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Neural Network Based Model to Estimate Dynamic Modulus E* for Mixtures in Costa Rica

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ABSTRACT

Several dynamic modulus (E*) predictive models of asphalt mixtures have been developed as an alternative to laboratory testing. The 1999 I-37A Witczak equation is one of the most commonly used alternatives. This equation is based on mixtures laboratory results in the U.S. In Latin American significant differences in countries there are properties, traffic information, and environmental conditions compared to the U.S.; therefore, there is a limitation is the use of this equation using local conditions. The National Laboratory of Materials and Structural Models at University of Costa Rica (Lanamme UCR) has previously performed a local calibration of this equation based on results from different types of Costa Rican mixtures. However, there was still room for improvement using advanced regression techniques such as neural networks (NN). The objective of this study was to develop an improved and more effective dynamic modulus regression model for mixtures in Costa Rica using Neural Networks. Results indicated that the new and improved model based on neural networks (E* NN-model) not only met the model adequacy checking criteria but also exhibited the best goodness of fit parameters and the lowest overall bias.

1. Introduction

The most important asphalt concrete mixture property influencing the structural response of a flexible pavement is the dynamic modulus (E*). For a specific mixture, temperature, rate of

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loading and aging significantly influence this property. E* is also the primary hot-mix asphalt (HMA) material property input at all three hierarchical levels in the new AASHTOware Pavement ME Design Guide or formerly known as mechanistic empirical pavement design guide (MEPDG) [1].

Various E* predictive models have been developed to estimate E* as an alternative to laboratory testing. The most widely used model is the 1999 I-37A Witczak predictive model based on conventional multivariate regression analysis of laboratory test data. Because of this, the Witczak model has been evaluated using many different datasets and has been calibrated to several regions. However, use of the model with no calibration for local mixtures should be limited.

The results of a study conducted at MnROAD indicated that the Witczak predictive equation fitted the data relatively well in some locations at intermediate and low temperatures, but for other locations the differences were significant [2]. The authors concluded that the Witczak equation should be used with caution and they also recommended further research to adjust and validate this equation for mixtures and local conditions found in Minnesota.

A study at the University of Florida [3], evaluated the same equation using 28 mixtures from Florida. The results of this study indicated that the Witczak equation was slightly bias for the mixtures investigated. The results also allowed the correction of the bias between predicted and measured E* by means of statistical calibration. Authors also found that E* predicted values at higher temperatures generally were closer to measured values than predictions at lower temperatures. Authors pointed out that the database used to develop the Witczak model could be constrained to predicting the modulus of mixtures tested at higher temperatures.

41 mixtures commonly used in North Carolina were used to evaluate the prediction accuracy of the Witczak equation and the influence of some mixture variables in the prediction of E* [4]. The study showed that Witczak's predictions for cooler temperatures were better than at warmer temperatures. This is the opposite of what was observed in Florida and thus highlights the importance of proper calibration.

Another study by Schwartz in 2005 [5] evaluated the accuracy and robustness of the Witczak predictive equation through a set of sensitivity and validation analyses. The same database used to create the Witczak equation and an independent set of laboratory E* test data for 26 other mixtures were used for calibration purposes. The validation analysis of the Witczak equation against the independent set of data showed a good match between predicted and measured E* values that was nearly as good as for the calibration data set, but with a slight positive bias which was higher for lower stiffness/higher temperature conditions.

The University of Arkansas studied 12 commonly used mixtures in Arkansas and found a good correlation between Witczak predicted E* values and laboratory measured results [6]. The goodness-of-fit statistics showed that the prediction of E* for the mixtures used in the study ranged from very good to excellent, according to the subjective criteria used.

