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Utilization of response surface methodology and machine learning for predicting and optimizing mixing and compaction temperatures of bio-modified asphalt

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ABSTRACT

The optimization of energy consumption during asphalt mixture production and compaction is a challenge in producing durable, sustainable, and environmentally friendly asphalt products. This study investigated the effects of crude palm oil (CPO) and/or tire pyrolysis oil (TPO) on shear viscosity and mixing and compaction temperatures of asphalt. Moreover, the possibility of using response surface methodology (RSM) and machine learning (ML) to develop predictive models for the shear viscosity and mixing and compaction temperatures of CPO- and/or TPO-modified asphalt was studied and compared. The results showed that the mixing and compaction temperatures significantly decreased with increasing CPO and TPO, and the shear viscosity consequently declined because of the light components, resulting in softer binders. However, at 5% of both materials, a balance between the required temperatures and a similar or better viscosity compared to the base asphalt were demonstrated. RSM analysis showed that CPO had a significant effect on the viscosity and production temperatures of the base and modified asphalts compared with TPO, which had no significant effects. The developed predictive models based on RSM exhibited a correlation coefficient (R^2) of more than 0.82 for all responses. In addition, it was found that extreme gradient boosting (XGB) regression was the best among all evaluated algorithms for predicting shear viscosity, whereas random forest regression (RFR) was the best for mixing and compaction temperatures, with R^2 values greater than 0.93. The performance evaluations of XGB and RFR showed extremely small differences between the predicted and experimental data. ML outperformed RSM in terms of prediction accuracy.

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1. Introduction

Asphalt is a by-product of the crude oil refinery process and is known to be utilized as the main raw material in the construction and maintenance of flexible road pavements [1]. The demand for this material has dramatically increased with an increase in the demand for constructing new roads and maintaining existing roads [2]. At the same time, the reservation of crude oil has continuously decreased over time owing to the high consumption and limited resources of crude oil as a nonrenewable material [3]. Therefore, researchers, pavement industries, and governments have conducted extensive studies during the last decade seeking an alternative binder for petroleum-based asphalt that can be used as a partial or total substitute for conventional asphalt with adequate durability, environmental friendliness, and renewable properties. Recently, bio-asphalt has been proposed and investigated as a sustainable alternative to conventional asphalt. Bio-asphalt is a new road cementing material made from a mix of petroleum-based asphalt with biomaterials derived from biological systems to produce more sustainable binders that use fewer renewable resources and have lower costs and energy consumption than petroleum-based materials [4–6]. Bio-oils are commonly used as partial replacements for petroleum-based asphalt because of their outstanding compatibility with the base asphalt [7–9]. Palm oil is one of the most recommended bio-oils in the asphalt industry used to produce bio-asphalt owing to its universal availability in large quantities than other vegetable oils, inherent degradability, low toxicity, and economic potential [8,10]. Therefore, crude palm oil (CPO) was used in this study as a bio-oil to produce bio-asphalt.

On the other hand, the dramatic increase in the demand for automobiles worldwide has resulted in huge tire waste, which is considered one of the largest sources of waste that is difficult to treat and causes serious environmental problems [11,12]. To mitigate the harmful disposal of scrap tires, they have been used in various applications, including civil engineering materials, particularly as a modifier for asphalt in the form of crumb rubber (CR). Generally, there are several advantages to using CR in asphalt pavements, including improvements in rutting, fatigue, and thermal cracking resistance [13]. In addition, it enhances the skid resistance and reduces the noise of asphalt pavements and is also an eco-friendly and safe method for recycling tire waste [13,14]. In contrast, the use of conventional CR as a modifier for asphalt has drawbacks, such as high energy consumption and possible emissions during the modification and paving process because of the high operating temperatures, which may exceed 180 °C, low workability, and poor storage stability [15,16]. Therefore, tire pyrolysis oil (TPO) has been proposed as an alternative to conventional CR for asphalt modification to overcome the disadvantages of CR [15–17].

TPO is produced by the vacuum pyrolysis of waste tire scrap. The liquid part is removed, and the pasty residue is collected separately for use as a TPO [18]. Wu et al. and Presit et al. [16,19] found that the application of TPO in asphalt modification improved the storage stability at high temperatures with increasing amounts of rubber waste that could be incorporated into the asphalt compared with CR. It was also claimed that the production temperatures of TPO-modified asphalt showed a decrease of 30 °C with adequate low and intermediate rheological properties compared to CR-modified asphalt. Lightly pyrolyzed rubber (LPR) has also been used as an alternative to asphalt; its use in asphalt up to 50% by weight provides excellent low-temperature rheological performance [19]. Kumar et al. [20,21] reported that a composite of waste ethylene-propylene-diene monomer (EPDM) rubber and TPO as modifiers in asphalt improved the high- and intermediate-temperature performances of asphalt, which was attributed to the swelling of EPDM rubber with TPO. In another study, the addition of pyrolytic tire rubber as an alternative rejuvenator increased the amount of incorporated reclaimed asphalt in the asphalt mixture from 20% to 60%, with a slight deterioration in rutting performance and improvement in fatigue and moisture damage resistances [22]. It was also stated that further studies are needed to evaluate the possibility of using TPO as an alternative for CR in asphalt modifications [17]. Moreover, the effects of interactions between biomaterials and rubber-based modifiers are a research topic under consideration.

The incorporation of rubber waste into bio-asphalt to produce bio-modified asphalt (BMA) could maximize the utilization of biomaterials as a partial or complete replacement for conventional asphalt towards adequate bio-modified asphalt and mixture performance; it could also provide a hybrid environmental solution for rubber waste management [13,23]. Recently, Lyu et al. [24] conducted a study to introduce bio-modified asphalt as a clean and sustainable product. The cohesion and adhesion properties of the developed bio-modified asphalt were significantly improved towards better moisture damage resistance. They also stated that this improvement was due to the chemical reaction between the bio-oil and rubber in the asphalt matrix. Another study was conducted by Dong et al. [25] to investigate the composite modification mechanisms of bio-asphalt, styrene butadiene styrene (SBS), and CR. Microstructural analysis showed that the bio-asphalt enhanced the swelling and homogeneous distribution of polymers. In addition, rheological property tests showed that the composite bio-asphalt and polymers improved the high- and low-temperature performances of the bio-asphalt. Al-Sabaeei et al. [13] evaluated the aging and high-temperature rheological properties of bio-modified asphalts prepared using CPO and TPO as alternatives to conventional CR. It was found that 20% of conventional asphalt can be substituted by a composite of CPO and TPO while maintaining a similar performance grade and better aging resistance than the base asphalt. In addition, the composition of 5% CPO and 5% TPO showed PG64H compared to PG64S for nonmodified asphalt. Nevertheless, evaluating the interaction effects of biomaterials and polymers, such as rubber, on the viscoelastic behavior and production energy consumption of asphalt is still necessary and of high interest to researchers [2,26]. Specifically, few studies have investigated the possibility of using biomaterials and/or rubber technology, such as TPO, to optimize energy consumption in terms of the mixing and compaction temperatures of asphalt, reducing CO_2 emissions while maintaining adequate performance.

It is well known that asphalt must be sufficiently heated to guarantee that the aggregate is coated and lubricated during asphalt mixture production and compaction. By increasing the temperature, the fluidity of asphalt can be effectively increased. In contrast, high temperatures lead to asphalt degradation; consequently, excessive greenhouse gases are expected to be generated together with a general waste of energy [27,28]. Several approaches are available to determine the fluidity of asphalt at high temperatures in terms of mixing and compaction temperatures. The traditional equiviscous method is the most commonly used method for determining the rotational viscosity of unmodified asphalt at a fixed shear rate. However, it was found that the traditional equiviscous method results in unrealistic and excessively high mixing and compaction temperatures for modified asphalt, causing aging and degradation of the binders [27–29]. Therefore, several alternative methods have been suggested to determine the appropriate production temperatures for modified asphalt, as summarized in the NCHRP 648 report [30]. In this regard, a recent study was conducted by Almusawi et al. [28] to explore adequate procedures for determining the compaction and mixing temperatures of asphalt mixes incorporating polymers and warm mix additives. Compared to other methods investigated, it was found that the steady shear flow (SSF) method exhibited the lowest mixing and compaction temperatures while maintaining a similar performance to asphalt incorporating warm mix additives. Therefore, the SSF method was adopted in this study to investigate the effects of CPO and/or TPO on the mixing and compaction temperatures of asphalt.

Modeling and optimization of the mixing and compaction temperatures of modified asphalt and bio-asphalt have not yet received sufficient attention. Response surface methodology (RSM) is considered one of the well-known methods that has been used in several research areas, such as biomaterials science, concrete, and pavement materials, to establish a correlation between one or more independent variables and responses [31,32]. The applications of RSM in asphalt pavements have dramatically increased over the last few years owing to its flexibility in experimental design and excellent capability to perform modeling and optimization in a few experimental runs [33,34]. Del Barco et al. [15] used RSM to model and optimize the performance and cost of asphalt modified with TPO. It was found that RSM is an adequate technique for accurately predicting the performance of TPO-modified asphalt. Thus, RSM was adopted in this study to optimize the compaction and mixing temperatures of the CPO-, TPO-, and bio-modified asphalts. Recently, there has been significant interest among construction and pavement material researchers in using advanced computational modeling, such as machine learning (ML), owing to its higher accuracy and capability of developing prediction models with low cost and time consumption compared to conventional mathematical approaches [35–37]. ML algorithms have also been extensively used during the last decade to solve different types of engineering problems owing to their capabilities in knowledge processing and optimization [38–40]. The ML approach can also properly learn the complex behaviors of materials without requiring prior knowledge of the correlations between variables and responses [38]. In recent years, ML algorithms have been extensively used in predicting the performance of asphalt pavement materials [35,37,38]. Moreover, the need for developing predictive models using advanced techniques, such as ML algorithms, to predict the mixing and compaction temperatures of base and modified asphalt with different modifiers was also strongly recommended for future studies [41]. Although there has been extensive research on the possibility of using bio-asphalt as an alternative to conventional petroleum asphalt, no study has investigated the effects of CPO and TPO on the mixing and compaction temperatures of bio-asphalt and bio-modified asphalt using experimental or RSM- and/or ML-based approaches. Therefore, ML was adopted in this study in addition to RSM to identify the best method that represents the effects of CPO and TPO on the viscosity, mixing, and compaction temperatures of asphalt and to develop appropriate predictive models.

1.1. *Objectives and research significance*

This study aims to conduct experimental and modeling research on the possibility of using CPO and/or TPO as sustainable alternatives to conventional additives to optimize the mixing and compaction temperatures of asphalt while maintaining the desired performance. To achieve this, the following objectives have been identified:

- To investigate the possibility of using RSM and ML algorithms for developing predictive models that can predict the shear viscosity and mixing and compaction temperatures of the base and CPO- and/or TPO-incorporated bio-modified asphalts (BMA);
- To optimize the production temperatures of bio-modified asphalt using RSM and select the best ML models among the tested ones to develop predictive models;
- To compare the performance of the developed RSM and ML models in predicting the shear viscosity and production temperatures of the base and bio-modified asphalts.

This study can be useful for the pavement industry to estimate the production temperatures of bio-modified asphalt toward minimizing energy consumption and emissions and incorporate as many possible biomaterials and rubber waste in asphalt as possible.

Table 1
The physical and rheological properties of the base asphalt.

Test	Standard	Standard limit		Results
		Min.	Max.	
Penetration at 25 °C, 0.1 mm	ASTM D5–13	60	70	60
Softening Point, °C	ASTM D36–12	49	56	49
Ductility at 25 °C, cm	ASTM D113	100	-	>100
Penetration Index (PI)		-	-	-1.10
Mass loss, %	ASTM D2872	-	1	0.12
G^* /sinδ, kPa, at 64 °C and 10 rad/sec	AASHTO T315	1.0	-	1.03
RTFO - G^* /sinδ, kPa, at 64 °C and 10 rad/sec	AASHTO T315	2.2	-	3.20
J_{nr} at 3.2 kPa, kPa^{-1}	AASHTO T350	-	4.5	4.16
Jnr-difference, %	AASHTO T350	-	75	22.3

It can also be used by other interested researchers as a background for investigating the effects of other bio-oils and waste materials for sustainable bio-modified asphalt products. Compared to using experimental methods, which are costly and require professional skills and significant time for execution, using RSM and ML is a more cost-effective, faster, and easier alternative. In addition, the RSM and ML methods can be used to validate the findings of the experimental work, thus providing a better understanding of the observed phenomenon.

