

Advanced Hybrid AI Models for Predicting Softening Point and Penetration of Modified Bitumen

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Abstract

Ensuring bitumen quality is essential for the durability of asphalt pavements. Conventional laboratory tests for softening point (SP) and penetration (P) are reliable but labor-intensive and time-consuming, particularly for modified binders incorporating recycled additives. This study proposes an advanced hybrid machine learning (ML) framework integrating Neural Architecture Search (NAS) with Artificial Neural Networks (ANN) to predict the SP and P of modified bitumen containing crumb rubber (CR), coffee grounds (CG), and olive pomace (OP). A dataset of 49 laboratory-prepared samples was used to train and validate three models – Random Forest (RF), ANN, and NAS-ANN – evaluated through statistical indicators (MSE, RMSE, R^2 , R). The NAS-ANN achieved the best performance, with $R = 0.9665/0.9567$ for SP and $0.9726/0.8711$ for P (training/validation). Sensitivity analysis indicated that OP had the most significant influence on SP, followed by CR and CG. The optimized NAS-ANN model was implemented in a user-friendly interface named SmartBit-AI, designed to facilitate rapid prediction and mix-design preselection. Overall, the proposed NAS-ANN framework complements conventional laboratory testing, offering a practical and efficient tool for accelerating sustainable bitumen evaluation and design.

Keywords

bitumen, softening point, penetration, pavement, machine learning, neural architecture search

1 Introduction

The rapid expansion of transportation infrastructure worldwide has created increasing demands on the performance and durability of asphalt pavements [1]. Consequently, the quality of materials used – particularly bitumen, the primary binding agent in asphalt concrete – has become a central focus of pavement engineering research [2]. Although bitumen constitutes a relatively small proportion of the asphalt mixture, it has a significant impact on critical performance characteristics such as elasticity, temperature susceptibility, resistance to deformation, and long-term aging behavior [3]. To ensure its reliability, two fundamental tests are widely used to characterize bitumen: the softening point (SP), which reflects temperature sensitivity, and the penetration (P) value, which measures consistency or hardness at a specified temperature [4].

These parameters serve as early indicators of bitumen quality and its suitability for use under specific environmental and loading conditions [5]. However, conventional laboratory methods for determining these properties are often time-consuming, require specialized expertise, and

may be inefficient when applied to large datasets or diverse mix compositions. This challenge is particularly evident in the case of modified bitumen, where the incorporation of additives such as polymers, industrial by-products, or recycled materials introduces additional variability [6–8].

In recent years, significant advancements in Artificial Intelligence (AI) and machine learning (ML) have transformed materials engineering, particularly in the study and prediction of bituminous material properties. Driven by the growing need for more efficient and accurate evaluation methods, these developments have introduced powerful data-driven tools capable of modeling complex and nonlinear relationships between compositional variables and bitumen performance metrics without relying on explicit physical equations [9–10]. Such approaches streamline quality control, reduce dependence on time-consuming experimental procedures, and enable rapid and precise property estimation [11–15]. Several studies have already demonstrated the effectiveness of ML techniques in predicting bitumen characteristics.

For example, Stergiou et al. [16] provided a comprehensive review of how ML models are applied to predict the thermal, mechanical, and optical properties of building materials and to optimize production processes. Their review highlighted the ability of ML to reduce laboratory testing time and costs across various materials, including those incorporating waste, thereby underscoring its broad applicability and utility in materials science [16].

Numerous studies have highlighted the strong potential of ML techniques in predicting various bitumen properties. For example, Salehi et al. [8] developed ensemble machine learning (EML) models to predict the rheological behavior and aging performance of recycled plastic modified bitumen (RPMB). Four EML algorithms were applied – Random Forest (RF), eXtreme Gradient Boosting (XGBoost), Categorical Boosting (CatBoost), and Light Gradient Boosting Machine (LightGBM) – with CatBoost achieving the highest accuracy, yielding coefficient of determination (R^2) values of 0.98 for complex shear modulus and 0.93 for phase angle prediction. Additionally, SHapley Additive exPlanations (SHAP) analysis identified temperature, frequency of the dynamic shear rheometer test, polymer content, and base bitumen P as key influencing factors [8]. This study employed four EML models: RF, XGBoost, CatBoost, and LightGBM. The CatBoost model showed the highest accuracy, achieving a R^2 of 0.98 for complex shear modulus prediction and 0.93 for phase angle prediction. The study also utilized SHAP analysis to identify the impact of input variables, finding that the temperature and frequency of the dynamic shear rheometer test, the amount of polymer, and the P of the base bitumen are key factors influencing rheological properties. Similarly, Arifuzzaman et al. [17] explored ensemble modeling for predicting fundamental properties of bitumen incorporating plastic waste. They compared Decision Tree (DT), Adaboost Regressor (AR), and Bagging Regressor (BR) models to estimate parameters such as air voids (V_a), Marshall flow (MF), Marshall stability (MS), tensile strength ratio (TSR), and indirect tensile strength (ITS). Among them, the BR model exhibited the highest predictive accuracy, and SHAP analysis further clarified the influence of input variables. These studies confirm the effectiveness of ensemble learning in forecasting the properties of plastic-modified asphalt mixtures [17].

Further exploring alternative materials, Tiwari et al. [18] examined the use of seven waste-derived fillers as substitutes for ordinary Portland cement in asphalt concrete mixtures. Marshall, ITS, moisture susceptibility, and Cantabro

abrasion loss tests were performed, and a DT CatBoost model was developed to predict mechanical properties, achieving high correlation and determination coefficients. Their findings demonstrated the potential of ML in evaluating asphalt mixtures incorporating diverse alternative fillers [18]. Similarly, Upadhyaya et al. [19] investigated the prediction of MS in asphalt mixes modified with glass and carbon fibers using Artificial Neural Networks (ANN), Support Vector Machines (SVM), Gaussian Processes, and RF, reporting that the SVM model yielded the most accurate predictions, with bitumen content identified as a critical factor [19]. Althoey et al. [20] compared Multi-Expression Programming (MEP), ANN, Adaptive Neuro-Fuzzy Inference System (ANFIS), and ensemble Decision Tree Bagging (DT-Bagging) models for predicting MS and MF. The DT-Bagging model achieved superior performance, and sensitivity analysis highlighted the most influential input parameters [20]. Liu et al. [21] proposed an ML-based asphalt mix design procedure to predict the rut depth of asphalt concrete pavements. They utilized 27 input features and compared Support Vector Regression (SVR), RF, ANN, and Gradient Boosting (GB). GB emerged as the optimal model, demonstrating ML's capability to predict long-term pavement performance and optimize mix design [21]. Othman [22] applied a multilayer perceptron feedforward ANN to predict the Optimum Asphalt Content (OAC) of asphalt mixes based on aggregate gradation, optimizing hyperparameters to achieve high accuracy and demonstrating the efficiency of ANN in replacing labor-intensive OAC estimation procedures [22]. In a related study, Upadhyaya et al. [23] also applied ML techniques – including ANN, SVM, Gaussian Processes, and RF – to predict binder content in glass fiber-reinforced asphalt mixes, again confirming the superiority of SVM in MS prediction [23]. Extending the scope, Miani et al. [24] developed a hyperparameter-optimized ANN approach for predicting Marshall test outcomes, stiffness modulus, and V_a , using Bayesian optimization to semi-automatically configure ANN architecture, which significantly enhanced predictive performance [24]. Finally, Awan et al. [25] employed MEP to construct empirical predictive models for MS and MF of Asphalt Base Course (ABC) and Asphalt Wearing Course (AWC), further confirming the robustness of advanced ML techniques in predicting key Marshall parameters as efficient alternatives to traditional laboratory testing [25].

