Synergistic optimisation of fine coal oil agglomeration using response surface methodology and random forest coupled with decision trees

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Abstract. This study investigates the optimization of fine coal-oil agglomeration by focusing on critical parameters: pulp density, oil dosage, pH, agglomeration time, agitation rate, and oil type. The goal is to improve coal quality, specifically reducing ash value and moisture, while maximizing calorific value (CV), fixed carbon (Fixed C), and minimizing sulphur content. Using a combination of Response Surface Methodology (RSM), random forest, and decision trees, the study identifies optimal conditions for agglomeration. A pulp density of 20%$_{wt}$ yielded a relative 18% ash reduction and a 0.5% sulphur reduction. An oil dosage of 15% was found to be efficient, significantly enhancing the calorific value to 27.5 MJ/kg and fixed carbon to 48% and as dry (ad) moisture basis of 5.58%. The optimal pH of 4 preserves electrostatic properties crucial for effective agglomeration, while an agitation rate of 2800 rpm and agglomeration time of 12 minutes further improve coal recovery. The incorporation of advanced modelling techniques such as random forest and decision trees enhance predictive accuracy, ensuring reliable optimization of these parameters. These findings underline the potential of this approach to improve coal recovery processes. They also promote sustainable practices in the coal industry.

1. Introduction

The global shift towards sustainable energy production has necessitated the exploration of alternative methods for coal utilization. Fine coal-oil agglomeration has emerged as a promising technique to enhance the recovery of valuable coal resources from fine and ultra-fine coal particles (0.001 and 0.1 mm), which are often discarded as waste in traditional mining operations [D. , below]. This process improves coal quality by increasing its calorific value as well as minimizes waste and emissions to the environment [below]. This process utilizes the difference in surface hydrophobicity between coal particles and mineral matter,

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which is crucial for enhancing high-ash coal quality [below]. Agglomeration is a process whereby larger lumps are created by utilizing a bridging liquid (agglomerant) to cumulate fine particles [below]. Numerous bridging liquids such as sunflower oil, jatropha oil, kerosene, n-heptane, xylene, canola oil, and diesel have been studied in the past [belowbelowbelow]. Literature on oil agglomeration processes is primarily focussed on the treatment of lignite and sub-bituminous coal ranks. This process typically utilizes organic solvents, vegetable oils, and fossil oils as agglomerant [below]. However, the success of coal-oil agglomeration is highly dependent on process parameters such as oil dosage, agitation speed, and particle size. As such, optimizing these parameters is crucial to maximize efficiency and achieve desired outcomes [belowbelow].

This study aims to present an advanced optimization approach for the fine coal-oil agglomeration process using response surface designs (RSD) coupled with machine learning algorithms, specifically random forest regression. Response surface methodology is a statistical technique that provides a mathematical and probabilistic framework for optimizing processes. It enables researchers to model and analyse the relationships between multiple variables and a response variable, facilitating the identification of optimal conditions [below]. The incorporation of random forest regression, a robust machine learning technique, enhances the predictive capability of the model, allowing for a more accurate estimation of the agglomeration performance under varying conditions [below, below].

The application of response surface designs in conjunction with random forest regression offers several advantages over traditional optimization methods. Firstly, RSD allows for a systematic exploration of the design space, efficiently identifying the critical parameters that significantly influence the agglomeration process. This is particularly beneficial in a complex process like coal-oil agglomeration, where the intricate interactions between parameters such as pH, pulp density, agitation speed, agglomeration time, type of oil and their dosages, may not be straightforward [below]. Secondly, random forest regression provides a powerful tool for capturing non-linear relationships and interactions among variables without the need for a predefined functional form [below-below]. This flexibility enables the model to adapt to the inherent complexities of the agglomeration process, leading to more accurate predictions and better multi-objective optimization outcomes.

The integration of these methodologies allows for a more effective exploration of the parameter space, reducing the need for extensive experimental trials. This not only saves time and resources but also minimizes the environmental footprint associated with extensive laboratory experiments [below, below]. Through employing advanced statistical and machine learning techniques, this study seeks to establish a more efficient and sustainable mathematical modelling framework for optimizing the fine coal-oil agglomeration process.
The implications of this research extend beyond the enhancement of coal recovery processes. As the world continues to grapple with the challenges posed by climate change and resource depletion, the development of innovative and efficient methods for utilizing existing resources is paramount [below, below]. The findings of this study are expected to contribute significantly to the field of coal processing by providing insights into the optimization of agglomeration processes, ultimately supporting the transition towards more sustainable energy solutions.

2. Materials and methods

2.1.Material

Standard specification kerosene and diesel oil were obtained for the purposes of this study and no modifications were made to this material. Kerosene was obtained from Aric Oil (Pty)

Ltd, while the diesel oil was obtained from a local service station, BP Garage, in Johannesburg. Laboratory-grade sodium hydroxide and hydrochloric acid (32% purity) are chemicals that were procured from Merck®. The fine coal used in this investigation was sourced from a mine in Mpumalanga, South Africa. The coal's as-received characteristics, including particle size distribution (PSD), bulk chemical composition, ultimate and proximate analyses are presented in Figure 1, Table 1 and Table 2.

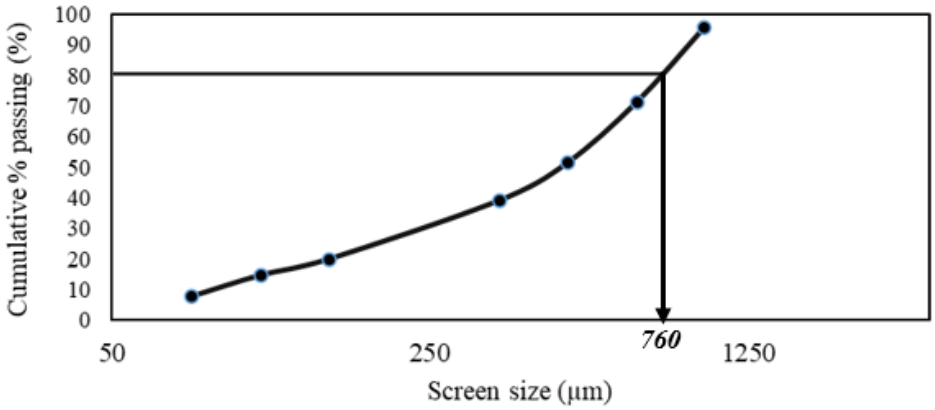

Fig. 1. Particle Size Distribution curve of the feed coal sample

Unal et al [below] and Laskowski [below] found that the feed must be adequately liberated to ensure effective coal cleaning. To achieve liberation particle size reduction is required, which generates a significant quantity of small particles in the final product. Fine particles are heavily influenced by the output of a single unit process which has led to emergence of various definitions for their size have emerged. In general, particles with sizes less than 1000 µm is termed fines [below]. Fig. **1** shows that about 80% of the feed material passes 760 µm.

