Modelling of Asphalt’s Adhesive Behaviour Using Classification and Regression Tree (CART) Analysis

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1. Introduction

The researchers usually modify the asphalt using different types of polymers to provide more durable and sustainable pavements. The polymers used for the modification of asphalt tend to have large chains (straight or cross-linked). The chemistry and structure of the chains affect the behaviour of the polymer as well as polymer-modified asphalt (PMA). The most commonly used polymers are elastomers and plastomers. The elastomers improve the elastic properties, while the plastomers provide a plastic matrix in the modified asphalt. In the following sections, the PMA indicates only styrene-butadiene-styrene (SBS) and styrene-butadiene (SB) modified asphalt following the scope of this study.

SBS is one of the most widely used polymers in the asphalt industry, followed by reclaimed tire rubber [1], which improves the mechanical, physical, and rheological properties of asphalt mixtures [2], increases the elasticity and tensile properties of asphalt [3], and lowers the creep stiffness [4]. The SB product is an SBS block copolymer and elastomeric in nature. The use of SB can affect different properties of asphalt, including viscoelastic properties (Jnr) [5], and provide increased resistance to permanent deformation at moderate temperature (25°C) [6], low-temperature ductility [7], etc. In addition to providing different aforementioned properties, it is observed that the use of SB and SBS significantly affects the adhesive properties of asphalt [7]. However, the effectiveness of the improved properties, including the adhesive properties, changes gradually over the service life. There could be different factors that affect the desired properties of PMA, and oxidation of asphalt is one of them. Oxidation can alter the
constituents, as well as the adhesion of the asphalt that subsequently erodes the viscoelastic properties and results in asphalt pavement failure [8, 9]. Therefore, it is imperative to have an explanatory insight to predict the adhesive property of the oxidized PMA.

In addition to the use of polymer, the increased traffic, the desired improved properties of the asphalt pavement, and the rapid development of nanotechnology have led the researchers to focus on introducing nanomaterials for asphalt modification. Nanomaterials are described as having at least one dimension within 1–100 nm. The properties of nanosized particles differ from those of traditional materials because of the increased ratio of surface to volume and nanometer-sized plates [10]. It was also observed that nanomaterials showed high sensitivity to temperature, high ductility, high surface area, high tension resistance, low electrical resistance, etc. [11–15]. Because of these favourable properties, a large number of nanomaterials have been used for asphalt modification, and carbon nanotube (CNT) is one of them. The CNT was found to improve the tracking resistance and thermal cracking [16, 17]. It can significantly improve the rheological and adhesive properties of asphalt, and the increase in the content of CNTs results in highly viscous and elastic coefficient values regardless of the type of binder [18–20]. However, it is observed that the presence of nanomaterials (or filler materials) affects the adhesive properties of asphalt [21]. In addition to this, the oxidation can also affect the adhesive properties of CNT-modified asphalt (CMA) [22]. Therefore, it is also important to visualize and predict the changes in adhesive properties of oxidized CMA.

Based on the above discussion, it is revealed that the adhesive properties play a significant role for oxidized asphalt regardless of the type of modified asphalt (PMA/CMA). However, none of the previous studies attempted to predict the adhesive properties of oxidized asphalt to the best of authors’ knowledge. Some of the studies that addressed the adhesive properties of the PMA [23–25] or CMA [26, 27] considered the effect of moisture rather than oxidation. In this regard, this study predicted the adhesive properties of oxidized asphalt (modified by polymers and CNTs) using a predictive modelling and machine learning technique, i.e., the classification and regression tree (CART). The model addresses the adhesive properties of modified asphalt simulating the real field oxidation and chemistry of asphalt at a nanoscale.

2. Research Approach

The flow chart describing the analysis steps involved in this study can be seen in Figure 1. It can be seen from the figure that the PMA will be modified using two different types of CNTs (each one comprises three different percentages). Once the PMA is modified by a CNT (named PCA), the samples are divided into two groups, such as fresh and oxidized. The adhesive properties of each sample are analysed using five different tips of AFM. The parameters (percentage and type of CNT, functional group, polymer type, etc.) that affect the behaviour of asphalt have been used to predict adhesive properties using the CART and were compared with the regression model. Further details can be observed in the following sections.