In recent years, the adoption of Neural Architecture Search (NAS) in civil engineering has shown remarkable progress, leading to the development of highly accurate

and adaptive predictive models. For example, Habal and Benbouras [26] successfully employed a NAS-based hybrid model to predict California Bearing Ratio (CBR) and compaction parameters of soils, achieving superior accuracy compared with conventional ANN and RF models [27]. Similarly, Fouchal et al. [14] enhanced the prediction of biological oxygen demand (BOD) by integrating ANN and RF models with NAS optimization, which significantly improved model generalization and convergence speed [14]. In geotechnical and geohazard studies, Mebirouk et al. [28] applied NAS to optimize hybrid metaheuristic models for landslide susceptibility mapping near major road networks in northern Algeria, demonstrating efficient performance and reduced computational cost [28]. Furthermore, Brahma et al. [29] proposed a NAS-based hybrid ML approach for predicting inelastic displacement ratios (IDR) in soil–structure interaction systems on very soft soils, obtaining outstanding predictive accuracy and stability under complex boundary conditions [29]. These examples clearly demonstrate that NAS has become a powerful optimization tool in civil engineering, enabling automated model design, improved predictive reliability, and faster computational performance. However, despite its success in geotechnical, structural, and environmental applications, the use of NAS in materials engineering – particularly in predicting bitumen or asphalt properties – remains scarce.

Despite the valuable contributions of previous studies, several critical research gaps remain. While ANN and conventional ML methods are widely applied, the existing literature shows a predominant reliance on standard ML algorithms or basic ANN architectures. Limited attention has been given to more advanced hybrid AI techniques, such as NAS, which can automatically generate optimal neural network structures. This approach has the potential to deliver superior predictive accuracy and computational efficiency compared to manually designed or traditionally optimized networks.

Building upon previous research, this study makes two key contributions: first, it systematically investigates the effects of multiple secondary raw materials (crumb rubber (CR), coffee grounds (CG), and olive pomace (OP)) on bitumen properties, in contrast to many studies that focus on a single type of modifier; second, it introduces a novel hybrid modeling approach that integrates Neural Architecture Search with Artificial Neural Networks (NAS-ANN). This innovative approach automates the design

of optimal neural network architectures, moving beyond conventional trial-and-error or predefined structures. As a result, it not only achieves superior predictive performance but also reduces reliance on human expertise in model design, providing a more efficient and robust framework for complex material prediction.

2 Materials and methods

2.1 Materials

2.1.1 Bitumen

In this study, a 40/50 P grade bitumen supplied by the Algerian oil refining company NAFTAL was used. The physical properties of the bitumen are presented in Table 1 [30–34].

2.1.2 Olive pomace

The OP used in this study was obtained from an olive oil factory located in the Tablat district of Medea province, Algeria.

2.1.3 Coffee grounds

CG are an abundant organic waste generated in large quantities by both the coffee industry and households. Owing to their fine particle size, porous structure, and high carbon content, spent coffee grounds (SCG) show strong potential as a sustainable additive for bitumen modification.

2.1.4 Crumb rubber

The CR used in this study was recovered from crushed rubber waste originating from shoe soles and vehicle carpets. It was supplied by the Algerian company SAEL (Company of Elastomers Application).

2.1.5 Preparation of modified bitumen samples

The base bitumen and additives were heated in a small container to a fluid state at 170 °C and blended using a mechanical stirrer at 1200 rpm for 60 min. The OP, CG, and CR were incorporated at proportions of 2, 4, 6, 8, 9, 10, 12, and 14% by weight of the bitumen.

Table 1 Base-binder properties (40/50 P grade)

Properties	Test method	Value	Specifications
P at 25 °C (0.1 mm)	EN 1426:2015 [30]	43.63	40–50
SP (°C)	EN 1427:2015 [31]	53.25	50–58
Flash point (°C)	EN ISO 2592:2017 [32]	300	> 250°
Ductility (cm)	NA 5223 [33]	>100	>100
Specific gravity (25 °C), g/cm ³	NF T66-007 [34]	1.039	1–1.1

2.2 Test methods

Both pure and modified bitumen samples were subjected to conventional binder tests. The P (Pen25) and SP tests were performed in accordance with EN 1426:2015 [30] and EN 1427:2015 [31] standards, respectively. Regarding test repeatability, the three P determinations were kept within 2 dmm, and the difference between two softening point results did not exceed 1.5 °C.

2.2.1 Penetration

The P of bitumen was determined following the EN 1426:2015 [30] procedure. The bitumen sample was first heated to a fluid state and then poured into a container to a minimum depth of 10 mm. After cooling to room temperature, the sample was placed in a water bath maintained at 25 °C for at least 1 h prior to testing. A penetrometer equipped with a clean standard needle was positioned vertically, with the needle tip just touching the surface of the bitumen without exerting additional pressure. The needle was then released to penetrate the bitumen for exactly 5 s, after which the depth of P was recorded in tenths of a millimeter (0.1 mm). This procedure was repeated three times on different points of the sample, and the final P value was calculated as the average of the three measurements.

2.2.2 Softening point

The SP of bitumen was determined in accordance with the EN 1427:2015 [31] Ring-and-Ball method. Two brass rings were filled with fluid bitumen, previously heated to a pourable state, and placed on a metal plate. After cooling, the samples were trimmed to remove any excess material. The rings were then immersed in a beaker containing either water or glycerin, depending on the expected SP range. The beaker was placed on a hot plate equipped with a magnetic stirrer, and the temperature of the liquid bath was increased at a controlled rate of 5 °C/min. A steel ball was positioned on top of each bitumen specimen, and heating was continued until the softened bitumen allowed the balls to fall and contact the bottom plate located 25 mm below. The temperature at this point was recorded as the SP.

2.3 Dataset

The selection of input variables is a critical step in ML modeling, as it directly influences predictive accuracy. The chosen inputs must adequately capture the essential characteristics of the studied phenomenon. In this research, a dataset comprising 49 samples obtained from laboratory experiments was used to develop computational models.

The input parameters were derived from experimental investigations on modified bitumen, specifically through SP and P tests. The primary additive variables considered include CR content, CG percentage, and OP percentage.

All SP and P tests were conducted in accordance with ASTM D36/D36M-12 [27] and ASTM D5-06 [35] standards to ensure consistency and reliability. Previous research has consistently demonstrated that these additives have a significant influence on the SP and P characteristics of bitumen. The selected variables are therefore appropriate for modeling purposes. Table 2 presents the input and output variables employed in the proposed model.

2.4 ML methods

In this study, multiple ML techniques were employed to conduct a comprehensive analysis and develop an optimal predictive model. The effectiveness of ML methods has been well documented across various disciplines, showing significant improvements in predictive accuracy and computational efficiency. Accordingly, Section 2.4 describes the ML models implemented in this research, while additional references are provided for readers seeking further methodological details.

The models utilized include ANN, RF, and a hybrid model based on NAS-ANN. All computational modeling and algorithm implementation were carried out using MATLAB [36].

NAS is a pioneering deep learning method designed to automate the process of neural network creation. By tailoring the construction of neural networks to specific tasks, NAS has the potential to significantly enhance the feasibility and efficiency of deep learning applications [26, 37, 38]. Unlike traditional approaches that rely on human expertise to manually design optimal network architectures, NAS employs advanced search algorithms to identify topologies that deliver the highest performance for a given task. This approach not only accelerates the development of deep learning models but also broadens their applicability across various domains. As illustrated in Fig. 1, the NAS method typically comprises two main stages [38–40]. The first stage, known as the *search stage*, involves exploring the vast search space using various techniques to

Table 2 Input and output variables used for ML modeling

Code	Parameter type	Variable type	Variable
X1	Input	Quantitative	% of CR
X2	Input	Quantitative	% of CG
X3	Input	Quantitative	% of OP
Y1	Output	Quantitative	SP
Y2	Output	Quantitative	P