Table 1. Bulk chemical composition of the feed coal sample

Component	Mass %
Al_2O_3	24.80
SiO_2	53.38
SO_3	4.24
CaO	3.86
TiO_2	2.16
Fe_2O_3	10.01
K_2O	1.55
Loss On Ignition (LOI) %	**75.00**

The bulk chemical composition of the coal sample summarised in Table 1 above reveals critical insights into its mineralogical characteristics and potential implications for utilization. Notably, silica (SiO_2) constitutes 53.38% of the composition, indicating substantial levels of

inert materials (ash forming minerals), which can influence the coal's thermal properties and ash behaviour during combustion. High silica content may lead to increased ash yield, complicating combustion processes [below – below]. Alumina (Al_2O_3), represented at 24.80%, suggesting the presence of clay minerals and indicates potentially lower combustibility due to the enhanced viscosity of molten ash, which can result in slagging issues [below, below]. Iron oxide (Fe_2O_3) is observed at 10.01%, playing a role in catalysing reactions during combustion and contributing to ash matrix stability [below]. The sulphur content, evidenced by sulphur trioxide (SO_3) at 4.24%, raises environmental concerns due to its potential to form sulphur dioxide (SO_2) upon combustion, which contributes to pollution and acid rain; [below – below]. Calcium oxide (CaO) at 3.86% acts as a fluxing agent in the ash, influencing melting behaviour and reducing slagging tendencies, while titanium oxide (TiO_2), present at 2.16%, can contribute to the stability of the ash but has limited implications for the coal's combustibility [below].

Table 2. Proximate and ultimate analysis of the feed coal sample

Ultimate	**Nitrogen %**	**Carbon %**	**Hydrogen %**	**Sulphur %**	**Oxygen %**	
	1.48	48.90	2.77	0.77	46.07	
Proximate	**Inherent moisture % (ad)**	**Total volatile matter %**	**Ash %**	**Fixed carbon %**	**Calorific value (MJ/kg)**	**Sulphur %**
	5.58	27.25	31.44	35.73	16.89	0.37

The ultimate analysis, captured in Table 2, reports a carbon content of 48.90%, which is typical for sub-bituminous coals with moderate calorific values [below, below]. The hydrogen content of 2.77% supports combustibility but is lower than that of higher-ranked coals. Nitrogen is present at 1.48%, which may influence nitrogen oxide (NOx) emissions, necessitating careful monitoring for regulatory compliance [below]. Sulphur content at 0.77% raises environmental concerns as it can lead to sulphur dioxide (SO_2) emissions during combustion, requiring effective management. An oxygen content of 46.07% suggests a reasonable portion of material consist of oxidizable compounds. This could adversely impact heating value, as oxygenated compounds contribute less energy to combustion compared to hydrocarbons, which indicates the need for effective pretreatment and process optimization [below].

The proximate analysis indicates a inherent moisture content of 5.58% (ad) in the feed coal sample, which falls within the requirements set out by the thermal sector of South Africa and may not require additional drying as pretreatment step [below]. The total volatile matter (TVM) indicates moderate potential for gas production, which is advantageous for gasification but complicates combustion efficiency [below]. High ash content at 31.44% (ad) suggests that substantial amount of incombustible material will remain, presenting challenges for ash management [below]. Fixed carbon at 35.73% offers a reasonable contribution to energy content but is lower than that of higher-ranked coals [below]. The calorific value of 16.9 MJ/kg positions this coal within a usable range, for electricity generation although it falls short of the higher energy profiles typical of bituminous coals; thus, highlighting characteristics of a subbituminous coal [below – below]. The sulphur content of 0.37% reinforces a relatively low environmental impact concerning sulphur emissions, which contrasts earlier findings in ultimate analysis.

2.2.Experimental

The set of experiments assesses the recovery of coal particles by employing an agglomeration method using diesel oil and kerosene as bridging agents [below]. Fig. **2** provides a flow diagram of the experimental setup.

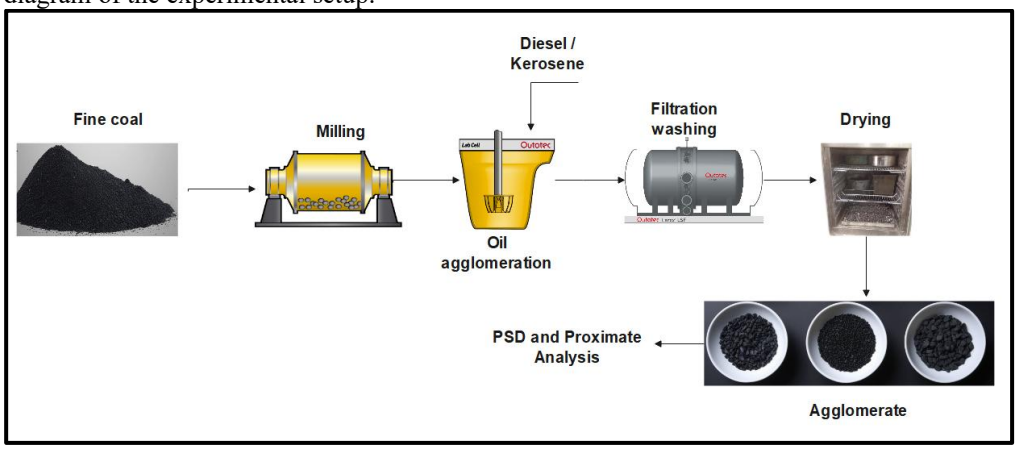

Fig. 2. Schematic representation of the experimental setup

The coal sample was prepared by milling for 20 minutes to ensure that all particles were <1 mm in size. A coal slurry, with varying pulp density, was subsequently prepared, after which it was stirred for 3 minutes to ensure good dispersion. The pH was measured and adjusted using sodium hydroxide for any increases or hydrochloric acid to reduce the pH, as per standard methodologies [below, below]. A proportional dosage of the relevant oil was introduced into the slurry, which was agitated at different speeds for various agglomeration times. After agitation, the agglomerated coal particles were recovered by screening and the non-agglomerated particles and removed by rinsing with water and thereafter filtered. The agglomerated particles were then dried in an oven overnight at 50°C for 12 hours. The mass fractions obtained from screening process were collected and the clean coal agglomerates were preserved for characterization.

