

**CHARACTERISING ASPHALT MIXTURES USING IMPROVED
MACHINE LEARNING APPROACHES BY OPTIMIZING MODEL
PERFORMANCE AND RANK BASED MODEL VARIABLES**

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PERFORMANCE AND RANK BASED MODEL VARIABLES**

by

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Submitted

In fulfilment of the Requirements of the Degree of Philosophy

to the



**INDIAN INSTITUTE OF TECHNOLOGY
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DEDICATED TO MY PARENTS, MY
FAMILY, MY GUIDE, AND MY
FRIENDS. I AM FOREVER
GRATEFUL FOR THEIR GUIDANCE
AND BELIEF IN ME.

CERTIFICATE

This is to certify that the thesis titled “**Characterising Asphalt Mixtures Using Improved Machine Learning Approaches by Optimizing Model Performance and Rank Based Model Variables**”, submitted by **Nishigandha Rajeshwar Jukte**, to the Indian Institute of Technology Delhi, for the award of the degree of **Doctor of Philosophy**, is a bonafide record of the research work done by her under my supervision and guidance, completed in February 2025. The thesis work, in my opinion, has reached the requisite standard, fulfilling the requirements for the degree of Doctor of Philosophy.

The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

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Nishigandha Rajeshwar Jukte

ABSTRACT

The dynamic modulus ($|E^*|$) and phase angle (ϕ) of asphalt mixtures are two essential parameters for predicting pavement performance. These parameters are helpful in evaluating fatigue cracking and rutting in Mechanistic Empirical Pavement Design Guidelines (MEPDG). In addition to this, these parameters are also used to assess low temperature cracking, moisture damage, international roughness index, and reflective cracking. Therefore, predicting these parameters at a given temperature and for a different range of loading frequencies is essential. To evaluate the effectiveness of the proposed methodologies in first three objectives, dynamic modulus and phase angle measurements reported in national cooperative highway research program (NCHRP Project) 9-19 were used. Eight binders and five aggregate gradations originating from 201 distinct asphalt mixtures were identified. Dynamic modulus and phase angle mastercurves were constructed for individual mixtures using three mastercurve (sigmoidal, generalized sigmoidal, and CAM mastercurve) functions and two temperature shift factor determination approaches (free shifting approach and second order polynomial approach).

In addition, for improving the accuracy of phase angle prediction, the first objective of the study proposes a rational model to describe the shape of phase angle mastercurve. The proposed model is a combination of two sigmoidal functions having seven parameters. The proposed 7-parameter model was compared with popular sigmoidal, generalized sigmoidal, and CAM mastercurve models. Results indicate that the proposed model accurately describes the shape of phase angle mastercurve than other described models. Statistical analysis showed reasonable correlation among phase angle mastercurve characteristics (peak phase angle and its location) and other variables (i.e. mixture volumetrics, mixture gradation).

Mixturewise regression models were also proposed to predict phase angle mastercurve characteristics. Goodness of fit indicators verified that the proposed predictive models were able to predict phase angle mastercurve characteristics well.

Further, the study proposes an efficient approach to arrive at Gene Expression Programming (GEP) based models for $|E^*|$ and ϕ prediction. The proposed methodology encompasses (i) construction of $|E^*|$ and ϕ mastercurves, (ii) ranking of GEP based predictive expressions that uses reduced frequency, aggregate gradation, asphalt binder content, binder properties, and mixture volumetrics as input, and (iii) selection of predictive model at optimal tree depth, and (iv) recalibration. Thus, proposed methodology strives to attain right balance among selection of highly influencing variables, predictive model complexity, and predictive accuracy. To validate the proposed methodology, database reported in NCHRP 9-19 study was used. With application of proposed approach with increasing tree depths, model complexity, predictive accuracy and computational time increased. However, beyond certain tree depth the increment in model accuracy was marginal. This can be attributed to incorporation of highly influencing variables in initial stages and limitation on model forms during GEP module execution. The robustness of the proposed GEP based predictive expressions was checked with independent database and competitor models. The numerical values of goodness of fit indicators showed improved predictive accuracy through proper selection of input variables, and predictive model. The predictive accuracy was further improved through mixturewise recalibration. The proposed predictive expressions can be conveniently utilized for $|E^*|$ and ϕ prediction through recalibration and subsequent preliminary design.