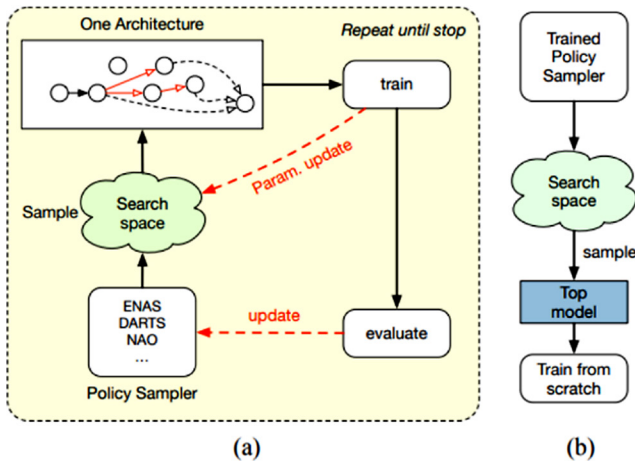


Fig. 1 Workflow of the NAS-ANN framework: (a) Search phase; (b) Standard evaluation phase

identify promising network architectures. In the second stage, referred to as the *evaluation stage*, the architectures discovered during the search are trained and evaluated on a target dataset. By iteratively cycling through these two stages, the architecture can be progressively refined and optimized. Despite its potential, NAS faces several challenges. The most significant obstacle is the immense size of the search space, which arises from the vast number of possible neural network architectures. Consequently, identifying the optimal architecture becomes a computationally expensive task. To address this limitation, researchers have proposed reducing the search space and utilizing predefined ground-truth architecture performances to evaluate the quality of the search process [41].

The first step in integrating a neural network with a NAS algorithm is to define a search space that encompasses all possible network configurations. This search space considers variables such as input data, target outputs, the number of layers, activation functions, and network operations. To navigate this extensive design space efficiently, various search strategies such as gradient-based methods, evolutionary algorithms, or reinforcement learning are employed. To mitigate the computational challenges of exploring a vast search space, researchers often opt to constrain the search to a smaller, more manageable subset of configurations.

This process involved using the "Tansig", "Logsig", and "Purelin" activation functions while limiting the number of nodes in each hidden layer. For each potential architecture, ground-truth performance metrics were obtained through repeated training using various random seeds. The NAS algorithm then generates and evaluates a large number of architectures. By training these architectures on a given dataset and assessing their performance, the algorithm identifies the most promising designs.

The selected architecture undergoes further optimization and refinement before being implemented in a real-world environment. Once deployed, the model is continuously monitored to ensure consistent performance and adaptability. By combining automated exploration with rigorous evaluation, NAS offers a powerful approach for discovering high-performing neural network topologies.

Table 3 illustrates the variations in the initial parameter settings for each approach. Manually designing a neural network or RF architecture for a specific task used to be a labor-intensive and time-consuming process [42, 43]. However, with the advent of NAS, this process has been significantly streamlined, drastically reducing the time required to identify the optimal model architecture [44]. NAS automates the selection of optimal network hyperparameters, such as the number of hidden layers, and the number of neurons per layer. This meticulous optimization enables the development of highly efficient models capable of capturing complex interactions between input features and target. By utilizing NAS, the time required to manually set up a model is significantly reduced, allowing resources to be allocated to other aspects of the study. The automation of the NAS process not only accelerates model development but also improves performance by systematically exploring a wide range of potential architectures and parameter configurations. This method ensures that the final model is optimally tuned to the specific characteristics of the dataset, leading to more accurate and reliable predictions.

Each candidate architecture combined one or two hidden layers with specific activation functions and neuron counts, while all input variables were normalized using a z-score transformation to ensure numerical stability and consistent learning behavior. A random-search strategy with parameter sharing was adopted for the NAS process, as it provides an effective balance between exploration efficiency and search coverage, particularly in small-scale

Table 3 NAS search space and initial parameter settings

Algorithms	Algorithm parameters	Value
NAS-ANN	Hidden layers	$H = [1-2]$
	Hidden neurons in the first layer	$N_1 = [1-20]$
	Hidden neurons in the second layer	$N_2 = [1-20]$
	Activation function in the first layer	"Tansig", "Logsig", and "Purelin"
	Activation function in the second layer	"Tansig", "Logsig", and "Purelin"
	Learning rate	0.001–0.05
	Training algorithm	Levenberg–Marquardt (LM)

datasets. The algorithm iteratively generated candidate networks from the defined search space and trained each configuration for up to 50 epochs, applying early stopping once the validation Mean Squared Error (MSE) showed no improvement for ten consecutive epochs.

The predictive performance of each candidate model was evaluated using the validation MSE and the R^2 , and the architecture yielding the minimum MSE was selected as the optimal network. In total, 500 candidate architectures were generated and evaluated during the NAS process. To mitigate stochastic variation, each configuration was retrained three times with different random seeds, and the average performance metrics were used for comparison.

The entire NAS experiment required approximately 3 h of computation time, with each candidate model taking around 20–25 s for training. This automated search procedure substantially reduced manual hyperparameter tuning while enhancing model efficiency and accuracy.

2.5 Statistical performance indicators

The predictive performance of the proposed models was assessed using a combination of statistical metrics and visual analyses. The statistical indicators employed include the MSE, Root Mean Squared Error (RMSE), R^2 , and the Pearson correlation coefficient (R). Together, these metrics provide a comprehensive evaluation of model accuracy by measuring both the magnitude of prediction errors and the strength of the correlation between predicted and observed values:

1. Mean Squared Error (MSE):

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^N (Y_{tar,i} - Y_{out,i})^2 \quad (0 < \text{MSE} < \infty). \quad (1)$$

2. Root Mean Squared Error (RMSE):

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^N (Y_{tar,i} - Y_{out,i})^2} \quad (0 < \text{RMSE} < \infty). \quad (2)$$

3. Coefficient of determination (R^2):

$$R^2 = 1 - \frac{\sum_{i=1}^N (Y_{tar,i} - Y_{out,i})^2}{\sum_{i=1}^N (Y_{tar,i} - \bar{Y}_{tar})^2} \quad (0 < R^2 < 1). \quad (3)$$

4. Pearson correlation coefficient (R):

$$R = \frac{\sum_{i=1}^N ((Y_{tar,i} - \bar{Y}_{tar})(Y_{out,i} - \bar{Y}_{out}))}{\sqrt{\sum_{i=1}^N ((Y_{tar,i} - \bar{Y}_{tar})^2 (Y_{out,i} - \bar{Y}_{out})^2)}} \quad (-1 < R < 1). \quad (4)$$

In Eqs. (1) to (4) $Y_{tar,i}$, $Y_{out,i}$, \bar{Y}_{tar} , and \bar{Y}_{out} represent the target values, predicted values, and their respective mean values across the 49 data samples. The proposed ML model achieved the lowest RMSE and MSE values, while simultaneously attaining the highest R^2 and R -values. These results indicate optimal predictive performance and a strong agreement with experimental observations.

The selection of the optimal model was based on these statistical performance metrics, ensuring both reliability and robustness. This advanced methodology demonstrates superior accuracy and resilience, effectively mitigating issues of overfitting and underfitting in predictive modeling [45]. The validation process was performed iteratively so that each subset served as the validation set once. A key advantage of this cross-validation technique is that all data points are used for both training and validation, thereby improving model stability and reliability [46].

2.6 Methodology

To determine the optimal model for predicting the SP and P, the following steps were undertaken:

1. Data collection: a dataset consisting of 49 samples was compiled from laboratory tests on the SP and P of modified bitumen.
2. Model development: the selected input parameters were modeled using three ML approaches – ANN, RF, and a hybrid NAS-ANN – to develop distinct predictive models.
3. Model evaluation: the optimal predictive model was identified by comparing the performance of the three approaches using statistical indicators including MSE, RMSE, R^2 , and R .
4. Model validation: to ensure generalization and mitigate overfitting, a five-fold cross-validation ($K = 5$) approach was applied to the best-performing NAS-ANN model. This step provided a more robust and unbiased estimate of model performance.
5. Sensitivity analysis: the relative influence of each input parameter (CR, CG, and OP) on the predicted outputs (SP and P) was quantified through a step-wise perturbation method, allowing the identification of the most significant modifiers affecting bitumen properties.

The overall research methodology for selecting the most suitable model is systematically illustrated in Fig. 2.