2.3.Response surface methodology (RSM), decision tree, and random forest algorithm

The methodology for integrating random forest and decision tree algorithms with RSM in the oil agglomeration process involves several key steps to enhance the predictive accuracy and optimization of the process parameters.

(1) Firstly, RSM is employed to identify significant process factors which influence responses.

RSM is a powerful statistical tool employed for optimization problems, potentially in processes such as fine coal oil agglomeration. RSM facilitates the modelling and analysis of the relationship between multiple input variables and corresponding responses, helping to identify the optimal conditions for enhanced recovery. In this context, Table 3 below represents the parametrisation of the input and output parameters which include pulp density, oil dosage, pH, agglomeration time, agitation rate, and oil type. The objective is to optimize responses (output parameters) such as ash value, moisture, calorific value (CV), sulphur content, and fixed carbon (Fixed C). The fundamental equation used in RSM can be expressed as follows:

$$Y = \beta_0 + \beta_1X_1 + \beta_2X_2 + \beta_3X_3 + \beta_{12}X_1X_2 + \beta_{13}X_1X_3 + \beta_{23}X_2X_3 + \beta_{11}X_1^2 + \beta_{22}X_2^2 + \beta_{33}X_3^2 + \varepsilon \quad (1)$$

Where Y represents the response under assessment, X_i are the independent variables, β coefficients (linear, quadratic, cubic) correspond to the regression coefficients, and ε is the error term [below]. The application of RSM will ensure that the current study builds a second-order polynomial model that captures the curvature of the response surface, allowing for the identification of the ideal settings for each parameter to minimize ash and moisture while maximizing CV and fixed carbon. These optimizations are pivotal for enhancing the efficiency and effectiveness of the fine coal oil agglomeration process. For the developed designed of experiment, the software Design Expert (DX) 13 was used.
The polynomial model of the highest order was selected based on specific criteria: a sequential p-value of ≤ 0.05, a lack of fit p-value greater than 0.05, and the highest adjusted and predicted R^2 values. Additional terms were assessed for significance to confirm that the chosen model was not aliased. The validation of the selected model was performed using Analysis of Variance (ANOVA). The optimal model was determined by checking the need for any modifications to satisfy statistical assumptions, as shown in the Box-Cox diagram. The interaction effects of the process parameters on the responses were represented through a regression equation derived from the statistical model, enhanced by RSM 3-D surface and 2-D contour plots.

Table 3 represents the parametrisation of the input parameters which include pulp density, oil dosage, pH, agglomeration time, agitation rate, and oil type.

Table 3. Parametrisation of the fine coal agglomeration design of experiment (DoE)

Factor	Name	Units	SubType	Minimum	Maximum
A	Pulp density	wt%	Discrete	10	30
B	Oil dosage	wt%	Discrete	10	20
C	pH		Discrete	2	7
D	Agglomeration time	min	Discrete	5	15
E	Agitation rate	rpm	Discrete	2000	3000
F	Oil type		Nominal	Diesel	Kerosene

(2) Secondly, Decision Tree models are developed to capture the decision rules based on the experimental data, providing interpretable insights into the interactions between the input variables and responses.

A Decision Tree is a hierarchical, tree-like structure used for classification and regression tasks, where each internal node represents a decision based on an attribute, each branch denotes the outcome of that decision, and each leaf node signifies a final decision or predicted value. Decision Trees are particularly valued for their interpretability and simplicity, allowing users to easily understand how decisions are made based on input features. The effectiveness of a Decision Tree relies heavily on its splitting criteria, which determine the best way to partition the dataset at each node. Two common splitting criteria are Gini impurity and Information Gain. These criteria guide the construction of Decision Trees by identifying splits that yield the most informative partitions of the data. Gini impurity measures the likelihood of misclassifying a randomly chosen element from the dataset if it were randomly labelled according to the distribution of labels in the subset. A lower Gini impurity indicates a purer node, meaning it contains instances predominantly from one class. Decision Trees use this criterion to choose splits that result in nodes with lower impurity,

thereby increasing the overall accuracy of the model. Information Gain quantifies the reduction in entropy (or uncertainty) achieved by partitioning the data based on a particular attribute. It measures how well a feature separates the classes. Higher Information Gain indicates that the attribute provides more information about the classification of instances, leading to more informative partitions. Decision Trees use this criterion to select attributes that maximize the gain in information, thus leading to more effective splits.

1. Gini Impurity is calculated as follows:

$$Gini\ (D) = 1 - \sum_{i=1}^{c} p_i^2 \qquad (2)$$

Where p_i represents the probability of a class occurring in the dataset D and c is the total number of classes.

2. Information Gain is defined as:

$$IG\ (D, A) = H(D) - \sum_{v\ \in\ Values\ (A)} \frac{|D_v|}{|D|}\ H(D_v) \qquad (3)$$

Where $H(D)$ is the entropy of the dataset D, A is the attribute being assessed for the split, and D_v is the subset of D where attribute A takes on the value v.

(3) Next, a Random Forest model is trained on the same dataset to enhance the robustness and predictive capability by aggregating multiple decision trees, thereby minimizing overfitting and increasing accuracy.

Random Forest is an ensemble learning technique that leverages multiple Decision Trees to improve predictive accuracy and reduce the risk of overfitting. As a result of constructing a collection of trees from random subsets of the training data and features, Random Forest captures a diverse range of patterns and relationships within the data. Each tree in the forest independently generates predictions, which are then aggregated to produce a final output, typically through majority voting for classification tasks or averaging for regression tasks. The equation for predicting the response from a Random Forest model can be expressed as follows:

$$\hat{Y} = \frac{1}{N} \sum_{n=1}^{N} T_n(X) \qquad (4)$$

where $\hat{Y}$ is the predicted response, T_n refers to the n-th decision tree in the ensemble, X is the feature set, and N is the total number of trees.