Robbins and Timm in 2011 [7], evaluated three E* predictive models (Witczak 1-37A, Witczak 1-40D, and Hirsch) with using 18 plant-produced, lab-compacted mixtures. These mixtures were placed at the 2006 National Center for Asphalt Technology Test Track. The Hirsch model for estimating asphalt mixture modulus is based on a law of mixtures for composite materials [8]

which utilizes the shear modulus of the binder, G*, and volumetric properties of the mix to predict E*. E* estimaded values were obtained at three temperatures and three frequencies for direct comparison with laboratory measured results. Results indicated that the Witczak equation had the greatest deviation from measured values, and the Witczak 1-40D model overestimated E* values by approximately 61%. The Hirsch model most accurately predicted the moduli for the 2006 Test Track mixtures.

Singh et al. in 2011 [9], also evaluated the Witczak equation for estimating the dynamic modulus of selected asphalt mixtures commonly used in Oklahoma. Analyses of the results indicated that a calibration factor was needed for the model to obtain an accurate estimates of dynamic modulus. El-Badawy et al. in 2012 [10], also indicated that the accuracy of this equation can be further enhanced by adding a local calibration factor.

In the case of Costa Rica, a similar analysis was performed to ensure that the Witczak model could be readily applied to local mixtures [11]. The Witczak model was identified to produce slightly biased predictions of E* when compared to several gradations, mostly of typical use in the country. As was the case with some of the previous studies, the model showed positive bias at higher stiffness/lower temperature conditions. Consequently, a calibrated Witczak model was fitted using nonlinear regression.

Far et al. in 2009 [12], developed a new, rational, and effective set of dynamic modulus E* predictive models. These predictive models used artificial neural networks (ANNs) trained with the same set of parameters used in the Witczak equation. E* values from several mixtures were collected from existing national efforts and from data obtained at North Carolina State University. The results showed that the predicted and measured E* values were in close agreement when ANN models were used.

A paper presented by Ceylan et al. in 2009 [13], discussed the accuracy and robustness of the various models including an ANN based models. The ANN-based E* models showed significantly better overall prediction accuracy, better local accuracy at high and low temperature extremes, less prediction bias, and better balance between temperature and mixture influences compared to the ordinary least squares (OLS) regression-based approach. Authors indicated that the ANN models were better able to rank mixtures in the same order as measured E* for fixed environmental and design traffic conditions.

In summary, the I-37A Witczak predictive model has worked well in some cases and not so well in others. Calibration of this equation has also been implemented by several researchers while others decided to utilize the 2006 Witczak model or decided to adopt a different approach such as the Hirsh model. Finally, the use of more advanced regression techniques has also proven to be a more attractive alternative to calibration of the Witczak equation.

2. Objective

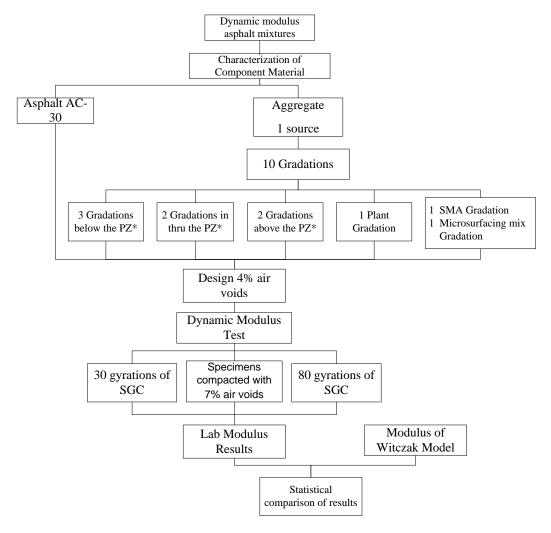
The objective of this study was to create a neural network (NN) based models to improved accuracy and reduce bias in the prediction of dynamic modulus (E*) for asphalt mixtures in Costa Rica.

3. Mixture characterization and evaluation

In 2011, LanammeUCR conducted a laboratory evaluation of the applicability of the Witczak Model to a typical aggregate source and one type of asphalt binder produced in Costa Rica [11]. The flow chart presented in Figure 1 summarizes the experimental plan of the study, where 10 different gradations were selected using one aggregate source and specimens were compacted using the Superpave gyratory compactor.