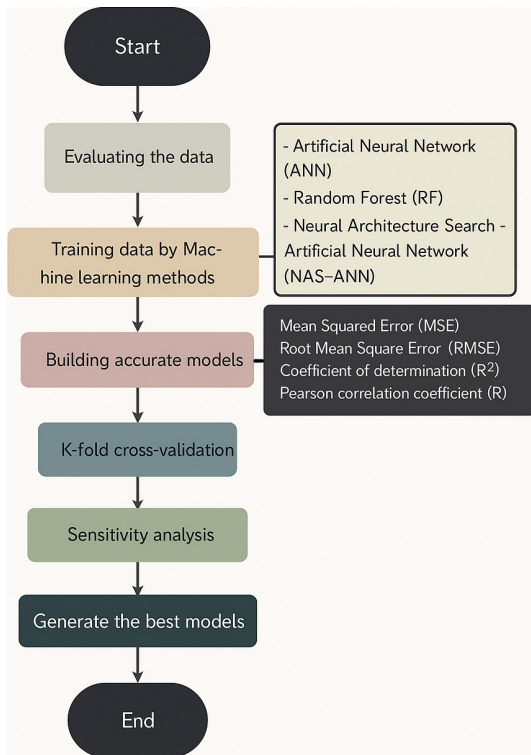


Fig. 2 End-to-end methodology for SP and P prediction

3 Results

3.1 Dataset compilation

In this study, a dataset of 49 samples was compiled to investigate the correlation between the type and percentage of different additives and their effects on the SP and P of bitumen. To ensure accuracy and reliability, the dataset was divided into 39 samples for training and 10 for validation. The data were randomly selected and treated as independent observations to avoid bias. Descriptive statistical analyses were performed using SPSS software, and the results,

presented in Table 4, include range, minimum, maximum, mean, standard deviation, variance, skewness, and kurtosis. The analysis revealed that the SP (Y1) ranged from 7.5 °C to 44 °C with a mean of 23.32 °C, while P (Y2) varied between 45 mm and 63 mm with a mean of 54.65 mm. The higher variability observed in Y1 compared to Y2 suggests that the additives exerted a stronger influence on thermal stability than on mechanical consistency. Furthermore, skewness values close to zero indicated nearly symmetric distributions, while negative kurtosis values suggested relatively flat distributions with fewer extreme deviations, confirming the representativeness of the dataset. Overall, these statistical characteristics demonstrate that the dataset is sufficiently diverse and balanced, providing a solid foundation for developing reliable ML models to predict the SP and P of modified bitumen.

3.2 Relationship between SP, P and input parameters

To statistically examine the relationship between the SP, P, and the selected input parameters, correlation analysis was carried out using SPSS software, with the results summarized in Fig. 3 and Table 5. The analysis revealed that the SP (Y1) showed a positive correlation with CR, indicating that increasing CR content generally enhances the thermal stability of bitumen. In contrast, SP exhibited a negative correlation with CG and OP, suggesting that higher proportions of these additives tend to reduce the SP, a trend consistent with experimental observations in bitumen modification studies. On the other hand, P (Y2) demonstrated a positive correlation with CR and OP, implying that higher amounts of these additives increase P values, whereas a negative correlation with CG indicated that greater CG content

Table 4 Descriptive statistics of the dataset (n = 49)

		X1	X2	X3	Y1	Y2
N	Valid	49	49	49	49	49
	Missing	0	0	0	0	0
Mean		3.5102	3.8571	3.7347	23.3233	54.6500
Median		0.0000	1.0000	3.0000	23.5000	54.5000
Mode		0.00	0.00	0.00	17.33a*	54.00a*
Standard deviation		4.60128	4.65922	3.37747	7.95471	3.94822
Variance		21.172	21.708	11.407	63.277	15.588
Skewness		0.931	0.784	0.212	0.139	-0.137
Standard error of Skewness		0.340	0.340	0.340	0.340	0.340
Kurtosis		-0.666	-0.914	-1.416	-0.198	-0.319
Standard error of Kurtosis		0.668	0.668	0.668	0.668	0.668
Range		14.00	14.00	9.00	36.50	18.00
Minimum		0.00	0.00	0.00	7.50	45.00
Maximum		14.00	14.00	9.00	44.00	63.00

* The meaning of "a" is that the multiple modes exist. The smallest values are shown in the marked cells.

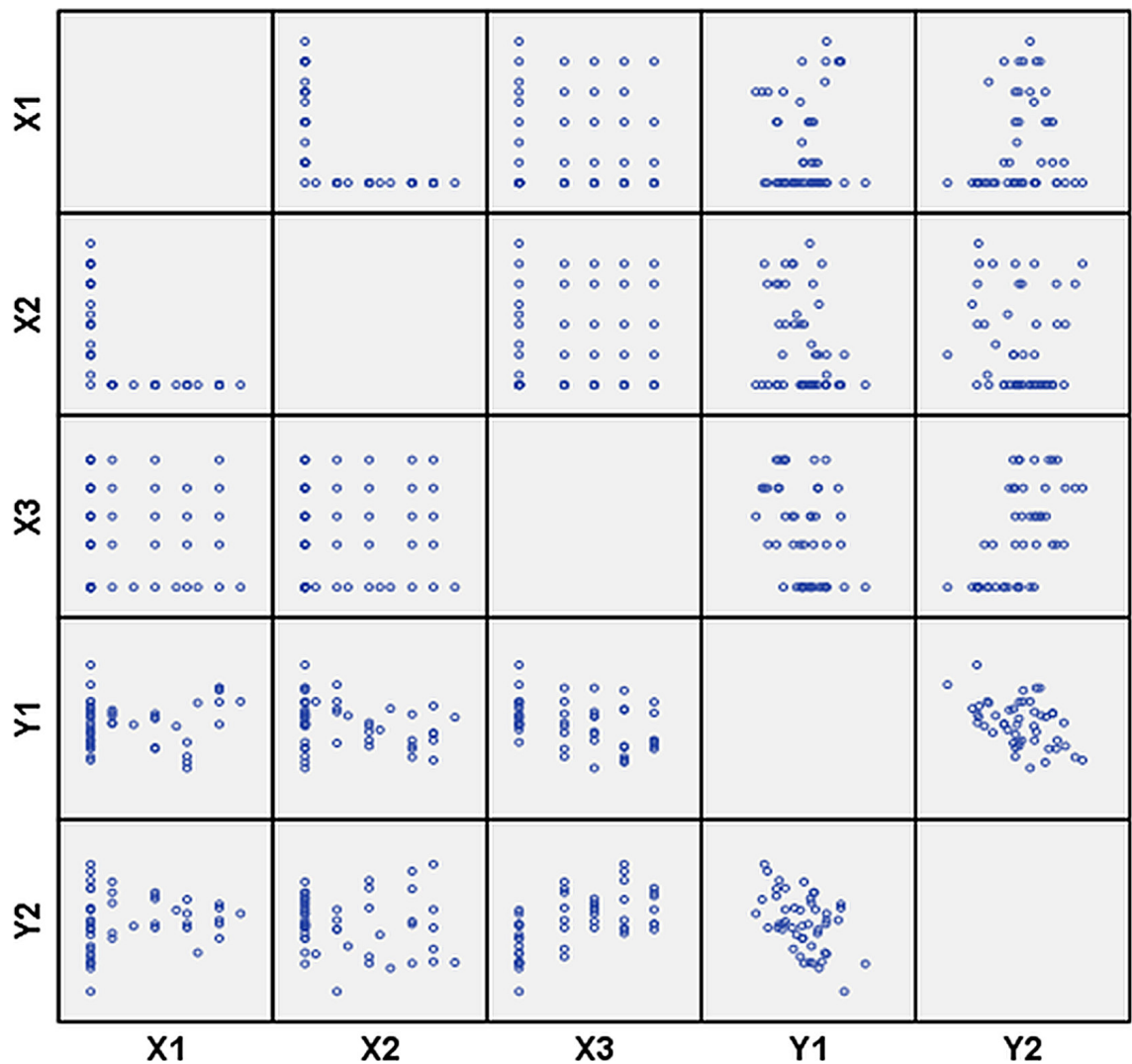


Fig. 3 Correlation matrix between inputs and targets ($n = 49$)