3. Materials and Procedure

The base asphalt collected from a local distributor was evaluated in the laboratory, and its properties are given in Table 1. The base asphalt was modified using 4% and 5% of SB and SBS following the usual practice in the industry [28]. Each polymer-modified asphalt was further modified using two different types of CNTs. The CNT is a one-atom thick graphite plate made into a seamless, one-nanometer diameter hollow cylinder. The synthesis and characterization of the helical microtubules of the fibre are performed on a molecular scale of the structures. The CNT exists in the form of coaxial tubes (multiwalled CNTs) and single tubes (single-walled CNTs). Young’s modulus of a CNT, depending on the radius of the tube, can be up to 1,000 GPa, and the tensile strength can be up to 150 GPa [29].

3.1. AFM Testing Description. Atomic force microscopy (AFM) can be a very important and suitable tool to assess the nanomechanical properties of asphalt such as contact force, friction, and van der Waals force. Several studies attempted to study different properties of asphalt using the AFM [30–33]. The AFM has also been used to evaluate different nanomechanical properties including adhesion and cohesion of asphalt binders [34]. Some of the studies observed the changes in adhesion of asphalt due to the presence of SBS.
was later on modified with ammine (-NH$_3$), hydroxy (-OH),
approximately 10 mm were placed on a glass substrate having a dimension of
the CNT. QX_he mixed samples modified with the CNT and binder was mixed with the polymer fraction chosen, as well
of 60°C for seven days that simulates the anticipated aging in
field condition.

3.2. Sample Preparation. The fresh asphalt sample was
heated inside a laboratory container at a temperature of around 164°C. After 30–45 minutes of duration, the asphalt
binder was mixed with the polymer fraction chosen, as well
as the CNT. The mixed samples modified with the CNT and
polymer are called dry conditioned samples. The samples
were placed on a glass substrate having a dimension of
approximately 10 mm × 10 mm × 1 mm. The dry samples
were placed inside a draft oven with an elevated temperature
of 60°C for seven days that simulates the anticipated aging in
the field condition.

4. Classification and Regression Tree
(CART) Analysis

The multiple regression model and the classification and
regression tree (CART) approaches were used to understand
the effect of different variables on the adhesion force of
asphalt. The use of regression models requires an assumption
regarding the underlying distribution of the data, and it
is a parametric method. On the contrary, the nonparametric
technique like artificial neural networks (ANNs) has also
been used that lacks the explanatory capability. The CART is
a nonparametric technique that can be used to include
variable(s) at more than one stage of the tree. Therefore,
complex interdependencies can also be uncovered among
the variables. The CART has successfully handled the
complex nonlinearity between the predictors and response
with its adaptive interpretation skills [39]. It can handle the
multicollinearity problems of the data more appropriately
compared to the regression models. In addition to this, the
CART analysis provides a model that can be interpreted
through logical statements to understand the effect of dif-
ferent variables on the target variable that is often not found
in other data mining tools [40]. The application of the CART
was successfully used not only to understand and predict
consumers’ behaviour but also in the road safety research
(i.e., car seat belt use). It was also used in different sectors of
pavement engineering, such as evaluation of the field ser-
viceability of pothole patches [41], factors influencing per-
meability of the rigid pavement [42], and roughness of the
asphalt pavement [43], field prediction of maintenance
probability, and selection of certain maintenance ap-
proaches following the existing condition [44, 45]. However,
the studies in which predictive models are used for pre-
dicting adhesion force of asphalt were found to be very few,
and the use of the CART technique has not been found in
these studies. Therefore, this technique has been applied for
predictive modelling of oxidized asphalt for the first time.
The details of the variables used in the model are presented
in Table 2.

5. Results and Discussion

The CART analysis incorporated 240 samples where one
hundred sixty samples were used for training and eighty
samples were used for testing. Table 3 presents the accuracies
for training and test samples in CART analysis.

The accuracy was calculated via the coefficient of cor-
relation, root mean square error (RMSE), and mean absolute
percentage error (MAPE) for samples used for the training
and testing of the model. These values were calculated by
using the actual/target values from the lab test and model
predictions. It can be observed from the table that the co-
efficient of correlation (CC) was reasonable for training as
well as test samples. The error was approximately 27% (mean
absolute percentage error (MAPE)) for the test samples
which amounts to 53 kN (root mean square error (RMSE))
in terms of adhesion force. The accuracy measures of the
CART were found to be acceptable for training as well as test
samples. However, there was no drastic change in the error
values which indicates that the model did not overfit
the training samples. Different artificial intelligence (AI) tech-
niques, such as multilayer perceptions (MLPs), support
vector machines (SVMs), and adaptive network fuzzy in-
ference systems (ANFISs), have been used for predicting

| Table 1: Asphalt properties. |
|-----------------------------|
| Properties                  | Values     |
| Specific gravity            | 1.02       |
| Viscosity (centipoise)      | 500        |
| Performance grade           | 66-22      |
adhesion force for asphalt [46]. However, for pavement design, these techniques cannot explain the relationship between the variables considered in the study, which makes the use of the proposed model in decision-making difficult. The gap can be fulfilled by the CART which explains the relationships between variables.