The study involved one aggregate source (from a northeast region of the country called Guápiles). The aggregate is extruded from igneous deposits along a river. The aggregate properties are shown in Table 1.

In Costa Rica only one type of asphalt is produced. The binder viscosity classification corresponds to an unmodified AC-30. Based on the Superpave specification, the binder classifies as a PG64-22. The properties for the asphalt binder are shown in Table 2.



PZ*: "prevention zone" or SUPERPAVE's restricted zone

Fig. 1. Flow Chart for the Experimental Plan.

Table 1Physical Properties of the Aggregates Used in the Study.

Property	Test Method	Value	Unit	Specifications				
Coarse Aggregate								
L.A. Abrasion	AASHTO T 96	21.21	%	37% max. ¹				
Specific Gravity	AASHTO T 85	2.652		2.85 max. ¹				
Absorption	AASHTO T 85	1.69	%	4% max. ¹				
Faces Fractured		100	%	90% min. ²				
1 face	ASTM D 5821							
2 or more		99.8	%	75% min. ²				
	Fine Aggre	gate						
Plasticity index	AASHTO T 90	NP		10% max. ¹				
Sand equivalent	AASHTO T 176	78		=				
Angularity	AASHTO TP 304	37.2	%	-				
Specific Gravity	AASHTO T 84	2.549		2.85% max. ¹				
Absorption	AASHTO T 84	3.283	%	-				

¹ Nevada DOT Standard Specifications for Road and Bridge Construction, 2001.

Table 2 Physical Properties of the Used Asphalt Binder.

Aging State	Property	Unit	Asphalt Binder AC-30
	Density at 25°C	g/cm ³	1.030
	Absolute viscosity at 60°C	Poise	3330
	Kinematic viscosity at 125°C	centiPoise	961
Original	Kinematic viscosity at 135°C	centiPoise	565
	Kinematic viscosity at 145°C	centiPoise	347
	VTS, regression slope of viscosity temperature susceptibility	-	3.43
	Regression intercept	-	10.26
	Absolute viscosity at 60°C	Poise	11512
RTFO	Kinematic viscosity at 125°C	centiPoise	1712
	Kinematic viscosity at 135°C	centiPoise	938
	Kinematic viscosity at 145°C	centiPoise	550

3.1. E* specimen preparation

Ten different types of asphalt mixtures were designed in the laboratory. Three dense graded mixtures (G1, G2 and G3) below the "prevention zone" (also called Superpave's restricted zone); two dense graded mixtures (G6 and G7) above the "prevention zone"; two dense graded mixtures (G4 and G5) thru the "prevention zone"; one Stone Matrix Asphalt (SMA) mixture (G9); one micro surface asphalt mixture (G8), and a typical plant dense graded mixture (G10). The gradations are presented in Table 3. The design air void content was fixed to 4%. Two mixture design methodologies were used: Marshall and Superpave. The optimum asphalt content by dry weight of aggregate (DWA) and by total weight of mixture (TWM), voids in the mineral aggregate (VMA), the voids filled with asphalt (VFA), and the effective asphalt content (Pbe) based on both methodologies are shown in Table 4.

² Standard Specifications for Constructions of Roads and Bridges on Federal Highways Projects, FP-03

Table 3 Studied Aggregate Gradations.

	-888		Studied Gradation								
ASTM Sieve	Sieve (mm)	Below the prevention zone		ention zone			Above the prevention zone		SMA	Plant	
		G1	G2	G3	G4	G5	G6	G7	G8	G9	G10
3/4	19.0	100	100	100	100	100	100	100	100	100	100
1/2	12.5	95	100	90	95	95	98	90	100	90	95
3/8	9.5	88	95	78	90	90	92	65	81	45	79
N°4	4.75	37	62	40	45	70	67	45	32	28	48
N°8	2.36	28	33	32	37	50	47	42	27	23	32
N°16	1.18	20	23	20	29	27	32	37	22	22	22
N°30	0.60	13	16	14	22	15	23	30	18	19	16
N°50	0.30	9	12	9	14	8	17	20	14	16	12
N°100	0.15	7	9	7	9	6	12	12	10	13	8
N°200	0.075	5	7	6	6	5	8	5	8	10	5

Table 4Summary Volumetric Properties of the Mix for All the Aggregate Gradations Studied.