Table 5 Pearson correlation matrix with significance

		X1	X2	X3	Y1	Y2
X1	R	1.000	−0.833**	−0.014	0.131	0.236
	Sig. (2-tailed)		0.000	0.926	0.369	0.102
	N	49	49	49	49	49
X2	R	−0.833**	1.000	0.040	−0.252	−0.171
	Sig. (2-tailed)	0.000		0.784	0.081	0.240
	N	49	49	49	49	49
X3	R	−0.014	0.040	1.000	−0.370**	0.594**
	Sig. (2-tailed)	0.926	0.784		0.009	0.000
	N	49	49	49	49	49
Y1	R	0.131	−0.252	−0.370**	1.000	−0.368**
	Sig. (2-tailed)	0.369	0.081	0.009		0.009
	N	49	49	49	49	49
Y2	R	0.236	−0.171	0.594**	−0.368**	1.000
	Sig. (2-tailed)	0.102	0.240	0.000	0.009	
	N	49	49	49	49	49

** Correlation is significant at the 0.01 level (2-tailed).

decreases P . These results highlight that the relationships between the input variables (CR, CG, OP) and the output properties (SP and P) are inherently complex and nonlinear. Consequently, conventional statistical approaches may be insufficient to capture such intricate interactions, underscoring the necessity of implementing advanced ML techniques to achieve accurate predictive modeling.

3.3 SP and P prediction through ML models

The process of selecting the most suitable ML model for predicting the SP and P involved several stages, beginning with the identification of relevant input parameters and followed by the development and evaluation of predictive models. In this study, three approaches – ANN, RF, and a NAS-ANN – were implemented using three input variables (X_1 , X_2 , X_3) and two output variables (Y_1 , Y_2). The dataset was divided into training (80%) and validation (20%) subsets, and model performance was evaluated using four statistical indicators: MSE, RMSE, R , and R^2 .

During the training phase, the results showed that SP prediction yielded values ranging from MSE = 4.4272–20.9215, RMSE = 2.1041–4.5740, R = 0.8872–0.9665, and R^2 = 0.7871–0.9341. For P , values ranged from MSE = 0.8145–6.1083, RMSE = 0.9025–2.4715, R = 0.8215–0.9726, and R^2 = 0.6749–0.9460. In the validation phase, SP prediction recorded MSE = 7.1551–37.2686, RMSE = 2.6749–6.1048, R = 0.8395–0.9567, and R^2 = 0.7048–0.9153, while P values ranged from MSE = 4.4952–9.7963, RMSE = 2.1202–3.1299, R = 0.8109–0.8712, and R^2 = 0.6576–0.7590.

Among the tested models, NAS-ANN consistently achieved the best performance, providing the lowest error values and the highest accuracy in both training and validation phases. For SP prediction, NAS-ANN achieved MSE = 4.4272/7.1551, RMSE = 2.1041/2.6749,

R = 0.9665/0.9567, and R^2 = 0.9341/0.9153 (training/validation). Similarly, for P prediction, NAS-ANN achieved MSE = 0.8145/4.4952, RMSE = 0.9025/2.1202, R = 0.9726/0.8712, and R^2 = 0.9460/0.7590. These findings confirm that NAS-ANN is the most effective and robust model for predicting both SP and P , outperforming ANN and RF, which showed relatively weaker predictive capabilities. The overall performance hierarchy was established as NAS-ANN > ANN > RF. Table 6 summarizes the detailed performance values of the models across training, validation, and combined datasets.

3.4 SP and P prediction through ML models

The NAS process systematically evaluated multiple candidate architectures to identify the most efficient configuration for predicting the SP (Y_1) and P (Y_2) of modified bitumen. Each candidate network combined one or two hidden layers with selected activation functions and neuron counts, and all input variables were normalized using a z-score transformation to ensure numerical stability. A random-search strategy with parameter sharing was adopted, and a total of 500 candidate architectures were evaluated, each trained for up to 50 epochs with early stopping applied when the validation MSE plateaued for ten consecutive epochs.

The optimal hyperparameters for the NAS-ANN model, identified through the NAS process, correspond to a two-hidden-layer configuration with 10 neurons in the first layer and 12 in the second, both using the tansig activation function for Y_1 , and 8 neurons in the first layer and 10 in the second, both using the tansig activation function for Y_2 .

This configuration achieved the lowest validation MSE and highest R among all tested networks, confirming its superior predictive accuracy and generalization capability.

Fig. 4 presents the comparison between target and predicted values of the SP obtained using the NAS-ANN model.

Table 6 Model performance indicators for SP (Y_1) and P (Y_2)^{*}

		Y1				Y2			
		MSE	RMSE	R	R^2	MSE	RMSE	R	R^2
Training	ANN	9.9800	3.1591	0.9284	0.8619	4.1200	2.0298	0.8657	0.7494
	RF	20.9215	4.5740	0.8872	0.7871	6.1083	2.4715	0.8215	0.6749
	NAS-ANN	4.4272	2.1041	0.9665	0.9341	0.8145	0.9025	0.9726	0.9460
Validation	ANN	10.4222	3.2283	0.9211	0.8484	5.1749	2.2748	0.8699	0.7567
	RF	37.2686	6.1048	0.8395	0.7048	9.7963	3.1299	0.8109	0.6576
	NAS-ANN	7.1551	2.6749	0.9567	0.9153	4.4952	2.1202	0.8712	0.7590
All	ANN	10.0684	3.1730	0.9269	0.8592	4.3310	2.0788	0.8665	0.7509
	RF	24.1909	4.8802	0.8777	0.7707	6.8459	2.6032	0.8194	0.6714
	NAS-ANN	4.9728	2.2183	0.9645	0.9304	1.5507	1.1460	0.9523	0.9086

^{*} Bold values in Table 6 represent the best (optimal) performance for each metric.

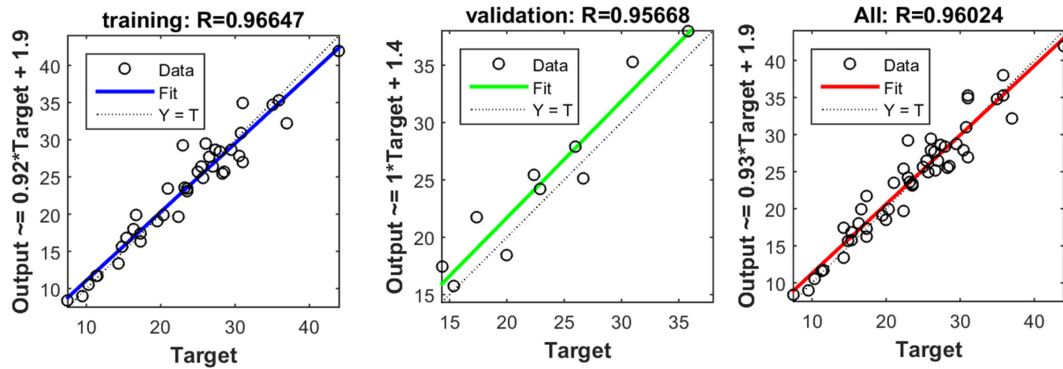


Fig. 4 NAS-ANN performance for SP

The results indicate a strong correlation, with coefficients of determination of $R_{training} = 0.9665$, $R_{validation} = 0.9567$, and $R_{all} = 0.9602$, which, according to Smith's classification, confirm the excellent predictive capability of the model for SP estimation. Fig. 5 illustrates the best performance epoch of the NAS-ANN model for SP prediction, where the lowest MSE was achieved at epoch 14 out of 20 tested, with values of $MSE_{training} = 4.4211$, $MSE_{validation} = 7.1549$, and $MSE_{all} = 4.9679$.