(4) Finally, synergistic application of RSM, decision tree, and random forest creates a comprehensive analytical framework that not only optimizes the oil agglomeration process but also elucidates complex relationships among variables, leading to more informed and effective decision-making.

To assess the performance of the combined methodologies of RSM, decision trees, and random forest, various performance metrics were employed. The common metrics include Mean Squared Error (MSE) for regression tasks, which quantifies the average squared difference between actual and predicted values. Additionally, R^2 was used for regression analysis to determine the proportion of variance in the dependent variable that is predictable from the independent variables. The visual outputs were obtained as a function of a python code which was ran on Google colab and Datacamp. The overall developed multi objective optimisation model is represented below. This function displays maximisation functions (blue slope), minimisation functions (red slope), and ranged functions (horizontal line). The

position of the dots on the line function represents the optimum location for the respective parameter.

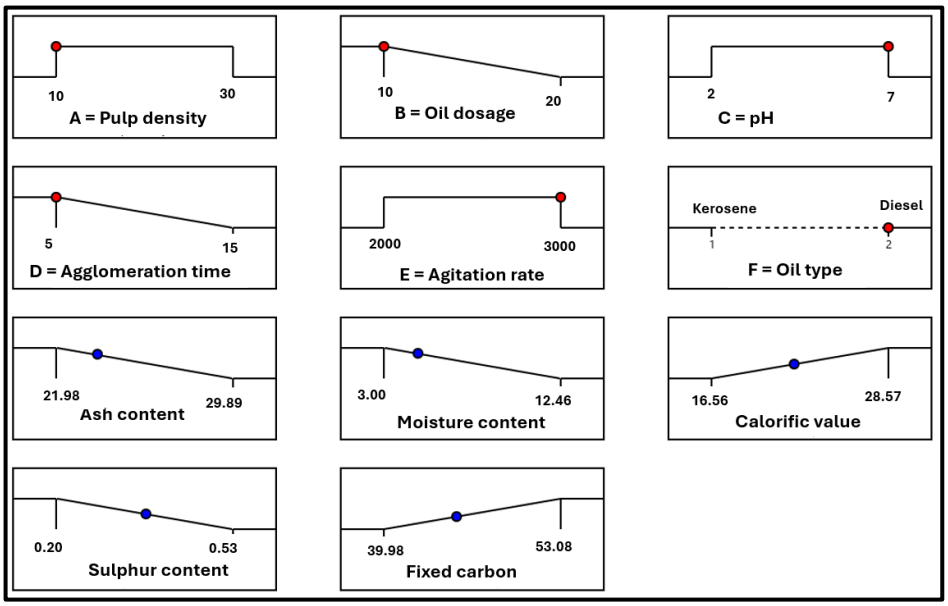

Fig. 3. Graphical multi objective optimisation with respective constraints.

3. Results and discussion

3.1.RSM optimisation

The goal of the developed RSM model is to ensure ideal settings for each parameter to minimize sulphur, ash, and moisture while maximizing CV and fixed carbon. In this instance, the results are based on a comparison between 2 bridging agents which are kerosene, and diesel.

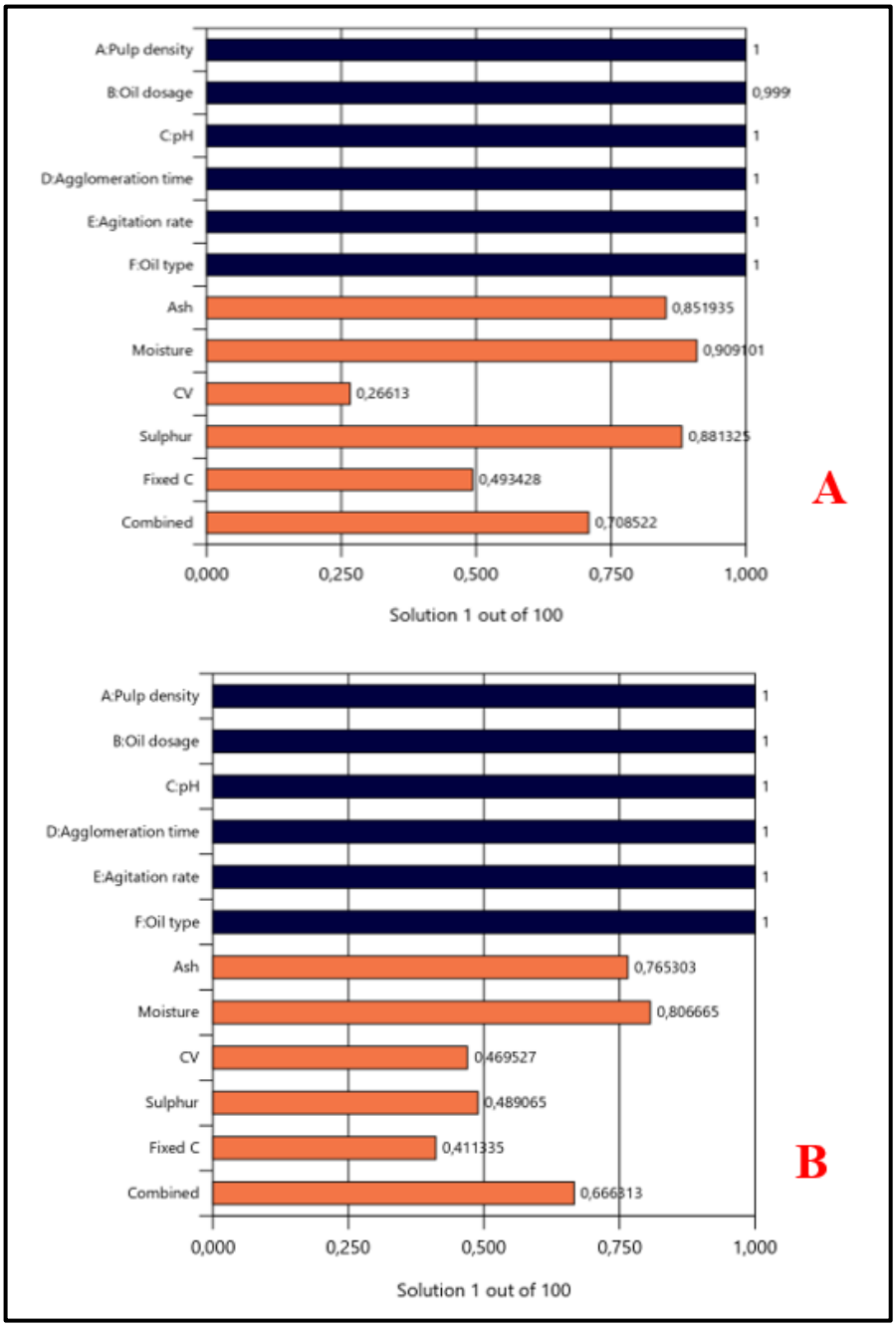

Fig. 4. Desirability function bar graph of the RSM model for the Kerosene oil (A) and Diesel oil (B)