2. Materials and methods

2.1. Materials

A base asphalt with a 60/70 penetration grade was used in this study. It was supplied by Petronas Research and Scientific Services (PRSS), Malaysia. The physical and rheological properties of the base asphalt are listed in Table 1. The bio-oil used in this study is crude palm oil (CPO) provided by Palm Oil Manufacturing, Perak, Malaysia. The CPO was used at concentrations of 0%, 5%, 10%, and 15% of the total weight of the blend. The physical and chemical properties of CPO are listed in Table 2. The tire pyrolysis oil (TPO) used in this study was the sludge of the processing of the conversion of scrap tires into bio-gas in bio-fuel manufacturing. This oil was supplied by Tyre Oil (M) Sdn. Bhd, Perak, Malaysia. Both CPO and TPO were used as partial replacements of the base asphalt at 0%, 5%, 10%, and 15% of the total weight of the blend. The CPO and TPO concentrations were selected based on relevant literature reviews [13,42] and past trials conducted by the authors. The physical and chemical properties of TPO are presented in Table 3, and the appearances of CPO and TPO are shown in Fig. 1.

2.2. Methods

2.2.1. Preparation of bio-modified asphalt samples

The base asphalt was heated in an oven at 160 °C for more than one hour to achieve sufficient fluidity. TPO was gradually added to the base asphalt, manually mixed for two minutes and left until an equilibrium mixing temperature of 140 °C was reached. Filtered CPO was then added to the blend and mixed using a high-shear mixer for one hour at 1000 rpm. The modification procedure adopted in this study followed that of Al-Sabaeei et al. [13]. Sixteen modified asphalt samples containing varying concentrations of CPO and/or TPO were prepared. The prepared samples were carefully stored and labeled as bio-modified asphalt (BMAX_1X_2), where X_1 and X_2 refer to the CPO and TPO contents, respectively. Subsequently, all the base and modified asphalts were used to conduct shear viscosity testing at various temperatures and analyze the mixing and compaction temperatures.

2.2.2. Dynamic shear viscosity test

The dynamic shear viscosity of asphalt is a measure of the resistance of a fluid to flow. As heating reduces viscosity, the viscosities of the base and BMA were determined using a Kinexus Pro+ dynamic shear rheometer in a range of temperatures from 76 °C to 88 °C with an increment of 6 °C. Several approaches are available to determine the fluidity of asphalt at high temperatures. The traditional equiviscous method (Brookfield) is the most commonly used method for determining the rotational viscosity of unmodified asphalt at a fixed shear rate. However, it results in unrealistic and excessive temperatures for modified asphalt [27–29]; furthermore, the temperature system and applied torque during the test were more accurate when using a rheometer than the Brookfield method [43]. Therefore, alternative efficient methods have been suggested, such as steady shear flow (SSF), which was applied in this study to determine the viscosity of the BMA at different levels of modification. Further details regarding the SSF method are provided in the mixing and compaction temperature section of the BMA in this paper. Based on the relationship that was established between the resultant viscosity and test temperatures at 76 °C, 82 °C, and 88 °C for each BMA binder, the adequate fluidity of BMA was identified, which indicates the effect on the workability of the bio-modified asphalt mixtures to be prepared with tested binders.

2.2.3. Mixing and compaction temperatures

The steady shear flow (SSF) is one of the common alternative approaches proposed by Reinke and the NCHRP 648 report for determining the mixing and compaction temperatures of modified asphalt [30,44]. In this study, it was used to determine the mixing

Table 2
The physical and chemical properties of the crude palm oil [13,42].

Characteristics	Value
Appearance	Deep orange-red in color
Density at 40 °C, g/cm^3	0.899
Dynamic viscosity, at 25 °C and 10 s^{-1} shear rate, mPa·s	60.603
Dynamic viscosity, at 25 °C and 100 s^{-1} shear rate, mPa·s	56.35
Softening point, °C	33–40
Flash point, °C	260
Carbon, %	76.44
Hydrogen, %	13.14
Nitrogen, %	0.41
Sulphur, %	0.019

Table 3
The physical and chemical properties of the tire pyrolysis oil [13].

Characteristics	Value
Appearance	Thick liquid with a dark color
Dynamic viscosity, at 60 °C and 10 s^{-1} shear rate, mPa·s	11,901
Dynamic viscosity, at 60 °C and 100 s^{-1} shear rate, mPa·s	1713
Carbon, %	78.77
Hydrogen, %	7.967
Nitrogen, %	1.105
Sulphur, %	0.0305
Others, %	12.13

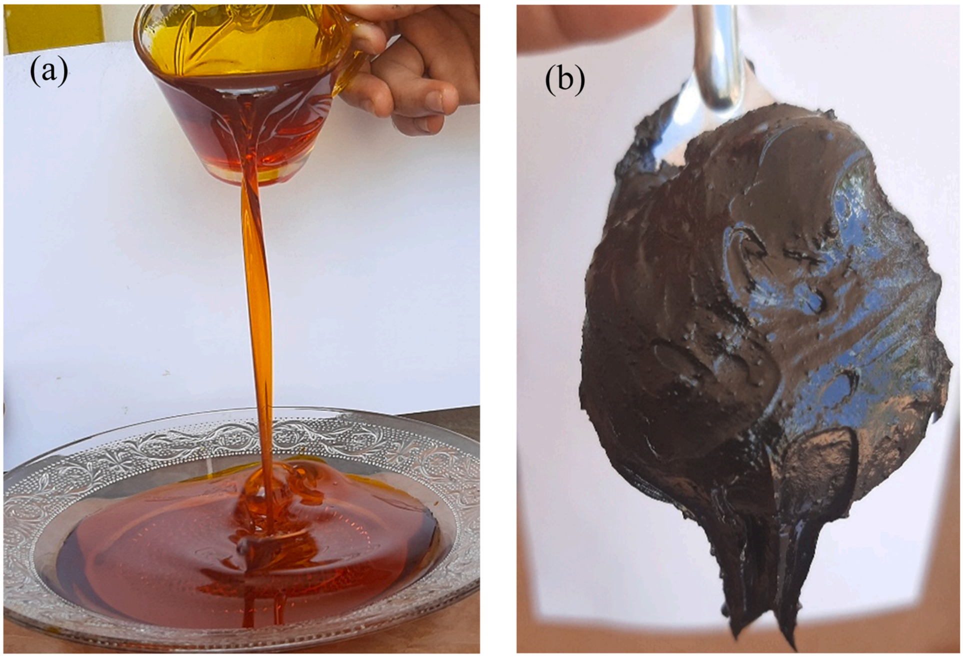

Fig. 1. Bio-oil and rubber aspects used in this study: (a) CPO and (b) TPO.

and compaction temperatures of the base and BMA. SSF was introduced based on the fact that the viscosities of various modified asphalts reach a steady state at a high shear stress of approximately 500 Pa [27,44]. The test was conducted using a Kinexus Pro+ dynamic shear rheometer with a 0.5-mm gap and a 25-mm plate diameter. The viscosities of the base and BMA were determined over a wide range of shear stresses (0.16–500 Pa) at several levels of temperature (76 °C, 82 °C, and 88 °C) and a constant shear mode. Test temperatures versus the viscosity values at 500 Pa were plotted on a log scale, and the temperatures corresponding to 0.17 ± 0.02 Pa·s and 0.35 ± 0.03 Pa·s were selected as the mixing and compaction temperatures, respectively. In this study, the rSpace software automatically performed the required calculations and extrapolated the results to determine the mixing and compaction temperatures at the required viscosity. The final values were reported. It can also be pointed out that the viscosities of the binder at which the SSF depends to determine the compaction and mixing temperatures were close to or similar to Superpave requirements. This was to determine the mixing temperature at an average of 0.17 Pa·s and compaction temperature at 0.32 Pa·s, which is equivalent to (0.28 + 0.03) for Superpave specification. The only difference is that the SSF used a different rheometer and shear rate, which is more accurate than the conventional method that is only valid for unmodified asphalt.

2.2.4. Design of experiment and method of analysis using RSM

RSM is a mathematical and statistical technique applied to experimental designs, statistical analysis and modeling, and numerical optimization [45]. It is commonly used for establishing the correlations among one or more responses and a set of independent variables in a few experimental runs [32,46]. A user-defined design (UDD) of the RSM was adopted in this study to design the experiment and perform the analysis and modeling using Design Expert 10.0.08 software. The UDD approach results in a higher number of runs compared to other RSM designs, which probably enhances the correlation and interaction influences of different variables on various responses. In this study, UDD was applied to conduct the statistical analysis and evaluate the correlations among the CPO and TPO contents as independent variables and shear viscosity, mixing temperature, and compaction temperature as responses. Based on previous research conducted by Al-Sabaeei et al. [13], the levels of CPO and TPO as independent variables were used at percentages of 0%, 5%, 10%, and 15% of the total weight of the blend for both modifiers. The experimental design adopted in this study is presented in Table 4.

Analysis of variance (ANOVA) was performed to evaluate the interaction effect between CPO and TPO and the appropriateness of the selected models. The fitness of the suggested models to the experimental data was assessed using the correlation coefficient (R^2). In addition, Fisher's test was used to check if the probability was within the 95% confidence interval. The standard deviation and coefficient of variance were determined to evaluate the spread of data from the mean and assess the reproducibility of the developed models, respectively. After ensuring that linear regression was inappropriate to represent the experimental data and the complex correlations between CPO and TPO as independent variables and shear viscosity, mixing temperature, and compaction temperature as dependent variables, appropriate high-order polynomial regression models were considered. The second-degree function presented in Eq. (1) is adopted in this study [31].

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \beta_{ii} X_i^2 + \sum_{i<j} \sum \beta_{ij} X_i X_j + \varepsilon, \tag{1}$$

where y is the predicted dependent variable, β is the y-intercept at $X_1 = X_2 = 0$, and k is the number of factors used in the analysis. X_i and X_j are the coded values of the independent variables, and i and j are the coefficients of the linear and quadratic equations, respectively. Lastly, ε denotes the error.

Multiobjective numerical optimization was performed for the shear viscosity and mixing and compaction temperatures after the statistical analysis and development of the predictive models. The main aim of the optimization was to determine the optimal contents of CPO and TPO that can produce bio-modified asphalt that incorporates as much CPO and TPO as possible, has adequate shear viscosity, and requires less production energy. Therefore, the multiobjective optimization criteria and goals were set in the range for all inputs and outputs. The optimization was performed, and the best solutions were selected according to the highest desirability proposed by the software. The optimum solution was experimentally validated, and the deviations in shear viscosity and mixing and compaction temperatures obtained from the experiment were compared with those from the developed predictive models to ensure that the difference was within the allowable error for pavement material applications.

2.2.5. *Machine learning analysis and modeling*

The machine learning (ML) method is currently considered the most common approach used to develop predictive models for the most complicated engineering problems [38–40]. This is an effective approach to solving civil engineering problems with a high degree of accuracy [47]. Recently, the applications of ML have become popular for developing predictive models for a wide range of material properties, including those of asphalt pavement materials [48–51].

In this study, three main steps were followed to optimize the ML models and select the best models that could accurately represent the experimental data obtained from the laboratory. First, the data obtained from the experiment were randomly shuffled and divided into 70% for training and 30% for testing and validation. The training dataset was used to develop the predictive models, and the accuracy of the developed models was assessed using testing and validation datasets. Based on the learning methods, ML can be classified as supervised, semi-supervised, unsupervised, or reinforcement learning. The primary goal of supervised learning is to achieve the desired outputs based on learning from a database that includes inputs and desired outputs to produce a model that can be used for predicting responses while minimizing variance errors [36,52]. Therefore, this study adopted supervised algorithms to develop predictive models that could accurately predict the shear viscosity and mixing and compaction temperatures of bio-modified asphalt at different CPO and TPO concentrations. During supervised learning, the predicted responses from the ML were compared

Table 4
Experimental design layout.