Similarly, Fig. 6 presents the comparison between target and predicted values of P using the NAS-ANN model. The results again show a strong correlation, with $R_{training} = 0.9726$, $R_{validation} = 0.8711$, and $R_{all} = 0.9478$, further validating the robustness of the model. The corresponding best performance epoch is shown in Fig. 7, where the lowest error was reached at epoch 8 out of 14

tested, with $MSE_{training} = 0.8150$, $MSE_{validation} = 4.4952$, and $MSE_{all} = 1.5510$. These results collectively demonstrate the strong learning ability and predictive accuracy of the NAS-ANN model for both SP and P values.

3.5 Evaluating the best fitted model using K -fold cross-validation approach

To enhance the reliability of the predictive performance assessment, a five-fold cross-validation ($K = 5$) procedure was applied to the optimized NAS-ANN model. This method divides the dataset into five mutually exclusive subsets (folds). Each fold is used once as the validation set while the remaining four serve as training data, ensuring that every observation contributes to both training and validation. Compared with a single train–test split, this procedure offers a more robust estimate

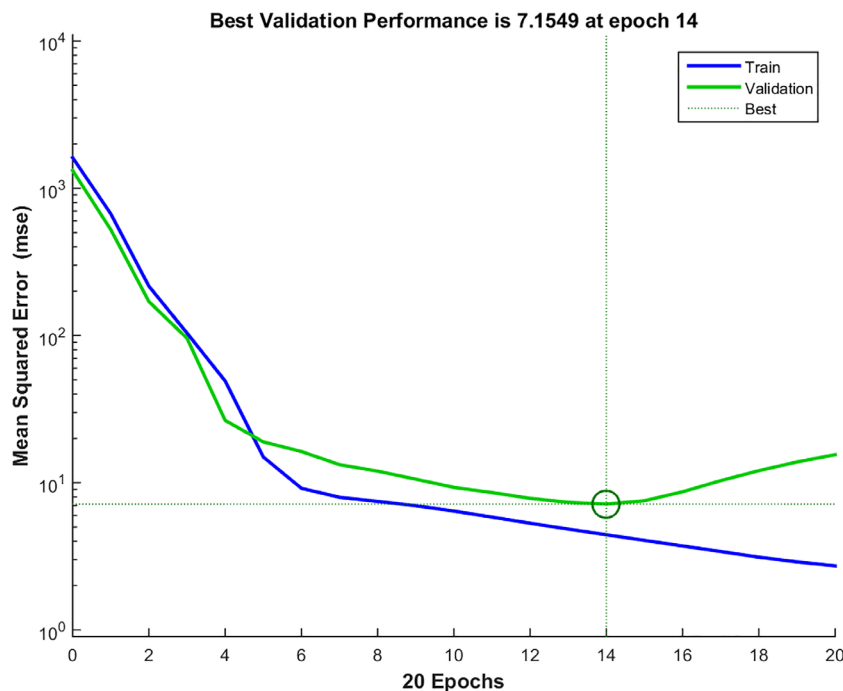


Fig. 5 Training history for SP: best epoch of the NAS-ANN

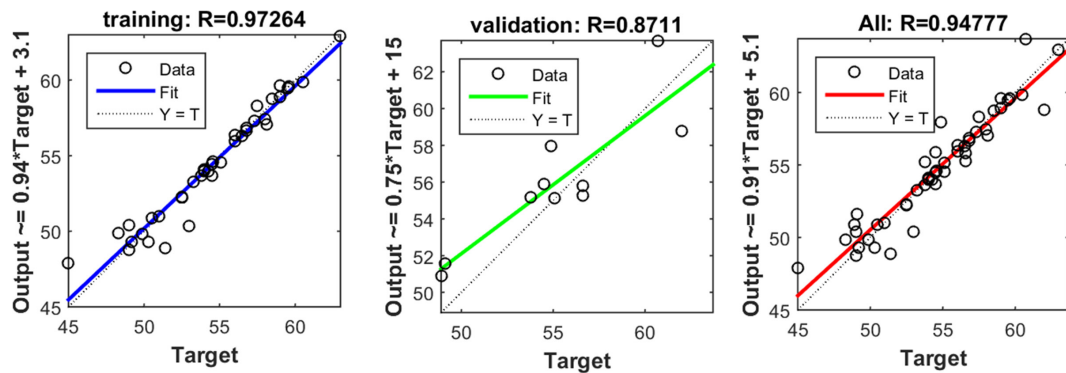


Fig. 6 NAS-ANN performance for P

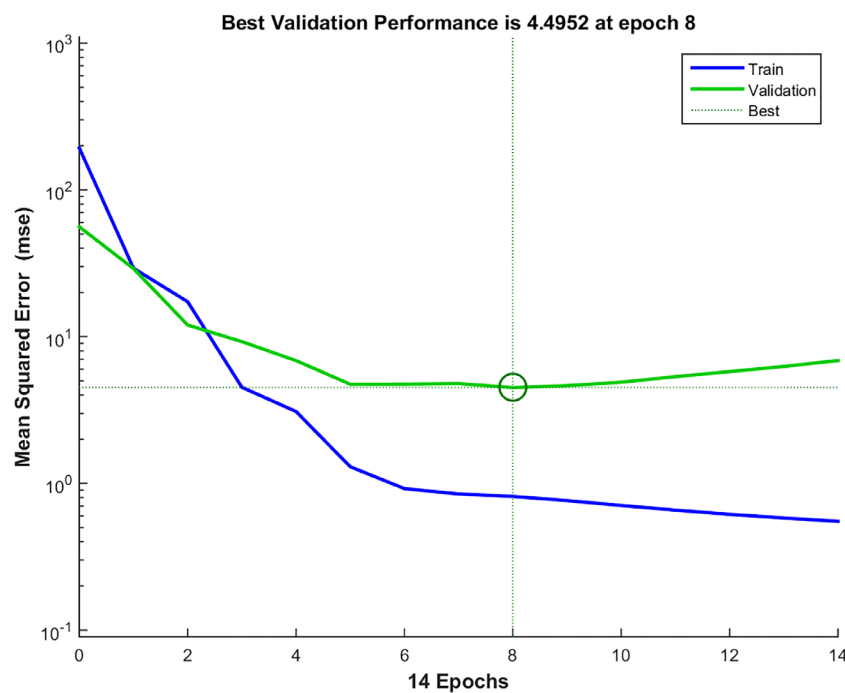


Fig. 7 Training history for P: best epoch of the NAS-ANN

of generalization capability and reduces dependence on a particular data partition.

Fig. 8 presents the performance metrics of the optimal ML models based on the fivefold cross-validation approach, displaying validation results for each data split. These results confirm the high predictive stability of the NAS-ANN model. R for softening-point prediction range from 0.928 to 0.975, while those for P vary between 0.856 and 0.923. All folds show strong positive correlations, demonstrating that the model generalizes well to unseen data. Minor fluctuations – especially the slightly lower R -values in folds 3 and 5 – likely reflect the limited sample size (49 records) and uneven representation of additive levels in those subsets.

Fig. 8 clearly indicates that the average R -values exceed 0.85 for both target variables, confirming that NAS-ANN provides consistent and accurate predictions under repeated

sampling. The modest decrease in R for P supports the interpretation that this output variable is more sensitive to data scarcity and noise, yet still remains within acceptable predictive accuracy for small-sample modeling. Overall, the K -fold cross-validation demonstrates that the proposed NAS-ANN architecture maintains robust generalization capability, effectively mitigating overfitting and ensuring reliability of the predicted softening-point and P values.

