Neural network modeling of SBS modified bitumen produced with different methods

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HIGHLIGHTS

► Mixing polymers into bitumen has important consequences on the engineering properties.
► Structural changes may be observed during processing of polymer-modified bitumens.
► Complex modulus determination of PMBs is important to select the performance grade.
► With the increase of experimental factors experimental trials increases exponentially.
► Complex modulus predicted accurately with the developed ANN model.

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ABSTRACT

Various types of polymers are added to bitumen in order to improve its properties under low and high temperatures. It is important to determine accurately the complex modulus of polymer-modified bitumen samples (PMBs) in order to make a suitable mix design. Moreover the determination of the complex modulus is important in order to evaluate the efficiency of the additives. However the manufacture processes of PMBs involve many factors. This study aims to model the complex modulus of styrene–butadiene–styrene (SBS) modified bitumen samples that were produced by different methods using artificial neural networks (ANNs). PMB samples were produced by mixing a 160/220 penetration grade base bitumen with 4% SBS Kraton D1101 copolymer at 18 different combinations of three mixing temperatures, three mixing times and two mixing rates. The complex modulus of PMBs was determined at five different test temperatures and at ten different frequencies. Therefore a total of 900 combinations were evaluated. Various different results were obtained for the same PMB produced at different conditions. In the ANN model, the mixing temperature, rate and time as well as the test temperature and frequency were the parameters for the input layer whereas the complex modulus was the parameter for the output layer. The most suitable algorithm and the number of neurons in the hidden layer were determined as Levenberg–Marguardt with 3 neurons. It was concluded that, ANNs could be used as an accurate method for the prediction of the complex modulus of PMBs, which were produced using different methods.

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1. Introduction

Various types of additives are added to bitumen in order to improve the low and high temperature properties. 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 [1]. SBS block copolymers are classified as elastomers that increase the elasticity of bitumen and they are probably the most appropriate polymers for bitumen modification by improving the temperature susceptibility of binder [2–4].

Mixing polymers into bitumen has important consequences on the engineering properties of bituminous binders. Thus, structural and chemical changes may be observed during processing of polymer-modified bitumens. Chemical compatibility and processing conditions are crucial to obtain suitable properties. Most polymers occur to be insoluble, in some degree, in the bitumen matrix, and phase separation may result. Lepe et al. tried different mixing rates such as 1200 rpm and 8200 rpm to produce polymer modified bitumen and concluded that a high energy mixing process is always necessary to stabilize and disperse a polymer

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in polymer-modified binders. However this process was mentioned to changes in the rheological response of such materials as a consequence of bituminous components oxidation [5]. Giuliani et al. used 180 °C and 4000 rpm mixing procedure for producing the eight different polymer modified bitumen [6]. Ouyang et al. used 170 °C, 25 min mixing time and 4000 rpm mixing rate for SBS modification [7]. Moillet et al. prepared the SBS and EVA modified binders at 180 °C, 2 h mixing time and 300 rpm mixing time [8]. Larsen et al. blended two SBS copolymers which differ in weight average molecular weight and two base asphalts with different asphalten contents under different experimental conditions. They used 4200 rpm and 5800 rpm mixing rate with different mixing times and observed important changes in rheological properties of bitumen [9]. Haddadi et al. denoted that bitumen-polymer mixing temperature and bitumen-polymer mixing time play a crucial role in determining the performance of polymer-modified asphalt concrete. They used 180 °C, 300 rpm mixing procedure for preparing the EVA modified binder. Since it was observed that the penetration decreases by increasing the mixing time to reach a constant value after 4 h duration whereas softening point increases then stabilizes after 4 h duration, they selected 4 h mixing time in this research [10]. Yılmaz and Kok used 170 °C, 500 rpm and 1.5 h mixing procedure in the study of determining the high temperature performance grade of SBS modified binders [11]. Navarro et al. modified the bitumen with different SBS contents at different mixing time and temperatures. They concluded that under severe processing conditions (180 °C and 1200 rpm) and low polymer concentration, the polymer influence is dampened and the glassy region appears at higher temperatures or lower frequencies. It was reported that at high polymer concentration, a phase inversion could be induced by processing 180 °C and 1200 rpm. [12].

