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Investigation of complex modulus of base and SBS modified bitumen with artificial neural networks

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ABSTRACT

This study aims to model the complex modulus of base and styrene–butadiene–styrene (SBS) modified bitumens by using artificial neural networks (ANNs). The complex modulus of base and SBS polymer modified bitumen samples (PMB) were determined by using dynamic shear rheometer (DSRs). PMB samples have been produced by mixing a 50/70 penetration grade base bitumen with SBS Kraton D1101 copolymer at five different polymer contents. In ANN model, the bitumen temperature, frequency and SBS contents are the parameters for the input layer where as the complex modulus is the parameter for the output layer. The variants of the algorithm used in the study are the Levenberg–Marquardt (LM), scaled conjugate gradient (SCG) and Pola-Ribiere conjugate gradient (CGP) algorithms. A tangent sigmoid transfer function was used for both hidden layer and the output layer. The statistical indicators, such as the root-mean squared (RMS), the coefficient of multiple determination (R^2) and the coefficient of variation (cov) was utilized to compare the predicted and measured values for model validation. The analysis indicated that the LM algorithm appeared to be the most optimal topology which gained 0.0039 mean RMS value, 20.24 mean cov value and 0.9970 mean R^2 value.

1. Introduction

Bitumen is a natural derivative of distillation of crude oil, which is particularly suitable as a binder for road construction due to their good adhesion to mineral aggregates and viscoelastic properties. Unfortunately, bitumen is a form of liquid at high temperature and becomes brittle at low temperatures, which can cause high temperature rutting, low temperature cracking of pavement and these functions limit its application (Yu, Zeng, Wu, Wang, & Liu, 2007). These deficiencies of bitumen can be decreased by the addition of polymers, which is closely connected with bitumen improved viscoelastic behavior (Yousefi, 2003). The rheological behavior of bitumen is very complex phenomenon, varying from purely viscous to elastic, depending on loading time and temperature. A considerable increase in complex modulus at high temperature (low frequency) is obtained by the addition of several contents of polymer, and further increasing the polymer content results in increased complex modulus (Lu & Isacsson, 1999; Ruan, Davison, & Glover, 2003). Besides the increased stiffness at high temperatures, polymer also causes a decreased complex modulus (G^*) in bitumen at low service temperatures (high frequency).

Currently, the most commonly used polymer for bitumen modification is the styrene–butadiene–styrene (SBS) followed by other polymers such as ethylene vinyl acetate (EVA), styrene butadiene rubber (SBR) and polyethylene (Sengoz & Isikyakar, 2008). SBS block copolymers are classified as elastomers that increase the elasticity of bitumen and they are probably the most appropriate polymers for bitumen modification. The polystyrene end-blocks impart the strength to the polymer while the polybutadiene, rubbery matrix mid-blocks give the material its exceptional elasticity (Airey, 2003; Gonzales, Munoz, & Santamaria, 2004).

In recent years, limited number of studies has been concentrated on artificial neural networks and bitumen. Ozsahin and Oruc (2008) developed a neural network model for predicting the resilient modulus of emulsified asphalt. Results indicated that neural networks predict the resilient modulus with high accuracy. Far, Sadat, Shane, and Richard (2009), presented a research effort to develop estimates of the dynamic modulus of hot mix asphalt layers, and their research showed that the predicted and measured dynamic modulus values are in close agreement using the ANN models. Specht, Khatchatourian, Brito, and Ceratti (2007) utilized the statistical analysis and artificial neural networks to create mathematical models for the prediction of the bitumen viscosity. The comparison between experimental data and simulated results with the generated models exhibited best performance of the neural networks analysis in contrast to the statistic models.

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In order to evaluate the efficiency of additives such as polymers the dynamic (oscillatory) mechanical analysis is used. These oscillatory tests are undertaken using dynamic shear rheometers (DSRs). The principal viscoelastic parameter obtained from the DSR is complex modulus which is strongly affected by the frequency, temperature, additive type and additive content. The test requires very accurate measurements and takes long times. In order to eliminate these drawbacks this paper represents an artificial neural networks (ANNs) approach which will provide an estimation of the complex modulus of SBS polymer modified bitumen.