The CART presented in Figure 3 highlights the following points. The most important parameter was found to be the tip type, i.e., NH$_3$, which is at the top of the tree. The use of NH$_3$ in the tip increases the adhesion force of asphalt. Hence, AFM tests need to be designed properly before using their results for mix design. The highest adhesion force was found when the NH$_3$ tip was used and SBS5 was used as the binder as this node has the highest mean adhesion force. The SBS5 binder was also found to increase the adhesion force when used with other tip types except CH$_3$. Therefore, it could be said that having dual styrene bonds increases the adhesion force of asphalt which can be attributed to a higher degree of internal bonding for the additive. Nodes for fresh samples were found to have a higher adhesion force as expected. The lowest mean adhesion force was observed for aged samples when the tip was made of OH. The CNT type was not found to have any effect on the adhesion force. However, it may have impact on other properties of asphalt such as elasticity, viscosity, and density. Hence, further research is required with regard to this modification in asphalt. The CART model provides the mean adhesion force for each combination of variables, and hence, it can be directly used to develop guidelines for mix design of asphalt and design of AFM experiments for asphalt.

Equation (2) represents the regression model developed for this study. It was developed by using the method of ordinary least squares. The coefficients were checked for their statistical significance, and the variables with statistically insignificant coefficients were omitted. The accuracy of this model is given in Table 4.

$$AF = 188.52 - 48.28(Si_3N_4) + 68.96(NH_3) - 81.6(OH) - 63.16(CH_3).$$

The following point was observed while comparing the regression model with the CART: the accuracy of the CART model (Table 3) is higher for training and test samples than that of the regression model (Table 4).

The tip type NH$_3$ was found to have the highest positive impact, and OH had the highest negative impact on the regression model (see equation (2)). Similar
observations can also be observed from the CART. The correlation of the tip type, binder type, and freshness of the samples and their combined impact on adhesion force are not captured by the regression model but were clearly shown in the CART.

6. Conclusions and Recommendations

This study investigated the aging behaviour of asphalts modified with SB, SBS, and CNTs. The aging behaviour is measured by evaluating the changes in adhesive properties of modified asphalt (SB, SBS, and CNTs) at the nanoscale. The test results were predicted by using classification and regression tree (CART) analysis including different parameters that affect the aging behaviour of modified asphalts. CART results were compared with the regression model results. The main findings from this study can be summarized as follows:

1. The CART analysis shows more explanatory relationships, at different levels of the tree, between different variables that affect the behaviour of oxidized asphalt.

2. The CART results were found to be more accurate (with higher CC and lower MAPE and RMSE values) than those of the regression model. It could be due to consideration of the interaction effect in the CART model that differs significantly from the usual regression techniques [47].

3. The functional group -NH$_3$ was the most important parameter for the tip type. The use of -NH$_3$ in the tip increases the adhesion force of asphalt. Hence, this effect should be considered when designing the AFM experiments for asphalt adhesion to avoid any biasness of the results due to the type of tip.

### Table 4: Accuracy measures of the linear regression model.

| Accuracy measure | Training sample | Test sample |
|------------------|-----------------|-------------|
| CC               | 0.67            | 0.64        |
| RMSE             | 44.81           | 62.52       |
| MAPE             | 24.29%          | 32.95%      |

**Figure 3:** CART for predicting asphalt adhesion force.
The highest adhesion force was found when the -NH₂ tip was used with the SBSS binder as this node has the highest mean adhesion force, whereas the lowest mean adhesion force was observed for aged samples when the tip was made of -OH.

(5) The CNT type was not found to have any effect on the adhesion force.

(6) In addition to this, scrutinizing the relation between the nanoscale adhesion and different macrostructural changes can provide a rigorous conclusion for hot mix asphalt (HMA).

Data Availability

The data are available from the corresponding author upon request.

Conflicts of Interest

The authors declare no conflicts of interest.

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