# Genetic Programming to Formulate Viscoelastic Behavior of Modified Asphalt Binder

Alireza Sadat Hosseini[a], Pouria Hajikarimi[b], Mostafa Gandomi[a], Fereidoon Moghadas Nejad[b],
and Amir H. Gandomi[c,*]

[a]School of Civil Engineering, College of Engineering, University of Tehran, Tehran, Iran, E-mail: {a.sadat, mostafa.gandomi}@ut.ac.ir

[b]Department of Civil & Environmental Engineering, Amirkabir University of Technology (Tehran Polytechnic), Tehran, Iran, E-mail: {phajikarimi, moghadas}@aut.ac.ir

[c]Faculty of Engineering & Information Technology, University of Technology Sydney, Sydney, Australia, E-mail: gandomi@uts.edu.au

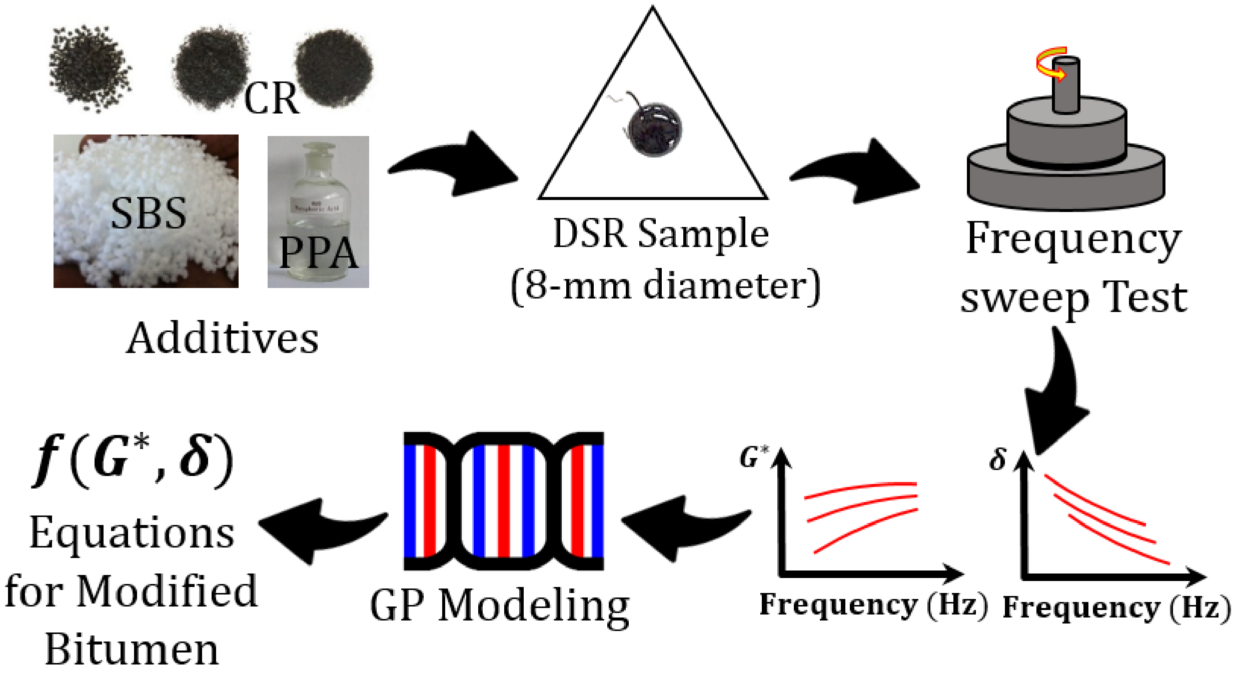
# Genetic Programming to Formulate Viscoelastic Behavior of Modified Asphalt Binder

## Abstract

The objective of this research was to develop prediction models for complex shear modulus (G*) and phase angle (δ) of bitumens modified with crumb rubber, styrene-butadiene styrene, and polyphosphoric acid at low and moderate temperatures. The experiments consisted of three different dosages of each modifier added to the original bitumen followed by measurement of G* and δ of the original and modified bitumen using the dynamic shear rheometer (DSR) test in frequency sweep mode (21 loading frequencies from 0.1 to 100 Hz) at seven test temperatures: -22, -16, -10, 0, 10, 16 and 22°C. Having the experimental database, a robust genetic programming (GP) method was used to develop an individual prediction model for each modifier based on temperature, loading frequency, the G* and δ of the original bitumen, and the dosage of the modifier. Results showed that GP successfully developed accurate and meaningful expressions for calculating G* and δ of the modified bitumen as two main constitutive components of the viscoelastic behavior of bituminous composites. Then, a parametric study and sensitivity analysis were performed on the developed models to better understand the effect of variables on the trend of the models. The modifier dosage is the most effective input variable of the model and the amount of G* and δ of the original bitumen accurately reflect the effect of temperature and loading frequency on viscoelastic behavior of the modified bitumen, as they behave linearly at the considered test temperatures.

**Keywords:** Genetic Programming, Modified Asphalt, Viscoelastic, Crumb rubber, SBS, PPA

## Graphical abstract



## 1. Introduction

Modification of original bitumen is a well-known method for improving its rheological and mechanical properties in order to meet the standard criteria and for increasing the life span of asphalt pavement. There are several additives used to enhance the low-, moderate-, and high-temperature performance of original bitumen, which can be selected based on climate conditions and dominant distress. Numerous previous publications investigated the effect of such additives on mechanical behavior, durability, and workability characteristics of original bitumen [1][2][3]. One of the major concerns regarding bitumen that is modified with different dosages of additives is precisely predicting its viscoelastic characteristics at the desired loading frequency, temperature, and additive concentration. Experimental and numerical modeling were used for this purpose, which assumed a simple thermo-rheological behavior of the original and modified bitumen.

Although such an assumption can work for relating time and temperature based on the time-temperature superposition principle (TTSP), it is difficult for these equations to account for additive dosage. Therefore, prediction models such as GP can be used to intelligently predict the viscoelastic behavior of modified bitumen that has additional dosage and viscoelastic characteristics relative to the original bitumen.

GP, which in general is defined as a specialization of genetic algorithm (GA), is a powerful method for optimizing complex problems and uses computer-based programs instead of binary strings to solve problems [4]. GP has an inherent superiority over conventional mathematical and statistical approaches and black-box algorithms such as ANN, which is the ability of GP to produce explicit equations without using initial prediction models that present the relation between the involved parameters. This ability can be easily implemented in the practical design of modified asphalt binders. A recent extension of GP is gene expression programming (GEP), which was proposed by Ferreira [5]. Computer programs of different sizes and shapes are encoded in linear chromosomes of fixed length and comprise the GEP solutions. In order to predict the complex relationships between inputs and outputs of a data source, researchers presented methodologies for using GP to generate prediction formulae for engineering problems [6].

Gholampour et al. [7] applied the GEP technique on a large test database to develop formulae with a wide range of applicability for predicting the mechanical properties of recycled aggregate concrete. To predict the dynamic modulus, which is one of the most important mechanical property parameters of asphalt concrete, Liu et. al [8] explored two different GEP approach models for hot mix asphalt (HMA) and mixtures containing recycled asphalt shingles. The GEP approach was implemented in order to develop a prediction model of density and viscosity of bitumen [9]. Results of the presented model were compared with traditional empirical models in order to investigate its performance. To predict fracture energy of asphalt concrete specimens, Majidifard et al. used GEP and hybrid artificial neural network/simulated annealing (ANN/SA) by implementing an experimental database containing results of disk-shaped compact tension (DC(T)) tests. More recently, fatigue life prediction of hot mix asphalt (HMA) was formulated using GP [10]. Although several research works used artificial neural network models to predict the rheological and mechanical characteristics of modified bitumens with different types of additives [11][12][13], the GEP has not been used for relating the percentage of additive and other effective parameters to the desired properties of modified bitumen as a closed form equation. Since the mechanism of the effect that different additives have on original bitumen varies regarding the type of its interaction (physical/chemical), intrinsic properties of the original bitumen, and testing conditions, particular equations for each type of additive must be derived. It is well-known that the original and modified bitumen behave as viscoelastic materials in which their characteristics depend on time, temperature, and loading rate. Therefore, an appropriate simple closed form equation should include constitutive properties of the original bitumen, the percentage of additives, and testing conditions to predict the rheological and mechanical characteristics of modified bitumen.

In this study, three different prevalent types of additives were selected and were used to modify the original bitumen, which included crumb rubber, styrene-butadiene-styrene (SBS), and polyphosphoric acid (PPA). Each modifier was added to the original bitumen at three different dosages: 10, 15, and 20 wt.% for crumb rubber, 2, 4, and 6 wt.% for SBS, and 0.5, 1, and 1.5 wt.% for PPA. Then, two constitutive viscoelastic parameters (complex shear modulus ($G^*$) and phase angle ($\delta$)) were measured by performing a frequency sweep test at seven different test temperatures: -22, -16, -10, 0, 10, 16, and 22°C. The purpose of this study is to use the GEP technique to predict G* and δ of modified bitumen based on these parameters measured for the original bitumen. Such a model will make it possible to find the optimum dosage of each additive in order to achieve the desired viscoelastic properties at low and moderate temperatures. In summary, Figure 1 illustrates the flow of work in this study.

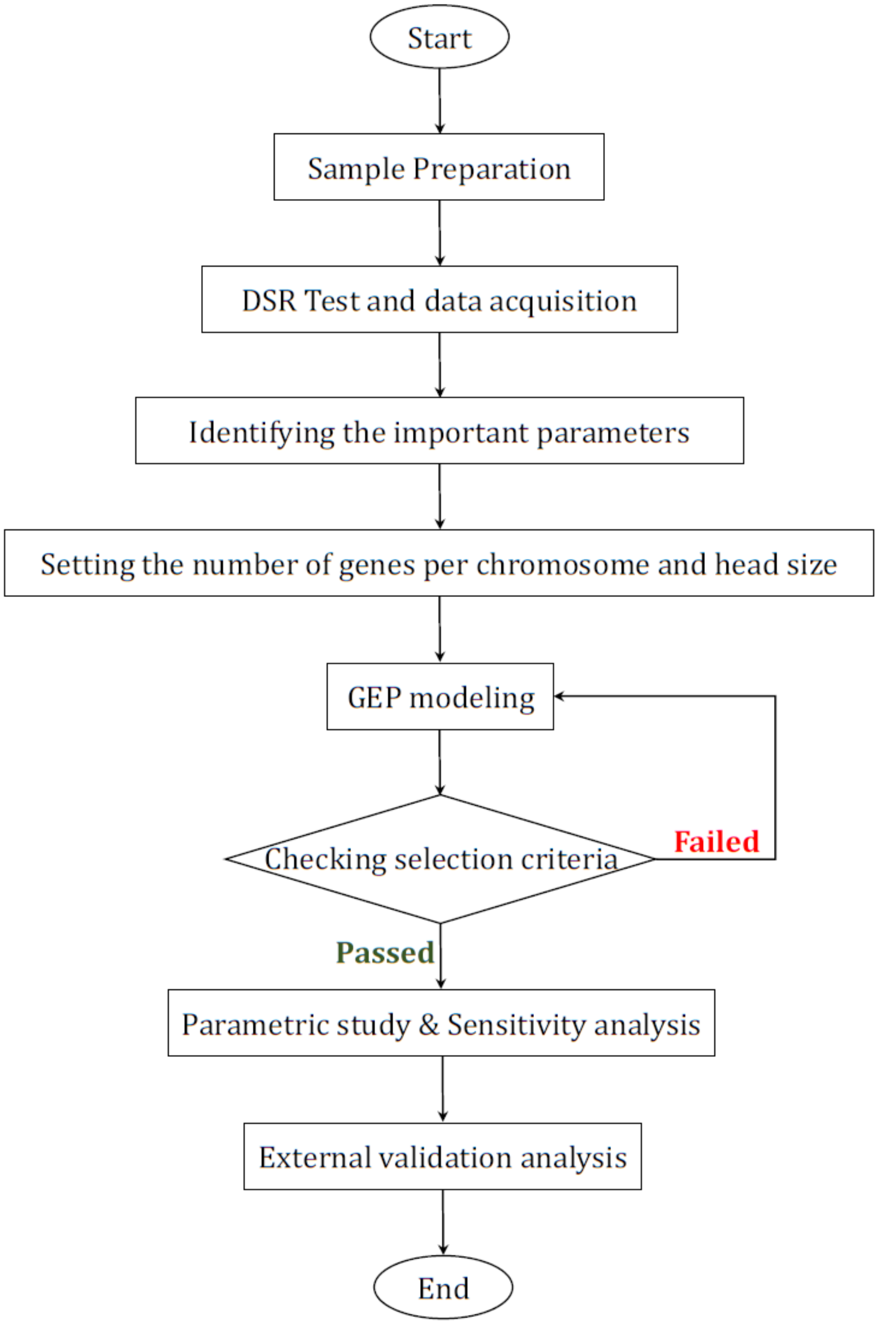


**Figure 1.** Flow of work in this study

# 2. Experimental Program

In this research, three common types of bitumen additives, including crumb rubber, styrene-butadiene-styrene (SBS) and polyphosphoric acid (PPA), were used to enhance the rheological and mechanical characteristics of the original bitumen. First in this section, these modifiers are briefly introduced; then, sample preparation, the test method, and generated results are presented.