In recent years, limited number of studies has been concentrated on artificial neural networks and bitumen. Ozsahin and Oruc 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 [13]. Far et al. 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 [14]. The statistical analysis and artificial neural networks were used 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 [15]. It was reported that the ANN model gives satisfactory results for estimating the deflection of pavement according to layer thickness [16].

It is very important to determine accurately the complex modulus of PMBs in order to select the high temperature performance grade. Moreover complex modulus determination is important to evaluate the efficiency of additives. However, the number of parameters such as mixing time, mixing rate and mixing temperature during the manufacture processes of polymer modified bitumen and test temperatures and frequencies during the determination of complex modulus and also the variables of these parameters are so much. With the increase of experimental factors, the number of experimental trials increases exponentially. In this study an ANN model was developed to determine complex modulus of PMBs produced with different methods to overcome this problem by carried out a serious of experiment including 900 patterns.

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 rheometer (DSR). 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. 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 [17].

The DSR test was performed on SBS modified bitumen prepared with different methods by using a Bohlin DSRII rheometer. The test was performed under controlled-stress loading conditions using frequency sweeps between 0.1 and 1 Hz at temperature between 40 and 80 °C. The tests were carried out with 25 mm diameter, 1 mm gap geometry. The stress amplitude for all the tests was confined within the linear viscoelastic response of the bitumen.

3. Materials and sample preparation

The base bitumen with a 160/220 penetration grade was procured from TUPRAS Oil Terminal of the Turkish Petroleum Refinery Corporation.

The SBS polymer used was Kraton D-1101 supplied by the Shell Chemicals Company. Kraton D-1101 is a linear SBS polymer in powder form that consists of different combinations made from blocks polystyrene (31%) and polybutadiene of a very precise molecular weight [18]. These blocks are either sequentially polymerized from styrene and butadiene and/or coupled to produce a mixture of these chained blocks.

Since 4% SBS content by weight of bitumen has been widely used in the application, this value was selected as a constant percentage in this study. The SBS modified bitumens were prepared by considering two different mixing rate such as 500 rpm and 1000 rpm, three different mixing time such as 30, 60 and 120 min, three different mixing temperature such as 170 °C, 180 °C and 190 °C. Thus 18 different combinations were evaluated. The PMBs were produced with a laboratory-scale mixing device (Fig. 1a) with a four-blade impeller (IKA) Fig. 1b.

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. 2.

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 [19].
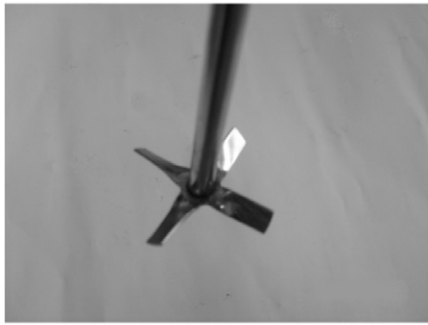
The output of the neuron net is given by:

$$y(t+1) = a\left(\sum_{j=1}^{n} w_{ij}x_j(t) - \theta_i\right)$$

$$f_i\Delta net_i = \sum_{j=1}^{m} w_{ij}x_j - \theta_i \quad (1)$$

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 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 SBS modified bitumen prepared with different methods 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. A multi-layer feed-forward neural network typically has an input layer, an output layer, and one or more hidden layers. The proposed ANN structure for estimating the complex modulus is given in Fig. 3. In input layer, there are mixing temperature, mixing time, mixing rate, test temperature and test frequency. In the output layer, there is complex modulus.

As it was mentioned before, an ANN model is proposed to determine complex modulus of PMBs produced with different methods including 900 patterns. Some statistical methods, such as the root-mean square (RMS), the coefficient of multiple determinations (R^2) and the coefficient of variation (COV) can be used to compare the predicted and actual values.

$$RMS = \sqrt{\frac{\sum_{i=1}^{n}(y_i^{pre} - y_i^{mea})^2}{n}} \tag{2}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i^{pre} - y_i^{mea})^2}{\sum_{i=1}^{n}(y_i^{mea})^2} \tag{3}$$

$$COV = \frac{RMS}{|t_i^{mea} -|} \times 100 \tag{4}$$

where n is the number of data patterns in the independent data set, y_i^{pre} indicates the predicted, y_i^{mea} is the measured value of one data point m, and $t_i^{mea} -$ is the mean value of all measured data points.