Run	Factor		Response		
	A: CPO (%)	B: TPO (%)	Shear Viscosity @ 88 °C (Pa·s)	Mixing Temp. (°C)	Compaction Temp. (°C)
1	0	0	8.37	154.43	140.55
2	0	5	11.79	157.74	137.68
3	0	10	8.65	154.11	133.71
4	0	15	7.5	151.94	131.91
5	5	0	7.66	150.58	130.95
6	5	5	16.04	158.94	139.12
7	5	10	10.49	155.97	135.83
8	5	15	9.15	150.09	130.91
9	10	0	2.94	136.03	114.39
10	10	5	7.55	148.6	129.37
11	10	10	5.2	141.98	122.19
12	10	15	4.25	142.85	122.85
13	15	0	1.77	124.51	103.22
14	15	5	6.49	144.37	125.2
15	15	10	2.32	131.77	109.44
16	15	15	3.27	137.09	115.74

with the experimental data, and the error to be used for adjusting the training process was calculated. This process was repeated until the desired error was achieved.

The next step was to use the supervised lazy regression algorithm to examine and compare various ML models that can be used to predict the shear viscosity and mixing and compaction temperatures of bio-modified asphalt based on the correlation coefficient (R^2) and root mean square error (RMSE). According to the Lazy learning optimization, the extreme gradient boosting regression (XGB regression) was found to be the best among the various ML models evaluated that could be used to represent the experimental shear viscosity of bio-modified asphalt with adequate accuracy. Furthermore, random forest regression (RFR) was found to be the best model for representing the experimental mixing and compaction temperatures of bio-modified asphalt among all the evaluated models, with the highest R^2 and lowest RMSE. Thus, the XGB regression and RFR models were adopted in this study to develop the final predictive models of the shear viscosity and mixing and compaction temperatures of CPO- and/or TPO-modified asphalt. The mathematical principles of both regression methods are briefly introduced in this study.

The extreme gradient boosting (XGBoost) model is an ML algorithm that belongs to the decision-tree-based model category. It was specifically developed for high computational and prediction accuracy and efficiency by combining a wide range of gradient-boosted decision trees [53]. XGBoost adopts ensemble learning that utilizes the sequence of decision trees on which each decision tree depends and learns from the previous decision tree to develop a strong learning process that improves the performance of the developed models [53–56]. The independent variables x_i and specifying dataset of n observations are typically used to develop XGBoost, where each of the independent variables has m unique features. There is a response (y_i) for each raw dependent variable. Based on the literature that used XGBoost for asphalt applications [53], the prediction model for XGBoost is shown in Eq. 2.

$$\hat{y}_i = \sum_{k=1}^{k} f_k(x_i), f_k \epsilon \mathrm{F} \tag{2}$$

where $\hat{y}_i$ is the predicted value of sample x_i, *and* f_k represents an independent tree structure identified by the leaf score of the k_{th} tree. F denotes the space of the regression trees.

The XGBoost classification model uses the following objective function, as shown in Eq. 3.

$$J(f_k) = \sum_{n=1}^{n} L(y_i, \hat{y}_i) + \sum_{k=1}^{k} \Omega(f_k) \tag{3}$$

where $\sum_{n=1}^{n} L(y_i, \hat{y}_i)$ represents the loss function, reflecting the degree to which the model fits the actual data; $\sum_{k=1}^{k} \Omega(f_k)$ denotes the regular term utilized to control the complication of the model; and n is the total number of data (samples). Ω is found based on Eq. 4 as follows:

$$\Omega(f) = \gamma^T + \frac{1}{2}\lambda\|\omega_i\|^2 \tag{4}$$

where T and ω_i represent the number of leaves and score of the i^{th} leaf, respectively.

As it is difficult to explain all the details of the XGBoost modeling process in this study, further detailed information on the XGBoost model can be found in the relevant literature [57].

Random forest is an advanced unbiased machine learning model that uses the bagging method to minimize variance and average noise [58]. It is an advanced version of the signal classification and regression tree algorithm that follows a simple nonparametric regression method [59]. Random forest works by aggregating the predictions of a certain number of similarly distributed decision trees that generate bootstrapped data [60]. Despite aggregating an extremely high number of trees, there is a limitation for bagging, which is the restriction of variances of prediction errors to shrink owing to the correlation between the pairs of variables. Random forest minimizes the influences of the correlation between each pair of variables by sampling random subsets of variables when each decision tree grows [60,61]. One of the most important benefits of RFR is its ability to correct overfitting, which can occur in ordinary regressions. Unlike a single decision tree, RFR can handle large datasets with abundant variables [61]. In addition, in RFR, each node is continuously divided into columns, and the optimum feature is selected until the tree building is stopped. The RFR then makes final predictions based on the average outputs of all the decisions.

In general, the number of trees (B) and random number of variables drawn in each decision tree (m) are considered the two main parameters in constructing the random forest [60]. Usually, these two variables can be determined from a grid search combined with cross validations [62]. The random forest regression can be constructed using the following steps [58,60]:

- For b = 1 to B:

(1) A bootstrap sample with N size from the training data is drawn.
(2) A random forest tree is grown to the bootstrapped data by repeating the following steps for each node of the tree until the minimum number of nodes is reached.

i. Randomly select m variables from the p total variables.
ii. Pick the best variable from the m variables.
iii. Split the nodes into subregions.

Subsequently, for regression problems, the prediction can be expressed as shown in Eq. (5), where $\hat{y}$ is the predicted value of sample x_i, B is the number of trees, and T_b is the random forest tree. For more details on random forest regression, refer to Breiman [58].

$$\hat{y} = \frac{1}{B}\sum_{b=1}^{B} T_b(x) \tag{5}$$

In this study, Anaconda Python 3.9.7 software was used to optimize and select the most appropriate ML algorithms and develop predictive models for the shear viscosity and mixing and compaction temperatures of CPO- and/or TPO-modified asphalt at various CPO and TPO concentrations. The input data used to develop the models were collected experimentally using a dynamic shear rheometer (DSR). The input parameters considered in this study were CPO as a bio-oil and TPO, with a content of 0–15% of the total weight of the blend for both parameters. Extensive training was conducted on a wide range of ML models, and the optimal ML model for each dependent variable that resulted in the highest accuracy was selected. The correlation coefficient (R^2) and root mean square error (RMSE) were used to evaluate the performance of the developed models.

A higher value of R^2 and its proximity to 1 indicate an excellent correlation between the actual data from the experimental work and the predicted data from the developed ML models. Additionally, a lower RMSE indicates better performance and a lower difference and error when the predicted data were compared with the experimental data. Therefore, a higher R^2 and lower RMSE reflect an appropriate accuracy of the developed models toward good performance.

A flowchart of the experimental design, in addition to the RMS and ML analysis and modeling, is presented in Fig. 2.

3. Results and discussions

3.1. Dynamic shear viscosity

Fig. 3 shows the results of dynamic shear viscosity at 500 Pa shear stress for the base and bio-modified asphalt obtained using a dynamic shear rheometer at 76 ºC, 82 ºC, and 88 ºC testing temperatures. In general, it can be observed that bio-asphalt modified with CPO exhibits lower shear viscosity over the temperature range than base asphalt, and the viscosity decreases as the CPO content increases. This result was expected because of the lightweight molecules and lower cohesion properties of CPO compared to asphalt, resulting in a softer bio-asphalt. However, at a lower bio-oil content (5% CPO), the shear viscosity of the CPO-modified asphalt was similar to that of the base asphalt. This can be ascribed to the polymerization of CPO at this lower content during the modification process [42]. In contrast, the TPO-modified asphalt showed an improvement in the shear viscosity of the base asphalt up to 10% TPO, with a slight reduction at 15% TPO at all testing temperatures. This slight reduction can be attributed to the aromatic content of TPO, which reduces the stiffness of the binder. BMA 05 showed the highest shear viscosity among the TPO-modified asphalts, with improvements of 43.5%, 36.48%, and 40.86% at 76 °C, 82 °C, and 88 °C, respectively; it also had higher shear viscosity compared to base asphalt.

From Fig. 3, it can also be observed that the composite of CPO and TPO exhibited a significant enhancement in the shear viscosity of the base asphalt compared to the individual modifications with CPO or TPO, particularly at a CPO content of 5%. This can be due to the interaction between CPO and TPO in the asphalt matrix, which results in a higher stiffness and shear resistance. BMA 55 showed the

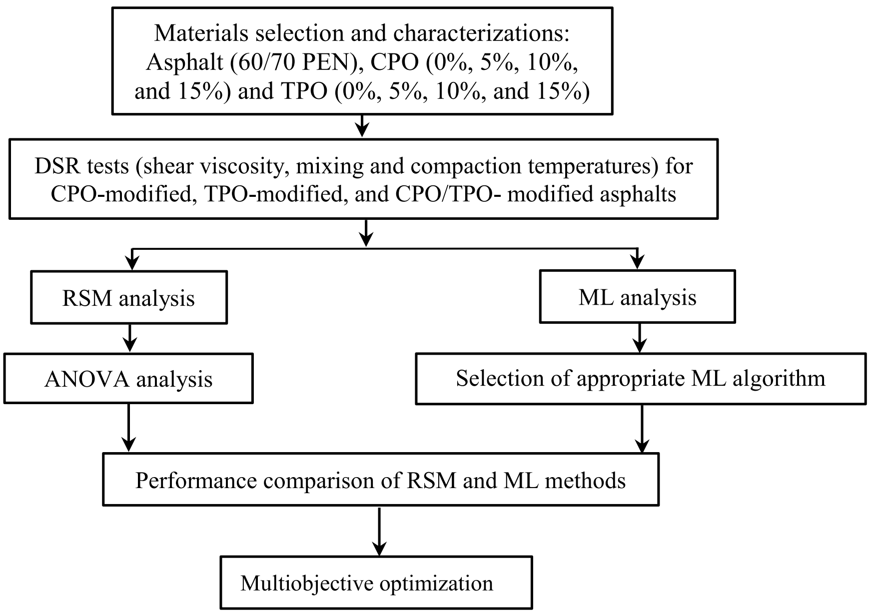

Fig. 2. Flowchart of the research.

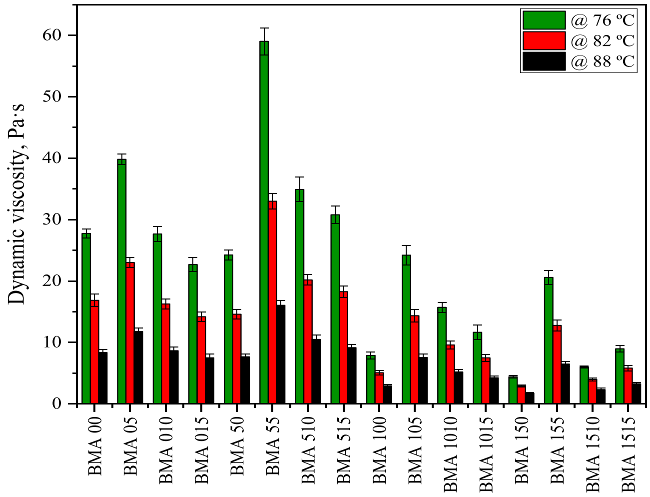

Fig. 3. Dynamic shear viscosity of base and modified binders at various temperatures.

highest shear viscosity among all the tested binders in this study, with improvements of 112.76%, 95.67%, and 91.64% at 76, 82, and 88 °C, respectively; it also had higher shear viscosity compared to base asphalt. In contrast, BMA 150 exhibited the lowest shear viscosity among all the tested binders, which was clearly due to its high CPO content that resulted in a softer binder. Meanwhile, BMA 515 had a higher shear viscosity than the base asphalt with 20% replacement for conventional asphalt by a combination of CPO and TPO. Overall, it was observed that BMA modified with up to 10% TPO and a composite of 5% CPO and various percentages of TPO showed viscosity values higher than or close to the conventional asphalt viscosity, which is a possible indicator that BMA binders (BMB 05, BMB 010, BMB 55, BMB 510, and BMB 515) can perform well in asphalt pavement applications exposed to shear at various temperatures.