Fig. **4**A and 4B demonstrate the integration of key parameters by the desirability function to analyse their interactions in oil agglomeration. A desirability value near 1 indicates an effective combination of factors, including pulp density, oil dosage, pH, agglomeration time, agitation rate, and oil type for optimizing outcomes. The combined reported desirability values of 0.71 for kerosene and 0.67 for diesel suggest that kerosene is a statistically more adequate to serve as bridging agent for minimizing ash, moisture, and sulphur while

maximizing fixed carbon and calorific value post-agglomeration. This aligns with previous studies, which showed a high internal phase water-in-oil emulsion containing 2.5 vol% kerosene generated fine coal agglomerates 17 times faster while requiring 10 times less organic liquid compared to pure oil binders [below]. The enhanced properties of the emulsion facilitated agglomeration, whereas kerosene was particularly effective in maintained agglomerate size during extended mixing, highlighting its suitability for fine coal agglomeration [below]. To improve agglomeration recovery, it is crucial to minimize the interaction between water and oil, also considering the binding agent's viscosity. Oil viscosity significantly influences agglomerate recovery, with higher viscosity oils demonstrating better potential due to lower oil-water interfaces that enhance hydrophobicity [below]. Lighter oils are generally used for higher rank coals, while heavier oils are preferred for lower rank coals like lignite, which can facilitate more effective particle collisions [below]. Additionally, using a more hydrophilic oil can improve the binding capacity of hydrophilic low-rank coal particles [below].

The 3-D analysis has been reported in Fig. **5** below. The 3-D analysis provides a visual representation of the interaction effects between process parameters and their impact on the responses. Through examining the surface plots, regions of optimal performance and understanding of how changes in input variables influence the output are identified. Peaks in the surface indicate higher response values, while valleys suggest lower performance. This visualization aids in pinpointing the best parameter settings for achieving desired outcomes, facilitating more informed decision-making in the optimization process. A pivotal observation regarding pulp density stems from [below], who assert that when pulp density subceeds 20%$_{wt}$, the slurry becomes too dilute. This dilution reduces the likelihood of interactions between the binding agent and coal particles, resulting in insufficient oil coverage over the coal. Consequently, this impacts the agglomeration rate, prolonging the time needed to reach equilibrium. The aforementioned relationship is further reinforced by findings from [below]. Conversely, when pulp density rises above 20%$_{wt}$, the slurry becomes excessively concentrated, thus hindering collisions between oil droplets and coal particles. This inefficacy leads to unutilised oil and unwarranted waste of resources and a subsequent decrease in coal recovery [below]. These findings align with experimental observations, where lower pulp densities adversely influenced both recovery rates and the quality of the agglomerated coal.

In reviewing the results from the proximate analysis across the initial experiments, a clear trend emerged in ash content. Specifically, an increase in pulp density correlated with a reduction in ash percentage. However, surpassing a certain pulp density threshold led to an uptick in ash content, a phenomenon described by [below]. Higher pulp densities result in the entrapment of ash-bearing minerals, decreasing the selectivity of the agglomeration process. This observation underscores the importance of optimizing pulp density for effective coal recovery.

The calorific value of the coal corroborated theoretical expectations across all nine experiments. Notably, the experiments conducted at a pulp density of 20% by weight exhibited the highest calorific values. This phenomenon has been attributed to the closer proximity between coal particles at increased solid ratios [below]. This proximity facilitates enhanced interactions between coal and oil, promoting more effective agglomeration and higher recovery of combustible material.

Examining sulphur content, experiments demonstrated that the lowest sulphur levels occurred at a pulp density of 20% by weight. This finding suggests that the oil agglomeration process is effective at recovering cleaner coal, with reduced pyritic sulphur content [50]. The relationship between the solid-solid ratio and increasing pulp density results in the unwelcome entrapment of higher ash and pyritic sulphur particles. This finding reinforces

the notion that maintaining an optimal pulp density is crucial for enhancing the recovery of coal with desired properties.