2. Dynamic mechanical analysis

At present the most commonly used method of fundamental rheological testing of bitumen is by means of dynamic mechanical methods using oscillatory-type testing, generally conducted within the region of linear viscoelastic (LVE) response. These oscillatory tests are undertaken using dynamic shear rheometers (DSRs). The DSR function is based on sandwiching the bitumen between two plates, in which the lower plate is fixed and the top plate oscillates at a frequency shown in Fig. 1 (Roberts, Kandhal, Brown, Lee, & Kennedy, 1996). The principal viscoelastic parameters that are obtained from the DSR are the magnitude of the complex shear modulus (G^*) and the phase angle (δ). G^* is defined as the ratio of maximum (shear) stress to maximum strain. It contains elastic and viscous components, which are designated as the (shear) storage modulus (G') and (shear) loss modulus (G''), respectively. These two components are related to the complex (shear) modulus and to each other through the phase (or loss) angle (δ) which is the phase, or time, lag between the applied shear stress and shear strain responses during a test (Airey, 2003).

3. Sample preparation and experiment

The base bitumen with a 50/70 penetration grade was procured from Aliaga/Izmir Oil Terminal of the Turkish Petroleum Refinery Corporation. In order to characterize the properties of the base bitumen, conventional test methods such as; penetration test, softening point test, ductility test, etc. were performed. These tests were conducted in conformity with the relevant test methods that are presented in Table 1.

The SBS polymer used was Kraton D-1101 supplied by the Shell Chemicals Company. SBS modified bitumen samples were prepared by means of a high shear laboratory type mixer rotating at 1100 rpm. In preparation, the base bitumen was heated to fluid condition (180–185 °C), and has been poured into a 2000 ml spherical flask. The SBS polymer was then added slowly to the base bitumen. The concentrations of SBS Kraton D-1101 in the base bitumen were chosen as 2–6% by an increase of 1% by weight. The temperature was kept constant at 185 °C, and the mixing process continued for 2 h.

The DSR test was performed on SBS PMB by using a Bohlin DSRII rheometer. The test was performed under controlled-stress loading conditions using frequency sweeps between 0.01 and 10 Hz and at temperatures between 10 and 80 °C. The test was carried out with 8 mm diameter, 2 mm gap parallel plate testing geometry between 10 and 30 °C, and with 25 mm diameter, 1 mm gap geometry between 30 and 80 °C. The stress amplitude for all the tests was confined within the linear viscoelastic response of the bitumen. The DSR test machine is seen in Fig. 2.

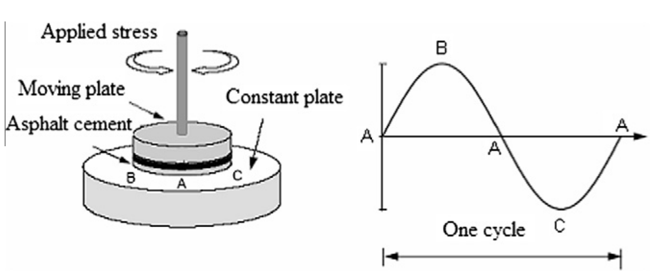

Fig. 1. Schematic representation of DSR.

Table 1
Properties of the base bitumen.

Test	Specification	Results	Specification limits
Penetration (25 °C; 0.1 mm)	ASTM D5 EN 1426	63	50–70
Softening point (°C)	ASTM D36 EN 1427	49	46–54
Viscosity at (135 °C), Pa s	ASTM D4402	0.51	–
Thin film oven test (TFOT); (163 °C, 5 h)	ASTM D1754 EN 12607-1		
Change of mass (%)		0.07	0.5 (max)
Retained penetration (%)	ASTM D5 EN 1426	51	50 (min)
Softening point after TFOT (°C)	ASTM D36 EN 1427	51	48 (min)
Ductility (25 °C), cm	ASTM D113	100	–
Specific gravity, gr/cm^3	ASTM D70	1.030	–
Flash point (°C)	ASTM D92 EN 22592	+260	230 (min)

4. Artificial neural networks (ANNs)

An ANN is an information processing idea that is inspired by the way of biological systems such as the brain. The key element of this idea is the novel structure of the information processing system. It is composed of large number of highly interconnected processing elements (neurons) working in unison to solve specific problems. A schematic diagram for an artificial neuron model is presented in Fig. 3.

