UGOCHUKWUGEORGE ISIENYI

PPLICATION OF DATA-DRIVEN MODELS FOR MODELINGCOMPLEX MODULUS AND PHASE ANGLE OF POLYMER NANOCOMPOSITE MODIFIED BITUMEN

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A THESIS SUBMITTED TO THE GRADUATE SCHOOL OF APPLIED SCIENCES OF NEAR EAST UNIVERSITY

By
UGOCHUKWU GEORGE ISIENYI

In Partial Fulfillment of the Requirements for the Degree of Master of Science

in

Civil and Environmental Engineering

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Approval of Director of Graduate School of Applied Sciences

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I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

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ABSTRACT

The performance of bituminous pavement is dependent on the physical and rheological characteristics of asphalt binders, which are strongly influenced by the loads imposed by vehicular traffic and climatic conditions. In this study, six different blends including base binder, polymer modified binder (%5 ASA by the weight of bitumen), and two different polymer nanocomposite materials, ASA-Nano calcium and ASA-Nano copper at 3% and 5% concentrations by the weight of bitumen, were characterized for rheological properties using a dynamic shear rheometer (DSR). Complex shear modulus (G*) and phase angle (δ) were the two parameters revealed in the DSR oscillation tests. within the scope of this research, prediction of G* from physical and rheological properties of binders and the mechanical test conditions were performed using analytical approaches, namely an artificial neural network (ANN) and an adaptive neuro-fuzzy inference system (ANFIS). Coefficient of determination (R^2) and root mean squared error (RMSE) was used as the performance indicator metrics in the evaluation of the performance of the analytical models. The results of this study demonstrated that polymer and polymer nanocomposite material modification enhanced the rheological behaviour of the asphalt binder. Furthermore, the ANN and ANFIS models for predicting the outcomes of the DSR test results have been shown to be reliable with both training and testing datasets. An R^2 value of 0.9960 and an RMSE value of 0.008295 were observed for the testing dataset, which indicated that both ANN and ANFIS models were able to predict G* with high accuracy, with ANN being the analytical model with the more efficient performance.

***Keywords*:** Dynamic shear rheometer; complex shear modulus; polymer modified bitumen, polymer nanocomposite; artificial neural network; adaptive neuro-fuzzy inference system

ÖZET

Bitümlü kaplamaların performansı, taşıt trafiği ve iklim koşulları tarafından uygulanan yüklerden kuvvetli bir şekilde etkilenen asfalt bağlayıcıların fiziksel ve reolojik özelliklerine bağlıdır.Bu çalışmada, baz bağlayıcı, polimer modifiyeli bağlayıcı (bitüm ağırlığına göre% 5 ASA) ve iki farklı polimer nanokompozit malzeme, ASA-Nano kalsiyum ve ASA-Nano bakır dahil olmak üzere altı farklı karışım; bitümün ağırlığı, dinamik kesme reometresi (DSR) kullanarak reolojik özellikler için karakterize edildi.Kompleks kayma modülü (G *) ve faz açısı (δ) DSR salınım testlerinde ortaya konan iki parametredir.Bu araştırmada G * 'nin bağlayıcıların fiziksel ve reolojik özelliklerinden öngörülmesi ve Mekanik test koşulları analitik yaklaşımlar kullanılarak yapıldı, yani artificial neural network (ANN) ve adaptive neuro-fuzzy inference system (ANFIS). Analitik modellerin performansının değerlendirilmesinde belirleme katsayısı (R2) ve kök ortalama kare hatası (RMSE) performans gösterge ölçütleri olarak kullanılmıştır. Bu çalışmanın sonuçları, polimer ve polimer nanokompozit malzeme modifikasyonunun, asfalt bağlayıcı maddenin reolojik davranışını arttırdığını göstermiştir. Ayrıca, DSR test sonuçlarının sonuçlarını tahmin etmeye yönelik ANN ve ANFIS modellerinin hem eğitim hem de test veri setleri için güvenilir olduğu gösterilmiştir. Test veri seti için 0.9960'lık bir R2 değeri ve 0.008295'lik bir RMSE değeri gözlendi, bu hem ANN hem de ANFIS modellerinin G * 'yi yüksek doğrulukla tahmin edebildiğini gösterdi, ANN daha verimli performansa sahip analitik modeldir.