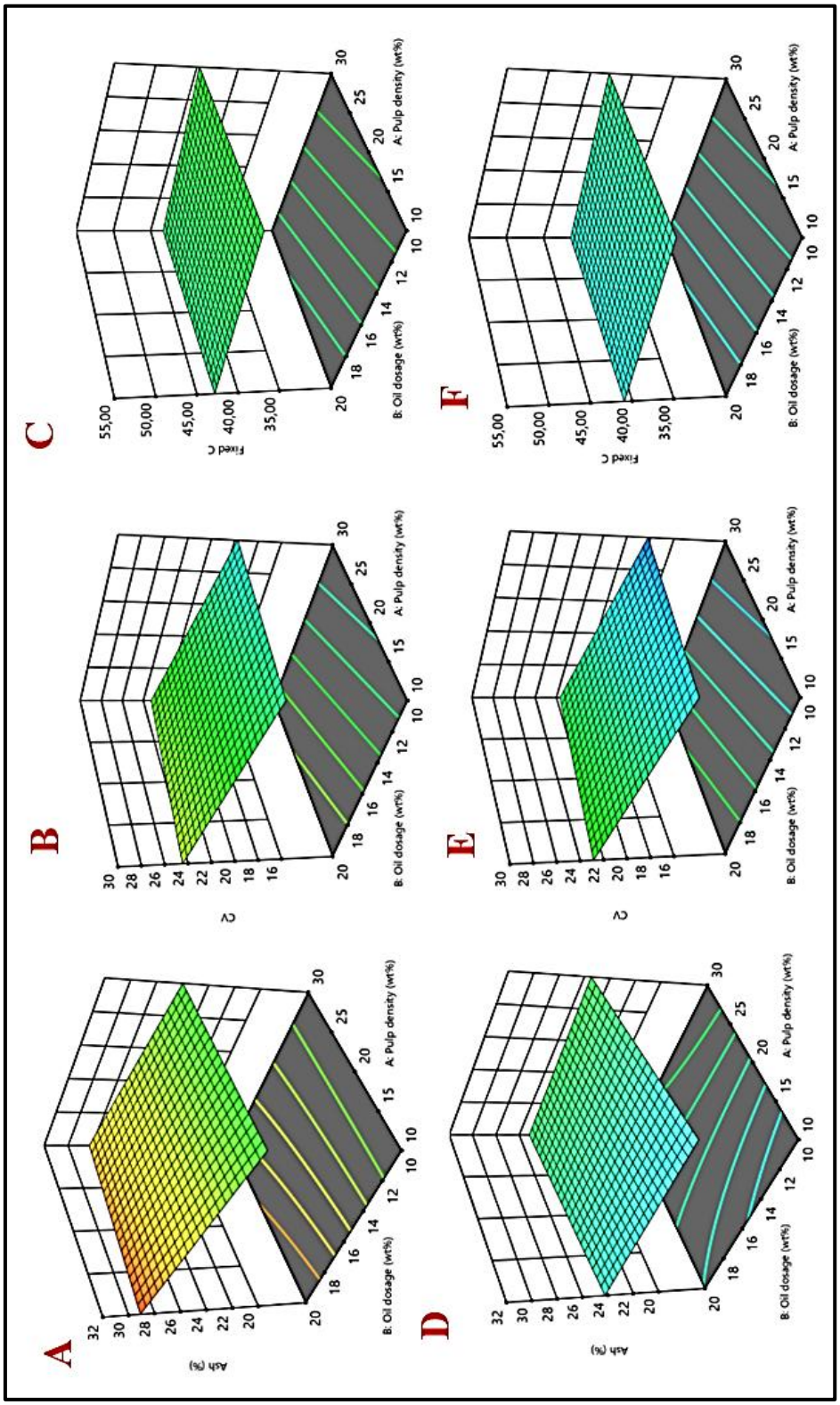

Fig. 5. Response surface plots of the different key parameters for Kerosene oil (A, B, and C) and Diesel oil (D, E, and F)

From the observations, it is evident that a pulp density of 20% by weight is critical for maximizing coal particle recovery during the oil agglomeration process. This optimal pulp density consistently yielded favourable conditions in terms of coal recovery metrics, calorific value, sulphur, and ash value. Additionally, an agglomeration time of 12 minutes is generally sufficient for effective separation [below] and [below]. Minor variations in calorific values between concentrates and tailings indicate that some combustible materials were still retrieved from the tailings. This suggests that the agitation rate and pH significantly influenced the separation effectiveness. Acidic pH values around 4 enhance the selectivity of the agglomeration process. Literature indicates that electrostatic repulsive forces between positively charged particles decrease, along with the hydrophilic nature of the coal surface. The reduction of electrostatic repulsive forces between positively charged coal particles, coupled with a decrease in the hydrophilic nature of the coal surface, significantly impacts the agglomeration process. Weakened repulsion allows particles to come into closer contact, promoting their aggregation into larger clumps or agglomerates. This increased agglomeration can affect the flowability and transport of coal, potentially leading to inconsistent heating during combustion or gasification processes [25, 51]. This dual reduction results in a significant decrease in sulphur content from 0.4 to 0.2% (ad) and ash value in the concentrates to 13% (ad) from the initial head sample reported at 31% (ad). Using the information from equation 5 below, the yield to product was observed to be 74%. This yield is recorded when mass of concentrate is 500g and mass of initial sample is 370g. The conditions observed during the RSM tests affirm the optimal nature of these settings, achieving an effective separation of waste from combustible material as evidenced by the increased calorific value in the concentrates. Lastly, a stirring speed of 2800 rpm and extended agglomeration times were found to maximize achievable calorific values while minimizing sulphur and ash in the product.

$$Yield = \frac{Mass\ of\ Concentrates}{Mass\ of\ initial\ sample} \times 100 \qquad (5)$$

3.2. Random forest and decision tree modelling

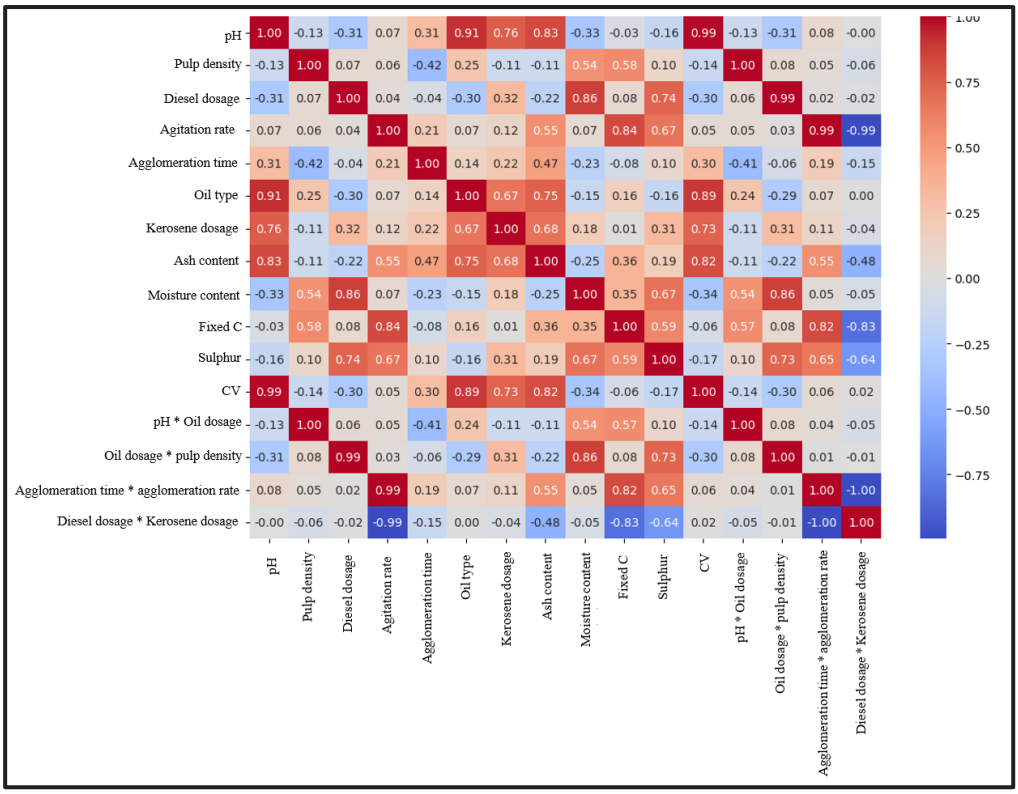

Fig. 6. Correlation heatmap developed for the interactions on the random forest model