The neurons are connected with connection link. Each link has a weight that is multiplied with transmitted signal in network. Each neuron has an activation function to determine the output. There are many kinds of activation functions. Usually nonlinear activation functions such as sigmoid, step are used. Neural Networks are trained by experience. When an unknown input is applied to the network, a new result is produced based on past experiences (Hanbay, Turkoglu, & Demir, 2008; Haykin, 1994). The output of the neuron net is given by Eq. (1).

$$y(t+1) = a\left(\sum_{j=1}^{n} w_{ij}x_j(t) - \theta_i\right) \quad \text{and} \quad f_i \underline{\underline{\Delta}} net_i = \sum_{j=1}^{m} w_{ij}x_j - \theta_i \qquad (1)$$

where, $X = (X_1, X_2, \ldots X_m)$ represent the m input applied to the neuron, W_i represent the weights for input X_i, θ_i is a bias value, $a(.)$ is activation function.

There are numerous algorithms available for training neural network models; most of them can be viewed as a straightforward application of optimization theory and statistical estimation. Most of the algorithms used in training artificial neural networks are employing some form of gradient descent. This is done by simply taking the derivative of the cost function with respect to the network parameters and then changing those parameters in a gradient-related direction. The most popular of them is the back propagation algorithm, which has different variants. Standard back propagation is a gradient descent algorithm. It is very difficult to know which training algorithm will be the fastest for a given

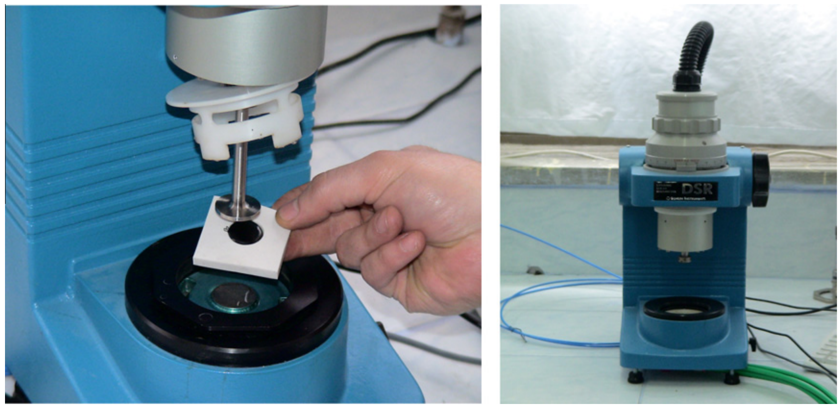

Fig. 2. DSR test machine.

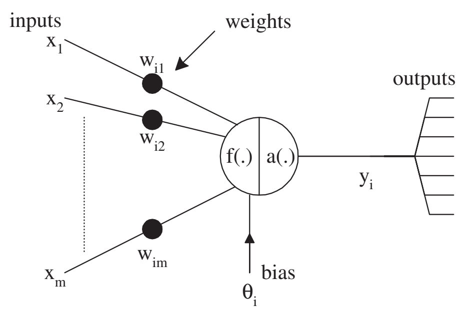

Fig. 3. Artificial neuron model.

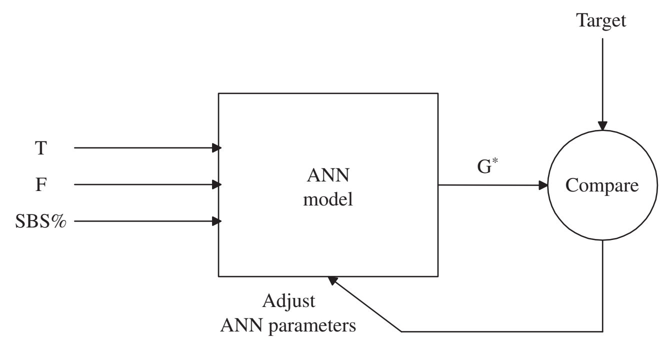

Fig. 4. Proposed model block diagram.

problem, and the best one is usually chosen by trial and error. An ANN with a back propagation algorithm learns by changing the connection weights, and these changes are stored as knowledge.

