482B−0.1576C−0.2434AB+0.0575AC−0.1965BC−0.1595A2−0.5145B2+0.1260C2Compressive Strength=+2.83+0.3339A+0.2482B−0.1576C−0.2434AB+0.0575AC−0.1965BC−0.1595A2−0.5145B2+0.1260C2 |

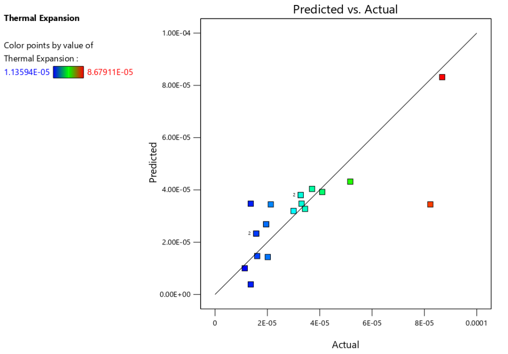
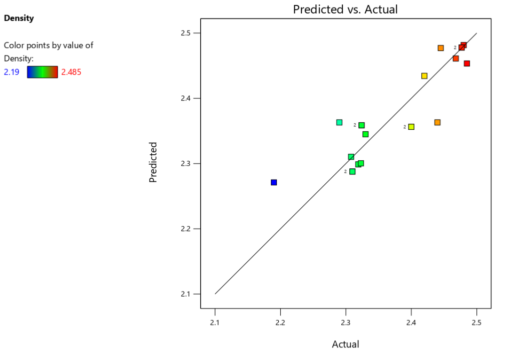
| | |
|---|---|
| Thermal Conductivity | Thermal Conductivity=+4.22+0.7410A+0.4286B+0.1390C+0.7474AB−0.3308AC−0.3252BC+0.9200A2−0.4555B2−0.0663C2Thermal Conductivity=+4.22+0.7410A+0.4286B+0.1390C+0.7474AB−0.3308AC−0.3252BC+0.9200A2−0.4555B2−0.0663C2 |
| Thermal Expansion | Thermal Expansion=+0.0000+4.105E−06A+1.033E−06B+7.975E−06C−3.919E−06AB+0.0000AC−0.0000BC−0.0000A2+6.841E−06B2+0.0000C2Thermal Expansion=+0.0000+4.105E−06A+1.033E−06B+7.975E−06C−3.919E−06AB+0.0000AC−0.0000BC−0.0000A2+6.841E−06B2+0.0000C2 |
| Density | Density=+2.36+0.0893A−0.0000B+0.0093C+0.0055AB−0.0076AC+0.0158BC+0.0239A2−0.0058B2+0.0010C2Density=+2.36+0.0893A−0.0000B+0.0093C+0.0055AB−0.0076AC+0.0158BC+0.0239A2−0.0058B2+0.0010C2 |

*Notes: Coded factors (A: Kaolin Clay, B: Granite, C: Borosilicate Glass) are scaled between -1 (low level) and +1 (high level). While the Actual factor equations are in original units and should be used for direct predictions but not for assessing factor significance.*

### Predicted and Actual Graphs for Each Response Variabl

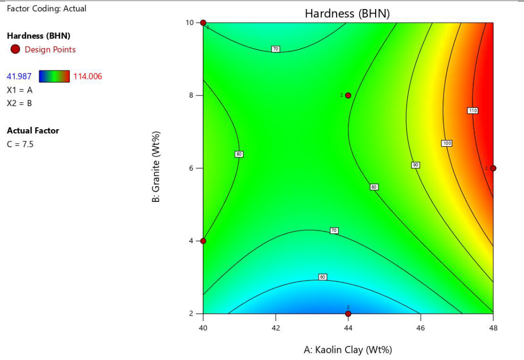
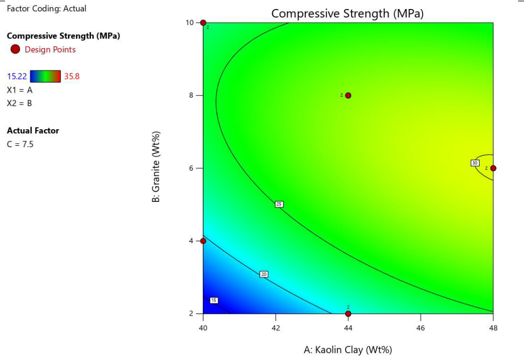
**Table 5:** Predicted and Actual Graphs for each response variable