## 2.1. Modifiers

### 2.1.1. Crumb rubber

Crumb rubber is one of the oldest modifiers of bitumen used for enhancing its low-temperature cracking resistance in cold regions, improving asphalt concrete fatigue and rutting performance, as well as resolving the difficulties associated with dumping used tire [14][15]. This modifier is generally produced by shredding used tires and classifying the product into different particle sizes. Liu et al. [16] investigated the effect of crumb rubber on the low-temperature performance of bitumen by implementing a bending beam rheometer test; the results showed that the optimum dosage of crumb rubber is between 15 and 20%. Aflaki and his coworkers [17] showed that modified bitumen containing 14% of rubber particles has a higher dissipated energy ratio and derivation of creep compliance. The crumb rubber used in this study was passed through sieve #50 obtained from Yazd Isatis Company. Table 1 shows the physical and chemical properties of the crumb rubber.

**Table 1.** Physical and chemical properties of crumb rubber

| Test Item | Result | Test Method |
|---|---|---|
| **Specific Gravity (gr/cm$^3$)** | 0.395 | ASTM-D70-03 |
| **Acetone Extract (wt%)** | 21.6 | ASTM-D494-11 |
| **Ash Content (wt%)** | 11 | ASTM-D4574 |
| **Percent Rubber Hydrocarbon (wt%)** | 49 | ASTM-D297 |
| **Mooney Viscosity at 100°C (ML)** | 56 | ASTM-D1646 |

| | | |
|---|---|---|
| **Tensile Strength (MPa)** | 48 | ASTM-D412 |
| **Elongation (%)** | 212 | ASTM-D1456 |
| **Hardness (Shore A)** | 63 | ASTM-D2240 |

### 2.1.2. Styrene-butadiene-styrene (SBS)

SBS is the most prevalent modifier of bitumen and has a wide range of applications [18]. It is an elastomer comprised of SBS tri-block chains with a two-phase morphology of spherical polystyrene block domains within a matrix of polybutadiene. A continuous polymer phase is formed within the bitumen structure if an appropriate SBS dosage (commonly 5-7% by mass of the original bitumen) is added to the original bitumen. The SBS used in this study was C-502 that has a linear structure and was acquired from Dynasol. Table 2 shows the physical, chemical, and thermo-mechanical characteristics of the SBS.

**Table 2.** Physical, chemical and thermo-mechanical properties of SBS

| Property | Value | Comment |
|---|---|---|
| **Volatiles** | <= 0.40 % | ASTM D-5668 |
| **Viscosity** | 1600 cP @Temperature 180 °C | Modified Bitumen Property in waterproof membranes (150/200 bitumen + 12% polymer) |
| **Brookfield Viscosity** | 5000 cP | 25% toluene solution; MA 04-3-064 |
| **Ash** | <= 0.35 % | ASTM D-5667 |
| **Styrene Content** | 31% | ASTM D-5775 |
| **Hardness, Shore A** | 76 | ASTM D-2240 |
| **Penetration** | <= 55 | at 25°C dmm, modified bitumen property in waterproof membranes (150/200 bitumen+12% polymer); ASTM D-5-86 |
| **Ring & Ball Softening Point** | >= 115 °C | Modified bitumen property in waterproof membranes (150/200 bitumen +12% polymer); ASTM D-36 |

### 2.1.3. Polyphosphoric acid (PPA)

PPA is a mineral liquid polymer of generic composition $H_{n+2}P_nO_{3n+1}$ [19]. Before the introduction of the Superpave protocol, PPA was being used to improve the penetration index and softening point of bitumen and, after introduction of this protocol, it has been used extensively to enhance binder PG (increasing the interval between high and low service temperatures). Several previous studies investigated the effect of adding PPA on the rheological and mechanical properties of original bitumen, which showed that PPA modification improves the behavior of bitumen in high service temperature [1]. Baldino et al. [20] reported that the effect of PPA on the low-temperature characteristics of bitumen is remarkably dependent on the amount of asphaltene and wax within the original bitumen. Therefore, the type of original bitumen affects the efficiency of PPA modification. The PPA used in this research program was obtained from Merck Millipore. Table 3 depicts the conventional, physical, and chemical properties of PPA.

**Table 3**. Conventional physical and chemical properties of PPA

| **Property** | **Value** |
|---|---|
| Boiling point@ 1013 hPa | 530°C |
| Density@ 20°C, gr/cm$^3$ | 2.06 |
| Melting Point | -20°C |
| Vapor pressure@ 20°C, hPa | 2 |
| Assay (acidimetric, calc. as $P_2O_5$) | 83 – 87% |

### 2.2. Sample Preparation

The original bitumen used in this study was PG 58-22, acquired from Pasargad Oil Company located in Tehran, Iran. All modifications were performed based on the weight of the original bitumen. Three different concentrations of each additive were used (Table 4). The dosage of each additive was based on the dosages reported in the technical literature [21][17] shown to improve the high, moderate, and low-temperature performance of an original bitumen, which are consistent with best practices in the pavement industry. Thus, one original and nine modified samples were fabricated. According to the type of modifier, different blending conditions were used, which are presented in Table 4. The type of mixer used to mix the additive with the original bitumen to achieve a homogeneous blend (high shear homogenizer or low shear conventional mixer), the rotational velocity of the mixer, the time, and the temperature of mixing are given as blending conditions.

**Table 4.** Sample code, modifier dosages and blending conditions of all modified bitumen samples

| Sample Code | Modifier | Dosage (wt% of original bitumen) | True PG | Blending Conditions (rpm:min@°C) | Type of Mixer |
|---|---|---|---|---|---|
| **BASE** | - | - | 58.3-25.0 | - | - |
| **CR10** | Crumb rubber | 10% | 68.3-26.6 | 4500:60@180 | High Shear Mixer |
| **CR15** | | 15% | 73.6-28.7 | | |
| **CR20** | | 20% | 75.4-30.8 | | |
| **SBS2** | SBS | 2% | 64.4-26.1 | 5500:90@180 | High Shear Mixer |
| **SBS4** | | 4% | 71.7-20.1 | | |
| **SBS6** | | 6% | 77.8-17.6 | | |
| **PPA05** | PPA | 0.5% | 70.5-21.2 | 50:45@150 | Low Shear Mixer |
| **PPA1** | | 1% | 77.1-17.7 | | |
| **PPA2** | | 2% | 82.2-14.7 | | |

## 2.3. Methodology

Two constitutive viscoelastic properties of the original and modified bitumens, including complex shear modulus (G*) and phase angle (δ), were measured by using an Anton Paar A-101 dynamic shear rheometer (DSR). The frequency sweep mode was performed over a frequency range of 0.1 to 100 Hz (21 frequencies) and at a strain amplitude of 0.01% (0.0001 mm/mm). Use of such a low strain amplitude ensures remaining of the bitumen within the linear viscoelastic range. A sinusoidal shear strain was applied on the bitumen sample at each frequency and the corresponding shear stress was determined as follows [22]:

$$\gamma(t)=\gamma_0 e^{i(\omega t-\delta)} \tag{1}$$

$$\tau(t)=\tau_0 e^{i\omega t} \tag{2}$$

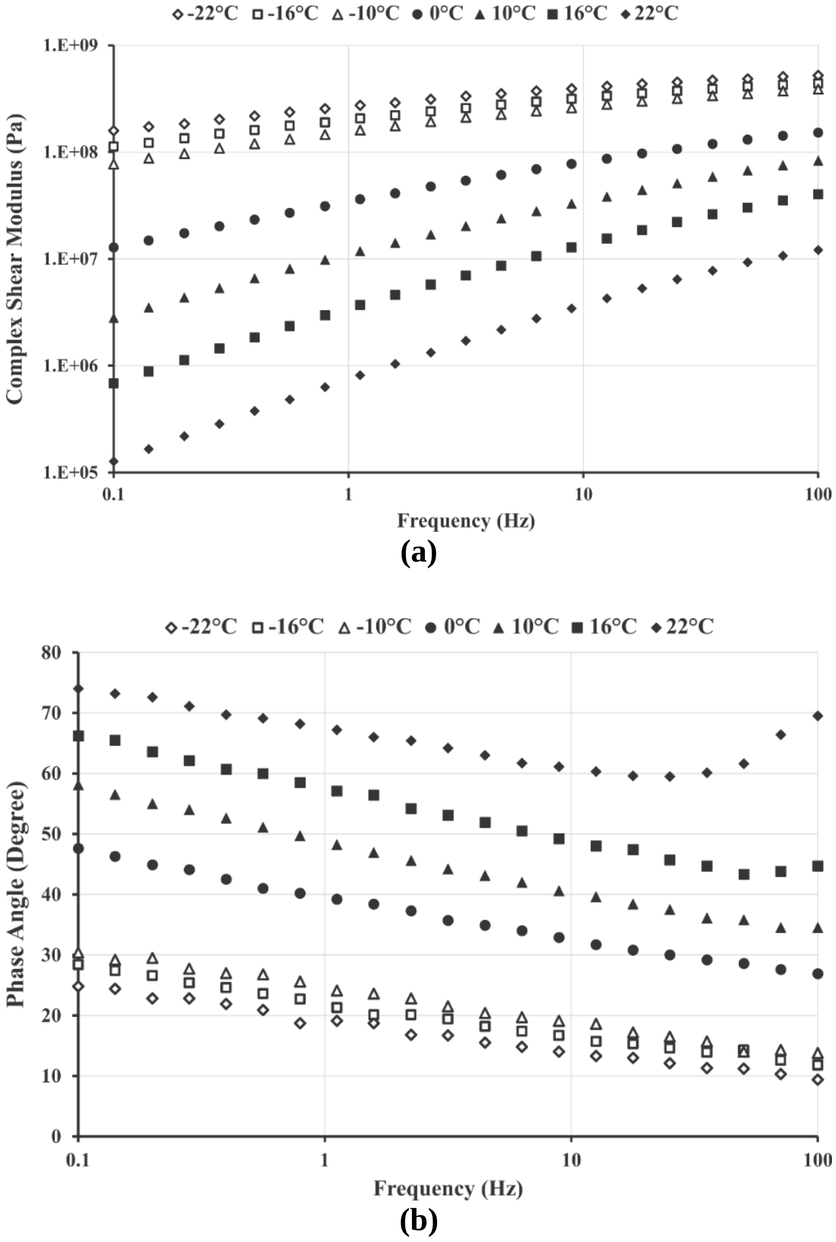
in which γ(t) and τ(t) are the applied shear strain and captured shear stress, $\tau_0$ and $\gamma_0$ are stress and strain amplitude, respectively, $\delta$ is phase angle, $\omega$ is the angular frequency, and $t$ is time. Complex shear modulus is defined as:

$$G^* = \frac{\tau_0}{\gamma_0} \tag{3}$$

To investigate the thermo-mechanical behavior of modified bitumens, seven different test temperatures were selected: -22, -16, -10, 0, 10, 16 and 22°C. These test temperatures are consistent with ASTM D 7175. The DSR sample had a diameter of 8 mm and a gap of 2 mm was set up between two parallel plates. While ASTM D 7175 can be used for test temperatures between 4 to 88°C, it was shown that a similar test setup can be used for sub-zero temperatures [23].

## 2.4. Database

Figure 2 shows typical results generated by the test method described in section 2.2 for the original bitumen at all test temperatures. As can be seen in Figure 2, the amount of both G* and δ are depended on the applied loading frequency and the test temperature. Increasing the test temperature decreased the complex shear modulus (G*) and increased the phase angle (δ). Also, increasing the applied loading frequency caused an increase in G* and a decrease in δ, since the bituminous sample had less time to relax the stress due to the applied strain. It is evident that adding different types of additive at various dosages altered the viscoelastic behavior of the original bitumen. For each type and percentage of additive, the complex shear modulus and phase angle curves versus frequency were captured.



(a)

(b)

**Figure 2.** Results of the frequency sweep test for (a) complex shear modulus, and (b) phase angle of the original bitumen at different test temperatures

## 3. Gene Expression Programming (GEP)

Using GP, which was originally introduced as a useful prediction algorithm by Koza [24], the relationships between the involved parameters of a problem are predicted based on the principle of Darwinian natural selection. The commonly used mechanisms of genetic algorithm (GA) can also be utilized in GP; nevertheless, the solution representation is different. The result of GA is in the form of a fixed-length binary string; however, an evolving GP results in a computer code of prediction  can be represented in the form of a tree that varies in length. This is the definition of the classical GP approach, called tree-based GP, which comprises a hierarchically-structured tree of functions and terminals [25]. GEP is basically a natural development of GP and has five main components: (1) a function set, (2) a terminal set, (3) a fitness function, (4) control parameters, and (5) a terminal condition. Unlike the traditional GP, GEP makes use of fixed-length character strings for solution representation. Parsing trees of various sizes, named expression trees (ETs), are a graphical representation of GEP. Because these genetic mechanisms work at the chromosome level, the main advantage of this method is the extreme simplicity of creating genetic diversity. The other positive aspect of GEP is its multi-genic nature, which makes it possible to evolve complex programs of a high degree of nonlinearity that comprise several subprograms [4].