Furthermore, the third objective proposed a deep learning approach to predict $|E^*|$ and ϕ . The input variables for deep learning model consisted of information regarding reduced frequency, binder properties, aggregate gradation, and mixture volumetrics. When

compared to other input variables, reduced frequency and binder properties were highly correlated with dynamic modulus and phase angle. Further, recursive feature elimination was used to rank all input variables. Using these ranked input variables, deep learning based models for predicting dynamic modulus and phase angle were developed. The deep learning architecture (finalized through exhaustive optimization) dependent on parameter under consideration, and mastercurve construction approach was adopted. Detailed statistical analysis indicated dynamic modulus predictive models performed better when compared to phase angle predictive models. The numerical values of goodness of fit indicators showed that accuracy of deep learning based model was dependent on mastercurve construction approach adopted. Overall results indicated that the deep learning based models can predict dynamic modulus and phase angle with good accuracy. The output from the proposed deep learning models can be used as direct input into pavement design framework, which can result in accurate prediction of pavement performance.

The fourth objective of the study was to propose a machine learning based cost optimization of Marshall mix design. To develop the machine learning based cost optimization framework, different aggregate gradations in terms of D_i values from D_{90} to D_{10} , binder content, and bulk specific gravity of aggregate were used to predict Marshall test results and mix volumetrics. However, along with the aggregate gradation, coefficient of uniformity (C_u) and curvature (C_c) were used to develop the framework. To account for all shape factors at all the points on a gradation curve, new C_u 's and C_c 's were developed. The new C_u 's and C_c 's showed better correlation with mixture volumetrics. The four approaches were used for optimization with different machine learning predictive models using input independent variables as: (i) Approach 1: D_i values from D_{90} to D_{10} (ii) Approach 2: D_i values and traditional C_u C_c (iii) Approach 3: new developed C_u and C_c (iv) Approach 4: new developed C_u 's and

C_c 's developed and traditional C_u C_c . The cost optimization algorithm was developed for these four approaches by providing constraints on aggregate gradation and mixture volumetrics. The approaches with new C_u 's and C_c 's resulted in lower binder content when compared to approaches with D_i values. Also, the approaches with traditional C_u C_c provided similar aggregate gradation curves.

सार

डामर मिश्रण का गतिशील मापांक ($|E^*|$) और चरण कोण (ϕ) फुटपाथ प्रदर्शन की भविष्यवाणी के लिए दो आवश्यक पैरामीटर हैं। ये पैरामीटर एमईपीडीजी डिज़ाइन में थकान क्रैकिंग और रटिंग के आकलन में सहायक हैं। इसके अलावा, इन मापदंडों का उपयोग कम तापमान क्रैकिंग, नमी क्षति और सूचकांक और परावर्तक क्रैकिंग का आकलन करने के लिए भी किया जाता है। इसलिए, किसी दिए गए तापमान पर और लोडिंग आवृत्तियों की एक अलग श्रृंखला के लिए इन मापदंडों की भविष्यवाणी करना आवश्यक है। चरण कोण भविष्यवाणी की सटीकता में सुधार करने की दिशा में, अध्ययन का पहला उद्देश्य चरण कोण मास्टरवक्र के आकार का वर्णन करने के लिए तर्कसंगत मॉडल का प्रस्ताव करता है। प्रस्तावित मॉडल सात पैरामीटर वाले दो सिग्मोइडल फ़ंक्शन का संयोजन है। प्रस्तावित मॉडल की प्रभावशीलता का मूल्यांकन करने के लिए, एनसीएचआरपी प्रोजेक्ट 9-19 में रिपोर्ट किए गए चरण कोण माप का उपयोग किया गया था। 201 अलग-अलग डामर मिश्रणों से उत्पन्न आठ बाइंडरों और पांच समुच्चय ग्रेडेशन की पहचान की गई। प्रस्तावित 7-पैरामीटर मॉडल की तुलना प्रसिद्ध सिग्माइडल, सामान्यीकृत सिग्माइडल और सीएएम मास्टरकर्व मॉडल से की गई थी। परिणाम दर्शाते हैं कि प्रस्तावित मॉडल अन्य मॉडलों की तुलना में चरण कोण मास्टरवक्र के आकार का सटीक वर्णन करता है। सांख्यिकीय विश्लेषण ने चरण कोण मास्टरवक्र विशेषताओं (शिखर चरण कोण और उसका स्थान) और अन्य चर (यानी मिश्रण वॉल्यूमेट्रिक्स, मिश्रण ग्रेडेशन) के बीच उचित सहसंबंध दिखाया। चरण कोण मास्टरवक्र विशेषताओं की भविष्यवाणी करने के लिए मिश्रणवार प्रतिगमन मॉडल भी प्रस्तावित किए गए थे। फिट संकेतकों की