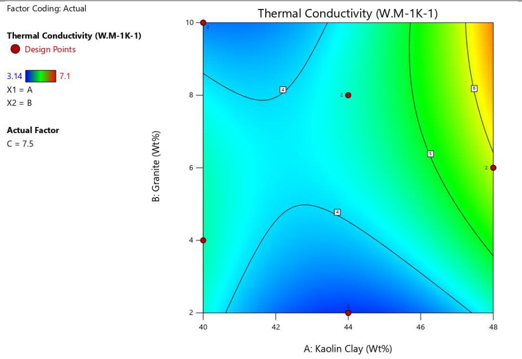
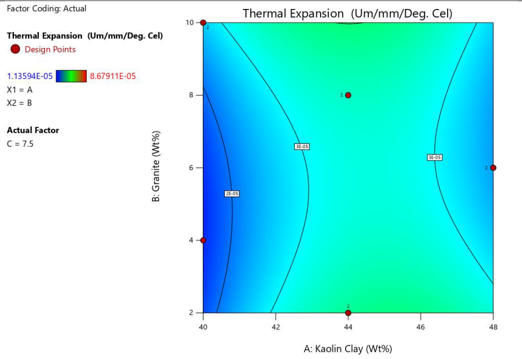
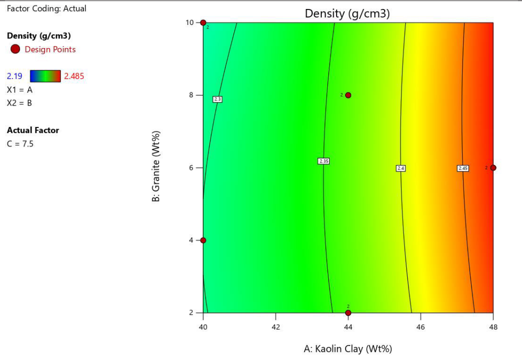
| **Response** | **Description** | **Graphical Representation** |
|---|---|---|
| Hardness (BHN) | The coded equations predicted hardness values closely matching actual measurements, confirming model accuracy. |  |
| Compressive Strength (MPa) | Predicted compressive strength values show high similarity with actual experimental data, indicating good predictive capability. |  |
| Thermal Conductivity (W·m$^{-1}$·K$^{-1}$) | Both predicted and actual thermal conductivity values align well, validating the model's prediction accuracy. |  |

| | | |
|---|---|---|
| Thermal Expansion (µm/mm/°C) | Predicted thermal expansion values closely follow actual data, demonstrating a reliable model fit. |  |
| Density (g/cm³) | The model accurately predicts density values, confirmed by the strong agreement between predicted and actual values. |  |

## Effect of the Additives on the Response

**Table 6:** Effect of the Additives on the Response

| Response | Key Findings | Contour Diagram |
|---|---|---|
| Hardness | Kaolin Clay (A) has the greatest positive influence on the hardness of the composite. |  |
| Compressive Strength | Both Granite (B) and Kaolin Clay (A) significantly contribute to compressive strength. |  |

| | | |
|---|---|---|
| Thermal Conductivity | Granite (B) and Kaolin Clay (A) are the major contributors to thermal conductivity. |  |
| Thermal Expansion | Borosilicate Glass (C) mostly influences thermal expansion properties. |  |
| Density | Kaolin Clay (A) primarily affects the composite's density. |  |

## Finite Element Analysis (FEA) Results

The graph represents a thermal analysis of a crucible pot, illustrating temperature distribution. A colour gradient scale on the right indicates temperatures in degrees Celsius: red areas signify the highest temperatures (up to 2,000°C), while blue areas represent the lowest (1,819.96°C). Green