GEP consists of genes in which each one contains a list of arbitrary fixed-length symbols comprising the terminal set. Therefore, the chromosomes, as an inherent part of GEP, represent a single parse tree. Karva [26] developed a new language that allows the chromosomes’ information to be read. Genes that are K-expressions [5] in Karva language are simply comprised of letters representing the problem variables (such as A, B, C, etc.) and constant numbers. K-expressions can also be presented in the form of parse trees that are capable of providing information regarding the mathematical as well as the logical complexity of a gene. For instance, Eq. (4) consists of the gene in Karma language as: ×.-.-.+.Ln.A.B.C.5, and can be alternatively illustrated as the ET shown in Figure 3, which starts from the root and reads through the string by sequence.

$$\exp\left(5\times A\times B\right)\times\frac{C}{A+B} \tag{4}$$

For a given problem, each GEP gene has a predetermined fixed length. However, the useless excessive elements for genome mapping in ETs can change the size of tree [26].

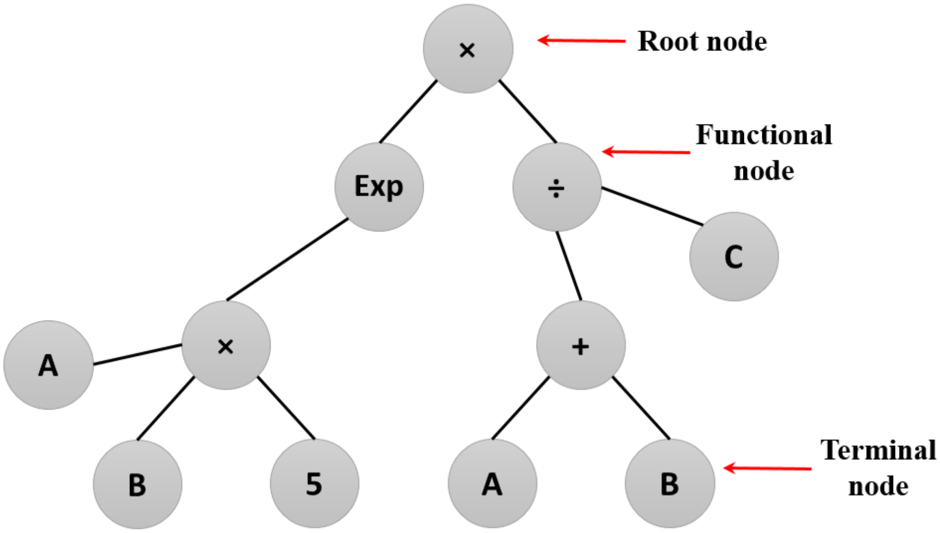


**Figure 3.** Tree representation of Eq. (1)

The GEP algorithm starts with random generation of fixed-length chromosomes of the initial population. Then, k-expressions for each chromosome are produced and evaluated regarding their fitness. Having been selected by roulette wheel sampling with elitism based on the fitness criteria, chromosomes are modified and reproduced. This selection criterion guarantees the maintenance and cloning of the best chromosomes from the previous generation to the next. The new generation experiences the same process from the beginning. This procedure is repeated up to a certain number of iterations, or until a solution has been found [5].

# 4. Model development

In order to develop a GP prediction model for estimating the complex shear modulus (G*) and phase angle (δ) of modified asphalt bitumens, all of the effective input parameters that were part of the experimental program have to incorporated into the models. It is well-known that the original bitumen, as well as modified ones, behave like viscoelastic materials and their mechanical behavior depends on time (frequency of applied load) and temperature. The additive dosage used to modify the original bitumen and inherent characteristics of the original bitumen significantly affect the viscoelastic properties of modified bitumen as well. Therefore, G* and δ, as two constitutive viscoelastic parameters, are functions of the input parameters, as follows:

$$G^* = f\left(G_0^*, T, \omega, P\right) \tag{5-1}$$

$$\delta = f\left(\delta_0, T, \omega, P\right) \tag{5-2}$$

where $G^*_0$ (Pa) and $\delta_0$ (degree) are the complex shear modulus and phase angle of the original bitumen, respectively, T is the test temperature (°C), ω is the loading frequency (Hz), and P is the percentage (%) of the specific additive (CR, SBS and PPA) that was introduced in order to modify the original bitumen.

## 4.1. Statistical analysis of the experimental data

As per the explanations given in subsection 2.3, the results of the test experiments at different test temperatures and loading frequencies consisted of 1,281 data points for all three modifiers at three different dosages. In order to analyze the data, each set of data for each modifier was randomly divided into Training and Validation subsets. The training subset for each modifier was used to develop the GP algorithm while the validation data were used to examine how general the predictions of each model were on data that were not used in the training procedure. The best top ten GP models were selected amongst all the developed models using the criteria of having the highest performance in training.Having been selected, the selected models, in terms of learning, were validated against the validation data subset to measure their performance on the data that had no contribution to the model development process. Here, two-thirds of data were used in the training process, while validation analysis was conducted on the remaining one-third.

Table 5 illustrates the ranges and statistics of the involved input and output parameters used for model development.

**Table 5.** Statistics of input and output variables used for the GP model development

| Statistical Parameter | Common inputs | | | | Percentage of additive, P (%) | | | G* (Pa) | | | δ (s) | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | T (°C) | ω (Hz) | $G^*_0$ (Pa) | $\delta_0$ (s) | CR | SBS | PPA | CR | SBS | PPA | CR | SBS | PPA |
| Range | 44.0 | 99.90 | 522873000 | 64.61 | 10.0 | 4.0 | 1.5 | 371053497 | 510452633 | 487596944 | 69.19 | 81.01 | 63.53 |
| Minimum | -22.0 | 0.10 | 127000 | 9.39 | 10.0 | 2.0 | 0.5 | 237622 | 113448 | 184139 | 10.38 | 8.98 | 9.25 |
| Maximum | 22.0 | 100.00 | 523000000 | 74.00 | 20.0 | 6.0 | 2.0 | 371291119 | 510566080 | 487781083 | 79.57 | 90.00 | 72.79 |
| Mean | 0.0 | 16.29 | 132949626 | 36.99 | 15.0 | 4.0 | 1.2 | 76239355 | 113434501 | 98416435 | 32.04 | 35.78 | 36.03 |
| Standard error | - | - | 6964564.82 | 0.88 | - | - | - | 4159385 | 6151394 | 6132163 | 0.67 | 0.85 | 0.74 |
| Standard deviation | - | - | 146089944 | 18.39 | - | - | - | 87248004 | 129032738 | 122336259 | 14.07 | 17.80 | 14.69 |
| Variance | - | - | 2.1342E+16 | 338.02 | - | - | - | 7.612E+15 | 1.665E+16 | 1.497E+16 | 197.89 | 316.97 | 215.80 |
| Confidence level (95.0%) | - | - | 13634810.9 | 1.72 | - | - | - | 8142997 | 12042834 | 12003747 | 1.31 | 1.66 | 1.44 |

## 4.2. Evaluation of model performance

As explained above, all data were divided into Training and Validation groups. Checks of validation and training performance of GP models was performed based on three main objectives: 1) the best fitness value and the least amount of error for the training subset, 2) the best fitness value and the least amount of error for the validation subset on the trained model, and 3) model simplicity. The latter was not a predominant and highly determining parameter and was controlled by setting the genes and head size of each model for the runs. The first and second criteria were controlled for the models in order to examine how accurate the predictions were, using correlation coefficient (R), the relative root mean squared error (RRMSE), and Performance index (PI), as follows:

$$R = \sum\left(O - \bar{O}\right)\cdot\left(P - \bar{P}\right) \Big/ \sqrt{\sum\left(O - \bar{O}\right)^2 \cdot \sum\left(P - \bar{P}\right)^2} \tag{6-1}$$

$$RRMSE = \sqrt{\frac{1}{n}\sum\left(O - P\right)^2} \tag{6-2}$$

$$PI = \frac{RRMSE}{1 + R} \tag{6-3}$$

where *O* and *P* are experimental and predicted outputs, respectively; $\bar{O}$ and $\bar{P}$ are the average of actual and calculated outputs, respectively, and *n* is the number of samples. These criteria indicate the prediction accuracy of GP models for the training subset.

A higher R together with lower RRMSE and PI values result in more accurate model predictions.

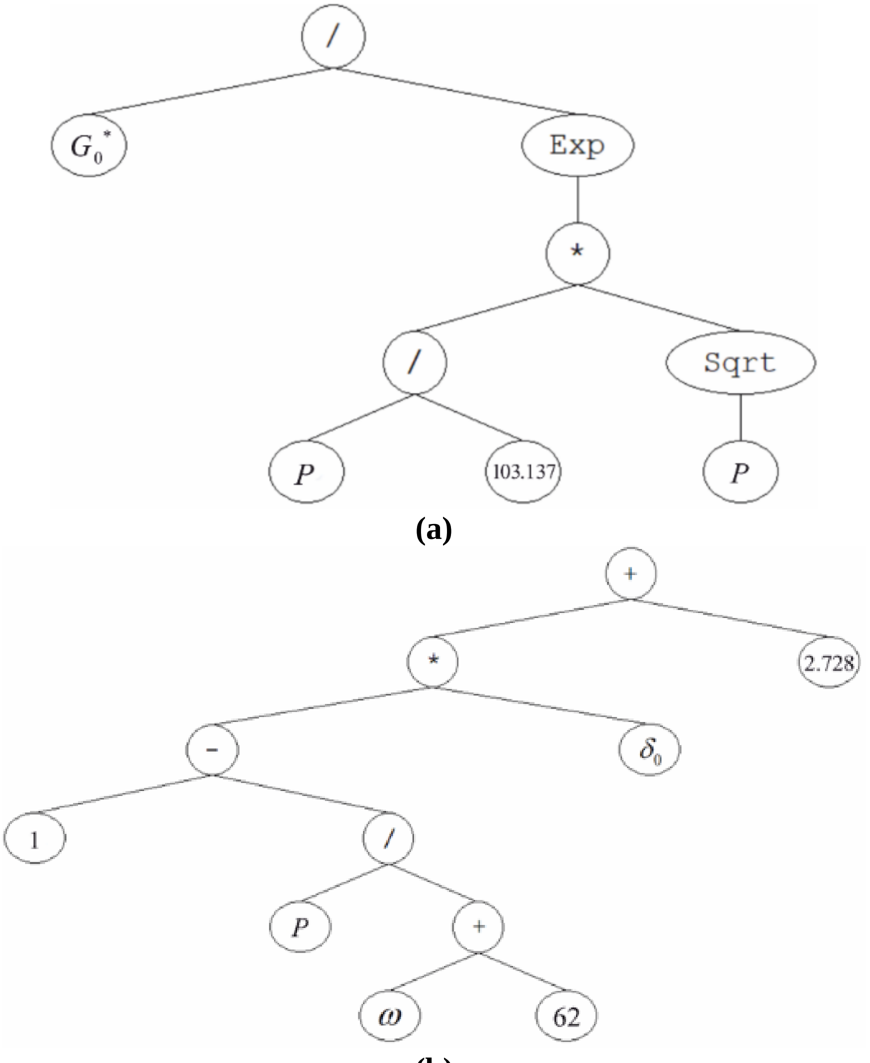
### 4.3. GEP modeling and Formulation

The GEP models were generated using five input parameters for each additive: T, ω, $G_0^*$, $\delta_0$, and P, since each additive had a special effect on the viscoelastic behavior of the original bitumen due to its inherent characteristics. In order to derive an accurate GEP model for each target parameter, several runs were conducted using R and the RRMSE as the accuracy controllers. In GP modeling, the population size (number of chromosomes) determines the number of evolved programs. Meanwhile, the appropriate population size depends on the complexity of the problem and the number of possible solutions for the problem. In the analyses, three sets were set for the population number (50, 150, and 300).

The number of genes per chromosome and head size, known as architectural parameters of the GEP, can determine the structure of each term in each model. The former is used for determining the number of terms in the model, while the latter determines the complexity of each term in the model. Three genes (1, 2, and 3), and three optimal levels of head size (3, 5, and 8) were selected. For a number of genes greater than 1, an extra linking function was used in order to link the encoded mathematical terms of each. With three sets for population size (three genes and three head sizes), a total of 27 different combinations of the parameters existed. Since ten replications for each combination were performed, the overall number of GEP runs was 270.