3.6 Evaluation of the proposed model in comparison to available models in the literature

To further assess the performance and effectiveness of the proposed NAS-ANN model, a comparative analysis was conducted against several state-of-the-art regression and ML models previously reported in the literature for predicting asphalt and bitumen-related properties. Table 7 [18, 20–25] summarizes the best-performing models from

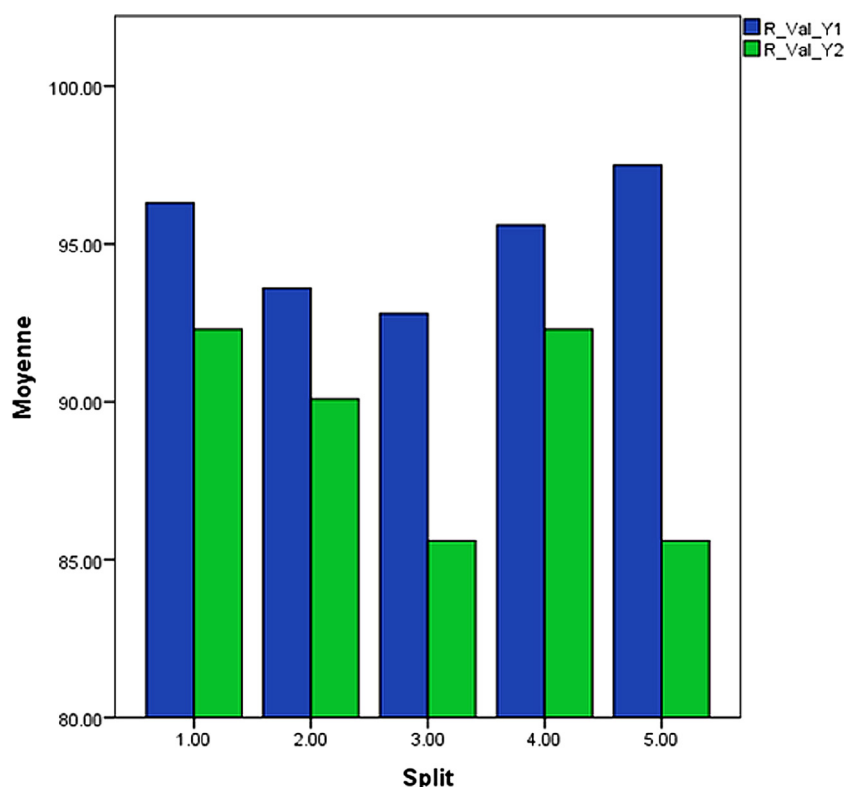


Fig. 8 Five-fold cross-validation (K = 5) of NAS-ANN

Table 7 Comparison of the proposed NAS-ANN model with existing models in the literature

Authors	Best models	Best Pearson correlation (R)
Tiwari et al. [18]	Boosting model	0.9724
Upadhyaya et al. [23]	SVM	0.8392
Althoey et al. [20]	ANFIS	0.960
Liu et al. [21]	GB	0.920
Othman [22]	ANN	0.962
Miani et al. [24]	Hyperparameter-optimized ANN	0.868
Awan et al. [25]	MEP	0.900
Our study	NAS-ANN	Y1 = 0.9602 and Y2 = 0.9500

recent studies together with their reported Pearson R , allowing a direct comparison with the present work.

The results clearly demonstrate that the NAS-ANN model developed in this study performs competitively with or better than most previously published models. For SP prediction (Y1), the R ($R = 0.9602$) is comparable to those achieved by the most advanced algorithms in the literature, such as the Boosting model (Tiwari et al. [18]; $R = 0.9724$) and the standard ANN (Othman [22]; $R = 0.962$). For P prediction (Y2), the proposed NAS-ANN obtained a similarly strong correlation ($R = 0.95$), outperforming other hybrid and ensemble approaches such as GB (Liu et al. [21]; $R = 0.92$) and MEP (Awan et al. [25]; $R = 0.90$). This comparative analysis confirms that integrating NAS with ANN optimization yields a robust

predictive framework capable of achieving accuracy comparable to or exceeding more complex ensemble and fuzzy-logic models. Therefore, the proposed hybrid NAS-ANN can be considered an efficient and reliable tool for predicting the SP and P of modified bitumen, bridging the gap between traditional ANN models and more computationally intensive ensemble techniques.

3.7 Sensitivity analysis

To identify the most influential input parameters affecting the model outputs, a sensitivity analysis was performed using the NAS-ANN model through the step-by-step perturbation technique [47]. In this method, each normalized input variable was varied individually while all other variables were kept constant at their mean values. For each

input, the relative percentage change in the predicted output was calculated, and the overall sensitivity level of each variable was obtained using Eq. (5):

$$\text{Sensitivity level of } X_j (\%) = \frac{1}{K} \sum_{i=1}^K \left(\frac{\% \text{ change in output}}{\% \text{ change in input}} \right)_i, \quad (5)$$

where $K = 49$ represents the number of samples used in the dataset. Fig. 9 summarize the sensitivity results for the NAS-ANN model. For softening-point prediction, the NAS-ANN indicates that OP is the dominant factor (54.22%), followed by CR (34.46%), whereas CG has a comparatively minor influence (11.32%).

For the original feature analysis, the same ordering is observed but with higher dominance of OP: OP = 63.09%, CR = 27.59%, and CG = 9.32%. These results confirm that variations in olive-pomace content have the strongest effect on the predicted softening behavior, with CR

contributing moderately and CG exerting a smaller effect. Fig. 9 summarizes these sensitivities.

3.8 Graphical user interface (GUI) design

The optimized NAS-ANN model developed in this study was integrated into a user-friendly graphical interface to ensure practical accessibility for researchers and civil engineers. Unlike traditional ML approaches that depend on complex coding or mathematical formulations, the proposed interface allows users to easily predict SP and P values without requiring prior expertise in programming or AI. By providing an intuitive and interactive platform, the SmartBit-AI tool enhances usability, facilitates real-world applications, and streamlines the decision-making process in bitumen characterization and pavement material design.

In this study, a graphical interface was designed using the optimal parameters derived from the NAS-ANN model (Fig. 10). The developed tool, named "SmartBit-AI" (Smart Bitumen AI), was implemented in MATLAB [36] to

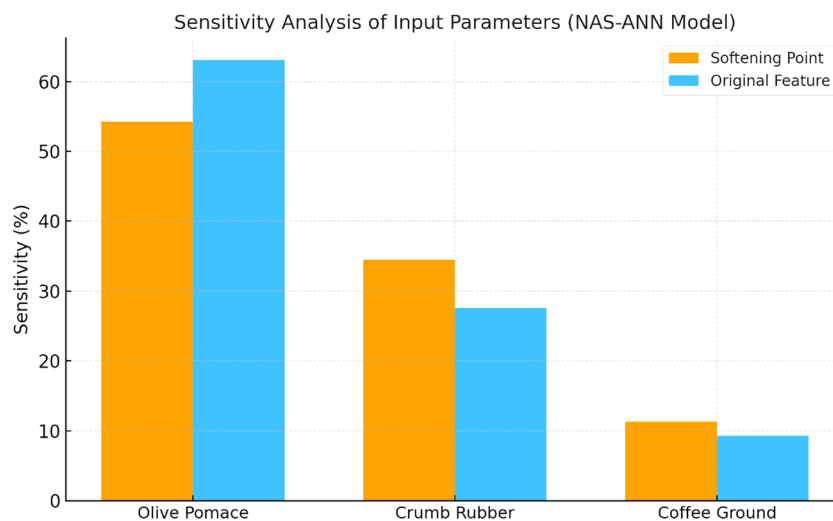


Fig. 9 Sensitivity analysis of inputs on model outputs

SmartBit-AI

Interactive Prediction Interface for Bitumen Properties

Modifier Contents	Predicted Properties
% of Crumb Rubber (CR) <input type="text" value="0"/>	Softening Point (SP) <input type="text" value="14.12"/>
% of Coffee Ground (CG) <input type="text" value="10"/>	Penetration (P) <input type="text" value="58.56"/>
% of Olive Pomace (OP) <input type="text" value="3"/>	
<input type="button" value="Predict"/>	

Fig. 10 "SmartBit-AI": user-friendly interface of the optimized NAS-ANN model for predicting SP and P given CR, CG, and OP contents (example inputs: CR = 0, CG = 10, OP = 3; outputs: SP = 14.12, P = 58.56)

enable flexible and efficient use. The interface includes three input fields – % of CR, % of CG, and % of OP – and two output fields displaying the predicted SP and P. Once the "Predict" button is activated, the system processes the input data through the trained NAS-ANN architecture and instantly presents the corresponding bitumen property values.