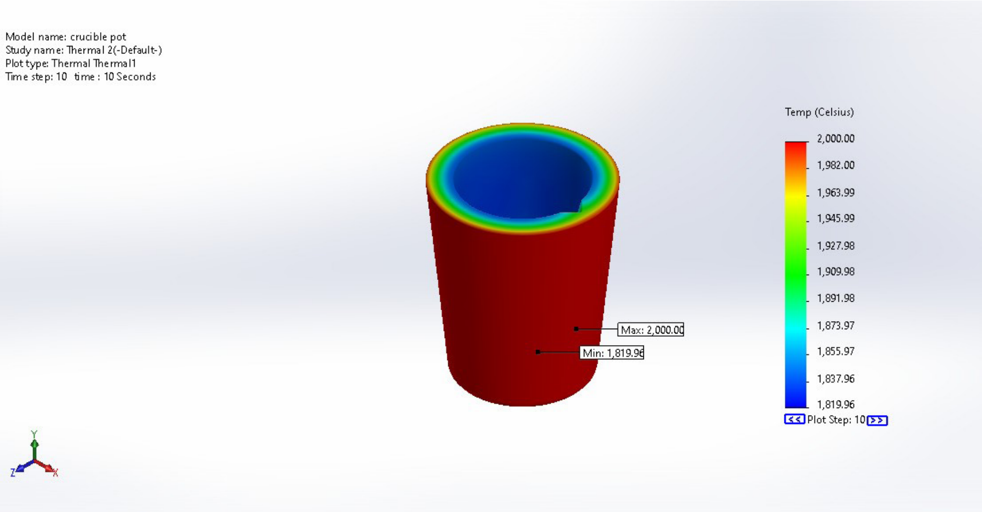


**Figure 6:** Finite Element Analysis (FEA) Thermal Simulation of the Crucible Pot

and yellow regions indicate moderate temperatures. This analysis, simulating 10 seconds, reveals how heat flows and dissipates within the pot, highlighting hot spots and cooler regions critical for evaluating thermal performance. The crucible is likely used for processes such as melting metals, making it essential to understand its thermal characteristics for effective operation under stress. Cooler areas may indicate insufficient insulation or heat retention, suggesting that improvements could be made to enhance temperature maintenance. Additionally, awareness of maximum temperatures is crucial for safety, as the 2,000°C region approaches the melting point of some materials, necessitating careful monitoring to prevent overheating. Overall, this thermal analysis provides valuable insights into the crucible pot's behaviour, informing operational planning, safety measures, and material selection in high-temperature applications.

## Research Validation

### Comparative Analysis of EQ-CB-G001015-LD Commercial Graphite Crucible and Optimized Graphite Composite Crucible

A comparative analysis between the EQ-CB-G001015-LD Commercial graphite crucible (referred to as Commercial Crucible) and the Optimized Graphite Composite Crucible was carried out to determine how the newly developed crucible pot can compete with the commercial crucible pots. The analysis focused on key properties including density, compressive strength, temperature resistance, and coefficient of thermal expansion (CTE).