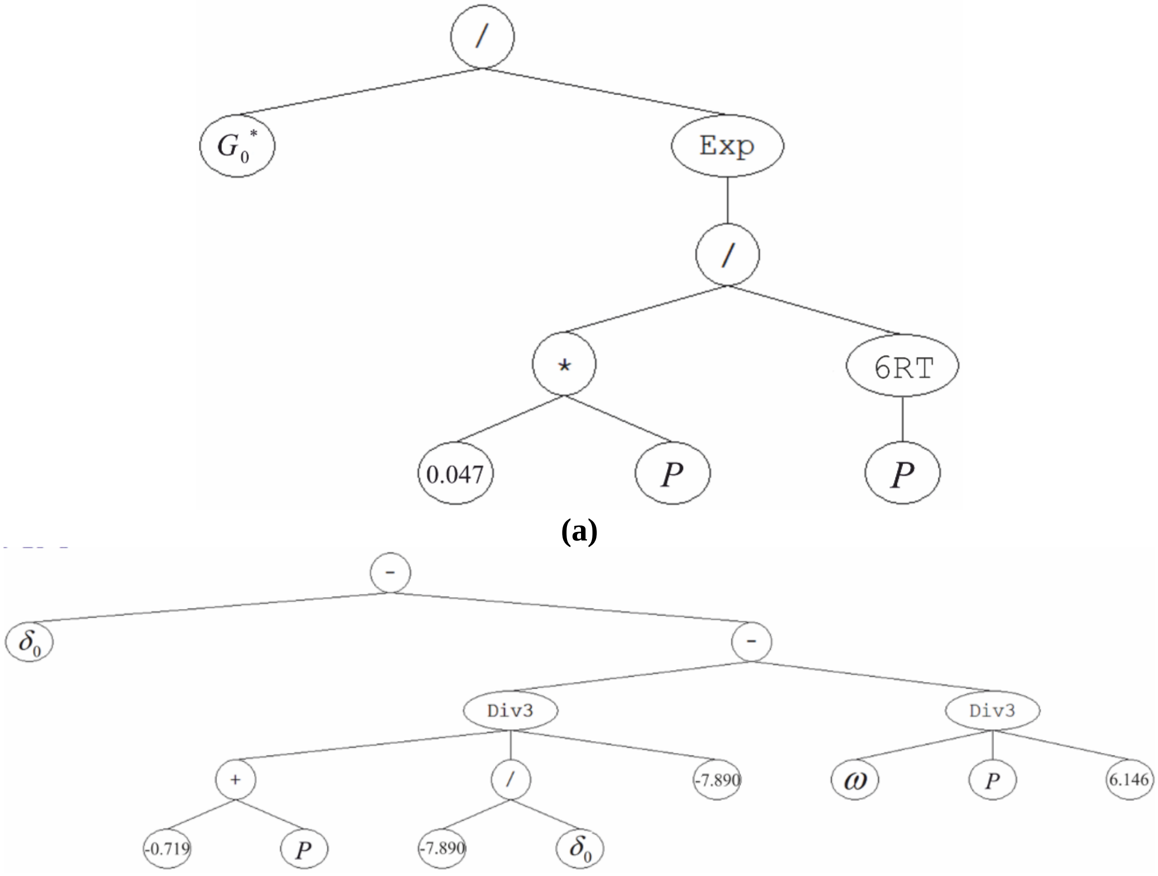
Basic arithmetic operators together with the most common mathematical functions were used to derive the GEP models for each target parameter. Amongst the generated models for each modified bitumen, those with the highest R and the lowest RRMSE were selected. Between the top ten statistically selected models, one model for each target parameter was selected, based on the theoretical fundamentals of the problem explained in the experimental program section. The GEP algorithm was implemented using GeneXproTools [27].

The best GEP models were selected according to the previously mentioned criteria of selection. Figures 4 to 6 show the ETs for the best models developed for CR, SBS, and PPA additives, respectively. It is worth noting that the exponential operator was observed in all the selected top ten models of G* prediction for all three additives. This interesting outcome amongst a great number of generations of GEP training can be attributed to the ideal form of the exponential operator for prediction of the modified complex shear modulus of modified bitumen.



**(b)**

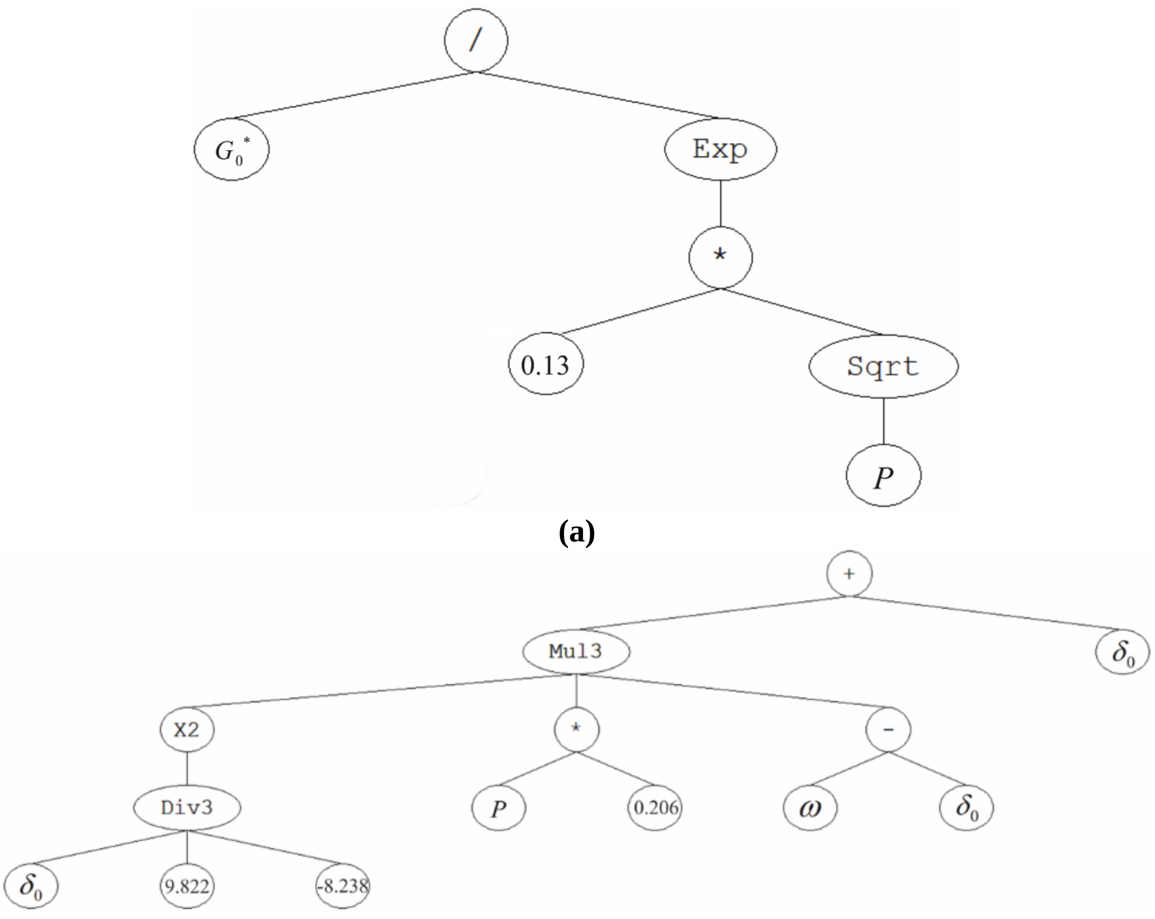
**Figure 4.** The best GEP model Tree representation for crumb rubber modified bitumen a) Complex shear modulus, b) Phase angle; *Note: "Eep" and "sqrt" are the exponential function and the square root.*



(a)

(b)

**Figure 5.** The best GEP model Tree representation for SBS modified bitumen a) Complex shear modulus, b) Phase angle; *Note: "6RT" and "Div3" are the 6th root and triple division, respectively*.



**(a)**

**(b)**

**Figure 6.** The best GEP model Tree representation for PPA modified bitumen a) Complex shear modulus, b) Phase angle; *Note: "Mul3" and "Div3" are the multiplication of three terms and triple division, respectively.*

The formulations for the prediction of complex shear modulus and phase angle in the CR, SBS, and PPA modified bitumen are as follow:

*Crumb rubber modified bitumen:*

$$G^* = G_0{}^* \cdot \exp\left(-\frac{P^{1.5}}{103.137}\right) \tag{7-1}$$

$$\delta = \delta_0\left(1 - \frac{P}{\omega + 62}\right) + 2.728 \tag{7-2}$$

*SBS modified bitumen:*

$$G^* = G_0^* \cdot \exp\left(-0.047 \times P^{5/6}\right) \tag{8-1}$$

$$\delta = \delta_0 + \frac{\omega}{6.146P} - \frac{\delta_0 \left(P - 0.719\right)}{\left(7.89\right)^2} \tag{8-2}$$

*PPA modified bitumen:*

$$G^* = G_0^* \cdot \exp\left(-0.13 \times P^{0.5}\right) \tag{9-1}$$

$$\delta = \delta_0 + 3.149 \times 10^{-5} \times \left[\delta_0^{\,2}.P.\left(\omega - \delta_0\right)\right] \tag{9-2}$$

Based on the experimental program, the ranges of validity of the proposed formulas (Eq. 7~9) are as follows:

$$\begin{aligned} &127\,kPa \le G_0^* \le 523000\,kPa \\ &9.39^\circ \le \delta_0 \le 74^\circ \\ &0.1\,Hz \le \omega \le 100\,Hz \\ &10\% \le P_{CR} \le 20\% \\ &2.0\% \le P_{SBS} \le 6.0\% \\ &0.5\% \le P_{PPA} \le 2.0\% \end{aligned} \tag{10}$$

## 5. Validity of the proposed models

As per the recommendation by Frank and Todeschini [28], a model can be safely acceptable if the ratio of the number of data sets to the number of input parameters is greater than five. Here, the mentioned ratio for CR, SBS, and PPA modified bitumen are 88, 88, and 80, respectively, which indicates the validity of the number of data. Moreover, for a valid model, it is necessary for the error value (e.g., RRMSE) to be at its minimum, and R to be higher than 0.8 [29]. In all of the selected prediction models, these statistical parameters were checked for the training and validation sets. A very good correlation between the predictions of the GP models and the experimental data can be seen in the scatter diagrams (Figures 7 to 9). Meanwhile, for the external validation of the proposed formulae on the verification dataset, the Golbraikh and Tropsha [30] criteria were checked. This criterion suggests that at least one of the regression line slopes (*k* and *k'*), which passes through the origin, should be close to one (i.e. $0.85<k, k'<1.15$).

$$k = \frac{1}{O^2}\sum O \times P \tag{11-1}$$

$$k' = \frac{1}{P^2}\sum O \times P \tag{11-2}$$

where $O$ and $P$ are the experimental observations and GP predicted values, respectively. Table 6 presents the calculated validation criteria (Eq. 7) for GP models (Eq. 4, 5, and 6). According to this table, all formulae met the criteria. Table 7 illustrates the calculated statistical indices from Eq. 6 for all proposed formulae. Based on the $R^2$, RRMSE, and PI values in this table, the results of training and testing are very close, which shows that the models did not overfit.

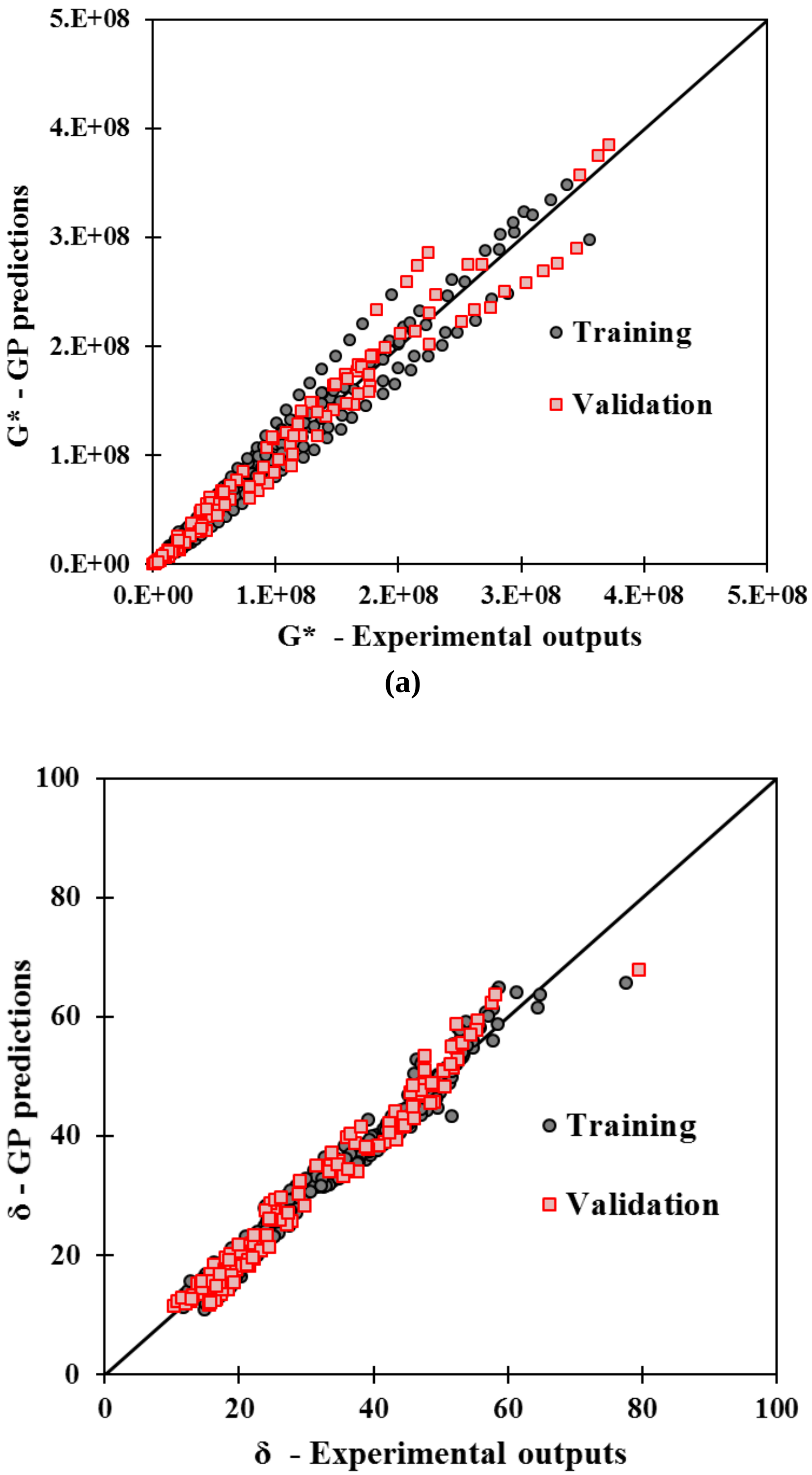
**Table 6.** External validation of GEP models

| | $k$ | | $k'$ | |
|---|---|---|---|---|
| Additive | $G^*$ | $\delta$ | $G^*$ | $\delta$ |
| CR | 1.0017 | 1.0016 | 0.9828 | 0.9926 |
| SBS | 0.9957 | 1.0003 | 0.9884 | 0.9949 |
| PPA | 1.0013 | 0.9596 | 0.9902 | 1.0393 |