Summary volumetric Properties of the Mix for All the Aggregate Gradations Studied.								
Description	Gradation	Mix design	Va	Pb (DWA)	Pb (TWM)	Pbe	VMA	VFA
	G1	Superpave	4.0%	7.20	6.80	5.69	17.32	77.66
		Marshall	4.0%	6.41	6.02	5.18	15.74	74.66
Below the	G2	Superpave	4.0%	7.40	6.90	6.06	17.44	76.12
prevention zone	G2	Marshall	4.0%	6.84	6.40	5.49	16.51	75.78
	G3	Superpave	4.0%	6.40	6.00	5.25	15.68	73.40
	U3	Marshall	4.0%	6.01	5.67	4.83	15.15	71.93
	G4	Superpave	4.0%	5.50	5.30	4.31	12.14	73.20
Thru the	G4	Marshall	4.0%	5.44	5.16	4.17	13.90	69.53
prevention zone	G5	Superpave	8.0%	7.50	7.00	6.00	20.90	61.60
		Marshall	8.8%	6.50	6.10	5.12	20.08	55.50
	G6 G7	Superpave	4.0%	5.50	5.20	4.35	14.10	72.10
Above the		Marshall	4.0%	5.84	5.52	4.41	14.52	70.50
prevention zone		Superpave	4.0%	5.00	4.80	3.32	12.32	63.20
		Marshall	4.0%	5.50	5.21	4.13	13.74	70.50
Miono gunfo sin o	G8	Superpave	4.0%	5.60	5.30	4.29	14.06	78.68
Micro surfacing		Marshall	4.0%	5.99	5.65	4.51	14.82	71.00
SMA	G9	Superpave	4.0%	4.90	4.70	3.74	12.44	68.86
		Marshall	4.0%	5.19	4.93	4.01	13.34	71.00
Dlant	C10	Superpave	4.0%	6.00	5.70	4.76	15.00	73.00
Plant	G10	Marshall	4.0%	5.65	5.35	4.46	14.50	71.10

4. Dynamic modulus of asphalt mixtures

In order to evaluate the dynamic modulus of the different mixes, all specimens were prepared following the standard method ASTM D3496 "Practice for Preparation of Bituminous Specimens for Dynamic Modulus Testing". The testing was performed according to ASTM D3497 "Standard Test Method for Dynamic Modulus of Asphalt Mixtures" and AASHTO T 62 "Determining Dynamic Modulus of Hot Mix Asphalt".

The experimental design included four factors; the first factor was the gradation with the ten levels (G1, G2, G3, G4, G5, G6, G7, G8, G9 and G10), the second factor was the temperature with five levels (-5, 5, 20, 40 and 55°C), the third factor was the loading frequency with six levels (0.1, 0.5, 1, 5, 10 and 25 Hz), and the fourth factor was the compaction effort with three levels (30 gyrations of the Superpave gyratory compactor (SGC), 80 gyrations of SGC, and specimens compacted with 7% air voids).

4.1. Master curves

The master curves and the corresponding shift factors were developed directly from the dynamic modulus tests. Microsoft Excel Solver was used to optimize the calibration coefficients. It involved nonlinear optimization using the sigmoidal function shown in Equations 1 and 2. Both equations describe the time dependency of the modulus. As summary of the regression parameters is shown in Table 5 and Figure 2 shows the Dynamic Modulus Master Curves of all 10 gradations used in the study.

$$Log |E^*| = \delta + \frac{\alpha}{1 + e^{\beta + \gamma(\log t_r)}}$$
 (1)

where.