In multi-layer feed-forward 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 contributes to the output signal directly. Other layers between input and output layers are called hidden layers. The back propagation-learning algorithm has been used 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
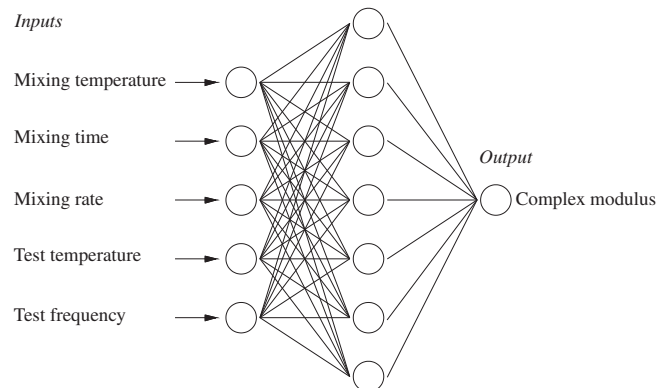

Fig. 1. Laboratory-scale mixing device (a) and four-blade impeller (b).

Fig. 2. Artificial neuron model.

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

Fig. 3. The ANN structure of the complex modulus estimation system.
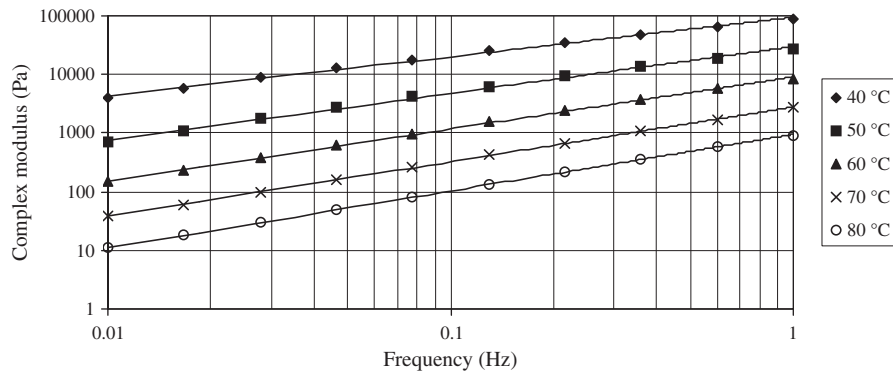
Fig. 4. The effects of temperature and frequency on complex modulus.

gradient (SCG) and Pola–Ribiere conjugate gradient (CGP) algorithms. In the training phase, a variable number of neurons 3, 5, and 7 were used in the hidden layer to define the output accurately. The data set included 900 data patterns. From these, 600 data patterns were used for training the network, and the remaining 300 patterns were randomly selected and used as the test data set.

5. Results and discussion

5.1. Dynamic mechanical analysis test results

In this study two groups of variables were evaluated to determine the complex modulus of SBS modified binder. The former is related to DSR test conditions and the latter is related to polymer modified bitumen manufacturing conditions. DSR test conditions include test temperature and frequency. These factors affect significantly the complex modulus of bitumen as it depicted in Fig. 4. This figure represent the complex modulus results of PMB prepared at 170 °C, 500 rpm and 30 min. Figure shows the variation on complex modulus versus frequency at different test temperatures. It was observed that the complex modulus increased with the increase in frequency and this was due to the rheological behavior of the bitumen samples since bitumen samples exhibit elastic behavior under shorter loading periods. Besides, for the same frequency level, the increase in temperature caused a decrease in the complex modulus number. However the effect of frequency was greater than that of the temperature.

Polymer modified bitumen manufacturing conditions include mixing temperature, mixing rate and mixing time. Fig. 5 shows