4.1. Modeling of base and SBS modified bitumen using ANN

There are many types of ANN architectures in the literature; however, multi-layer feed-forward neural network is the most widely used for prediction (Esen, Inalli, Sengur, & Esen, 2008a). A multi-layer feed-forward neural network typically has an input layer, an output layer, and one or more hidden layers (Esen, Inalli, Sengur, & Esen, 2008b). In these networks, neurons are arranged in layers and there is a connection among the neurons of other layers. The input signals are applied to the input layer, the output layer directly contributes to the output signal. The layers between input and output layers are defined as hidden layers. Input signals are propagated in gradually modified form in the forward direction, finally reaching the output layer (Palau, Velo, & Puigjaner, 1999).

In this study, the temperature of the bitumen (*T*), frequency (*F*) and SBS content are the parameters chosen as the input layer and complex modulus of bitumen (G^*) as the output layer. The related illustration is given in Fig. 4. The back propagation learning algorithm has been performed in a feed forward, single hidden layer neural network. The variants of the algorithm used in the study are the Levenberg–Marquardt (LM), scaled conjugate gradient (SCG) and Pola-Ribiere conjugate gradient (CGP) algorithms. A tangent sigmoid transfer function has been utilized for both the hidden layer and the output layer.

In training, several number of neurons (2, 3, 4, and 5) were applied in the hidden layer to define the output accurately. The data set for the G^* of system consisted of 192 data patterns.

The efficiency of the proposed method was demonstrated by using the 5-fold cross validation test. In 5-fold cross validation test, the data set is randomly split into five exclusive subsets ($X_i, \ldots X_5$) of approximately equal size and the holdout method is repeated 5 times. Four folds contain 38 samples and the last fold contains 40 samples. At each time, one of the five subsets is used as the test set and the other four subsets are put together to form a training set. The advantage of this method is that it is not important how the data is divided. Every data point appears in a test set only once, and appears in a training set two times. Therefore, the verification of the efficiency of the proposed method against to the over-learning problem should be demonstrated.

Model validation is the utilization of the test data in trained network to see the prediction capability by comparing the output and target pairs. The statistical parameters, such as the root-mean squared (RMS), the coefficient of multiple determinations (R^2) and the coefficient of variation (cov) may be used to compare predicted and measured (target) values for model validation.

The error estimated by the RMS is defined by the following equation:

$$\mathrm{RMS} = \sqrt{\left[\sum_{m=1}^{n}(y_{pre,m} - t_{mea,m})^2\right] \Big/ n} \tag{2}$$

In addition, the coefficient of multiple determinations (R^2) and the coefficient of variation (cov) in percent are defined as follows:

$$R^2 = 1 - \left[\sum_{m=1}^{n}(y_{pre,m} - t_{mea,m})^2\right] \Big/ \left[\sum_{m=1}^{n}(t_{mea,m})^2\right] \tag{3}$$

$$\mathrm{cov} = (RMS/|\bar{t}_{mea,m}|) \cdot 100 \tag{4}$$

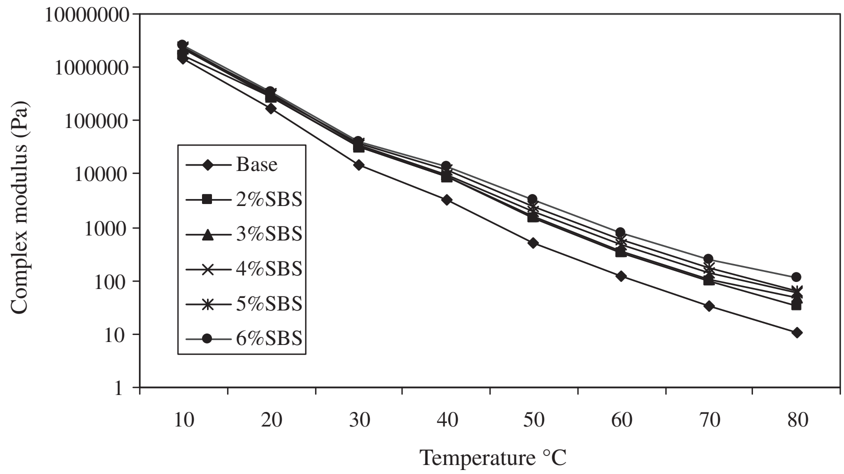

Fig. 5. Variations on complex modulus at 0.1 Hz.