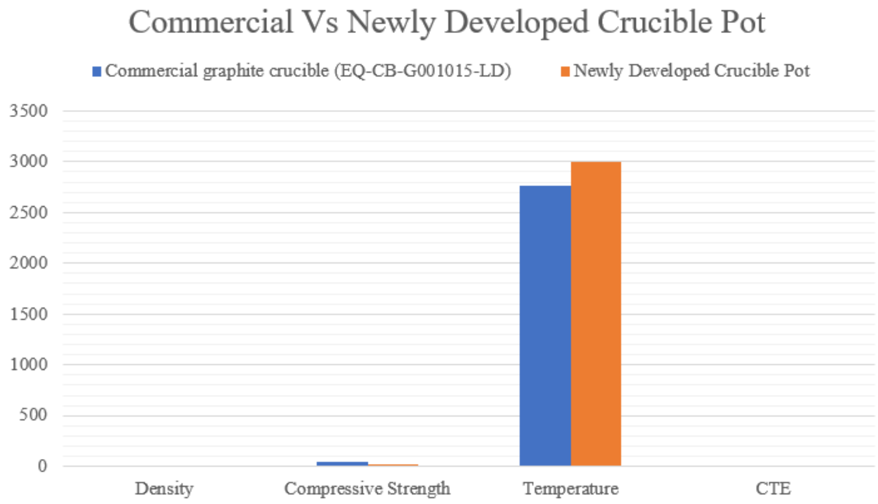


**Figure 7:** Comparing the various properties of the commercial and newly developed material

From Figure 7, it can be noted that the density of the Commercial Crucible was found to be 1.74, while the Optimized Crucible exhibited a density of 2.354. This indicates that the Optimized Crucible has a higher density compared to the Commercial Crucible, suggesting potential improvements in material characteristics. The compressive strength of the Commercial Crucible was measured at 42.7, whereas the Optimized Crucible showed a compressive strength of 25.02. The results indicate that the Commercial Crucible has a higher resistance to compressive forces compared to the Optimized Crucible. In addition, the temperature limit of the Commercial Crucible was determined to be 2760, while the Optimized Crucible exhibited a higher temperature limit of 3000. This suggests that the Optimized Crucible can withstand higher temperatures without significant degradation or failure. The Commercial Crucible demonstrated a CTE of 2.4E-6, whereas the Optimized Crucible showed a slightly higher CTE of 2.376E-6. This implies that the Optimized Crucible may have a slightly higher tendency to expand or contract with temperature changes compared to the Commercial Crucible. The results of the comparative analysis indicate that the Optimized Graphite Composite Crucible offers certain improvements over the EQ-CB-G001015-LD Commercial graphite crucible. The Optimized Crucible exhibited a higher density and temperature resistance, suggesting enhanced material properties. However, it is important to note that the Commercial Crucible demonstrated higher compressive strength and a slightly lower CTE. These findings suggest that the Optimized Crucible may be suitable for applications that prioritize density and temperature resistance, while the Commercial Crucible may be better suited for applications that require higher compressive strength and lower thermal expansion.

## CONCLUSION

This study successfully optimized the composition of graphite crucible pots using kaolin clay and functional additives (granite and borosilicate glass) through predictive modelling and experimental validation. The optimal formulation—43.5721% kaolin clay, 3.31722% granite, and 7.05904% borosilicate glass—demonstrated superior mechanical strength (compressive strength of 25.02 MPa, hardness of 55.78 BHN) and thermal performance (thermal conductivity of 3.32 W/mK, thermal expansion of 2.3760E-5 per °C). Finite Element Analysis (FEA) confirmed the crucible's ability to withstand temperatures exceeding 2000°C, while comparative analysis revealed its advantages over commercial alternatives, including higher density (2.354 g/cm³) and enhanced temperature resistance. The integration of Response Surface Methodology (RSM) and computational simulations provided a robust framework for material optimization, ensuring reliability and performance for high-temperature industrial applications.

## Recommendations for Future Work

[1] Expanded Additive Exploration: Investigate other functional additives (e.g., alumina, zirconia) to further enhance thermal shock resistance and chemical inertness.

[2] Long-Term Durability Testing: Conduct cyclic thermal shock tests and prolonged exposure studies to evaluate the crucible's lifespan under repetitive heating-cooling conditions.

[3] Cost-Benefit Analysis: Assess the economic feasibility of large-scale production, including raw material sourcing and energy consumption during sintering.

[4] Advanced Computational Models: Incorporate multi-physics simulations (e.g., coupled thermal-structural analysis) to predict crack propagation and failure modes under operational stresses.

[5] Industrial-Scale Validation: Partner with foundries or metallurgical industries to test the optimized crucible in real-world melting processes, comparing performance with conventional crucibles.

[6] Environmental Impact Study: Evaluate the sustainability of the production process, including waste management and energy efficiency, to align with green manufacturing practices.

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