how these factors affect the complex modulus of PMBs. The complex modulus in Fig. 5 were taken from the master curves which was constructed from the data like in Fig. 4 for all manufacturing conditions using a time temperature superposition procedure. In this process the data sets for all test temperatures are combined to produce a single composite curve at a single reference temperature, which was selected as 50 °C in this study. Thus the effects of manufacturing conditions on complex modulus can be assessed from Fig. 5 for 0.1 Hz by considering a single test temperature. It is seen from the figure that the mixing temperature has a slight effect on complex modulus. An increment of 10 °C increased the complex modulus a maximum of 1.2 times among the PMBs that were prepared at the same mixing time and rate. There is no significant effect that was observed between the 30-min and 60-min mixing times. However the complex moduli of PMBs that were prepared at the 120 min mixing time were much greater than those that were prepared at 30 and 60-min mixing times at a constant rate of mixing. The complex modulus of the PMBs that were prepared at 500 rpm for a 60 min mixing time was at most 1 times greater than that, which was prepared at 500 rpm for 30 min for all mixing temperatures. However the complex moduli of the samples that were prepared at 500 rpm for 120 min were 1.34, 1.31 and 1.18 times greater than those that were prepared at 500 rpm for 30 min at 170 °C 180 °C and 190 °C, respectively. The effect of mixing rate became apparent distinctly at high mixing times and temperatures, while it was not so effective at low mixing times and temperatures. The complex modulus at the conditions of 1000 rpm, 30 min and 190 °C was only 5% greater than that at 500 rpm, 30 min and 190 °C. However the complex modulus at 1000 rpm, 120 min and 190 °C was 1.2 times greater than that at 500 rpm, 30 min and 190 °C.
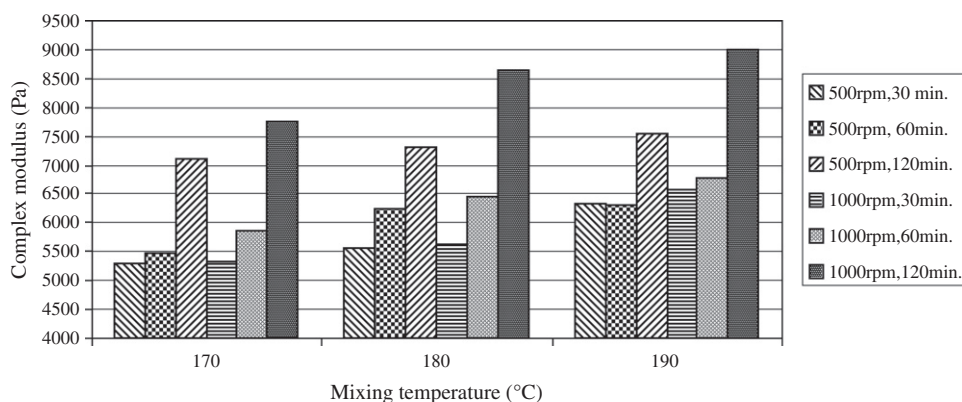

Fig. 5. Effects of mixing conditions on complex modulus.

Table 1
Statistical parameters for various ANN structures.

	R^2	RMS	COV
LM-3	0.9961	0.0066	13.6807
LM-5	0.9931	0.0086	17.9946
LM-7	0.9916	0.0097	20.0909
SCG-3	0.9293	0.0269	56.6680
SCG-5	0.9605	0.0203	42.1943
SCG-7	0.9721	0.0174	36.7023
CGF-3	0.8365	0.0374	80.2529
CGF-5	0.8600	0.0396	80.8972
CGF-7	0.9349	0.0273	55.7323

5.2. ANN model results

In order to achieve the optimal result, different algorithms and different numbers of hidden neurons were used. Statistical values such as root-mean squared (RMS), fraction of variance (R^2) and coefficient of variation (COV) are given in Table 1.

As seen in Table 1, 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−005) takes more
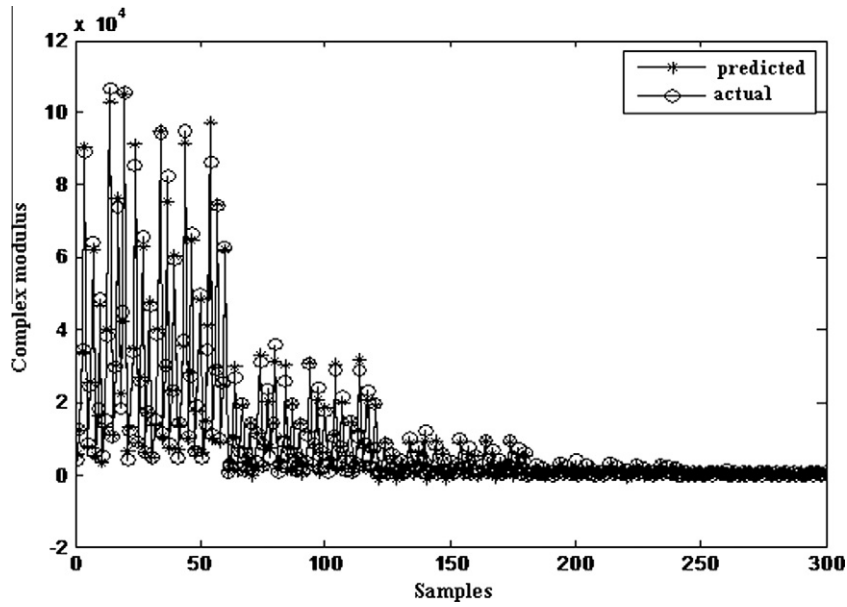