अच्छाई ने सत्यापित किया कि प्रस्तावित पूर्वानुमानित मॉडल चरण कोण मास्टरकर्व विशेषताओं की अच्छी तरह से भविष्यवाणी करने में सक्षम थे।

इसके अलावा, गतिशील मापांक ($|E^*|$) और चरण कोण (ϕ) भविष्यवाणी के लिए जीन एक्सप्रेसन प्रोग्रामिंग (जीईपी) आधारित मॉडल पर पहुंचने के लिए एक कुशल दृष्टिकोण। प्रस्तावित पद्धति में (i) $|E^*|$ का निर्माण शामिल है और ϕ मास्टरकर्व्स, (ii) जीईपी आधारित पूर्वानुमानित अभिव्यक्तियों की रैंकिंग जो इनपुट के रूप में कम आवृत्ति, समग्र ग्रेडेशन, डामर बाइंडर सामग्री, बाइंडर गुण और मिश्रण वॉल्यूमेट्रिक्स का उपयोग करती है, और (iii) इष्टतम पेड़ की गहराई पर पूर्वानुमानित मॉडल का चयन, और (iv) पुनर्अंशंकन. इस प्रकार, प्रस्तावित पद्धति अत्यधिक प्रभावशाली चर, पूर्वानुमानित मॉडल जटिलता और पूर्वानुमानित सटीकता के चयन के बीच सही संतुलन प्राप्त करने का प्रयास करती है। प्रस्तावित पद्धति को मान्य करने के लिए, एनसीएचआरपी 9-19 अध्ययन में रिपोर्ट किए गए डेटाबेस का उपयोग किया गया था। पेड़ की गहराई बढ़ाने के साथ प्रस्तावित दृष्टिकोण के अनुप्रयोग के साथ, मॉडल जटिलता, पूर्वानुमान सटीकता और कम्प्यूटेशनल समय में वृद्धि हुई। हालाँकि, पेड़ की निश्चित गहराई से परे मॉडल सटीकता में वृद्धि मामूली थी। इसका श्रेय प्रारंभिक चरणों में अत्यधिक प्रभावशाली चर को शामिल करने और जीईपी मॉड्यूल निष्पादन के दौरान मॉडल रूपों पर सीमा को दिया जा सकता है। प्रस्तावित जीईपी आधारित भविष्य कहनेवाला अभिव्यक्तियों की मजबूती की जांच स्वतंत्र डेटाबेस और प्रतिस्पर्धी मॉडल के साथ की गई थी। फिट संकेतकों की अच्छाई के संख्यात्मक मूल्यों ने इनपुट चर और पूर्वानुमानित मॉडल के उचित चयन के माध्यम से पूर्वानुमानित सटीकता में सुधार दिखाया।