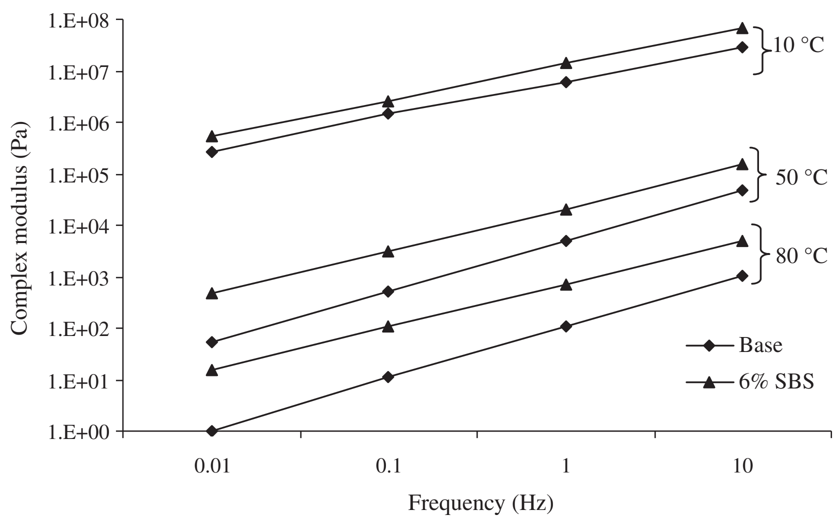

Fig. 6. Variation on complex modulus versus frequency.

where n is the number of data patterns in the independent data set, $y_{pre,m}$ indicates the predicted values, $t_{mea,m}$ is the target value of one data point m, and $\bar{t}_{mea,m}$ is the mean value of all target data points.

5. Results and discussions

5.1. Dynamic mechanical analysis test results

The variations on complex modulus versus temperature and SBS content at 0.1 Hz is presented in Fig. 5. It is seen that the complex modulus decreases significantly with the increase in temperature. The complex modulus of the PMB samples is greater than the complex modulus of base bitumen as depicted in Fig. 5. Besides, for the same level of temperature, the complex modulus increases with increase in SBS content.

The variation of complex modulus of the base and 6% SBS polymer modified bitumens with frequency and temperature are presented in Fig. 6.

As depicted in Fig. 6, which are drawn in log–log scale, for base and SBS PMB samples as the frequency increases, the complex modulus increases as well. This is due to the rheologic behavior of the bitumens since bitumens under shorter loading time exhibit elastic behavior. Besides, for the same frequency level, the increase in temperature decreases the complex modulus as presented in Fig. 6. This also indicates that, the temperature has a significant effect on the level of complex modulus.

5.2. Artificial neural networks model results

The computer program was performed on MATLAB (version 5.3. The MathWorks Inc., USA) environment by using the neural network toolbox. At first the data set is normalized within the range [0, 1] through the following transformation formula:

$$u_{nar} = \frac{u}{\vec{1}_N\left(\sqrt{diag(u^T u)}\right)^T} \tag{5}$$

where u are the input or output data set. $\vec{1}_N = [111\ldots1]^T$ is an N-dimensional vector. N represents number of patterns in the input or output set. $diag$ is diagonal values of the square matrix $(u^T u)$.

ANN topologies with various number of hidden layer neurons are then trained. An example of the training performance of the ANN for LM-2 topology (ANN type with LM algorithm including