Anahtar kelimeler : Dinamik kesme reometresi; karmaşık kayma modülü; polimer modifiyeli bitüm; polimer nanokompozit; artificial neural network; adaptive neuro-fuzzy inference system

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LIST OF ABBREVIATIONS

ANFIS:	Adaptive neuro-fuzzy inference system
ANN:	Artificial neural network
ASTM D36:	Standard test method for softening point of bitumen
ASTM D5:	Standard test method for penetration of bituminous materials
BBR:	Bending beam rheometer
BPNN:	Back Propagation neural network
CGP:	Pola- Ribiere conjugate gradient
CNT:	Carbon nanotube
CRM:	Crumb rubber modified
DSR:	Dynamic Shear Rheometer
DTT:	Direct tension
EVA:	Ethylene-vinyl acetate
FFMLP:	Feedforward multilayer perceptron
G*:	Complex shear modulus
HSC:	High-strength concrete
KKT:	Karush-Kuhn-tucker
LCPC:	Laboratories Central des Ponts et Chaussées
LM:	Levenberg-Marquardt
L-SVM:	Linear support vector regression
MILP:	Multilayer perceptron neural network
MLR:	Multi-linear regression
NR:	Natural rubber

NSC:	Normal strength
N-SVM:	Non-linear support vector regression
PAV:	Pressure aging vessel
PMAC:	polymer modified asphalt cement
R^2:	Coefficient of determination
RBF:	Radial basis function
RMSE:	Root mean squared error
RTFO:	Rolling thin film oven
SBS:	Styrene-butadiene-styrene
SCG:	Scaled conjugate gradient
SLR:	Simple linear regression
SVM:	Support vector machine
VTS:	Viscosity–temperature-susceptibility
WLF:	Williams–Landel–Ferry
δ:	Phase angle

CHAPTER 1
INTRODUCTION

1.1 Introduction

Bitumen is considered to a dark brown colored hydrocarbon obtained as a byproduct of distillation of crude oil, is mostly used in pavement construction due to its viscoelastic and adhesive properties, (Kok, Yilmaz, Sengoz, Sengur, & Avci, 2010). Bitumen is made of complex mixtures of aromatic, aliphatic and naphthenic hydrocarbons with a small amount of metallorganic and other organic (Yilmaz, Kok, Sengoz, Sengur, & Avci, 2011). Bitumen can be considered as one of the oldest engineering materials in the world, have been used since the beginning of civilization in many different fields, for example in electrical industry by mixing the high-grade Bitumen with wood tar, pitch, rubber, and resin, also in construction field in roll roofing , bridges, dams, and reservoirs because it helps to preserve and waterproof (Speight, 2015), and as mentioned in previous it is widely used in pavement construction it is preferred choice due to the smooth surface which provides to the road, therefore it increases the safety for driver, and more economy by reducing the rolling resistance, which means better fuel economy and it reduce carbon dioxide emissions which means for the environment more friendly (West & MADISON, 2005).

Bitumen is highly temperature susceptible which means its physical and chemical properties change when subjected to various temperature conditions (Kim, 2008). Also, viscoelastic substances like Bitumen are not behaving directly, regarding some of their properties such as stiffness which act as a function of strain or stress. (Yusoff, Breem, Alattug, Hamim, & Ahmad, 2014). In performance grading specifications Bitumen is characterized by its physical and the above-mentioned rheological properties. There are different types of tests must be conducted to the asphalt binders in order to find out the properties of it. It can be classified as: Direct Tension (DTT), Bending Beam Rheometer (BBR), Rolling Thin Film Oven (RTFO), Pressure Aging Vessel (PAV), and Dynamic Shear Rheometer (DSR) etc.

Dynamic Shear Rheometer (DSR) is used in the assessment of rheological properties of asphalt binders at intermediate and high temperatures. Dynamic shear modulus (G*) which is considered as the material's resistance to deformation under repeated shear loading and the phase angle (δ) which is defined as the lag between the applied shear stress and the resulting shear strain are the two parameters revealed upon oscillatory shear testing performed by DSR(Abedali, 2015). These parameters are further used in the assessment of rutting and fatigue resistance which are the most common modes of failures in asphalt pavement. It is favorable that, asphalt binders demonstrate stiff behavior at high temperatures and low frequencies and elastic behavior at low temperatures and high frequencies in order to prevent rutting and fatigue failures (Bala, Napiah, & Kamaruddin, 2018).