The correlation heatmap provides a comprehensive view of the relationships among key parameters influencing the oil agglomeration process. The values range from -1 to 1, reflecting the strength and direction of linear associations. Notably, a strong positive correlation exists between pulp density and oil dosage (0.99), indicating that higher oil dosages typically require increased pulp densities for effective agglomeration. This relationship suggests that a balanced combination of these parameters enhances the bonding among coal particles while optimizing liquid usage [below]. Another important finding is the correlation between agglomeration time and fixed carbon content (0.91), suggesting that extended agglomeration periods, especially approaching 12 minutes may yield higher levels of fixed carbon in the recovered product, which is crucial for improving the calorific value of the final product [below, below].

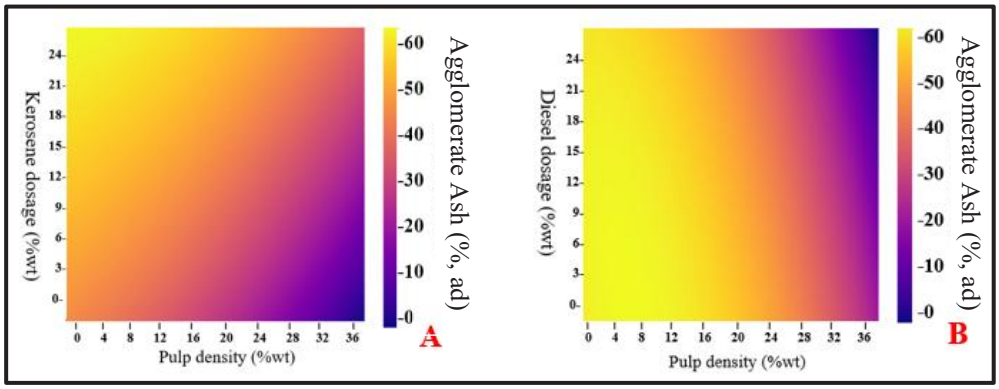

Fig. 7. Sensitivity analysis plots for the kerosene oil (A) and diesel oil (B)

Further insights are provided by the sensitivity analysis plots depicted in Fig. 7. Plot A reveals that optimizing kerosene dosage while varying pulp densities leads to significant reductions in ash content, shown by the transition from purple to yellow zones. The observation further implies that that higher kerosene dosages improve the dispersion of hydrophobic coal particles is crucial for understanding their binding capacity. Increased kerosene enhances the hydrophobic nature of the coal, allowing particles to repel water and maintain better separation from ash and other impurities. This improved dispersion not only enhances the binding capacity of the coal particles but also reduces the likelihood of agglomerate breakup during mixing [below]. Such improvements are crucial, as they contribute to the material's strength and wear resistance in processing.

Plot B indicates that increasing diesel dosage significantly lower ash content, suggesting that diesel may not be as effective for agglomeration as kerosene. This aligns with findings that lighter oils like kerosene possess properties that facilitate better coal particle agglomeration compared to heavier oils. The implications of using less effective oils are critical from a metallurgical standpoint; they can lead to inefficient separation processes, resulting in increased material loss and handling challenges.

These analyses underscore the importance of optimizing parameters in the oil agglomeration process, particularly from metallurgical perspectives. Enhanced coal quality through optimized agglomeration leads to higher fixed carbon levels and lower ashvalues, both essential for producing high-quality thermal coal. Such coal quality significantly impacts the efficiency of blast furnace operations in iron and steel production. Additionally, reducing sulphur and ash content not only improves metallurgical properties but also minimizes environmental pollutants, aligning with regulatory requirements and sustainability efforts within the coal industry [below].

3.3. Model performance analysis

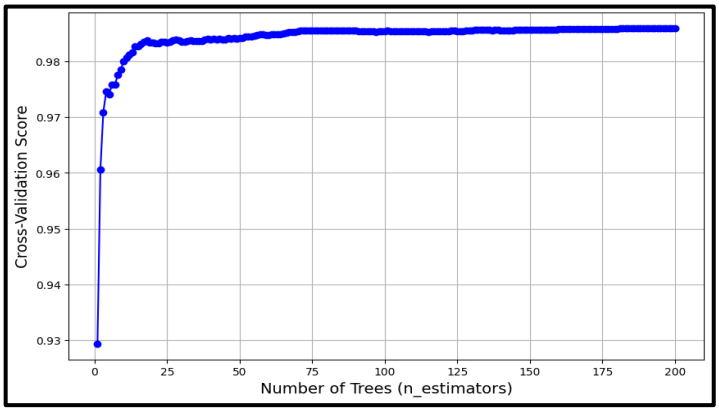

Fig. 8. Cross validation scores of the random forest model as a function of the tree numbers

Fig. **8** illustrates the relationship between the number of trees in the random forest model (n_estimators) and the corresponding cross-validation score. The cross-validation score stabilizes around 0.98, signifying excellent predictive accuracy. This high score reflects the ensemble nature of random forests, which operate by aggregating predictions from multiple decision trees to achieve a more robust model. Each tree is trained on a random subset of the data (using bootstrapping) and a random subset of features, which enhances diversity and reduces overfitting common in single decision trees. The nearly flat curve beyond a certain number of trees indicates the phenomenon of diminishing returns; adding more trees beyond this point contributes little to the model's accuracy. This saturation point is crucial, as it allows practitioners to balance model complexity with computational efficiency. Random forests are known to effectively manage the trade-off between bias and variance [below, 17].