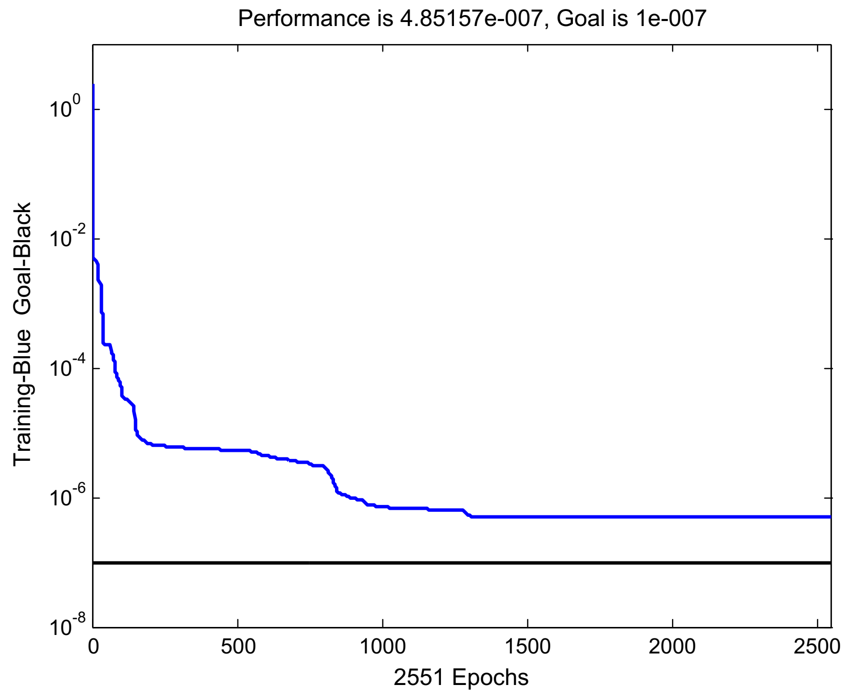

Fig. 7. The training performance of the ANN (LM-2 topology).

two hidden neurons) is given in Fig. 7 where the variation of mean-square error with training epochs is illustrated.

Fig. 8 presents the comparison of calculated and ANN predicted G^* values of modelling system for LM-2.

The ANN topologies with various number of hidden layer neurons are trained with the statistical weighting pre-processed inputs. The related test results (RMS, cov and R^2) are represented in Table 2.

As seen in Table 2, the training accuracy is improved by decreasing the number of hidden neurons as indicated by the smaller RMS and cov values and R^2-values approaching 1. On the other hand, beyond a certain number of hidden layers the obtained errors begin to increase together with the complexity of the ANN. Besides, the convergence to the target error rate (1e-007) takes more iteration which is very time consuming.

Based on the statistical data presented in Table 2, the LM algorithm gained promising results compared to SCG and CGP algorithms and among the LM algorithms, the LM-2 algorithm appeared to be most optimal topology. This topology gained 0.0039 mean RMS value, 20.24 mean cov value and, 0.9970 mean R^2 value, respectively.

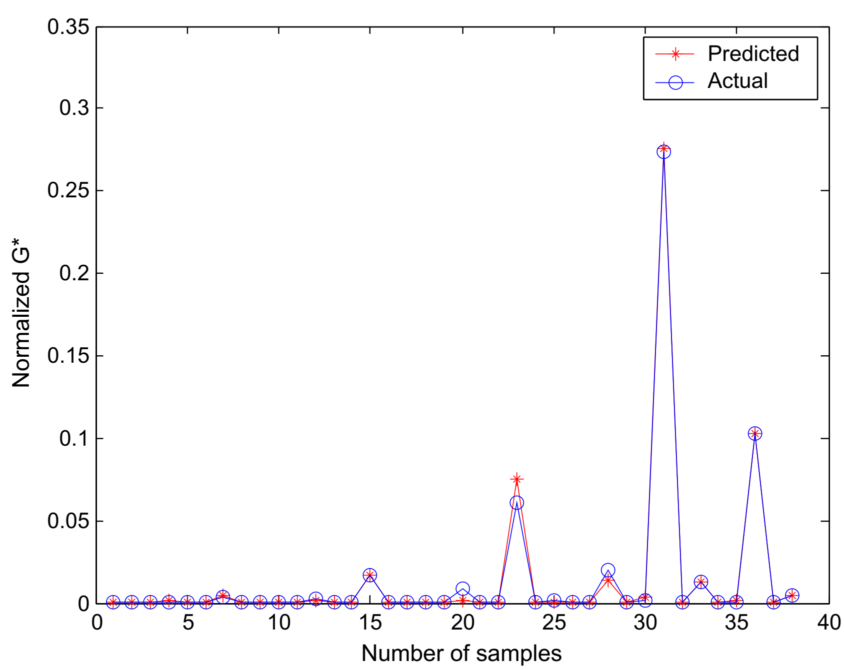

Fig. 8. The comparison of actual and ANN (LM-2 topology) predicted G^*.