 $E^* = \text{dynamic modulus}.$

 t_r = time of loading at the reference temperature.

 δ , α = estimated parameters; for a given set of data, δ represents the minimum value of E* and $\delta + \alpha$ represents the maximum value of E*.

 β , γ = parameters describing the shape of the sigmoidal function.

$$a(T) = \frac{t}{t_r} \quad , \quad \log(t_r) = \log(t) - \log[a(T)] \tag{2}$$

 t_r = time of loading at the reference temperature.

t =time of loading at a given temperature of interest.

a(T) = Shift factor as a function of temperature.

T = temperature of interest.

Table 5 Summary of the Fitting Parameters for the Construction of the E*Master Curves.

Gradation	Parameter							
	δ	α	β	γ				
G1	1.8155	2.3618	-0.5631	0.4766				
G2	1.8647	2.4533	-0.3800	0.5018				
G3	1.8542	2.3952	-0.3458	0.4784				
G4	1.8013	2.5136	-0.7055	0.4589				
G5	2.1775	1.8860	-0.1475	0.5982				
G6	1.7743	2.7039	-0.5207	0.4182				
G 7	2.1687	2.3301	-0.5388	0.4960				
G8	2.0420	2.0748	-0.6264	0.5309				
G9	2.0682	2.3802	-0.6617	0.5529				
G10	1.5471	2.7260	-0.7342	0.4276				

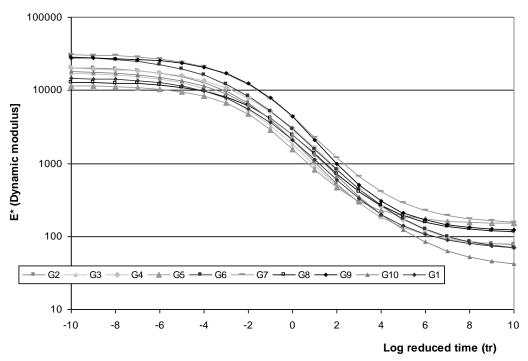


Fig. 2. Dynamic Modulus Master Curves for the Gradations Used in the Study.

5. Quality of fitted Witczak model on Costa Rican mixes

 $\rho 200 = \%$ passing the No. 200 sieve.

For Level 2 and Level 3 analysis of the mechanistic-empirical design guide, the master curves would be developed directly from the dynamic modulus Witczak I-37A predictive equation shown in equation 3. This equation is intended to predict E* values of asphalt mixtures over a wide range of temperatures, rates of loading, and aging conditions based on information that is readily available from material specifications or volumetric design of the mixture [1].

$$\log E^* = 3,750063 + 0,02932\rho_{200} - 0,001767(\rho_{200})^2 - 0,002841\rho_4 - 0,058097V_a$$

$$-0,802208\left(\frac{V_{beff}}{V_{beff}+V_a}\right) + \frac{3,871977 - 0,0021\rho_4 + 0,003958\rho_{38} - 0,000017(\rho_{38})^2 + 0,005470\rho_{34}}{1 + e^{(-0,603313 - 0,31335\log(f) - 0,393532\log(\eta))}}$$
where:
$$E^* = \text{dynamic modulus, psi,}$$

$$\eta = \text{bitumen viscosity, } 106 \text{ Poise,}$$

$$f = \text{loading frequency, Hz,}$$

$$Va = \text{air void content, } \%,$$

$$Vbeff = \text{effective bitumen content, } \% \text{ by volume,}$$

$$\rho 34 = \text{cumulative } \% \text{ retained on the } \frac{3}{4} \text{ in sieve,}$$

$$\rho 38 = \text{cumulative } \% \text{ retained on the } 3/8 \text{ in sieve,}$$

$$\rho 4 = \text{cumulative } \% \text{ retained on the No. 4 sieve,}$$

Overestimation of E* values for mixtures in Costa Rica (Figure 4) was first reported by Loría and his associates in 2011 [11]. The application of this model on mixtures in Costa Rica not only over predicted E* values but also failed to comply one of the assumptions of OLS regression and ANOVA: a constant variance of the error term. In the residual versus the fitted values plot, the errors should have constant variance when the residuals are scattered randomly around zero. In this case, the residuals increase or decrease with the fitted values in a pattern that looks like a funnel or uneven spreading of residuals across fitted values, the errors may not have constant variance (Figure 3). A curvilinear pattern in the residual versus fitted values plot also indicated that a higher-order term to has to be added model.