मिश्रणवार पुनर्अंशांकन के माध्यम से पूर्वानुमानित सटीकता में और सुधार किया गया। प्रस्तावित भविष्यसूचक अभिव्यक्तियों का उपयोग $|E^*|$ के लिए आसानी से किया जा सकता है और पुनर्अंशांकन और उसके बाद प्रारंभिक डिजाइन के माध्यम से ϕ भविष्यवाणी।

इसके अलावा, तीसरे उद्देश्य ने डामर मिश्रण के गतिशील मापांक और चरण कोण की भविष्यवाणी करने के लिए एक गहन शिक्षण दृष्टिकोण का प्रस्ताव दिया। प्रस्तावित दृष्टिकोण को मान्य करने के लिए राष्ट्रीय सहकारी राजमार्ग अनुसंधान कार्यक्रम 9-19 में रिपोर्ट किए गए गतिशील मापांक और चरण कोण डेटा का उपयोग किया गया था। इस डेटाबेस में 201 विशिष्ट डामर मिश्रणों का चयन किया गया। दो सिग्मॉइडल कार्यों और दो तापमान बदलाव कारक निर्धारण दृष्टिकोणों के संयोजन का उपयोग करके व्यक्तिगत मिश्रण के लिए गतिशील मापांक और चरण कोण मास्टरकर्व का निर्माण किया गया था। गहन शिक्षण मॉडल के लिए इनपुट चर में कम आवृत्ति, बाइंडर गुण, समग्र उन्नयन और मिश्रण वॉल्यूमेट्रिक्स के बारे में जानकारी शामिल थी। जब अन्य इनपुट चर की तुलना की जाती है, तो कम आवृत्ति और बाइंडर गुण गतिशील मापांक और चरण कोण के साथ अत्यधिक सहसंबद्ध होते हैं। इसके अलावा, सभी इनपुट चर को रैंक करने के लिए पुनरावर्ती सुविधा उन्मूलन का उपयोग किया गया था। इन रैंक किए गए इनपुट चर का उपयोग करके, गतिशील मापांक और चरण कोण की भविष्यवाणी के लिए गहन शिक्षण आधारित मॉडल विकसित किए गए थे। गहन शिक्षण वास्तुकला (संपूर्ण अनुकूलन के माध्यम से अंतिम रूप दिया गया) विचाराधीन पैरामीटर पर निर्भर है, और मास्टरकर्व निर्माण दृष्टिकोण अपनाया गया था। विस्तृत सांख्यिकीय विश्लेषण से संकेत मिलता है कि चरण कोण पूर्वानुमानित मॉडल

की तुलना में गतिशील मापांक पूर्वानुमानित मॉडल ने बेहतर प्रदर्शन किया। फिट संकेतकों की अच्छाई के संख्यात्मक मूल्यों से पता चला कि गहन शिक्षण आधारित मॉडल की सटीकता अपनाए गए मास्टरकर्व निर्माण दृष्टिकोण पर निर्भर थी। समग्र परिणामों से संकेत मिलता है कि गहन शिक्षण आधारित मॉडल अच्छी सटीकता के साथ गतिशील मापांक और चरण कोण की भविष्यवाणी कर सकते हैं। प्रस्तावित गहन शिक्षण मॉडल के आउटपुट का उपयोग फुटपाथ डिजाइन ढांचे में सीधे इनपुट के रूप में किया जा सकता है, जिसके परिणामस्वरूप फुटपाथ प्रदर्शन की सटीक भविष्यवाणी हो सकती है।