Table 2
Statistical values of ANN model.

Algorithm-neurons	RMS					Cov					R^2					Mean values		
	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	RMS	Cov	R^2
LM-2	0.0041	0.0034	0.0021	0.0034	0.0067	19.85	19.47	14.79	20.21	26.89	0.9975	0.9968	0.9983	0.9974	0.9950	**0.0039**	**20.24**	**0.9970**
LM-3	0.0053	0.0053	0.0031	0.0048	0.0057	25.33	30.65	21.39	28.83	22.63	0.9960	0.9921	0.9965	0.9946	0.9962	0.0048	25.76	0.9951
LM-4	0.0062	0.0062	0.0061	0.0051	0.0091	28.32	36.48	47.16	29.77	37.90	0.9947	0.9899	0.9812	0.9942	0.9896	0.0065	35.92	0.9899
LM-5	0.0107	0.0111	0.0046	0.0072	0.0048	47.72	59.09	32.39	44.37	19.01	0.9855	0.9705	0.9912	0.9874	0.9973	0.0077	40.51	0.9864
SCG-2	0.0048	0.0078	0.0048	0.0040	0.0068	26.81	39.94	32.78	23.56	26.97	0.9938	0.9907	0.9916	0.9965	0.9951	0.0056	30.01	0.9935
SCG-3	0.0053	0.0060	0.0056	0.0048	0.0089	29.67	29.26	41.39	29.37	34.95	0.9928	0.9948	0.9859	0.9932	0.9920	0.0061	32.92	0.9917
SCG-4	0.0052	0.0085	0.0057	0.0054	0.0075	30.84	42.79	43.8	32.15	29.35	0.9923	0.9897	0.9857	0.9946	0.9940	0.0065	35.78	0.9913
SCG-5	0.0073	0.0087	0.0049	0.0061	0.0107	38.82	46.60	36.29	38.25	44.57	0.9861	0.9880	0.9893	0.9911	0.9867	0.0075	40.90	0.9882
CGP-2	0.0160	0.0099	0.0062	0.0164	0.0131	68.81	48.61	45.36	98.24	51.25	0.9595	0.9848	0.9830	0.9350	0.9803	0.0123	62.45	0.9685
CGP-3	0.0159	0.0127	0.0130	0.0082	0.0154	86.44	68.68	88.86	47.83	63.96	0.9331	0.9729	0.9152	0.9851	0.9657	0.0130	71.15	0.9544
CGP-4	0.0151	0.0148	0.0109	0.0141	0.0143	90.34	76.34	74.85	76.43	49.76	0.9259	0.9595	0.9480	0.9604	0.9832	0.0138	73.54	0.9554
CGP-5	0.0179	0.0120	0.0066	0.0178	0.0239	97.04	57.56	44.26	112.85	109.28	0.9101	0.9795	0.9836	0.9281	0.9257	0.0156	84.19	0.9454

6. Conclusion

The estimation of damage accumulation over the service life of the new pavement is based on empirical rutting and cracking performance equations, which require the complex modulus as an input parameter. The complex modulus is dependent upon temperature and loading frequency, and thus allows for a more accurate representation of traffic load effects on pavements. In the light of the findings from laboratory experiments, it is possible to consider that SBS polymer modification increases the complex modulus of the base bitumen. Besides, the complex modulus decreases significantly with the increase in temperature and decrease in frequency.

The Levenberg–Marquardt (LM), scaled conjugate gradient (SCG) and Pola-Ribiere conjugate gradient (CGP) are the algorithms used to model the G^* of the base and SBS PMB. Among them LM algorithm appeared to be most optimal topology.

Based on the results of the study, it can be concluded that both artificial neural networks method and statistical methods can be used for modelling and predicting the complex modulus of bitumen under varying temperature and frequency with high accuracy. Results also indicate that ANN is an excellent method that can reduce the time consumed and can be used as an important tool in evaluating the factors affecting complex modulus of asphalt mixture at the design stage.

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