3.2. Mixing and compaction temperatures

Fig. 4 shows the mixing and compaction temperatures of the base, CPO-modified, TPO-modified and bio-modified asphalts obtained using the SSF method. Overall, the mixing and compaction temperatures of the CPO-modified asphalt decreased as the CPO content increased compared with those of the base asphalt. In addition, BMA150 showed the lowest temperatures among all the tested binders. This can be attributed to the effect of CPO on the stiffness of the asphalt, which led to the lower energy required to achieve the desired workability. This reduction in mixing and compaction temperatures is useful for reducing emissions and energy consumption, particularly at a lower bio-oil content (5% CPO), which maintains mechanical properties similar to the base asphalt [42,49] and

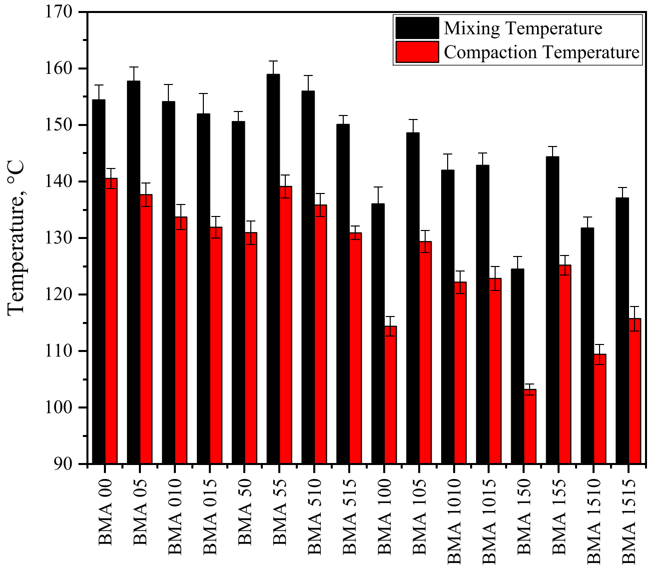

Fig. 4. Mixing and compaction temperatures of base and modified binders.

simultaneously requires lower mixing and compaction temperatures. BMA 50 showed 3.85 °C and 9.6 °C reductions in the mixing and compaction temperatures of base asphalt. On the other hand, the mixing and compaction temperatures of the TPO-modified asphalt decreased as the TPO content increased, with a slight increase at 5% TPO. Among the tested TPO-modified asphalts, BMA 015 exhibited the lowest mixing and compaction temperatures. The mixing and compaction temperatures of the base asphalt were reduced by 2.49 °C and 8.46 °C, respectively, due to the addition of 15% TPO. At the same time, based on the literature, BMA 015 showed mechanical properties similar to those of base asphalt with a performance grade of PG64S [13]. Thus, BMA 015 is an adequate alternative binder for base asphalt to reduce the energy consumption and emissions while maintaining the desired mechanical properties.

From Fig. 4, it can be observed that the combination of CPO and TPO reduced the mixing and compaction temperatures with an increase in CPO. However, at lower contents of CPO and TPO, there was a slight increase compared to the base asphalt, which can be due to the interaction of CPO and TPO at these lower contents that resulted in stiff binders. Based on the shear viscosity results shown above and those of a previous study by Al-Sabaeei et al. [13], BMA 515 has mechanical properties similar to those of the base asphalt with a performance grade of PG64S. In addition, it showed a 4.34 °C and 9.64 °C reduction in mixing and compaction temperatures compared to base asphalt with 20% replacement of asphalt with a combination of CPO and TPO. These findings reflect the feasibility of using CPO and TPO to produce sustainable bio-modified asphalt with adequate mechanical properties and low energy consumption and emissions.

3.3. Response surface methodology results

3.3.1. Statistical analysis and ANOVA

Statistical analysis and modeling were performed using the RSM after the shear viscosity and mixing and compaction temperatures were experimentally tested to validate the findings of the experimental work. This can provide a clear understanding of the behavior of bio-modified asphalt at different percentages of CPO and TPO towards developing predictive models for shear viscosity and mixing and compaction temperatures. Based on the R-square and predicted R-square and using model summary statistics (MSS) and the sequential model sum of squares (SMSS), cubic polynomial regressions were suggested as the most appropriate for modeling the shear viscosity, while the quadratic polynomial was the most suitable for modelling the mixing and compaction temperatures. For further evaluation, ANOVA was performed.

A summary of the ANOVA for the shear viscosity (SV), mixing temperature (MT), and compaction temperature (CT) responses of CPO- and/or TPO-modified asphalt is presented in Tables 5–7, respectively. The F-values of the shear viscosity, mixing temperature, and compaction temperature were 30.75, 11.21, and 9.49, respectively, reflecting the significance of the developed models. The p-values for all models and most of their terms were less than 0.05, indicating statistical significance within the 95% confidence interval. The model terms with p-values greater than 0.1, indicates that they were not statistically significant. To develop the models, only significant terms or terms necessary for maintaining the hierarchy were included.

The quality and fitness of the models were evaluated using their correlation coefficients (R^2). As shown in Tables 5–7, the R^2 values for shear viscosity, mixing temperature, and compaction temperature were 0.9535, 0.849, and 0.826, respectively. These results indicate that the developed models have a high degree of correlation because the R^2 values are close to unity. This also indicates that almost 95%, 85%, and 82.6% of the changes in the shear viscosity and mixing and compaction temperatures of the bio-modified asphalt were due to the addition of CPO and/or TPO. Moreover, this also suggests that the developed models can represent more than 80% of the viscosity and production temperatures of the BMA. Tables 5–7 also shows that the adjusted R^2 values of the shear viscosity, mixing temperature, and compaction temperature were 0.9225, 0.773, and 0.739, respectively. These values are close to the R^2 values, with differences of less than 0.2, indicating that the predicted responses of the developed models are expected to be extremely close to the actual values obtained from experimental work [31]. To evaluate the variability of the experimental data, the standard deviation (Std. Dev.) and the coefficients of variation (C.V.) were reported. It was found that Std. Dev. and C.V. values for all the developed models were low compared to their mean, indicating a higher fitness and correlation of the predicted values with the actual data from the experiments. To verify the satisfaction of the developed models, adequate precision (AP) is also presented in Tables 5–7. It can be observed that the AP values for all models are greater than four, which is the desired value by the design approach used in the RSM, indicating that each of the developed models can be used to traverse the design space.

The cubic and quadratic polynomial regressions generated from the ANOVA for the shear viscosity, mixing temperature, and compaction temperature of the CPO- and/or TPO-modified asphalt are shown in Eqs. 6–8. All model terms and their interactions that did not significantly affect the viscosity and mixing and compaction temperatures were excluded, and only the terms that were

Table 5
ANOVA results for shear viscosity.

Source	Sum of squares	df	Mean square	F Value	p-value prob > F	
Model	207.52	6	34.59	30.75	< 0.0001	Significant
A-CPO	63.58	1	63.58	56.52	< 0.0001	R^2 = 0.9535
B-TPO	29.36	1	29.36	26.11	0.0006	Adj R^2 = 0.9225
A^2	10.76	1	10.76	9.56	0.0129	Std. Dev. = 1.06
B^2	34.87	1	34.87	31.00	0.0003	C.V. = 14.96%
A^3	28.49	1	28.49	25.33	0.0007	A.P. = 18.040
B^3	30.09	1	30.09	26.75	0.0006	

Table 6
ANOVA results for mixing temperatures.

Source	Sum of squares	df	Mean square	F Value	p-value prob > F	
Model	1265.70	5	253.14	11.21	0.0008	Significant
A-CPO	1033.63	1	1033.63	45.77	< 0.0001	$R^2 = 0.849$
B-TPO	6.87	1	6.87	0.30	0.5934	Adj $R^2 = 0.773$
AB	40.32	1	40.32	1.79	0.2111	Std. Dev. = 4.75
A^2	52.85	1	52.85	2.34	0.1571	C.V. = 3.25%
B^2	132.02	1	132.02	5.85	0.0362	A.P. = 10.896

Table 7
ANOVA results for compaction temperatures.

Source	Sum of squares	df	Mean square	F Value	p-value prob > F	
Model	1508.62	5	301.72	9.49	0.0015	Significant
A-CPO	1270.10	1	1270.10	39.97	< 0.0001	$R^2 = 0.826$
B-TPO	0.56	1	0.56	0.018	0.8969	Adj $R^2 = 0.739$
AB	78.04	1	78.04	2.46	0.1482	Std. Dev. = 5.64
A^2	49.56	1	49.56	1.56	0.2402	C.V. = 4.46%
B^2	110.36	1	110.36	3.47	0.0920	A.P. = 10.03

necessary to maintain the hierarchy were included. The final regression models presented in Eqs. 6–8 can be utilized to predict the shear viscosity and mixing and compaction temperatures of the base and bio-modified asphalt within CPO and TPO contents of 0–15%. According to the RSM, normalization of the factors to (−1 to +1) should be performed in using these developed regressions.

$$Shear viscosity at 88^{\circ}C = 9.96 - 9.52A - 6.47B - 1.84A^2 - 3.32B^2 + 6.71A^3 + 6.90B^3 \tag{6}$$

$$Mixing\ temperature = 152.17 - 10.78A + 0.88B + 2.86AB - 4.09A^2 - 6.46B^2 \tag{7}$$

$$Compaction\ temperature = 131.92 - 11.95A + 0.25B + 3.98AB - 3.96A^2 - 5.91B^2 \tag{8}$$

3.3.2. Response surface contour plots

Diagnostic plots were graphically constructed to ascertain normal distribution and adequacy of the data. Normal probability plots of the shear viscosity, mixing temperature, and compaction temperature based on the distribution of data points are shown in Fig. 5a, 5b, and 5c, respectively. The normal plots of residuals presented values that were closely aligned along the inclined straight line, indicating that the data were normally distributed. The residual versus run-order plots of the shear viscosity, mixing temperature, and compaction temperature are shown in Fig. 5d, 5e, and 5f, respectively. All points were plotted inside the red boundaries of the graphs, and none of the points exceeded the upper or lower boundaries. This indicates that there was no apparent drift in the model during the process. This also implies that the values predicted by the developed models are expected to be accurate [63]. In addition, to understand the behavior of the developed models, the predicted values obtained from the developed models were plotted against those from the experimental work, as shown in Fig. 6a, 6b, and 6c, for the shear viscosity, mixing temperature, and compaction temperature, respectively. Almost all points of the responses spread close to the equality line, indicating that the predicted viscosity and production temperatures were in good agreement with the experimental values obtained using the dynamic shear rheometer. This reflects the precision of the developed models. The aforementioned discussion suggests that the diagnostic plots validating the developed models are appropriate and applicable in predicting the shear viscosity and mixing and compaction temperatures of bio-modified asphalt.

To illustrate the graphical relationships between the CPO and TPO contents as independent variables and the shear viscosity and mixing and compaction temperatures as responses, Fig. 7a – 7f show the 2D and 3D plots. From Fig. 7a and 7d, it can be observed that the shear viscosity of the binders decreased with increasing CPO and TPO beyond 5%. This can be because of the light components of CPO and TPO, which led to softer binders. However, the combination of CPO and TPO improved the shear viscosity to a certain extent, which can be ascribed to the chemical interactions between CPO and TPO in the asphalt matrix. Furthermore, Fig. 7b and 7e show that the compaction temperature decreased with increasing CPO content and TPO beyond 5%, which can be attributed to the reduction in the stiffness and viscosity of the binders, particularly with high CPO content. Similarly, the compaction temperature showed a significant reduction at high CPO and/or TPO percentages, as shown in Fig. 7c and 7f. However, at lower contents (<5%), there was a slight increase in the mixing and compaction temperatures. These findings can be useful for maintaining the viscosity of binders within the desired range and minimizing the production temperatures toward more sustainable bio-modified asphalt than conventional asphalt.

3.4. Machine learning analysis and modelling results

The results of using different ML algorithms to develop predictive models for the shear viscosity, mixing temperature, and compaction temperature of the base and bio-modified asphalt are presented in this section.