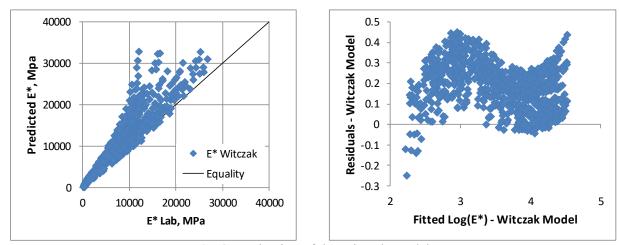


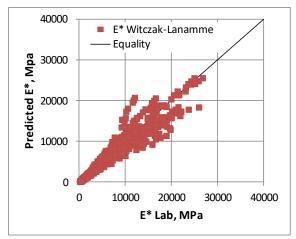
Fig. 3. Evaluation of the Witczak Model.

As mentioned previously, the Witczak-Lanamme model was developed to adjust or calibrate the Witczak model based on the E* results of several mixtures used in Costa Rica. This new model was suggested based on a nonlinear approach that significantly improved the model fit (R²=0.9355, standard deviation of error term=1,494.4 and SSE=5.1997). The model is shown in Equation 4.

$$\log E^* = 5,535833 + 0,002087 \rho_{200} - 0,000566 (\rho_{200})^2 - 0,002590 \rho_4 - 0,078763 V_a$$

$$-1,865947 \left(\frac{V_{beff}}{V_{beff} + V_a}\right) + \frac{2,399557 + 0,000820 \rho_4 - 0,013420 \rho_{38} + 0,000261 (\rho_{38})^2 + 0,005470 \rho_{34}}{1 + e^{(0,052941 - 0,498163 \log(f) - 0,691856 \log(\eta))}}$$
 (4)

The application of the Witczak-Lanamme model not only fixed the overestimation of E* values but also in the residual versus the fitted values plot, the errors had constant variance with the residuals scattered randomly around zero (Figure 4). However, further investigation showed that high errors were still obtained from some mixtures and the variance of the predictions was not uniform. Ideally, in the plot of actual E* values versus predicted ones, a small and random deviation from the line of equality is desired for all data points. As an attempt to reach this ideal scenario, the artificial neural networks (NN) methodology was implemented using the same dataset.



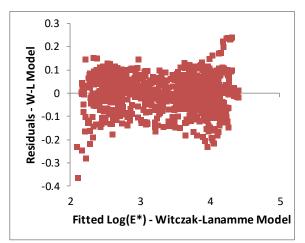


Fig. 4. Evaluation of the Witczak-Lanamme Model.

6. Development of the E* - NN model

A neural network is a massively parallel distributed processor that has a natural propensity for storing experimental knowledge and making it available for use [14]. Knowledge is acquired by the network through a learning (training) process. The strength of the interconnections between neurons is implemented by means of the synaptic weights used to store the knowledge. The learning process is a procedure of adapting the weights with a learning algorithm in order to capture the knowledge. In other words, the aim of the learning process is to map a given relation between inputs and outputs of the network.