*k* and *k'* are regression line slopes

**Table 7.** Statistical indices (Eq. 6) for the training and validation subsets of all formulae

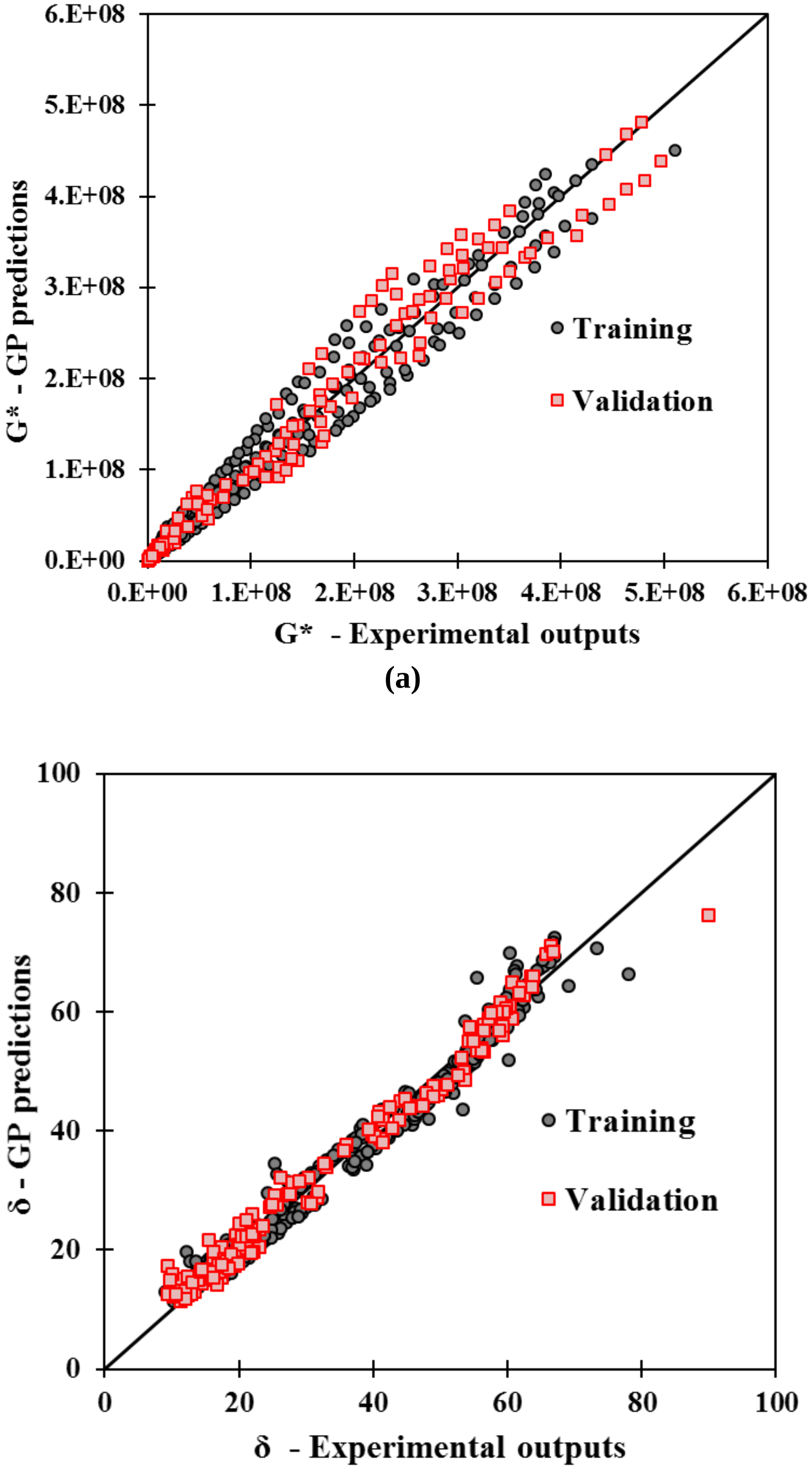
| Additive | Equation | Training | | | Validation | | |
|---|---|---|---|---|---|---|---|
| | | $R^2$ | RRMSE (%) | PI | $R^2$ | RRMSE (%) | PI |
| CR | G* | 0.974 | 19.4 | 0.098 | 0.971 | 18.2 | 0.091 |
| | δ | 0.974 | 7.0 | 0.035 | 0.973 | 8.5 | 0.043 |
| SBS | G* | 0.972 | 20.0 | 0.101 | 0.970 | 18.1 | 0.091 |
| | δ | 0.981 | 7.2 | 0.036 | 0.981 | 8.0 | 0.040 |
| PPA | G* | 0.990 | 13.2 | 0.066 | 0.985 | 13.9 | 0.070 |
| | δ | 0.956 | 8.5 | 0.043 | 0.974 | 7.0 | 0.035 |



**(a)**

**(b)**

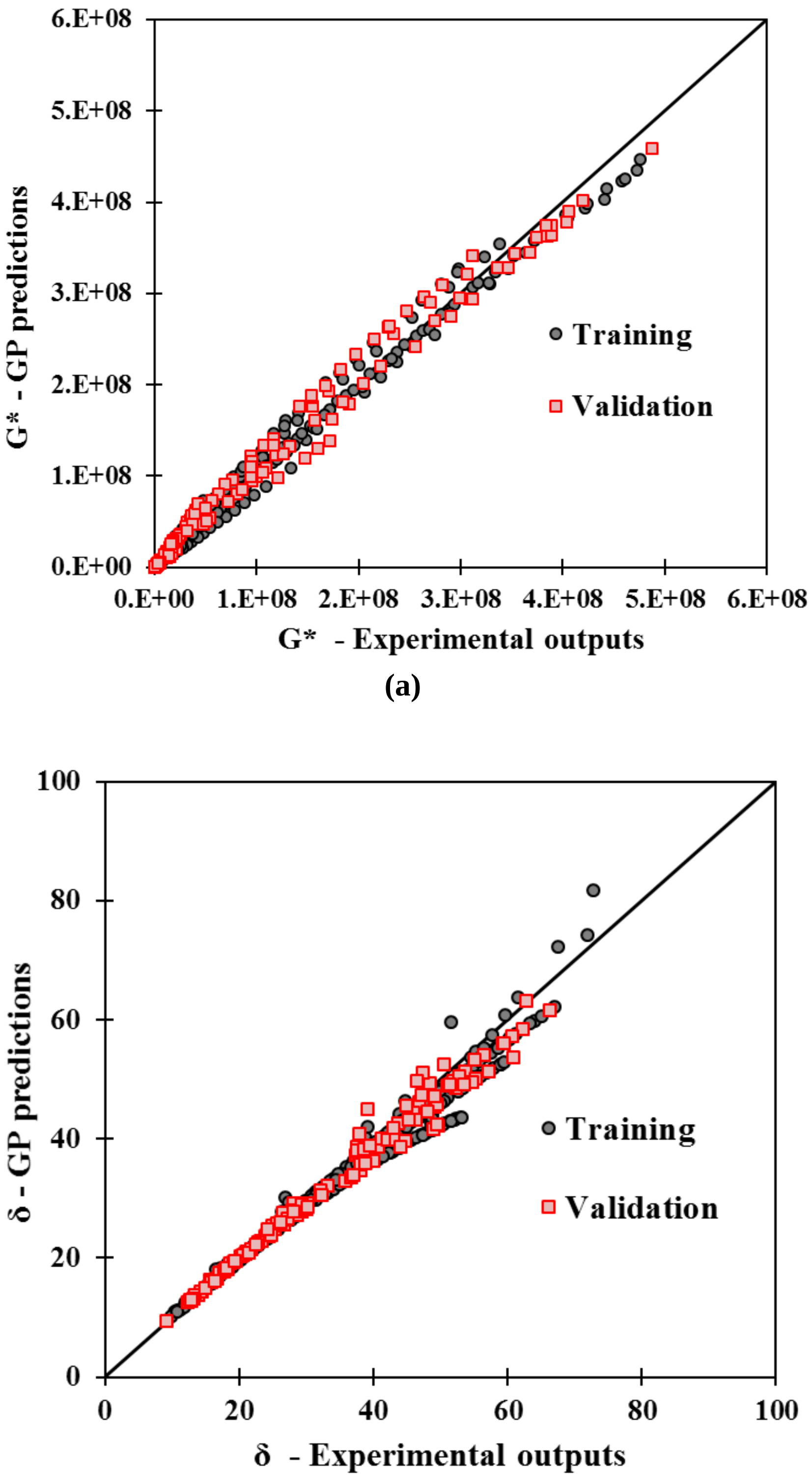
**Figure 7.** Experimental versus GEP model predictions for crumb rubber modified bitumen a) Complex shear modulus, b) Phase angle



(a)

(b)

**Figure 8.** Experimental versus GEP model predictions for SBS modified bitumen a) Complex shear modulus, b) Phase angle



(a)

(b)

**Figure 9.** Experimental versus GEP model predictions for PPA modified bitumen a) Complex shear modulus, b) Phase angle

An external validation analysis was conducted to examine the performance of the proposed formulae on the prediction of the complex shear modulus and phase angle of the modified bitumens. For this purpose, the experimental data from Hajikarimi et al. [31], Moghadas Nejad et al. [32] and Samieadel and Fini [33] were used for the validation of the formulae on crumb rubber, SBS and PPA-modified bitumens. The statistical parameters of the external data are presented in Table 8. Scatter diagrams of the external validation study are illustrated in Table 9 and Figure 10 to 12. According to the results, most of the data points are very close to the ideal correlation line. Therefore, according to Table 9 and Figure 10 to 12, GEP models showed a very good performance in the prediction of complex shear modulus and phase angle on the unseen experimental data.

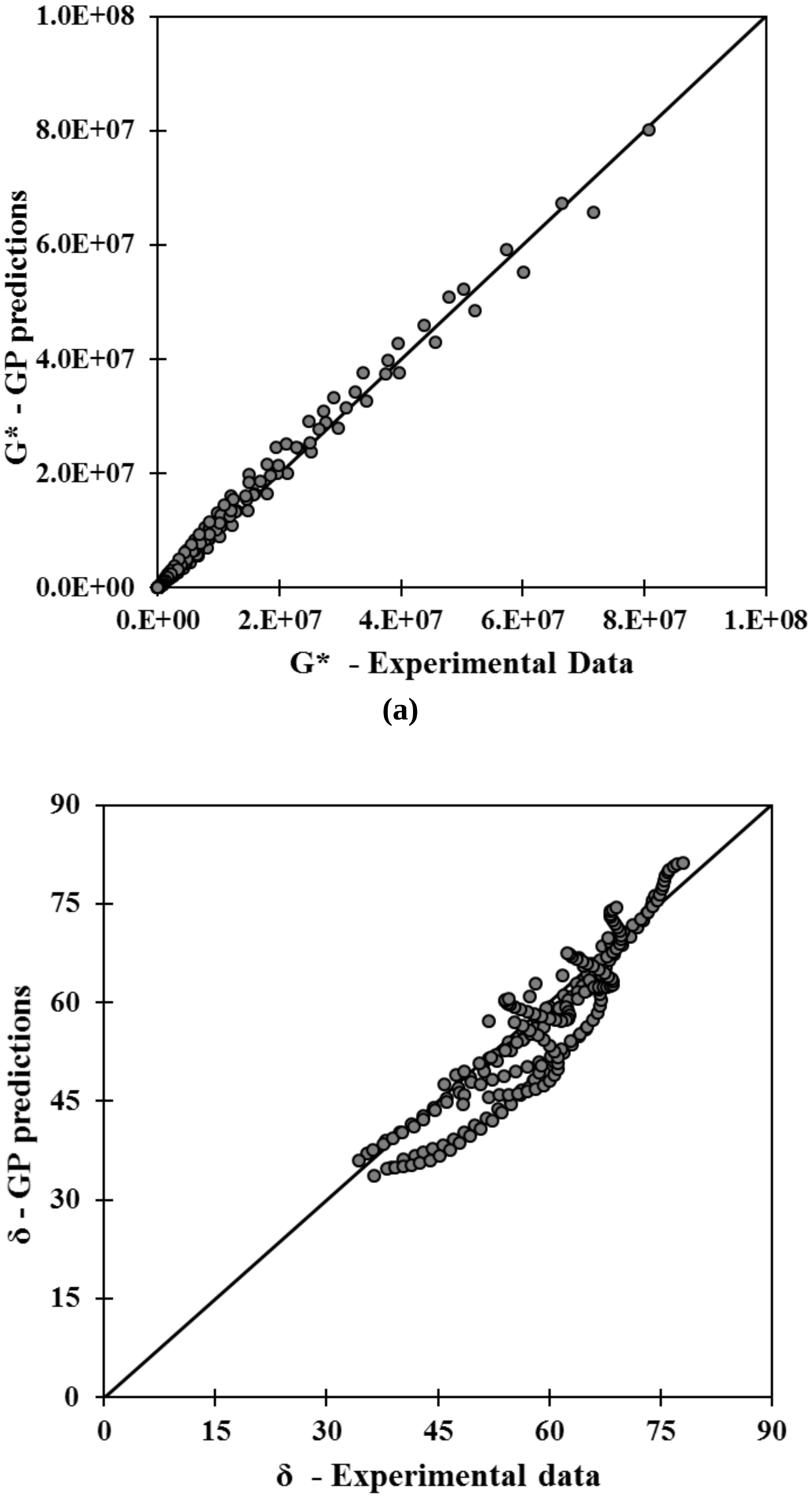
**Table 8.** Statistics of input and output variables of the external data