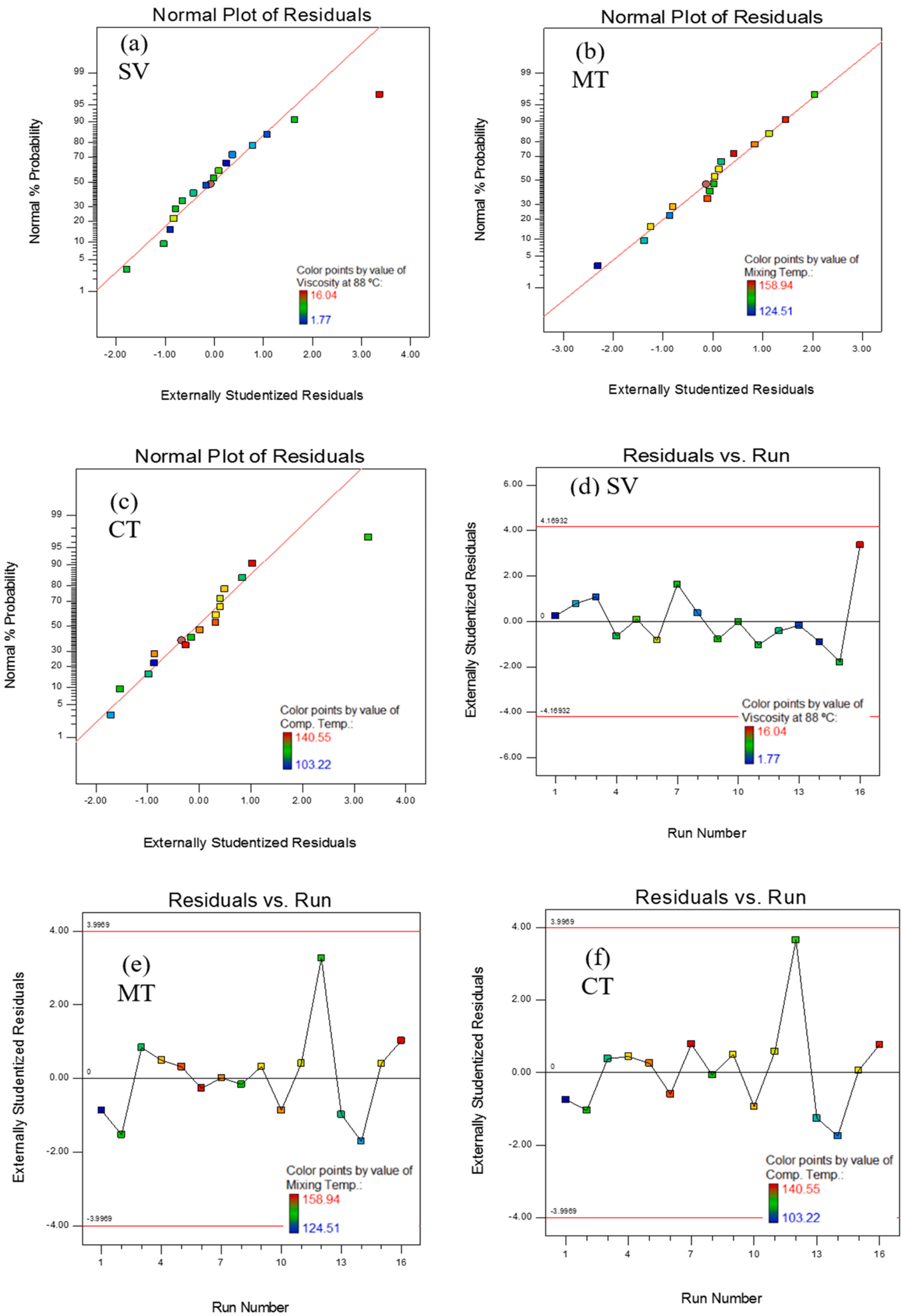

Fig. 5. Diagnostic plots for shear viscosity, mixing temperature, and compaction temperature responses.

3.4.1. Dynamic shear viscosity

The selection of an appropriate ML algorithm is essential for determining the accuracy of the predictions of the dependent variables. However, it is well known that there is no specific standard for selecting the most appropriate ML models for civil engineering materials modeling, including the rheological and production temperatures of base and modified asphalts. Therefore, extensive

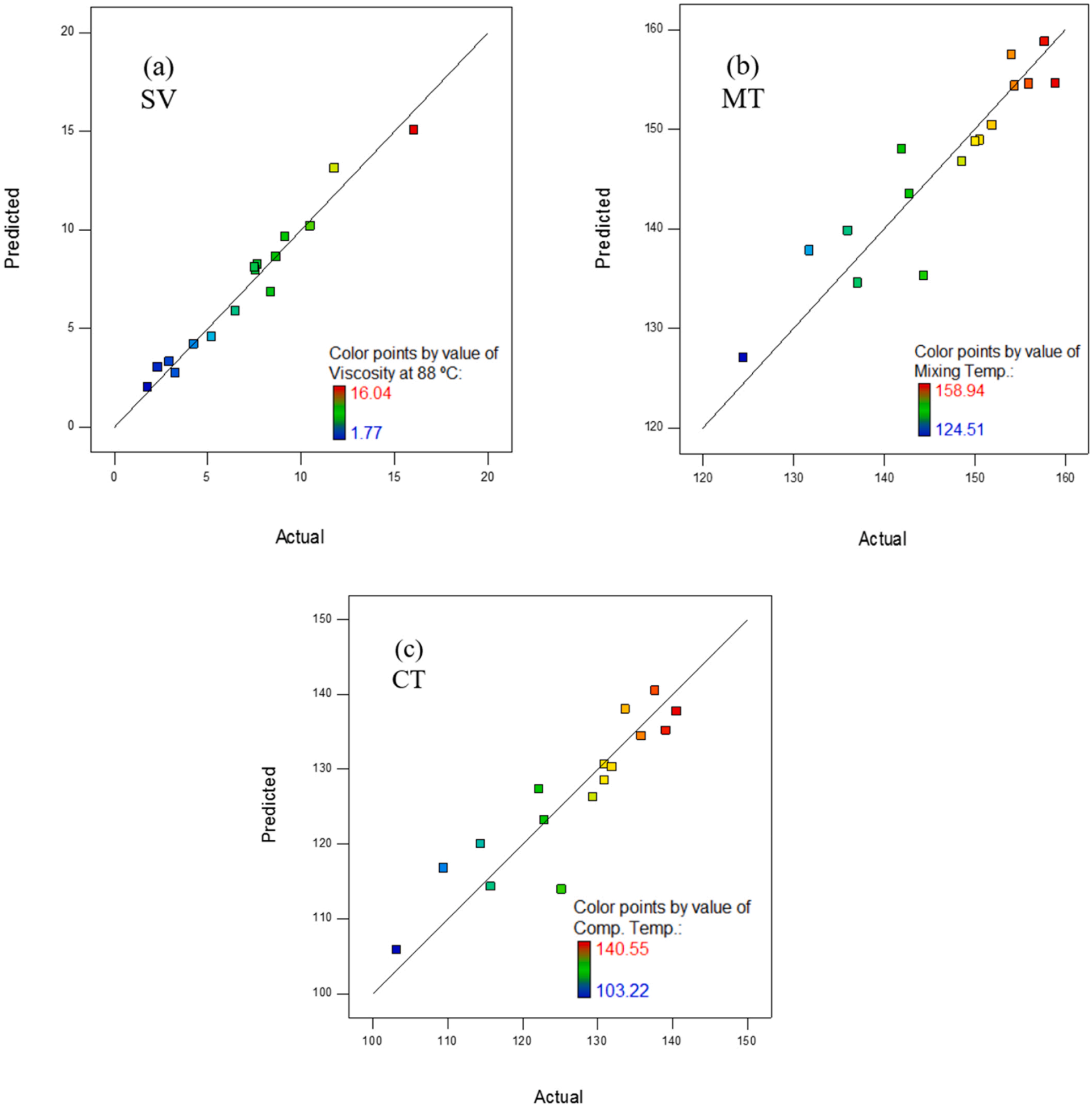

Fig. 6. Actual versus predicted plots: (a) shear viscosity, (b) mixing temperature, and (c) compaction temperature.

training was conducted on shear viscosity data obtained from experimental work to select the best ML algorithm that can represent the behavior of the shear viscosity of bio-modified asphalt. The results of the training are presented in Fig. 8a and 8b in the form of R^2 and RMSE values, respectively. From Fig. 8a, it can be observed that the XGB regression had the highest R^2 value of 0.912 among all evaluated models. This indicates that approximately 91% of the shear viscosity of the CPO- and/or TPO-modified asphalt obtained from the DSR experimental work can be represented by XGB regression. Meanwhile, Fig. 8b shows that the XGB regression had the lowest RMSE value of 0.999 Pa·s for shear viscosity among all investigated ML models. The aforementioned discussion suggests that XGB regression is accurate for predicting the shear viscosity of asphalt. Therefore, XGB regression was selected in this study to develop predictive models for the shear viscosities of the base and modified asphalts.

Fig. 9a shows the relationship between the predicted shear viscosity obtained from the XGB regression and the experimentally obtained actual shear viscosity of the CPO-and/or TPO-modified asphalt. Almost all points were very close to the equality line, indicating a high degree of agreement between the predicted shear viscosity from the ML model and the shear viscosity from the laboratory. This also reflects the strong correlation between CPO and TPO as independent variables and shear viscosity as a response. An R^2 value of 0.97847 indicates the capability of the developed XGB regression model to predict almost 98% of the shear viscosity of

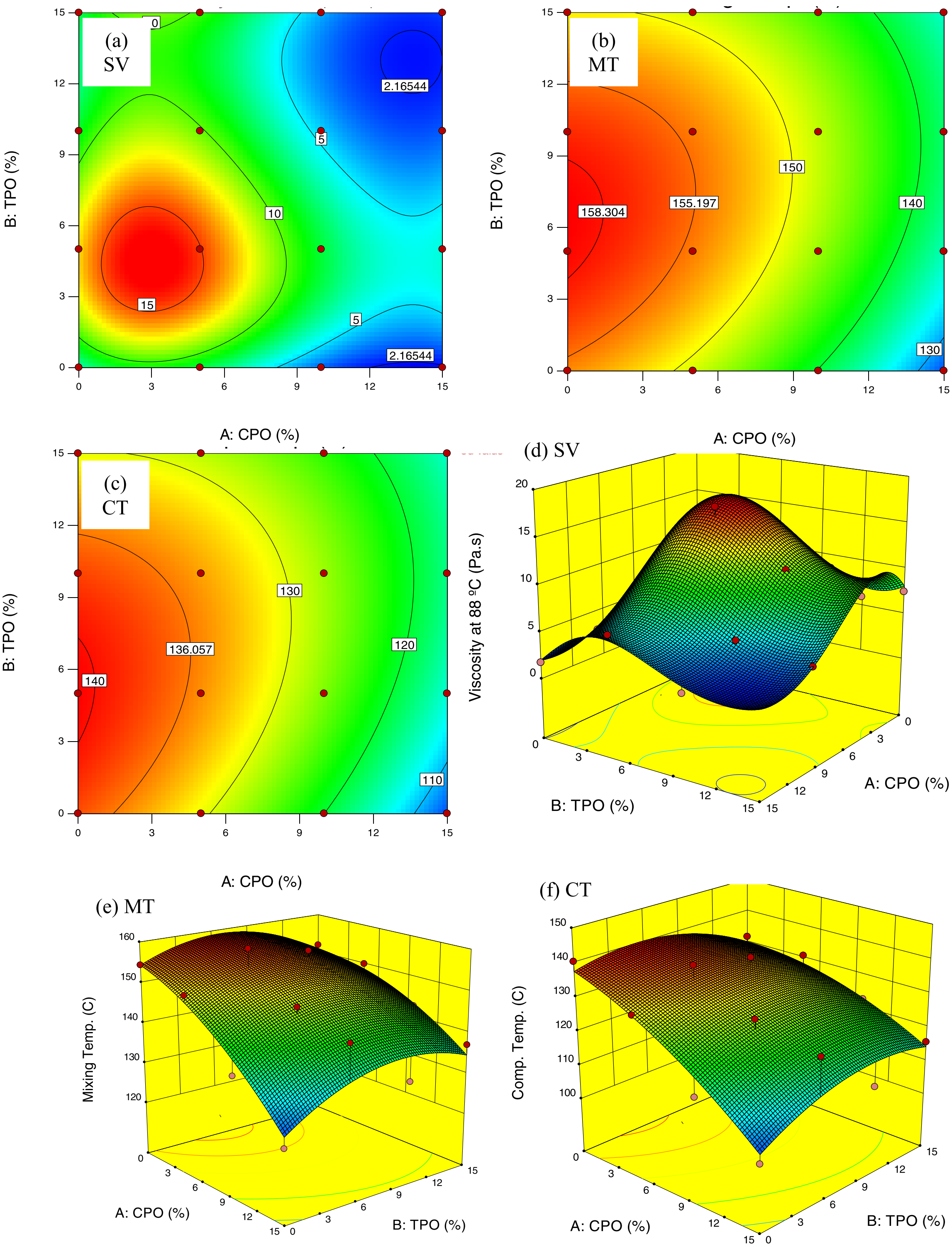

Fig. 7. 2D and 3D plots of shear viscosity, mixing temperature, and compaction temperature responses.