The learning method used to develop the NN model was a feed-forward back propagation with the sigmoidal function (Equation 5) as the transfer function. It was found that the two-layer network with 10 nodes in the hidden layer was the most appropriate for this dataset (Figure 5). The structure of the network is given by Equations 5 through 7. A single index indicates an array; dual indices represent a matrix with the first letter indicating the values in the row and the second letter indicating the values in the column. The index i represents the input parameters and the index k represents the hidden layer.

$$f(T) = \frac{2}{1 + e^{-2T}} - 1 \tag{5}$$

$$H_k^1 = B_k^1 + \sum_{i=1}^m W_{ik} P_i \tag{6}$$

$$Output = Ln(E^*) = f(B_O + \sum_{i=1}^m H_k^1 W_k)$$
(7)

where;

T =placeholder variable,

 H_k^1 = transferred value of nodes at the hidden layer,

 P_i = input variables (ρ 200, ρ 4, ρ 38, Va, V_{beff}, loglog(η), temperature and frequency),

 W_{ik} = weight factors for the hidden layer,

 W_k = weight factors for the output layer,

 B_k^1 = bias factors for first layer, B0 = bias factor for outer layer,m = number of nodes in hidden layer $Ln(E^*)$ = natural logarithm of E^* .

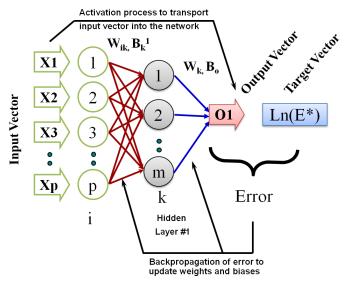


Fig. 5. Schematic of model development process.

6.1. Model weights and bias values

Weight matrices and bias vectors of the NN model are shown as follows:

Bias factors for first layer,

 $B_k^1 = \begin{bmatrix} 2.3134 & 4.0247 & 2.1380 & -11.9793 & 0.3330 & -6.3721 & -5.0298 & -0.2873 & -10.6756 & 10.3805 \end{bmatrix}$ Weight factors for the hidden layer,

Weight factors for the output layer and bias factor for outer layer,

$$W_k = \begin{bmatrix} 0.2402 \\ 0.0377 \\ 0.0410 \\ 0.0722 \\ 6.6041 \\ -0.0695 \\ -0.2727 \\ 7.6429 \\ -13.6531 \\ 0.0456 \end{bmatrix}$$

$$B_0 = -13.6918$$

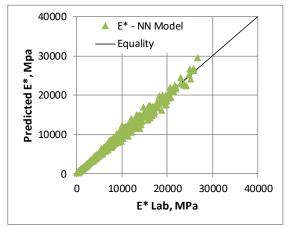
Relative importance based on Garson's formula indicated that all input variables can be considered significant to explain output variable. Temperature was found to be the most important input variable. This was expected since dynamic modulus of asphalt mixtures are highly susceptible to small changes in temperature. Relative importance results were computed in percentage format as follows:

14.9%
11.7%
12.3%
15.6%
9.2%
9.1%
17.5%
9.8%

Potential overfitting on the model was controlled by constraining the complexity of the model and by monitoring the performance of the model during training. The first one was accomplished by changing the network structure (number of weights). The second one was accomplished by evaluating performance on both a training dataset and on a holdout validation dataset. Learning curves will show a line for the training dataset that drops and may plateau and a line for the validation dataset that drops at first, then at some point begins to rise again. This was an indication of potential overfitting.

As an example, if these parameters are substituted into Equations 5 through 7 with $\rho 200 = 5$, $\rho 4 = 63$, $\rho 38 = 12$, $V_a = 7.41$, $V_{beff} = 5.69$, $\log \log(\eta) = 3.7859$, temperature = -3.4 and frequency = 25, the predicted $\ln(E^*)$ value of 9.31415 and the E* value of 11,402 MPa would be calculated from this recommended model.

The results of the application of the NN model on the entire E* database are shown in Figure 6. In the plot of actual E* values versus predicted ones, a small-constant deviation from the line of equality was acquired for all data points. In addition, in the residual versus the fitted values plot, the errors had constant variance with the residuals scattered randomly around zero.