अध्ययन का चौथा उद्देश्य मार्शल मिक्स डिज़ाइन के मशीन लर्निंग आधारित लागत अनुकूलन का प्रस्ताव करना था। मशीन लर्निंग आधारित लागत अनुकूलन ढांचे को विकसित करने के लिए, मार्शल परीक्षण परिणामों की भविष्यवाणी करने और वॉल्यूमेट्रिक्स को मिश्रित करने के लिए D_{90} से D_{10} तक D_i मानों, बाइंडर सामग्री और समुच्चय के थोक विशिष्ट गुरुत्व के संदर्भ में विभिन्न समुच्चय ग्रेडेशन का उपयोग किया गया था। हालाँकि, समग्र उन्नयन के साथ-साथ रूपरेखा को विकसित करने के लिए एकरूपता और वक्रता के गुणांक का उपयोग किया गया था। ग्रेडेशन वक्र पर सभी बिंदुओं पर सभी आकार कारकों को ध्यान में रखने के लिए नए C_u 's और C_c 's विकसित किए गए। नए C_u 's और C_c 's ने मार्शल परीक्षण परिणाम मिश्रण वॉल्यूमेट्रिक्स के साथ बेहतर सहसंबंध दिखाया। चार दृष्टिकोणों का उपयोग इनपुट स्वतंत्र चर का उपयोग करके विभिन्न मशीन लर्निंग पूर्वानुमानित मॉडल के साथ अनुकूलन के लिए किया गया था: (i) दृष्टिकोण 1: D_{90} से D_{10} तक D_i मान (ii) दृष्टिकोण 2: D_i मान और

पारंपरिक $C_u C_c$ (iii) दृष्टिकोण 3: नए विकसित $C_u's$ और $C_c's$ (iv) दृष्टिकोण 4: नए विकसित $C_u's$ और $C_c's$ के विकसित और पारंपरिक $C_u C_c$ । कुल ग्रेडेशन और मिश्रण वॉल्यूमेट्रिक्स पर बाधाएं प्रदान करके इन चार दृष्टिकोणों के लिए लागत अनुकूलन एल्गोरिदम विकसित किया गया था। नए $C_u's$ और $C_c's$ के दृष्टिकोणों के परिणामस्वरूप D_i मानों वाले दृष्टिकोणों की तुलना में कम बाइंडर सामग्री प्राप्त हुई। इसके अलावा, पारंपरिक $C_u C_c$ के दृष्टिकोण समान समग्र उन्नयन वक्र प्रदान करते हैं।

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List of Notations

$ E^* $	Dynamic modulus of asphalt mixture, MPa
ϕ	Phase angle of asphalt mixture, °
T	Loading temperature, °C
f	Loading frequency, Hz
σ_o	Peak applied stress
ε_o	Peak resulting strain
$ G^* $	Complex shear modulus of asphalt binder, MPa
δ_b	Binder phase angle of asphalt binder, °
$\rho_{3/4}$	% weight of aggregates retained on the ¾-inch sieve
$\rho_{3/8}$	% weight of aggregates retained on the 3/8 -inch sieve
ρ_4	% weight of aggregates retained on the No. 4 sieve
ρ_{200}	% weight of aggregates passing through the No. 200 sieve
AC	Asphalt binder content, %
V_a	Air voids in the mix, %
V_{beff}	Effective asphalt binder content, %
VMA	Voids in mineral aggregates, %
VFB	Voids filled with the bitumen, %
DV	Dependent variable
MV_i	Mixture indicator i ($i = 1$ through 5)
AGP_j	Aggregate gradation property indicator j ($j = 1$ through 4)
BP_k	Binder property indicator k ($k = 1$ through 2)
aT	Temperature shift factor
f_r	Reduced frequency, Hz
NoC	Number of coefficients
QoF	Quality of fit indicators
$SQFI$	Sum of quality of fit indicators
IVP	Independent variable proportion
R^2	Coefficient of determination

$Adj R^2$	Adjusted coefficient of determination
SSE	Sum of squared error
$RMSE$	Root mean squared error
C_u	Coefficient of uniformity
C_c	Coefficient of curvature
D_i	Aggregate particle size at every 10% interval from D_{90} to D_{10} , mm
V_a	Air voids, %
MAS	Maximum aggregate size, mm
$NMAS$	Nominal maximum aggregate size, mm
P_b	Binder content, %
C_i	Aggregate cost for bin i