This interface offers substantial benefits for both researchers and practitioners by transforming the NAS-ANN model into a practical predictive tool. It eliminates the need for complex computations, reduces human error, and supports sustainable pavement design by allowing rapid assessment of additive proportions and their effects on bitumen performance. Consequently, SmartBit-AI serves as an intuitive, reliable, and efficient modeling environment, bridging the gap between advanced AI techniques and their implementation in materials and pavement engineering.

4 Discussion

The present study provides new insights into the predictive modeling of bitumen properties by integrating NAS with ANN, resulting in a hybrid NAS-ANN framework. This integration enabled automatic optimization of the network's architecture and hyperparameters, producing models with superior accuracy and stability compared to conventional ANN and RF approaches. The NAS-ANN achieved the lowest prediction errors and the highest R in both training and validation phases, confirming its capability to capture nonlinear interactions between modifier content and bitumen performance.

A comparative analysis against recent ML models for bituminous materials (Table 7) reveals that the NAS-ANN model performs competitively with, or better than, several state-of-the-art approaches such as GB, CatBoost, ANFIS, and MEP. While models like boosting (Tiwari et al. [18]; $R = 0.9724$) and ANN (Othman [22]; $R = 0.962$) show high accuracy, the proposed NAS-ANN achieved $R = 0.9602$ for SP and $R = 0.95$ for P, ranking among the top-performing algorithms. This demonstrates that automated neural architecture optimization can deliver accuracy comparable to complex ensemble and fuzzy systems, while requiring less manual tuning and computational effort. Moreover, NAS-ANN enhances interpretability and adaptability, offering a more accessible modeling framework for material prediction tasks.

The sensitivity analysis confirmed that the influence of each input parameter varies significantly depending on the target property. For softening-point prediction, OP was identified as the most influential factor ($\approx 54\%$), followed by CR ($\approx 34\%$), and CG ($\approx 11\%$). These results indicate that

OP strongly affects the thermal characteristics of bitumen, likely due to its polar organic compounds enhancing stiffness and temperature resistance. A similar pattern was observed for the original feature analysis, with OP remaining the dominant input ($\approx 63\%$). These outcomes highlight the model's physical coherence and validate its internal learning structure – factors that enhance confidence in its predictive reliability. Importantly, such sensitivity-based insights can guide formulation optimization and support decision-making in selecting modifier combinations for desired property outcomes.

To translate the model's predictive capacity into a practical engineering tool, the optimized NAS-ANN framework was embedded into a user-friendly application named "SmartBit-AI". The interface allows users to input modifier contents – CR, CG, and OP – and instantly obtain predicted SP and P values. By integrating AI-based prediction within an interactive environment, the tool bridges the gap between research and practice, facilitating rapid material evaluation without the need for complex programming knowledge. This implementation enhances accessibility for researchers, laboratories, and civil engineers, particularly for rapid screening and mix-design preselection, where laboratory testing may be limited by time or cost constraints. The model serves as a practical complement to conventional testing methods, supporting efficient preliminary assessments rather than replacing experimental verification.

The domain of applicability is limited to modifier contents between 2–14%, as higher concentrations were found to cause viscosity increases, dispersion issues, and phase instability. Extrapolation beyond this range is not recommended.

From a research perspective, the successful implementation of NAS-ANN paves the way for applying advanced hybrid models in other areas of civil engineering materials, such as predicting the rheological or fatigue behavior of modified binders. For practitioners, the developed model offers a valuable decision-support tool that can reduce reliance on trial-and-error experimentation during mix design [48–50]. This in turn translates into tangible economic and environmental benefits, as fewer raw materials and less energy are consumed during testing, while simultaneously promoting the reuse of industrial and agricultural wastes in road construction.

Despite the promising outcomes, several limitations must be acknowledged to ensure a balanced interpretation. First, the dataset consisted of only 49 experimental samples, sufficient for training but restricting generalization. Larger, more diverse datasets covering different climatic conditions, binder grades, and traffic categories are necessary

to enhance robustness. Second, the model was trained on laboratory-scale data, and thus does not explicitly account for temperature dependence, long-term aging, or field-scale variability. Third, while NAS-ANN demonstrated excellent predictive capability, it should be externally validated on independent datasets before practical deployment.

Future research should focus on expanding the dataset and incorporating additional modifiers such as polymers, nanomaterials, or industrial by-products to enhance the generalization capability of the proposed framework. Moreover, coupling the NAS-ANN architecture with Explainable AI (XAI) techniques – such as SHAP and Local Interpretable Model-Agnostic Explanations (LIME) – would provide deeper interpretability and reveal the underlying physical mechanisms governing additive–binder interactions. In addition, future investigations could explore the integration of metaheuristic–ML hybrid methods, such as Genetic Algorithms (GA), Particle Swarm Optimization (PSO), Grey Wolf Optimizer (GWO), and Thermal Exchange Optimization (TEO), to further refine the learning process and improve global search efficiency. These algorithms have demonstrated strong capabilities in optimizing neural network parameters, feature selection, and hyperparameter tuning in civil and materials engineering applications. Combining NAS with metaheuristic optimization could yield adaptive hybrid frameworks that balance accuracy, robustness, and computational efficiency, while offering deeper insights into the nonlinear behavior of modified bitumen systems. Such advanced hybridization of NAS, XAI, and metaheuristic algorithms would represent the next generation of intelligent modeling in pavement and materials engineering – merging automation, transparency, and optimization toward smarter, sustainable, and data-driven material design.

In summary, the proposed NAS-ANN model exhibits scientific novelty and practical relevance. It achieves high prediction accuracy for SP and P, provides interpretable insights through sensitivity analysis, and offers a functional engineering interface (SmartBit-AI) for efficient, sustainable material design. By merging computational intelligence with user-oriented implementation, this study contributes to the evolution of data-driven, resource-efficient, and sustainable pavement engineering.

5 Conclusions

This study introduced a novel ML framework for predicting the SP and P of modified bitumen, using three approaches: ANN, RF, and a hybrid NAS-ANN. A carefully designed dataset of 49 experimental samples was used, with CR, CG, and OP identified as the key influencing factors.

The NAS-ANN model consistently outperformed conventional ANN and RF models, demonstrating superior predictive accuracy and robustness across all statistical indicators. For SP, the model achieved $R = 0.9665$ (training) and 0.9567 (validation), while for P it reached $R = 0.9726$ (training) and 0.8711 (validation). These results confirm the ability of NAS-ANN to capture complex, nonlinear interactions between additive contents and bitumen properties while minimizing errors and avoiding overfitting.

When compared with models reported in the literature, such as GB, ANFIS, and MEP, the proposed NAS-ANN achieved comparable or better R , confirming its efficiency and reliability. Sensitivity analysis revealed that OP exerted the greatest influence on both SP and P, followed by CR and CG, consistent with their physical effects on binder performance.

To promote practical use, the optimized NAS-ANN model was implemented in a user-friendly graphical interface (SmartBit-AI), allowing users to input modifier contents (CR, CG, OP) and instantly obtain SP and P predictions. This digital tool provides a practical complement, rather than a replacement, to traditional laboratory testing – particularly useful for rapid mix-design screening and preselection.

The model's domain of applicability lies between 2–14% modifier content, beyond which excessive viscosity and poor dispersion may occur. Despite its strong performance, the limited dataset size and absence of field-scale validation represent constraints on generalization.

Future research should focus on expanding the dataset, incorporating additional modifiers such as polymers or nanomaterials, and validating the framework under diverse climatic and loading conditions. Integrating Explainable AI (XAI) methods (e.g., SHAP, LIME) and metaheuristic–ML hybrid algorithms could further enhance interpretability, optimization efficiency, and understanding of additive–binder interactions.

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