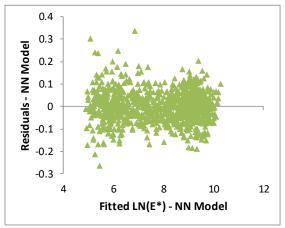


Fig. 6. Evaluation of the E* - NN Model.

The slope of the measured versus predicted curve for all three models was used to perform a bias analysis. As shown in Figure 7 the highest deviation from the line of equality in terms of the slope was obtained for the Witczak I-37A model. On average, predicted E* values were deviated from the equality line by 35%. In second place, the Witczak-Lanamme model predicted E* values with a slight deviation from the equality line (about 4%). Finally, the E* - NN had the lowest deviation from the line of equality with only 1%.

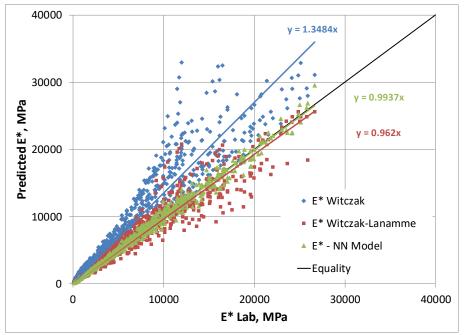


Fig. 7. Comparison of Predictive Models.

The accuracy of the three predictive models was also analyzed by means of goodness of fit parameters in arithmetic space. Table 6 shows the calculated parameters for all the models along with the respective criteria. The lowest coefficient of determination (R²) in arithmetic space and the highest standard error of the estimate/standard deviation value (Se/Sy) for the Witczak model confirmed its limited ability to predict E* values for mixtures in Costa Rica. A significant improvement in the prediction of E* values, with respect to the Witczak model was obtained with the use of the Witczak-Lanamme model (59% improvement in the R2 value and 29% reduction in the Se/Sy value). However, the best results were obtained for the E* - NN model with the highest R² and lowest Se/Sy values (69% improvement in the R² value and 77% reduction in the Se/Sy value with respect to the Witczak model).

Table 6 Goodness of Fit Parameters.

Parameters				Goodness of Fit (Witczak et al. 2002)			
Model	\mathbb{R}^2	R ² adj.	Se/Sy arithmetic	Criteria	\mathbb{R}^2	Se/Sy	
Witczak	0.592	0.589	0.372	Excellent	> 0.90	< 0.35	
Witczak-Lanamme	0.935	0.934	0.262	Good	0.70089	0.36 - 0.55	
E* - NN Model	0.993	0.992	0.086	Fair	0.40 - 0.69	0.56 - 0.75	
		Poor	0.20 - 0.39	0.76 - 0.90			

In summary, overestimation of E* values for Costa Rican mixtures by the Witczak I-37A model led to its local calibration (Witczak-Lanamme model). An additional model adequacy checking performed on these two models led to the construction of a new and improved model based on artificial neural networks (E* - NN model). This final model not only met the model adequacy criteria but also had the best overall goodness of fit parameters.

7. Conclusions and recommendations

The results of this study led the research team to the following conclusions:

- Even when a local calibration of the Witczak I-37A model was performed for 10 mixtures in Costa Rica, there was still room for improvement. Further investigation showed that high errors were still obtained from some mixtures when using the calibrated model.
- The data clearly indicated that calibration of the E* models, based on direct application of standard regression techniques such as OLS was not adequate since several of the assumptions made when using this technique were violated, rendering the estimated values as inefficient (variance in the model can be further improved).
- The application of artificial neural networks proved to be a most appropriate methodology to improve the predictability of E* values. The E* NN model complied with the model adequacy criteria, had the best goodness of fit parameters and exhibited the lowest overall bias (69% improvement in the R² value and 77% reduction in the Se/Sy value with respect to the Witczak model).
- In order to further improve this prediction model for Costa Rica, future calibration and verification efforts are necessary; therefore, it is recommended to increase the number of tests performed (increase the E* database).

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