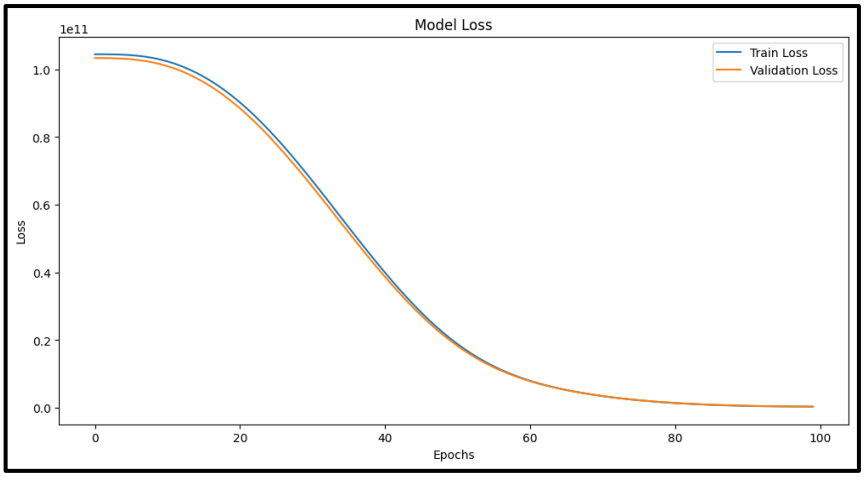

Fig. 9. Overall RSM, random forest, and decision tree model loss function for training and validation

The training and validation loss metrics are plotted against the number of epochs,which is considered as one complete pass through the entire training dataset during the training process of the machine learning model. This showcases the model's learning capabilities in relation to the dataset. The gradual decline in both training and validation loss indicates that the random forest model is effectively minimizing error during training. A close alignment of the training and validation loss curves suggests that the model generalizes well without

overfitting. Monitoring these loss metrics is crucial as it provides insights into model convergence and the efficacy of the optimization process. Ideally, one would expect both curves to converge toward a minimum loss value, confirming that the model's parameters are being optimized appropriately throughout the training process. A significant divergence between the two curves could indicate overfitting, where the model performs well on training data but poorly on validation data.

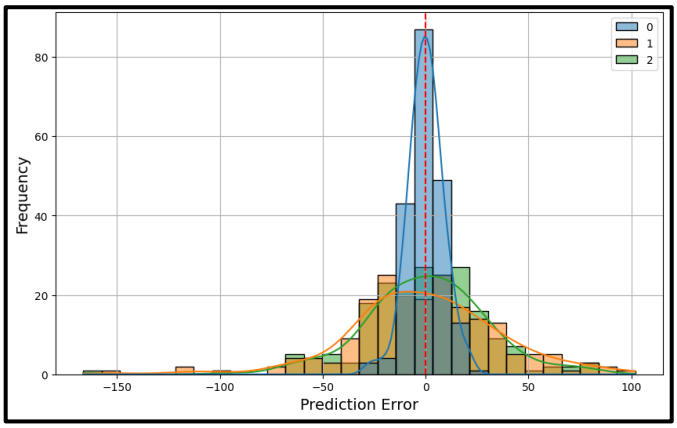

Fig. 10. Frequency histogram for the prediction error distribution of the overall model

The prediction error distribution histogram reveals the spread and central tendency of the prediction errors across instances in the dataset. The peak at zero indicates a high concentration of accurate predictions, while the spread captures variability in model performance. A symmetrical distribution around zero suggests that the model is unbiased, producing residuals that are evenly spread around the mean. This is a desirable outcome, as it implies that the model does not systematically overpredict or underpredict values, aligning with expectations in regression tasks.

The histogram also shows different colored lines corresponding to various categories or classes in the dataset. This visualization is valuable for identifying how well the model performs across different segments of data, allowing the researcher to assess whether the model treats all classes equitably.

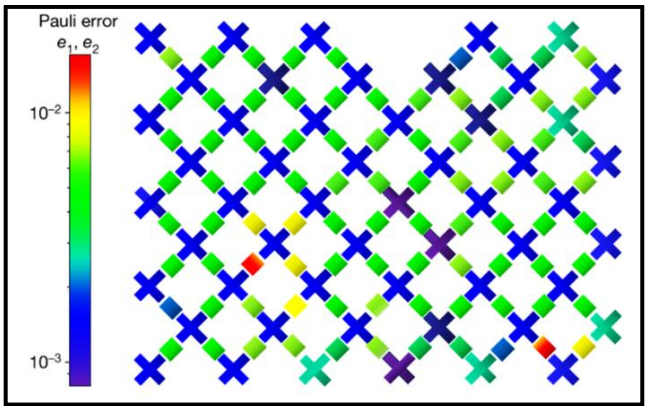

Fig. 11. Pauli error analysis of the developed overall model

The Pauli error representation provides a more nuanced view of prediction errors, displaying them in a grid format. This visualization technique breaks down errors at a granular level,

helping identify specific areas within the parameter space where the model struggles. Such detailed error analysis is invaluable for model refinement; understanding patterns in errors, informing decisions about feature engineering, hyperparameter tuning, or even model selection.

4. Conclusions and recommendations

The optimization of parameters affecting fine coal-oil agglomeration underscores the importance of a systematic approach to enhance coal processing efficiency. This study identifies a pulp density of 20% by weight as optimal, leading to a significant 18% relative reduction in ash value. An oil dosage of 15% positively influenced theCV, which reached 27.5 MJ/kg, alongside an increase in fixed carbon to 48%. The pH level of 4 was determined to be ideal for maximizing the effectiveness of the agglomeration process, while an agitation rate of 2800 rpm and an agglomeration time of 12 minutes were pivotal in achieving superior coal recovery. The outcomes clearly highlight that these optimized parameters effectively mitigate sulphur content, which decreased to 0.2% (ad), contributing to a cleaner end product. The integration of advanced statistical techniques facilitated better model predictions, thereby establishing a robust framework for future coal processing optimizations. This collective insight into parameter optimization is critical for enhancing coal recovery and promoting sustainable practices in coal utilization.

To enhance the understanding of coal-oil agglomeration processes and optimize recovery rates further, it is imperative to conduct a comprehensive analysis on the kinetics of the agglomeration in terms of the agglomerated particle size distribution. This critical assessment will aid in identifying how particle sizes impact agglomeration efficiency. Additionally, evaluating surface properties using Scanning Electron Microscopy (SEM) and Brunauer–Emmett–Teller (BET) analysis will reveal insights into surface morphology and porosity, vital for improving particle interaction during agglomeration. Furthermore, employing Fourier Transform Infrared Spectroscopy (FTIR) will assist in determining the types of chemical bonds formed during the agglomeration process. This multifaceted analytical approach will deepen the understanding of coal behavior under varying conditions, paving the way for tailored optimization strategies that enhance both the quantity and quality of coal recovery operations.

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