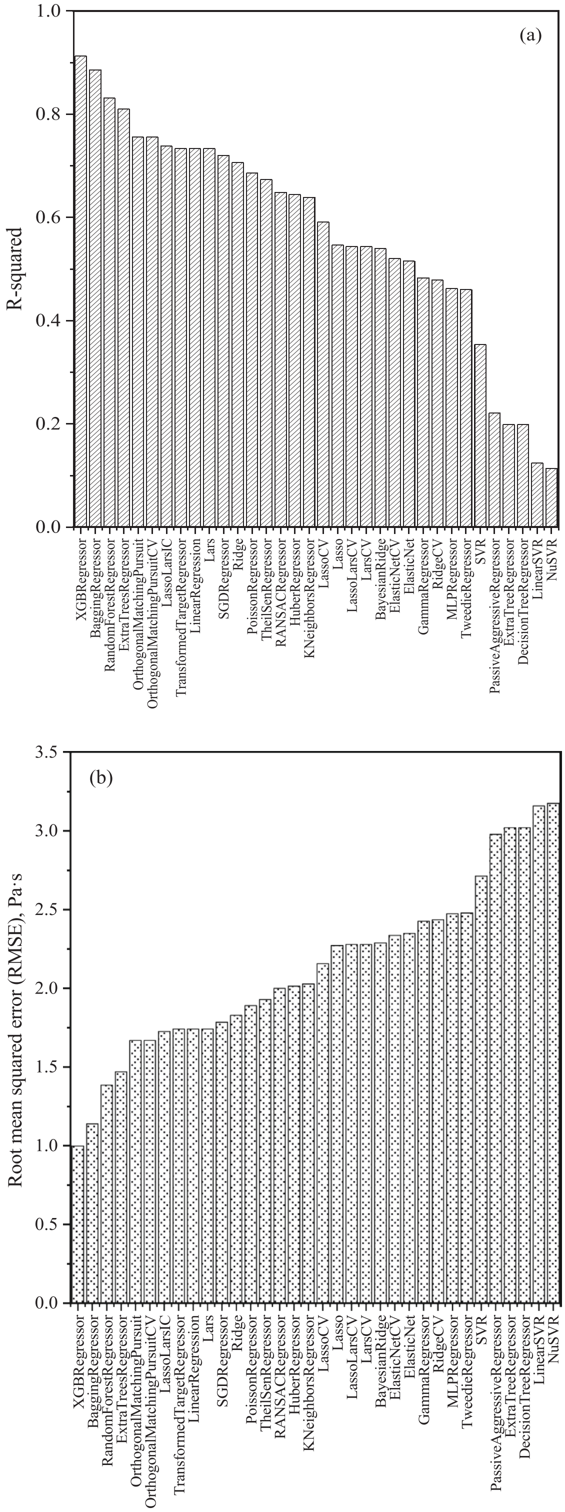

Fig. 8. The correlation coefficient and RMSE of shear viscosity obtained from various ML models.

the bio-modified asphalt with an adequate degree of accuracy. Furthermore, the performance of the developed ML model for the shear viscosity of the bio-modified asphalt is shown in Fig. 9b. It can be observed that most of the predicted values are almost identical to the actual values obtained from the experiment. This indicates the capability and accuracy of the developed XGB regression model in predicting the shear viscosity of the bio-modified asphalt investigated in this study.

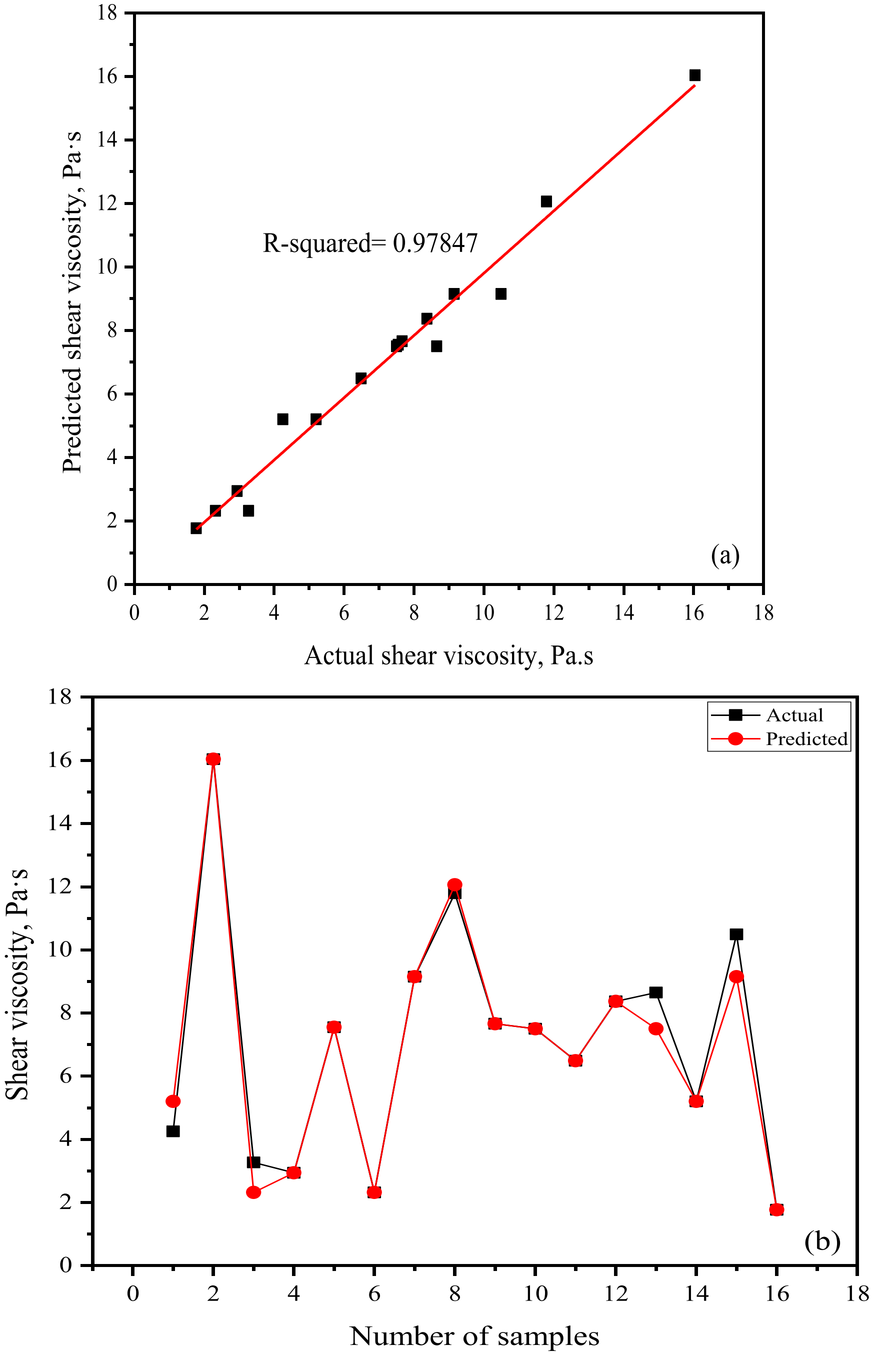

Fig. 9. Performance of the ML model for shear viscosity: (a) predicted versus actual plot and (b) point-to-point comparison plot.

3.4.2. Mixing temperature

The correlation coefficient (R^2) and root mean square error (RMSE) of the mixing temperatures of the BMA are presented in Figs. 10a and 10b, respectively. The most common ML models were used to train the experimental data of the mixing temperatures of the BMA to identify the optimal model that could successfully predict the mixing temperatures with adequate accuracy. From Figs. 10a and 10b, it can be noticed that random forest regression (RFR) shows the highest R^2 value of 0.96583 and the lowest RMSE value of 1.499 °C. This indicates that the RFR is the best model among all the evaluated ML models for predicting the mixing temperatures of bio-modified asphalt. Almost 97% of the changes in mixing temperatures due to CPO and/or TPO intervention can be represented by the RFR. Therefore, RFR was selected as the optimal ML algorithm to develop predictive models for the mixing temperatures of the base and modified asphalts evaluated in this study.

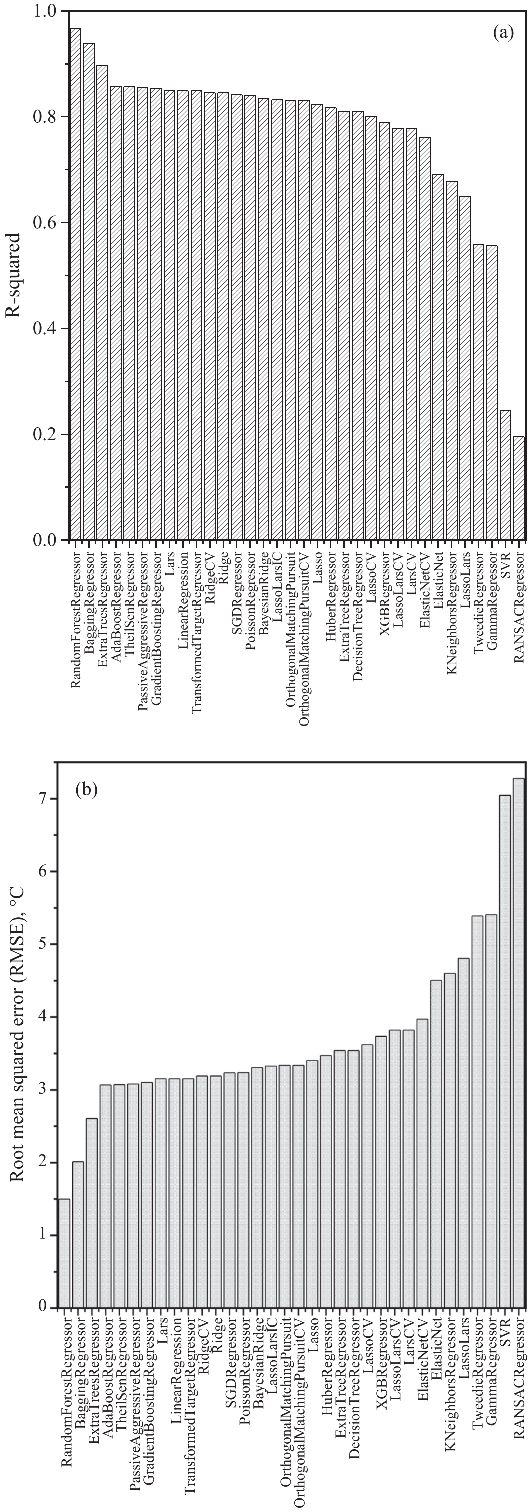

Fig. 10. The correlation coefficient and RMSE of mixing temperatures obtained from various ML models.