Fig. 6. Comparison of actual and ANN predicted values for LM-3 structure.
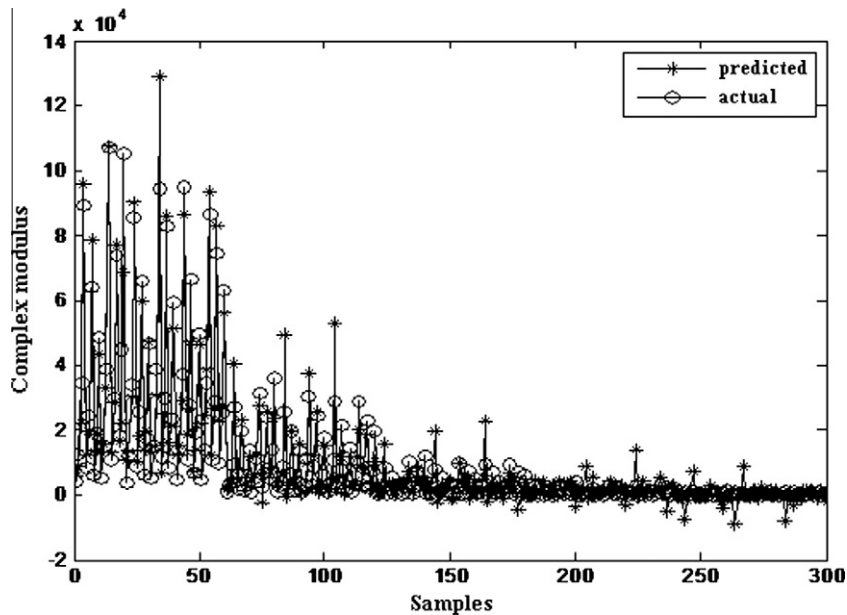

Fig. 7. Comparison of actual and ANN predicted values for CGF-5 structure.

iteration which is very time consuming. Based on the statistical data presented in Table 1, the LM algorithm gained promising results compared to SCG and CGP algorithms and among the LM algorithms, the LM-3 algorithm appeared to be most optimal topology. This topology gained 0.0066 mean RMS value, 13.68 mean COV value and, 0.9961 mean R^2 value, respectively.

The prediction comparison with the actual complex modulus of LM-3 based ANN structures, which is gained the best results, was given in Fig. 6. The worst topologies belong to CGF-5 were given in Fig. 7.

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. However the manufacturing processes of PMBs significantly affect its rheological properties. In this study the mixing temperature, time and the rate during the manufacturing process of PMBs and also the test temperatures and the frequency for determining the complex modulus were evaluated. It was determined that the complex modulus increased with the increase in frequency. Additionally the increase in temperature decreased the complex modulus at the same frequency level. However the effect of frequency was greater than that of the temperature.

It was observed that the mixing temperature during the manufacturing processes of PMBs had a slight effect on the complex modulus. There was no significant effect, which was observed between the 30-min and 60-min mixing periods while the 120 min mixing time had a large effect on the complex modulus. The effect of mixing rate was apparent distinctly at high mixing times and temperatures. The highest complex modulus was obtained at 190 °C, 120 min of mixing time and 1000 rpm rate of mixing conditions. This set of conditions would cause either good polymerization or increased viscosity due to oxidation under these manufacturing conditions.