| Additive | Statistical Parameter | T (°C) | ω (Hz) | $G^*_0$ (kPa) | $\delta_0$ (s) | P (%) | G* (kPa) | δ (s) |
|---|---|---|---|---|---|---|---|---|
| CR<br>(5, 10, 15, 20%) | Minimum | 10 | 0.1 | 17.555 | 35.4 | 5 | 7.375 | 34 |
| | Maximum | 30 | 100 | 89300 | 85.4 | 20 | 80126 | 81 |
| | Mean | 20 | 16.4 | 13052 | 65.6 | 12.5 | 8558 | 56.7 |
| | Range | 20 | 99.9 | 89282 | 50.0 | 15 | 80119 | 47.5 |
| SBS<br>(2, 4, 6%) | Minimum | 10 | 0.1 | 21.0 | 35.7 | 2 | 17.0 | 35.4 |
| | Maximum | 30 | 100 | 67303 | 80.9 | 6 | 61896 | 79.2 |
| | Mean | 20 | 16.4 | 9967801 | 60.3 | 4 | 8613 | 58.0 |
| | Range | 20 | 99.9 | 67282 | 45.2 | 4 | 61879 | 43.9 |
| PPA<br>(1%) | Minimum | 20 | 0.1 | 819.5 | 26.5 | 1.0 | 719.6 | 27.9 |
| | Maximum | 20 | 101.4 | 26253 | 72.8 | 1.0 | 23052 | 60.7 |
| | Mean | 20 | 15.6 | 9670 | 46.9 | 1.0 | 8491 | 43.7 |
| | Range | 0 | 101.3 | 25433 | 46.3 | 0.0 | 22333 | 32.8 |

* The base binder was PG58-22

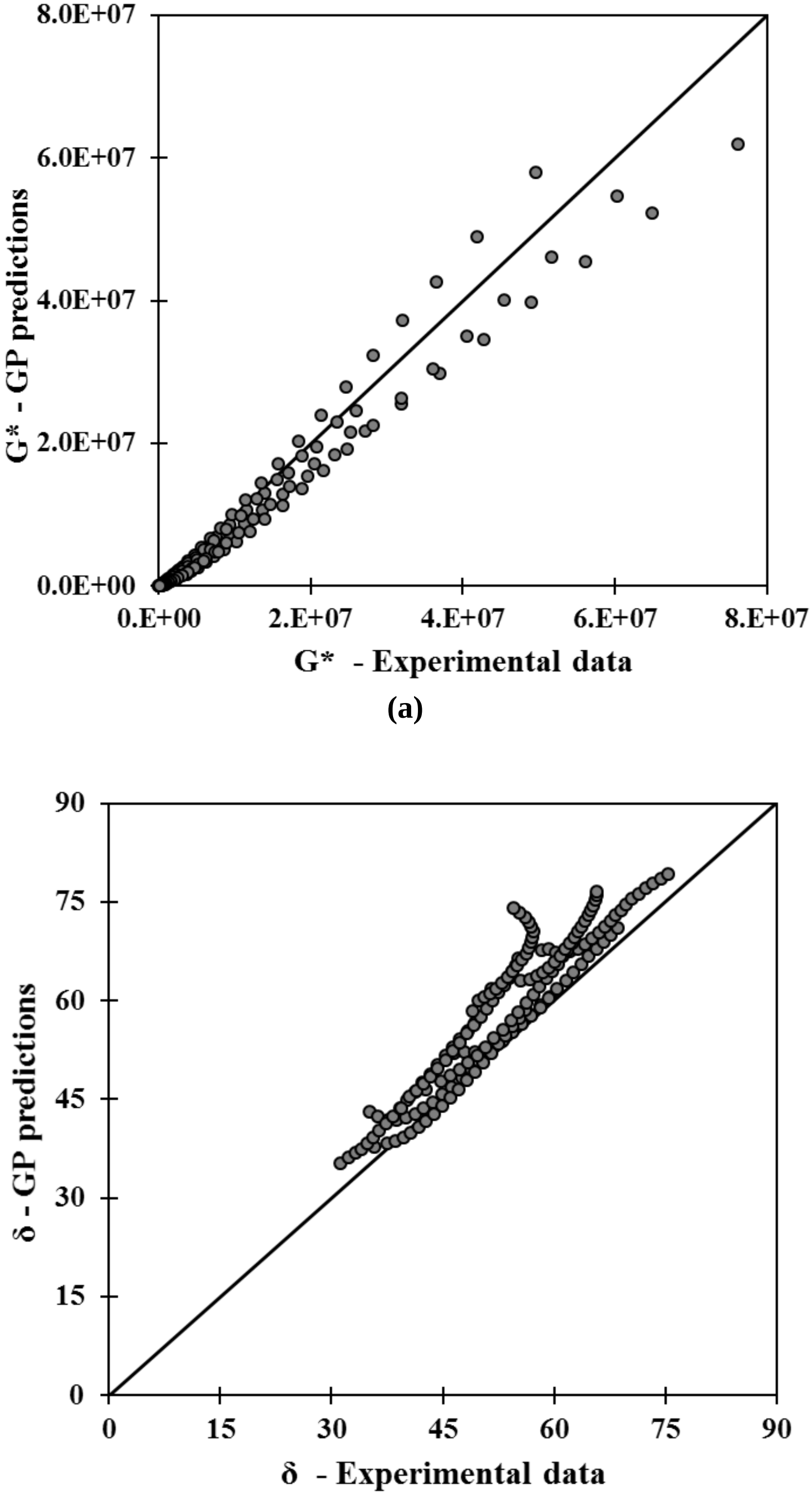
**Table 9.** Statistical indices (Eq. 6) for the prediction of all formula on the external datasets

| Additive | Equation | $R^2$ | RRMSE (%) | PI |
|---|---|---|---|---|
| CR | G* | 0.9911 | 0.1646 | 0.08 |
| | δ | 0.8576 | 0.1706 | 0.09 |
| SBS | G* | 0.9675 | 0.3036 | 0.15 |
| | δ | 0.8848 | 0.1193 | 0.06 |
| PPA | G* | 0.9966 | 0.1722 | 0.09 |
| | δ | 0.9685 | 0.1215 | 0.06 |



(b)

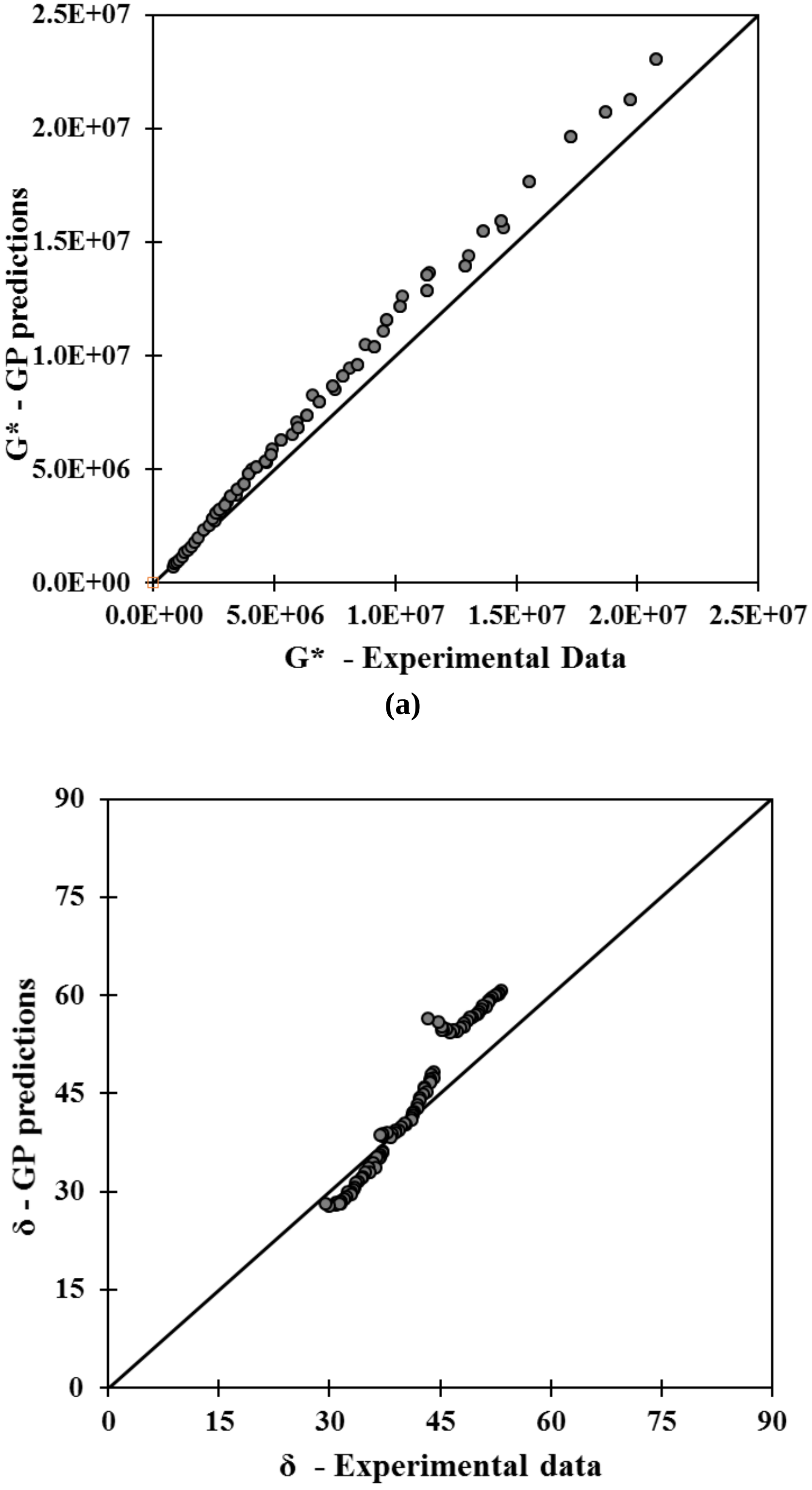
**Figure 10.** Experimental external data versus GEP model predictions for crumb rubber modified bitumen a) complex shear modulus, b) phase angle



**(a)**

**(b)**

**Figure 11.** Experimental external data versus GEP model predictions for SBS modified bitumen a) complex shear modulus, b) phase angle