The relationship between the predicted mixing temperatures of the BMA obtained from the RFR model and the actual values obtained from the experiment is presented in Fig. 11a. Almost all the predicted and actual data points were located close to the equality line. This result reflects the agreement between the predicted and actual mixing temperatures, indicating the satisfactory accuracy of the developed predictive model. It also revealed a high degree of correlation between CPO and TPO as independent variables and the

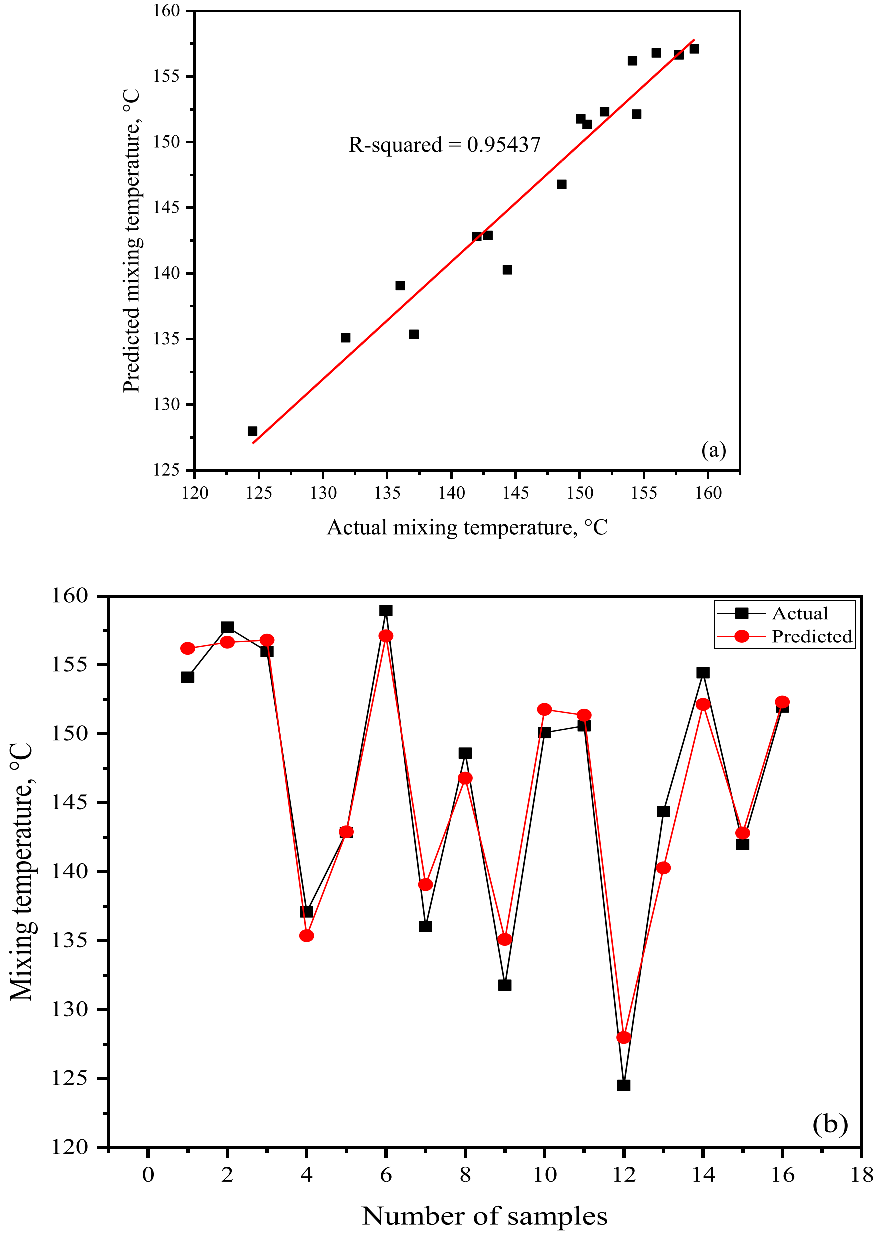

Fig. 11. Performance of the ML model for mixing temperatures: (a) predicted versus actual plot and (b) point-to-point comparison plot.

mixing temperatures of BMA as a response. This strong correlation also supports and validates the findings similar to those of the RSM. As shown in Fig. 11a, the R^2 value was 0.95437, indicating that the developed RFR model can successfully represent approximately 95% of the mixing temperatures of the base and modified asphalts obtained from the dynamic shear rheometer.

The performance of the developed ML model in predicting the mixing temperatures of the BMA is shown in Fig. 11b. Only a small difference was observed between the mixing temperature values obtained from the RFR model and those obtained from the experiment. This indicates the capability of the developed ML model to predict the mixing temperatures of the base and modified asphalts with an adequate degree of accuracy. These findings are consistent with the results obtained using RSM.

3.4.3. *Compaction temperature*

The R^2 and RMSE values of the compaction temperatures of the BMA obtained from the extensive training of various ML models are shown in Figs. 12a and 12b, respectively. Similar to the results for mixing temperatures, the random forest regression also showed the highest R^2 value of 0.96281 and lowest RMSE of 1.63 °C among all evaluated ML models for compaction temperature. This indicates that approximately 96% of the compaction temperatures of the base and bio-modified asphalts obtained from the experiment can be

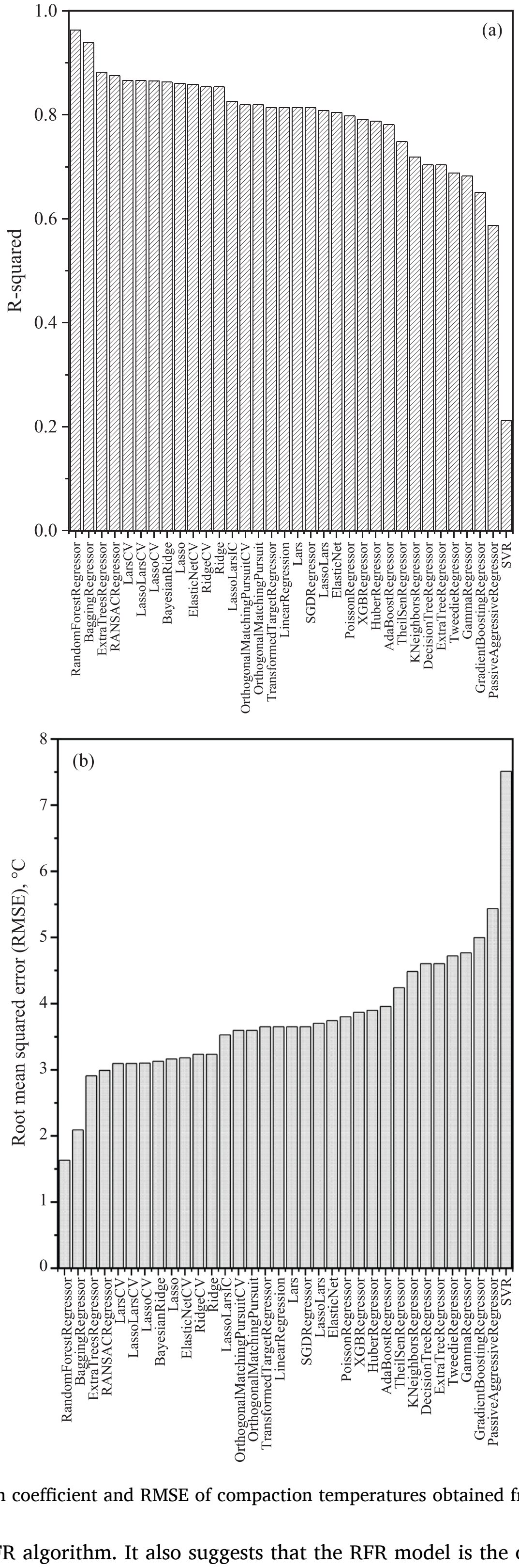

Fig. 12. The correlation coefficient and RMSE of compaction temperatures obtained from various ML models.

successfully represented using the RFR algorithm. It also suggests that the RFR model is the optimal and the most appropriate ML model among all investigated ML models for predicting the compaction temperatures of BMA. Therefore, the RFR was selected to develop a predictive model that can be used to predict the compaction temperatures of the base and modified asphalts within the CPO and TPO concentrations used in this study.

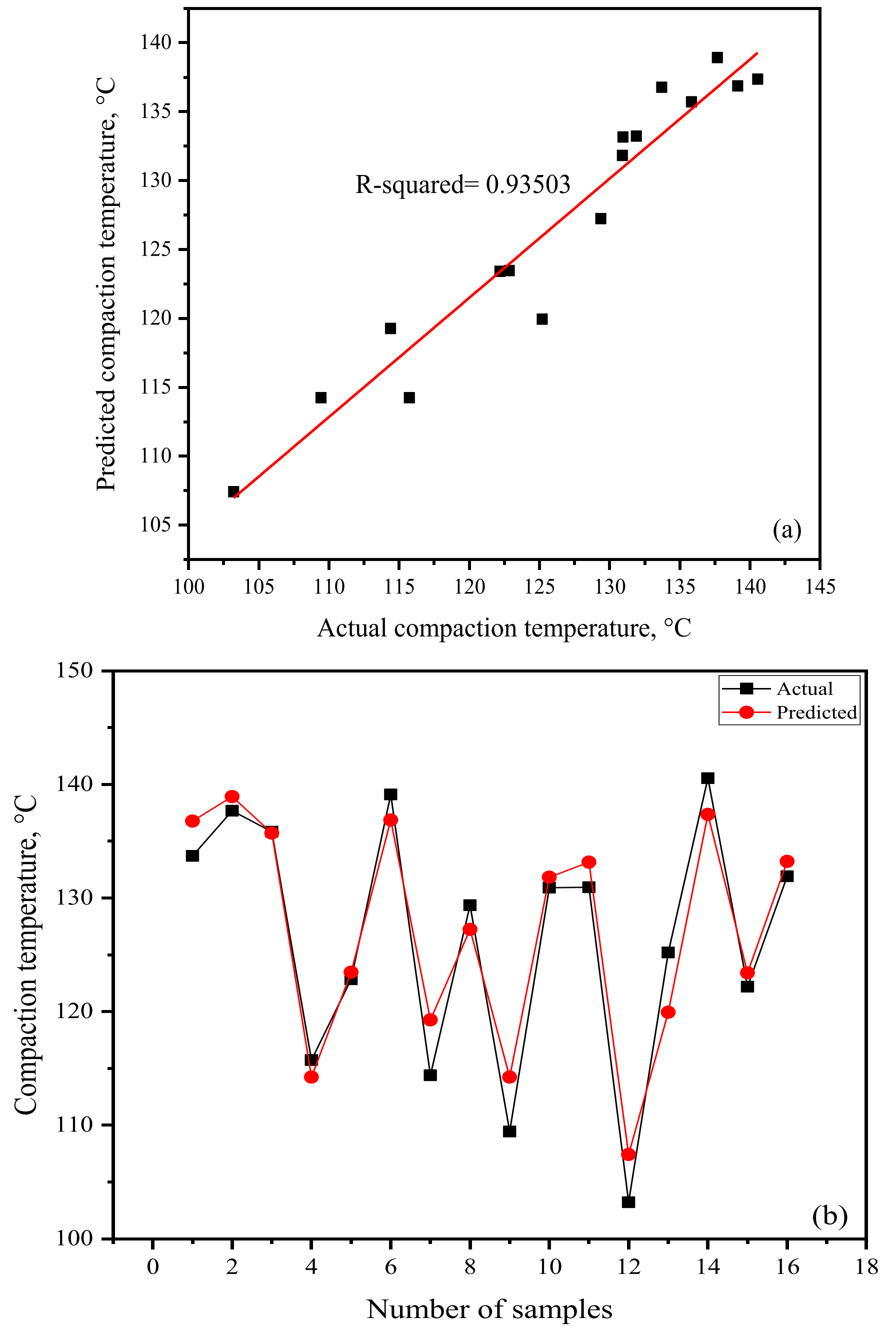

Fig. 13. Performance of the ML model for compaction temperatures: (a) predicted versus actual plot and (b) point-to-point comparison plot.

Fig. 13a shows the relationship between the predicted compaction temperatures obtained from the RFR model and actual values obtained from the dynamic shear rheometer. Almost all points were spread very close to the equality line, indicating adequate agreement between the compaction temperatures predicted by the ML approach and the actual values obtained from the experimental work. This also reflects the high correlation between CPO and TPO as independent variables and the compaction temperatures of the BMA as dependent variable. From Fig. 13a, it can also be observed that the R^2 value is 0.93503, which indicates that almost 93% of the changes in the compaction temperatures of the BMA are due to the effects of the CPO and TPO interventions. This also reflects the capability of the developed RFR model to represent 93.5% of the experimental data used to develop the model. Therefore, the RFR model is an appropriate model to be used for predicting the compaction temperatures of BMA within the limitations of the materials and standards used in this study.

The point-to-point performance of the developed RFR model for the compaction temperatures of the BMA binders in terms of the difference between the predicted and actual values is shown in Fig. 13b. It should be noted that the predicted values obtained from the ML model were very close to the actual values obtained from the experimental work, indicating the ability of the proposed RFR model to learn the correlation between CPO and TPO as independent variables and the compaction temperature as a response. This also reflects the capability of the developed model to generalize the variables within the boundaries applied in this study with a satisfactory degree of prediction. This behavior is in agreement with those of the RSM results. Therefore, the RSM and ML approaches validate the effects of CPO and TPO on the production temperatures of the BMA binders obtained from the dynamic shear rheometer.