Experimental results showed that the ANN could be used as an alternative way in these systems. Three algorithms (LM, SCG, and CGP) were tested and the best algorithm was determined as the LM algorithm in this application. The R^2 values in the three algorithms were about 0.90, which could be considered as very satisfactory. The most suitable neuron number in the hidden layer was determined as 3 neurons. For this level number in training, it the root-mean squared (RMS) value was determined as 0.0066, the absolute fraction of variance (R^2) value was determined as 99.61% and the coefficient of variation in percent (COV) value was determined as 13.68%. This study showed that the values that were predicted using the ANN, especially using the back propaga-tion learning algorithm along with feed forward, could be utilized in order to predict of the complex modulus of PMBs that were produced using different methods accurately.

Inherent bitumen properties can be considered as independent variables in determining the complex modulus for further studies.

References

[1] Airey GD. Styrene butadiene styrene polymer modification of road bitumens. J Mater Sci 2004;99:951–99.
[2] Valtorta D, Poulikakos LD, Partl MN, Mazza E. Rheological properties of polymer modified bitumen from long-term field tests. Fuel 2007;86:938–48.
[3] Wen G, Zhang Y, Sun K, Fan Y. Rheological characterization of storage-stable SBS-modified asphalts. Polym Test 2002;21:295–302.
[4] Wu S, Pang L, Mo L, Chen Y, Zhu G. Influence of aging on the evolution of structure, morphology and rheology of base and SBS modified bitumen. Constr Build Mater 2009;23:1005–10.
[5] Lepe AP, Boza FJM, Gallegos C, Gonzalez O, Munoz ME, Santamari A. Influence of the processing conditions on the rheological behaviour of polymer-modified bitumen. Fuel 2003;82:1339–48.
[6] Giuliani F, Merusi F, Filippi S, Biondi D, Finocchiaro ML, Polacco G. Effects of polymer modification on the fuel resistance of asphalt binders. Fuel 2009;88(9):1539–46.
[7] Ouyang C, Wang Y, Zhang Yinxi. Preparation and properties of styrene–butadiene–styrene copolymer/kaolinite clay compound and asphalt modified with the compound. Polym Degrad Stabil 2005;87:309–17.
[8] Mouillet V, Lamontagne J, Durrieu F, Planche JP, Lapalu L. Infrared microscopy investigation of oxidation and phase evolution in bitumen modified with polymers. Fuel 2008;87:1270–80.
[9] Larsen DO, Alessandrini JL, Bosch A, Cortizo MS. Micro-structural and rheological characteristics of SBS-asphalt blends during their manufacturing. Constr Build Mater 2009;23:2769–74.
[10] Haddadi S, Ghorbel E, Laradi N. Effects of the manufacturing process on the performances of the bituminous binders modified with EVA. Constr Build Mater 2008;22:1212–9.
[11] Yılmaz M, Kok BV. Stiren–butadien–stiren modifiyeli bitümlü bağlayicilarin superpeve sistemine göre yüksek sicaklik performans seviyesinin ve işlenebilirliliğinin belirlmesi. Gazi Ünv. Müh. Mim. Fak. Der. 2008;23(4):811–9.
[12] Navarro FJ, Partal P, Boza FM, Gallegos C. Effect of composition and processing on the linear viscoelasticity of synthetic binders. Eur Polym J 2005;41:1429–38.
[13] Ozsahin TS, Oruc S. Neural network model for resilient modulus of emulsified asphalt mixtures. Constr Build Mater 2008;22:1436–45.
[14] Far S, Sadat M, Shane UB, Richard KY. Application of artificial neural networks for estimating dynamic modulus of asphalt concrete. Transportation Research Board Annual Meeting; 2009. p. 3799.
[15] Specht LP, Khatchatourian O, Brito LAT, Ceratti JAP. Modeling of asphalt-rubber rotational viscosity by statistical analysis and neural networks. Int J Mater Res 2007;10(1):69–74.
[16] Saltan M, Terzi S. Modeling deflection basin using artificial neural networks with cross-validation technique in backcalculating flexible pavement layer moduli. Adv Eng Softw 2008;39:588–92.
[17] Airey GD. Rheological properties of styrene butadiene styrene polymer modified road bitumens. Fuel 2003;82:1709–19.
[18] Preparing Blends of Kraton D Polymers and Bitumen. Shell Technical, Bulletin; 1995.
[19] Esen H, Inalli M, Sengur A, Esen M. Performance prediction of a ground-coupled heat pump system using artificial neural networks. Expert Syst Appl 2008;35(4):1940–8.