**(a)**

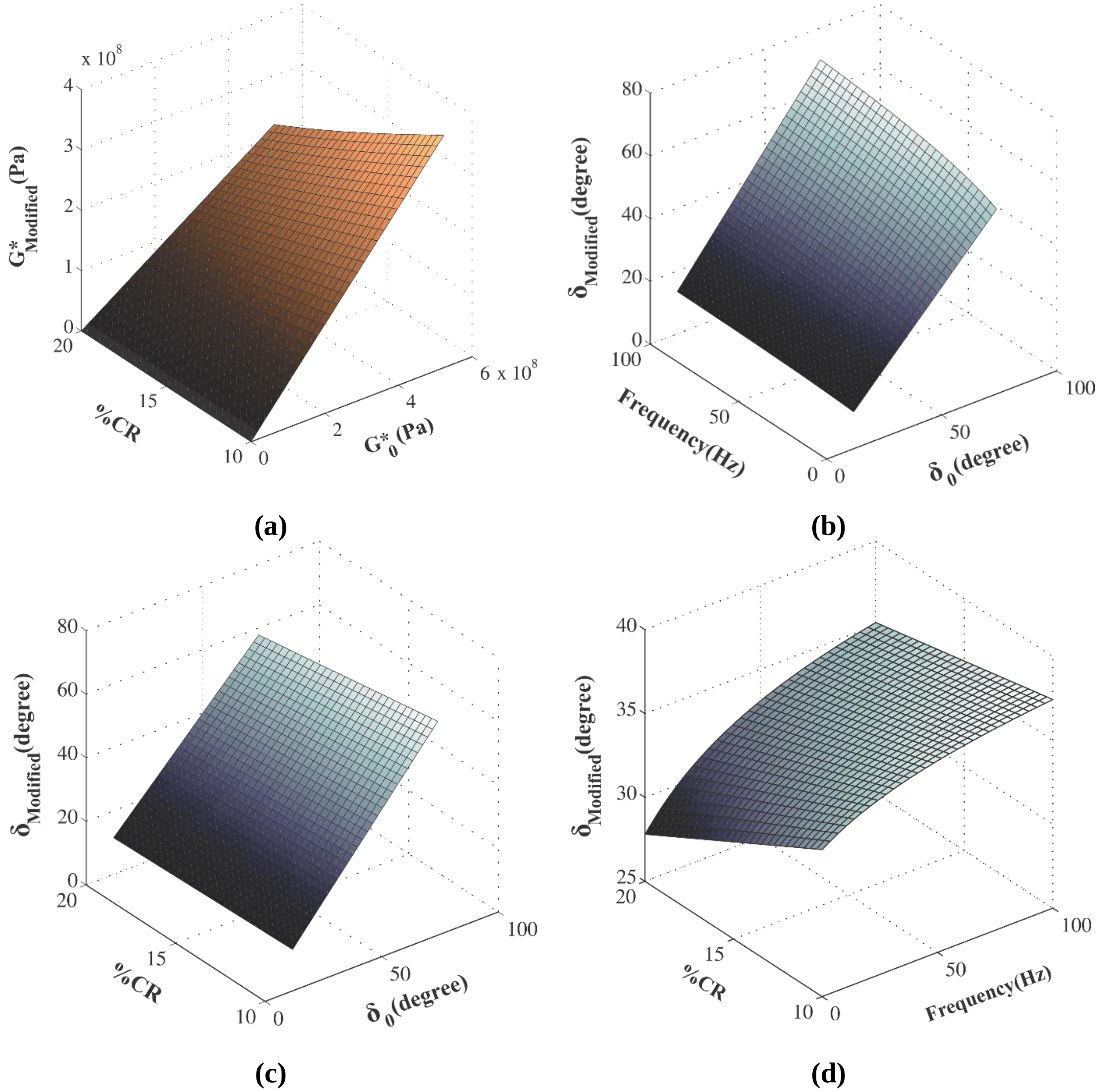
**(b)**

**Figure 12.** Experimental external data versus GEP model predictions for PPA modified bitumen a) complex shear modulus, b) phase angle

## 6. Parametric study and sensitivity analysis

A parametric study of the GEP models was conducted to examine the robustness of the prediction models for all three modified bitumens, and the response of each GEP model to its corresponding input parameters was investigated. The three-dimensional diagrams in Figures 13 to 17 illustrate the general trend of the models against pairs of input predictors for the presented formulae for CR, SBS, and PPA modified bitumens. As can be seen in Figures 13 to 15, the observed trends were in good agreement with the structure of the proposed formulae. For example, the increasing effect of complex shear modulus and phase angle on the base bitumen is obvious, and it can be seen that a higher percentage of modifier decreased the modified complex shear modulus. This effect can be clearly observed in Figure 13-a as well as in Figure 14-a and Figure 15-a. Figure 13-b, Figure 14-b, and Figure 15-b show that with an average additive percentage, the higher the loading frequency that is applied on the specimen, the sharper the effectiveness of the phase angle of unmodified bitumen. Meanwhile, the decreasing effect of additive percentage together with the boosting influence of phase angle of the original bitumen on the phase angle of the modified bitumen can be clearly seen in Figure 13-c, Figure 14-c, and Figure 15-c. Based on Figure 13-d, Figure 14-d, and Figure 15-d, which provide a better understanding of the influence of additive percentage and loading frequency: increasing the loading frequency enhanced the phase angle of the modified bitumen; however; this effect was stronger for crumb rubber additive as compared to the other additives. It can be observed in Figure 13-d that increasing the percentage of the modifier decreased the phase angle of the modified bitumen, and this effect increased in lower frequencies. Nevertheless, Figure 14-d shows that increasing the loading frequency intensified the decreasing effect of the percentage of SBS. Both crumb rubber and SBS increased the stiffness and viscosity of bitumen which resulted in increasing of the elastic characteristics of modified bitumen. A rather different behavior was observed for the PPA modifier against the loading frequency. As shown in

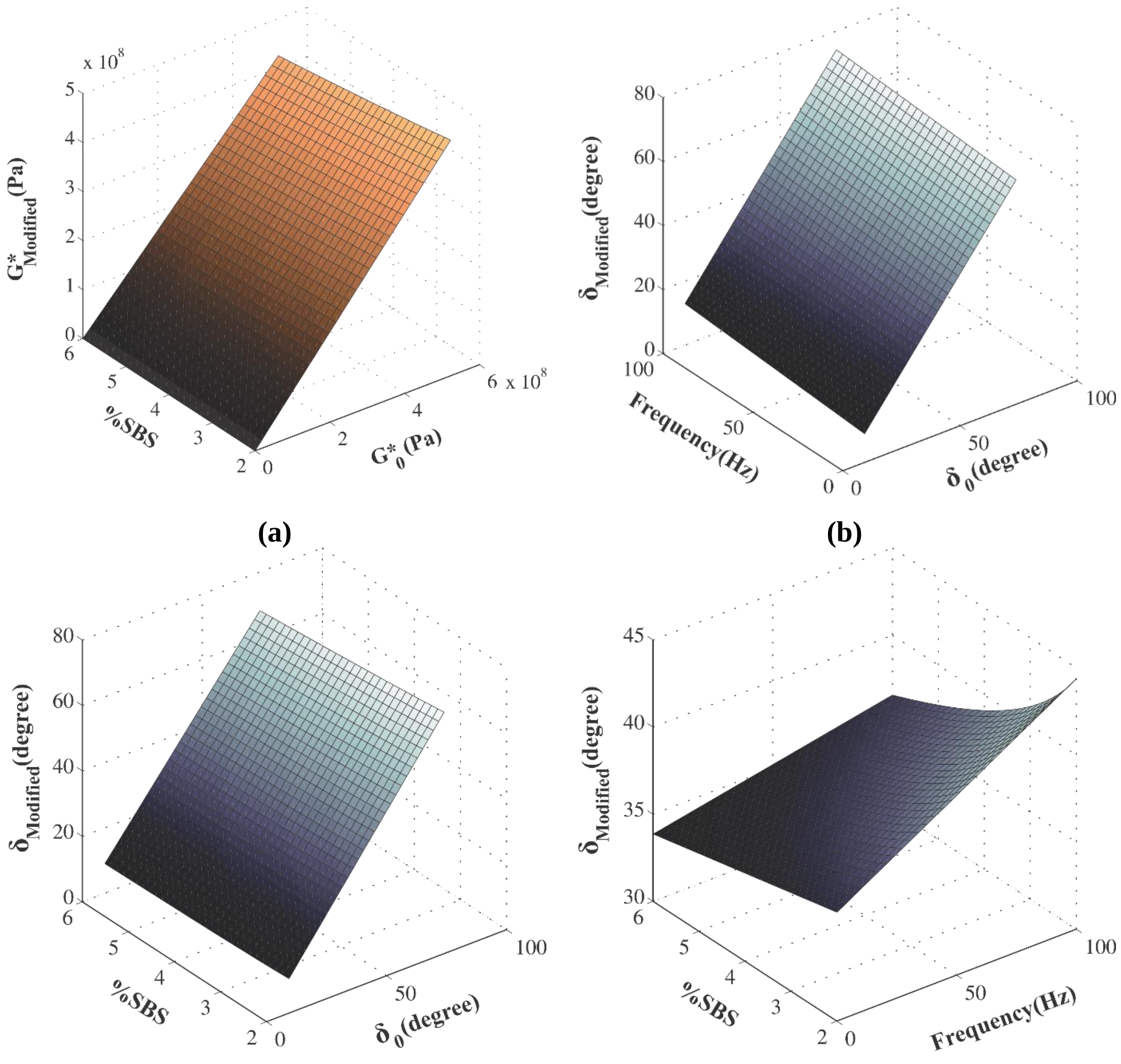
Figure 15-d, increasing the loading frequency changed the decreasing effect of the PPA modifier to an increasing effect. It is reported that adding PPA disturbs the hydrogen-bond network formation in bitumen which results in reduction of the effective molecular weight of asphaltenes accumulated through hydrogen bonds and disruption of the asphaltenes-maltenes equilibrium which can result in such a rheological behavior [34]. It is necessary to mention that the effect of PPA directly depends on the amount of wax and asphaltene of the original bitumen [20]. Overall, the parametric study confirmed that the prediction models (e.g., proposed equations) are capable of capturing the characteristics of the effective input parameters.



(a) (b)

(c) (d)

**Figure 13.** Parametric study of CR-modified bitumen viscoelastic behavior inputs and target parameters in the GEP models. a) Complex shear modulus in modified bitumen vs. unmodified bitumen and additive percentage, b) phase angle in modified bitumen vs. unmodified bitumen and loading frequency, c) phase angle in modified bitumen vs. unmodified bitumen and additive percentage, d) phase angle in modified bitumen vs. loading frequency and additive percentage



**(a)** **(b)**

**(c)** **(d)**

**Figure 14.** Parametric study of SBS-modified bitumen viscoelastic behavior inputs and target parameters in the GEP models. a) Complex shear modulus in modified bitumen vs. unmodified bitumen and additive percentage, b) phase angle in modified bitumen vs. unmodified bitumen and loading frequency, c) phase angle in modified bitumen vs. unmodified bitumen and additive percentage, d) phase angle in modified bitumen vs. loading frequency and additive percentage

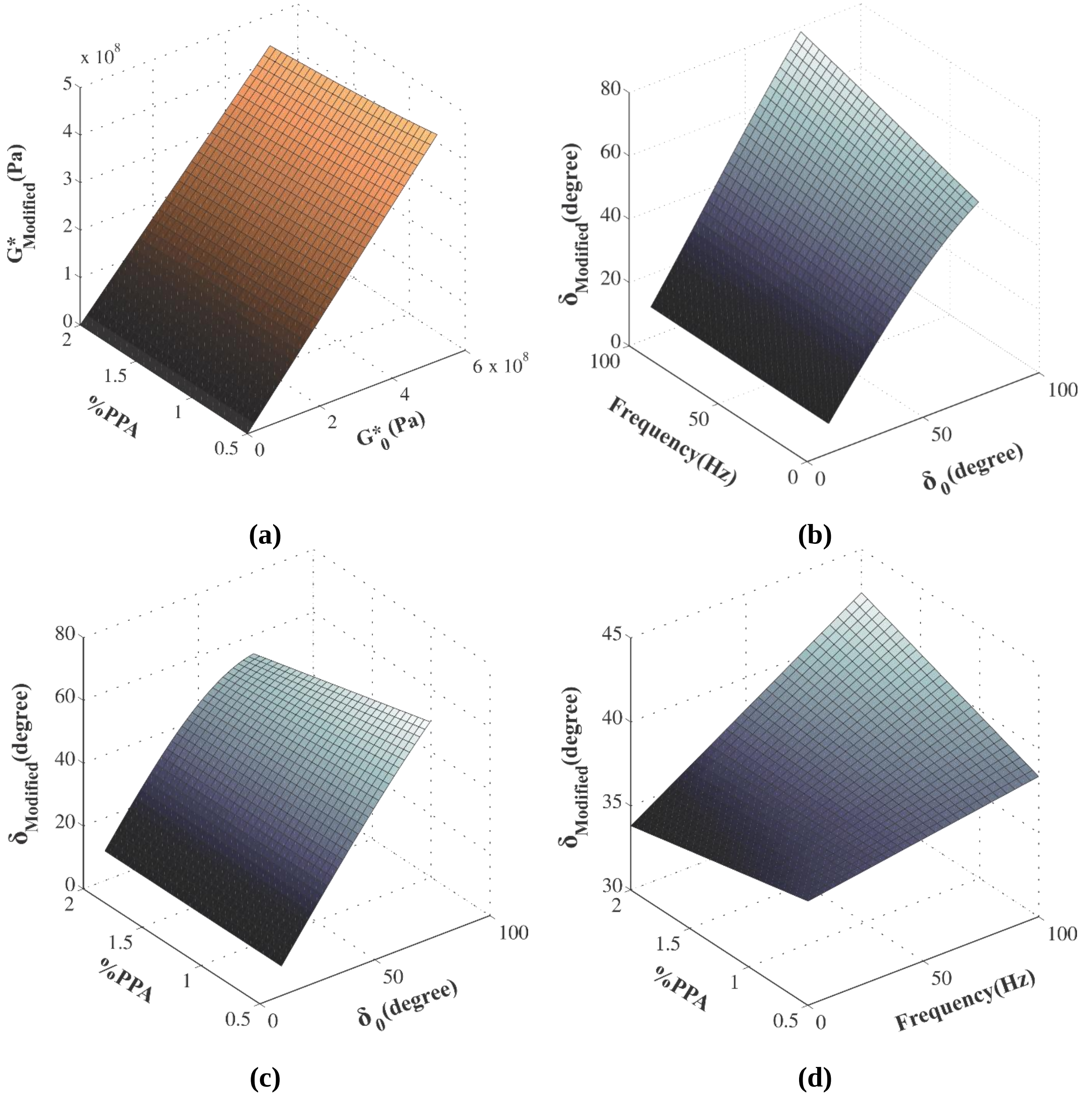


**Figure 15.** Parametric study of PPA-modified bitumen viscoelastic behavior inputs and target parameters in the GEP models. a) Complex shear modulus in modified bitumen vs. unmodified bitumen and additive percentage, b) phase angle in modified bitumen vs. unmodified bitumen and loading frequency, c) phase angle in modified bitumen vs. unmodified bitumen and additive percentage, d) phase angle in modified bitumen vs. loading frequency and additive percentage

The contribution rate of each input parameter was examined by sensitivity analysis. For this, the sensitivity percentage of each output parameter to each contributing input parameter was calculated using the following formulae [35].

$$D_i = f_{\max}(v_i) - f_{\min}(v_i) \tag{12-1}$$

$$S_i = \frac{D_i}{\sum D} \times 100 \tag{12-2}$$

where $S_i$ is the sensitivity percentage of the $i$th parameter and $f_{\min}(v_i)$ and $f_{\max}(v_i)$ are the minimum and maximum values, respectively, of the output calculated from the *i*th input parameter, while the mean value of other parameters were used. Results of the sensitivity analysis are presented in Table 10. It can be seen that the major contribution came from the viscoelastic parameters of the original bitumens (i.e., $G_0^*$ in $G^*$ formulae, and $\delta_0$ in $\delta$ the formulae).