3.5. Performance comparison of the RSM and ML approaches

In this study, user-defined design RSM and ML methods were used to predict the shear viscosity, mixing temperature, and compaction temperatures of bio-modified asphalt. Both methods were compared by assessing the relationship between the predicted and actual values to determine the prediction accuracy of the developed models. In addition, the absolute percentage error (APE) of both methods was calculated and compared. Tables 8–10 list the predicted and actual outcomes and their respective APE for the shear viscosity, mixing temperature, and compaction temperature, respectively.

Overall, the ML model predictions matched the experimental data better than the RSM models. Thus, the ML models are more capable of generalizing data than RSM models. Table 8 shows that the shear viscosity values of the BMA obtained from the ML models are extremely close to the actual values, with an APE of less than 0.05 for most of the binders. In contrast, the shear viscosity values obtained from the RSM are far from the actual values, with APE higher than 0.05 for most binders. This indicates that ML is a more appropriate technique than RSM for representing the experimental behavior of the shear viscosity of the base and modified asphalt with an adequate degree of accuracy. From Tables 9 and 10, it can be observed that almost all values of the mixing and compaction temperatures obtained from both methods (RSM and ML) are close to the experimental data, with an APE of less than 0.05. This reflects the capability of both methods to represent and predict the mixing and compaction temperatures of BMA at various CPO and/or TPO concentrations within the limitations and standards used in this study, with an adequate degree of accuracy. However, the ML models outperform RSM in the prediction of mixing and compaction temperatures, which are very close to those obtained from DSR, revealing the power of ML in modeling even with limited available data.

3.6. Multiobjective optimization of responses and prediction validation

The response surface was optimized to determine the best solutions for the shear viscosity, mixing temperature, and compaction temperature. The optimal asphalt was selected based on the highest desirability of 1.00 among the solutions obtained from the optimization process, as shown in Fig. 14. Each optimization ramp shows the criteria defined for the multiobjective optimization process, and the blue or red pointer indicates the optimized value for each response or factor. The multiobjective optimization resulted in bio-modified asphalt with 5% CPO and 15% TPO, which was the optimal asphalt that fulfilled the optimization criteria used in this study. The optimal asphalt was selected based on the highest desirability of 1.00 among the solutions obtained from the optimization process. The high desirability of the optimized solution indicates the quality of the optimization. Therefore, BMA 515 was used to validate the developed RSM and ML models by comparing the shear viscosity and mixing and compaction temperatures obtained from the experimental work with the predicted results from the RSM and ML, as presented in Table 11. Good agreement was observed between the data obtained from the DSR machine and the predicted results from the RSM and ML, as the measured APE was less than 10%. It can also be observed that the ML models exhibited a very low APE (less than 2%) for all responses compared to the RSM, indicating that ML is more reliable and accurate in predicting the shear viscosity and production temperatures of the base and bio-modified asphalts. The findings of this optimization are consistent with the literature results, showing that bio-modified asphalt with 5% CPO and 15% TPO has appropriate mechanical properties with a performance grade of PG64S [13]. Therefore, the optimal 5% CPO and 15% TPO combination obtained from this study has the potential to reduce the mixing and compaction temperatures and improve and maintain the desired mechanical properties of asphalt. Based on the desired feature requirements, multiobjective optimization is a powerful technique for resolving conflicting responses toward achieving an optimal solution.

4. Conclusions

In this study, the effects of crude palm oil (CPO) as a bio-oil and tire pyrolysis oil (TPO) as an alternative to conventional crumb rubber in separate and composite forms on the shear viscosity, mixing temperature, and compaction temperature of asphalt were evaluated and compared using RSM and ML approaches. This is to develop reliable and accurate predictive models. The main conclusions are as follows:

- The use of CPO and/or TPO as extenders in the base asphalt resulted in a lower shear viscosity, particularly at higher CPO percentages. However, at a content of 5% or less for both the materials, the viscosity was better than or similar to that of the base asphalt. BMA 55 showed the highest shear viscosity among all tested binders in this study, with 112.76% improvement at 88 °C compared to base asphalt.
- It was also noticed that the separate addition of CPO or TPO into the asphalt significantly reduced the mixing and compaction temperatures, and 15% CPO showed the lowest temperatures among all tested binders. Although the CPO/TPO composite resulted in a lower reduction in temperature than the base asphalt, a similar or better viscosity was maintained.

Table 8
Comparison of RSM and ML prediction performance for shear viscosity at 88 °C.

Binder	Actual SV, Pa·s	RSM predicted SV, Pa·s	% Error	ML predicted SV, Pa·s	% Error
BMA 00	8.37	7.17	-0.143	8.37	0.000
BMA 05	11.79	12.46	+0.057	12.06	+0.023
BMA 010	8.65	8.65	0.000	7.50	-0.133
BMA 015	7.5	8.03	+0.071	7.50	0.000
BMA 50	7.66	8.93	+0.166	7.66	0.000
BMA 55	16.04	14.21	-0.114	16.04	0.000
BMA 510	10.49	10.41	-0.008	9.15	-0.128
BMA 515	9.15	9.79	+0.070	9.15	0.000
BMA 100	2.94	3.08	+0.048	2.94	0.000
BMA 105	7.55	8.36	+0.107	7.55	0.000
BMA 1010	5.2	4.56	-0.123	5.20	0.000
BMA 1015	4.25	3.94	-0.073	5.20	+0.224
BMA 150	1.77	1.56	-0.119	1.77	0.000
BMA 155	6.49	6.84	+0.054	6.49	0.000
BMA 1510	2.32	3.04	+0.310	2.32	0.000
BMA 1515	3.27	2.41	-0.263	2.32	-0.291

Table 9
Comparison of RSM and ML prediction performance for mixing temperature.

Binder	Actual MT, °C	RSM predicted MT, °C	% Error	ML predicted MT, °C	% Error
BMA 00	154.43	154.38	0.000	152.14	-0.015
BMA 05	157.74	158.81	+ 0.007	156.65	-0.007
BMA 010	154.11	157.49	+ 0.022	156.20	+ 0.014
BMA 015	151.94	150.43	-0.010	152.31	+ 0.002
BMA 50	150.58	148.93	-0.011	151.35	+ 0.005
BMA 55	158.94	154.62	-0.027	157.11	-0.012
BMA 510	155.97	154.57	-0.009	156.80	+ 0.005
BMA 515	150.09	148.78	-0.009	151.77	+ 0.011
BMA 100	136.03	139.83	+ 0.028	139.07	+ 0.022
BMA 105	148.6	146.80	-0.012	146.79	-0.012
BMA 1010	141.98	148.02	+ 0.043	142.81	+ 0.006
BMA 1015	142.85	143.49	+ 0.004	142.90	0.000
BMA 150	124.51	127.10	+ 0.021	127.98	+ 0.028
BMA 155	144.37	135.34	-0.063	140.27	-0.028
BMA 1510	131.77	137.83	+ 0.046	135.09	+ 0.025
BMA 1515	137.09	134.58	-0.018	135.36	-0.013

Table 10
Comparison of RSM and ML prediction performance for compaction temperature.

Binder	Actual CT, °C	RSM predicted CT, °C	% Error	ML predicted CT, °C	% Error
BMA 00	140.55	137.73	-0.020	137.36	-0.023
BMA 05	137.68	140.50	+ 0.020	138.92	+ 0.009
BMA 010	133.71	138.02	+ 0.032	136.77	+ 0.023
BMA 015	131.91	130.28	-0.012	133.23	+ 0.010
BMA 50	130.95	130.63	-0.002	133.16	+ 0.017
BMA 55	139.12	135.17	-0.028	136.86	-0.016
BMA 510	135.83	134.45	-0.010	135.71	-0.001
BMA 515	130.91	128.49	-0.018	131.82	+ 0.007
BMA 100	114.39	120.01	+ 0.049	119.26	+ 0.043
BMA 105	129.37	126.32	-0.024	127.24	-0.016
BMA 1010	122.19	127.37	+ 0.042	123.41	+ 0.010
BMA 1015	122.85	123.17	+ 0.003	123.46	+ 0.005
BMA 150	103.22	105.87	+ 0.026	107.42	+ 0.041
BMA 155	125.2	113.95	-0.090	119.94	-0.042
BMA 1510	109.44	116.76	+ 0.067	114.24	+ 0.044
BMA 1515	115.74	114.33	-0.012	114.24	-0.013

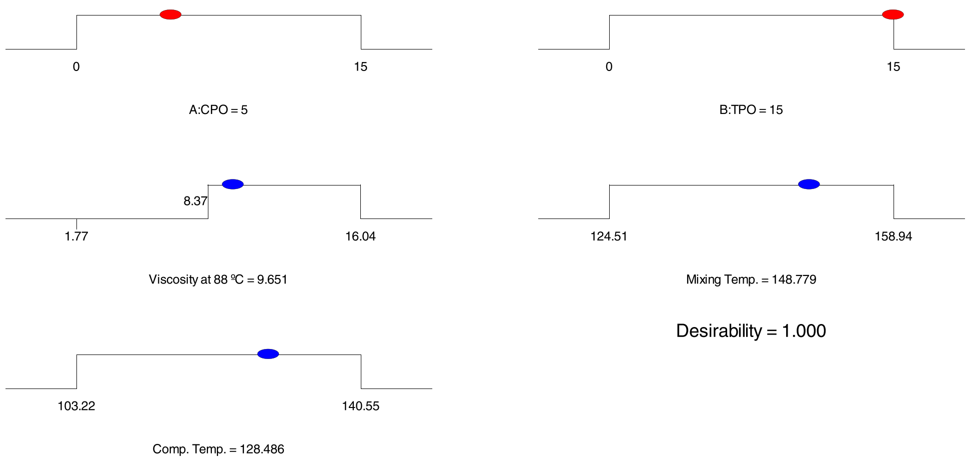

Fig. 14. RSM optimization ramps for shear viscosity, mixing temperature, and compaction temperature.

Table 11
Optimized BMA515 binder and validation of RSM and ML models.

Response	Experiment	RSM		ML	
	Actual	Predicted	% Error	Predicted	% Error
Shear viscosity, Pa·s	9.15	9.79	+ 6.99	9.15	0.00
Mixing Temp., °C	150.09	148.78	-0.873	151.77	+ 1.119
Compaction Temp., °C	130.91	128.49	-1.849	131.82	+ 0.695

- The RSM statistical analysis showed a correlation coefficient (R^2) of more than 0.82 for all responses, indicating that the RSM-developed models can accurately represent and predict at least 82% of the experimental data for the shear viscosity and mixing and compaction temperatures of the bio-modified asphalt.
- The multiobjective optimization resulted in asphalt with 5% CPO and 15% TPO, which can fulfill the requirements of reducing the mixing and compaction temperatures and maintaining the desired viscosity by incorporating bio-oil and waste from tire rubber recycling.
- The evaluation of a wide range of machine learning (ML) models showed that XGB regression was the best model among all tested ML models for predicting shear viscosity, whereas random forest regression (RFR) was the best for predicting mixing and compaction temperatures, with R^2 values of more than 93%.
- The point-to-point comparison between the experimental and ML-based predicted shear viscosity and mixing and compaction temperatures of the bio-modified asphalt showed that the predicted and actual values were extremely close, reflecting the reliability and capability of ML to predict the properties of CPO/TPO-modified asphalt.
- The comparison between the RSM and ML approaches demonstrated that both methods can make accurate predictions. However, ML outperformed RSM with a lower APE (less than 5%) for almost all binders and responses in this study.

Overall, it can be stated that ML is a powerful tool for predicting the shear viscosity and mixing and compaction temperatures of bio-modified asphalt with an adequate degree of accuracy. Future studies should investigate the effects of broader replacement percentages, modifiers, and binder grades, which were not considered in this study. Future research should quantitatively evaluate the environmental and economic impacts of different biomaterials on energy consumption and CO_2 emissions during the production and construction of asphalt mixtures. Additional parameters, such as life cycle cost and life cycle assessment, can also be incorporated into optimization models.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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