**Table 10.** Results of the sensitivity analysis (in percent) for the input parameters of the GEP models

| Formula | Additive | Input parameter | | | |
|---|---|---|---|---|---|
| | | $G_0^*$ | $\delta_0$ | ω | P |
| G* | CR | 88.8 | _ | _ | 11.2 |
| | SBS | 96.7 | _ | _ | 3.3 |
| | PPA | 98 | _ | _ | 2 |
| δ | CR | _ | 83.6 | 8.8 | 7.6 |
| | SBS | _ | 89.3 | 5.9 | 4.8 |
| | PPA | _ | 88 | 9.3 | 2.7 |

## 7. Summary and Conclusion

GEP, which is a robust and natural development of traditional GP, was used to develop formulae that can be used to predict the complex shear modulus and phase angle of modified asphalt bitumen. The input data consisted of results of an experimental program conducted on three different additives, namely crumb rubber, SBS, and PPA. It is necessary to mention that all experiments were performed at a low strain amplitude (0.01%), and consequently, all derived equations are valid for the linear viscoelastic behavior of modified bitumens. The validity and robustness of the formulae were investigated using various statistical indices for error calculation and other well-known criteria. Also, an external validation analysis was conducted in order to examine the performance of the proposed formulae against an unseen set of data. Moreover, a parametric study was performed that investigated the effect of each input parameter on model predictions and, through a sensitivity analysis, the level of dependency of the output parameters on each of the inputs was studied. It was generally found that the complex shear modulus and phase angle of modified bitumen were dependent mainly on the viscoelastic parameters of the original bitumen, rather than other parameters. Also, to provide additional insight into the meaningfulness of the derived formulae, results of the parametric study that evaluated the effect of the corresponding input variables on the target parameters were presented in the form of three-dimensional surface diagrams. These relationships were interpreted and compared with the experimental trends, which showed that the trend of GEP formulation is consistent with the material behavior observed in the tests.

## 8. Future Research Work

This research work presented a GEP model that can be used to predict complex shear modulus (G*) and phase angle (δ) as two constitutive parameters of bitumen modified with crumb rubber, SBS, and PPA, and three closed-form equations were derived for these additives. However, two main issues should be considered for future research works: 1) using original bitumens from different sources, and 2) running experiments under different test conditions. Original bitumens from different sources can be used to incorporate additional parameters into the prediction model; e.g., asphaltene or maltene content. Additionally, it is possible to run frequency sweep tests at temperatures higher than 22°C and applying strain that is greater than 0.01% in order to involve more testing conditions for predicting modified bitumen characteristics over a wide range of temperature and loading rates.

# 9. References

[1] S. Aflaki and N. Tabatabaee, “Proposals for modification of Iranian bitumen to meet the climatic requirements of Iran,” *Constr. Build. Mater.*, vol. 23, no. 6, pp. 2141–2150, 2009, doi: https://doi.org/10.1016/j.conbuildmat.2008.12.014.

[2] Y. Yildirim, “Polymer modified asphalt binders,” *Constr. Build. Mater.*, vol. 21, no. 1, pp. 66–72, 2007, doi: https://doi.org/10.1016/j.conbuildmat.2005.07.007.

[3] K. B. Vural, Y. Mehmet, and G. Alaaddin, “Evaluation of Low-Temperature and Elastic Properties of Crumb Rubber– and SBS-Modified Bitumen and Mixtures,” *J. Mater. Civ. Eng.*, vol. 25, no. 2, pp. 257–265, Feb. 2013, doi: 10.1061/(ASCE)MT.1943-5533.0000590.

[4] A. H. Gandomi, S. K. Babanajad, A. H. Alavi, and Y. Farnam, “Novel approach to strength modeling of concrete under triaxial compression,” *J. Mater. Civ. Eng.*, vol. 24, no. 9, pp. 1132–1143, 2012.

[5] C. Ferreira, “Gene expression programming: a new adaptive algorithm for solving problems,” *arXiv Prepr. cs/0102027*, 2001.

[6] A. H. Gandomi, A. H. Alavi, and C. Ryan, *Handbook of genetic programming applications*. Springer, 2015.

[7] A. Gholampour, A. H. Gandomi, and T. Ozbakkaloglu, “New formulations for mechanical properties of recycled aggregate concrete using gene expression programming,” *Constr. Build. Mater.*, vol. 130, pp. 122–145, 2017, doi: https://doi.org/10.1016/j.conbuildmat.2016.10.114.

[8] J. Liu, K. Yan, L. You, P. Liu, and K. Yan, “Prediction models of mixtures’ dynamic modulus using gene expression programming,” *Int. J. Pavement Eng.*, vol. 18, no. 11, pp. 971–980, Nov. 2017, doi: 10.1080/10298436.2016.1138113.

[9] A. Eleyedath and A. K. Swamy, “Prediction of density and viscosity of bitumen,” *Pet. Sci. Technol.*, vol. 36, no. 21, pp. 1779–1786, 2018.

[10] A. R. Azarhoosh, Z. Zojaji, and F. Moghadas Nejad, “Nonlinear genetic-base models for prediction of fatigue life of modified asphalt mixtures by precipitated calcium carbonate,” *Road Mater. Pavement Des.*, vol. 21, no. 3, pp. 850–866, 2020.

[11] B. V. Kok, M. Yilmaz, B. Sengoz, A. Sengur, and E. Avci, “Investigation of complex modulus of base and SBS modified bitumen with artificial neural networks,” *Expert Syst. Appl.*, vol. 37, no. 12, pp. 7775–7780, 2010, doi: https://doi.org/10.1016/j.eswa.2010.04.063.

[12] N. I. M. Yusoff, D. Ibrahim Alhamali, A. N. H. Ibrahim, S. A. P. Rosyidi, and N. Abdul Hassan, “Engineering characteristics of nanosilica/polymer-modified bitumen and predicting their rheological properties using multilayer perceptron neural network model,” *Constr. Build. Mater.*, vol. 204, pp. 781–799, 2019, doi: https://doi.org/10.1016/j.conbuildmat.2019.01.203.

[13] S. Han, Z. Zhang, Y. Yuan, and K. Wang, “Prediction of asphalt complex viscosity by artificial neural network based on Fourier transform infrared spectroscopy,” *Pet. Sci. Technol.*, vol. 37, no. 14, pp. 1731–1737, Jul. 2019, doi: 10.1080/10916466.2019.1605377.

[14] D. Lo Presti, “Recycled tyre rubber modified bitumens for road asphalt mixtures: A literature review,” *Constr. Build. Mater.*, vol. 49, pp. 863–881, 2013.

[15] T. Wang, F. Xiao, S. Amirkhanian, W. Huang, and M. Zheng, “A review on low temperature performances of rubberized asphalt materials,” *Constr. Build. Mater.*, vol. 145, pp. 483–505, 2017.

[16] S. Liu, W. Cao, J. Fang, and S. Shang, “Variance analysis and performance evaluation of different crumb rubber modified (CRM) asphalt,” *Constr. Build. Mater.*, vol. 23, no. 7, pp. 2701–2708, 2009, doi: https://doi.org/10.1016/j.conbuildmat.2008.12.009.

[17] S. Aflaki, P. Hajikarimi, E. H. Fini, and B. Zada, “Comparing effects of biobinder with other asphalt modifiers on low-temperature characteristics of asphalt,” *J. Mater. Civ. Eng.*, vol. 26, no. 3, 2014, doi: 10.1061/(ASCE)MT.1943-5533.0000835.

[18] B. Sengoz and G. Isikyakar, “Evaluation of the properties and microstructure of SBS and EVA polymer modified bitumen,” *Constr. Build. Mater.*, vol. 22, no. 9, pp. 1897–1905, 2008, doi: https://doi.org/10.1016/j.conbuildmat.2007.07.013.

[19] D. Fee, R. Maldonado, G. Reinke, and H. Romagosa, “Polyphosphoric acid modification of asphalt,” *Transp. Res. Rec.*, vol. 2179, no. 1, pp. 49–57, 2010.

[20] N. Baldino, D. Gabriele, C. O. Rossi, L. Seta, F. R. Lupi, and P. Caputo, “Low temperature rheology of polyphosphoric acid (PPA) added bitumen,” *Constr. Build. Mater.*, vol. 36, pp. 592–596, 2012, doi: https://doi.org/10.1016/j.conbuildmat.2012.06.011.

[21] S. Aflaki and P. Hajikarimi, “Implementing viscoelastic rheological methods to evaluate low temperature performance of modified asphalt binders,” *Constr. Build. Mater.*, vol. 36, 2012, doi: 10.1016/j.conbuildmat.2012.04.076.

[22] H. F. Brinson and L. C. Brinson, *Polymer engineering science and viscoelasticity: An introduction*. Springer, 2008.

[23] K. Santosh and Y.-R. Kim, “Investigation of DSR Test Methods to Determine Binder Low Temperature Properties,” 2019.

[24] J. R. Koza, *Genetic programming: on the programming of computers by means of natural selection*, vol. 1. MIT press, 1992.

[25] A. H. Gandomi, A. H. Alavi, M. R. Mirzahosseini, and F. M. Nejad, “Nonlinear genetic-

based models for prediction of flow number of asphalt mixtures," *J. Mater. Civ. Eng.*, vol. 23, no. 3, pp. 248–263, 2011.

[26] A. H. Alavi and A. H. Gandomi, "A robust data mining approach for formulation of geotechnical engineering systems," *Eng. Comput. Int J Comput. Eng.*, vol. 28, no. 3, pp. 242–274, 2011.

[27] GEPSOFT, "GeneXpro tools," *GEPSOFT*, p. Bristol., 2006.

[28] I. E. Frank and R. Todeschini, *The data analysis handbook*. Elsevier, 1994.

[29] G. N. Smith, "Probability and statistics in civil engineering," *Collins Prof. Tech. books*, vol. 244, 1986.

[30] A. Golbraikh and A. Tropsha, "Beware of q2!," *J. Mol. Graph. Model.*, vol. 20, no. 4, pp. 269–276, 2002.

[31] P. Hajikarimi, M. Rahi, and F. Moghadas Nejad, "Comparing different rutting specification parameters using high temperature characteristics of rubber-modified asphalt binders," *Road Mater. Pavement Des.*, vol. 16, no. 4, pp. 751–766, 2015.

[32] F. M. Nejad, M. Shahabi, M. Rahi, P. Hajikarimi, and S. Kazemifard, "An investigation on the effect of SBS+vacuum bottoms residue modification on rheological characteristics of asphalt binder," *Pet. Sci. Technol.*, vol. 35, no. 22, 2017, doi: 10.1080/10916466.2017.1384839.

[33] A. Samieadel and E. H. Fini, "Interplay between wax and polyphosphoric acid and its effect on bitumen thermomechanical properties," *Constr. Build. Mater.*, vol. 243, p. 118194, 2020.

[34] J. F. Masson and M. Gagné, "Polyphosphoric acid (PPA)-modified bitumen: disruption of the asphaltenes network based on the reaction of nonbasic nitrogen with PPA," *Energy & fuels*, vol. 22, no. 5, pp. 3402–3406, 2008.

[35] A. H. Gandomi, G. J. Yun, and A. H. Alavi, "An evolutionary approach for modeling of shear strength of RC deep beams," *Mater. Struct.*, vol. 46, no. 12, pp. 2109–2119, 2013.