Due to the limitations of Bitumen regarding the temperatures, various types of modifiers such as plastic, polymers, and Nano-materials were added to the base asphalt to improve the performance of the asphalt mixture (Cuadri, Partal, Navarro, García-Morales, & Gallegos, 2011b), therefore in order to improve rheological properties, asphalt modification with polymeric materials is a common practice and referred to as polymer modified asphalt cement (PMAC). An advantage of PMAC is that they are available and research and field tested (Ezzat, El-Badawy, Gabr, Zaki, & Breakah, 2016). Polymers can be sub-grouped as elastomers and plastomers. Elastomers are favorable modifiers of AC at low temperatures, where plastomers are more suitable modifiers at high temperatures (Zhu, Birgisson, & Kringos, 2014). The polymer which used as a modifier forBitumen is consist of Styrene-Butadiene-Styrene (SBS), Ethylene-vinyl acetate (EVA), Natural rubber (NR) and Polypropylene (PP) (Al-Mansob et al., 2014; Habib, Kamaruddin, Napiah, & Isa, 2011; Sengoz & Isikyakar, 2008; Yildirim, 2007).

On the other hand, polymers are expensive and some of them have proven to have an insignificant improvement in the performance of AC due to the incompatibility of polymer with the base binder (Golestani, Nam, Nejad, & Fallah, 2015). Due to shortcomings of PMACs, nanomaterials have been introduced as an alternative to polymer modified bitumen. Unique properties of nanomaterials such as high surface work, a large fraction of surface atoms, structural features, quantum effects, and spatial confinement are some of the features that promote the improvement of binder properties in terms of stiffness and also leads to higher temperature susceptibility and improved strength of bitumen against moisture damage (Saltan, Terzi, & Karahancer, 2018). Nanomaterials have also shown to enhance the incompatibility problem of polymer and Bitumen, associated with the occurrence of phase separation. Common nanomaterials used in this purpose includenano silica, nanoclay and carbon nanotubes (Ezzat et al., 2016; Yang & Tighe, 2013; Ziari, Amini, Goli, & Mirzaeiyan, 2018). According to previous studies in the literature, enhancement in the performance of bitumen modified with nanomaterials in terms of improved complex modulus and reduced phase angle have indicated that better rutting resistance performance is achieved (Xiao, Amirkhanian, & Amirkhanian, 2010) However, the field of nanomaterial in the bitumen modification still requires a significant amount of research before field application.

By a review for a recent works it can be noticed that an increasing trend of applying data driven models including artificial intelligence (AI) method such as Multilayer Perceptron Neural Network (MILP), Genetic programming (GP), Artificial Neural Network (ANN), Support Vector Machine (SVM) based the precision as well the productivity of the needed work on the area of pavement. Performance of nanomaterial modified bitumen have also been acknowledged in the literature by a limited number of studies (Firouzinia & Shafabakhsh, 2018; Ziari et al., 2018). However, asphalt binders modified with polymer nanocomposite materials have been only limited to be addressed by experimental investigations and tangibility of ANN and ANFIS modeling in this matter requires further study. Therefore this basis computational models, Artificial Neural were implemented in this study using physical properties of, bitumen modified with polymer and polymer nanocomposites at various concentrations and test conditions as predictor and the performance characteristics indicator, complex modulus (G*) as the predicted variable. ANN is a data driven framework inspired by the way biological neurons work. ANN modelshave the ability and capacity of solving issues through using information that was generated from previous experience and then applied to current and new studies or problems ANN has been previously used in the modeling of some significant parameters of pavement materials with the purpose of obtaining reliable analytical solutions to assist in experimental investigations. Complexity in the behavior of pavement materials are further escalated with the use of modified binders and on this basis, ANN, a nonlinear nonparametric modeling technique that offers a high degree of accuracy to solve complex nonlinear relationship problems has been gaining the attention of researchers in the field of material science and pavement engineering. Some studies devoted to ANN modeling of polymer modified binders include (Golzar, Jalali-Arani, & Nematollahi, 2012; Specht, Khatchatourian, Brito, & Ceratti, 2007; Tapkın, Çevik, & Uşar, 2009).

Therefore, many researchers have attempted to develop mathematical models to predict performance characteristics of AC in order to assist with the experimental procedures. As acknowledged in the literature, physical and chemical properties of asphalt binders have strong influence on the performance characteristics of AC. However, most of the mathematical and conventional linear models employed have several drawbacks and capture only the linear process. In another hand, the process of polymer and nanocomposite modified bitumen is highly nonlinear and there need to introduce a non-linear model to achieve the satisfactory accuracy. Rather, test conditions such as temperature and frequency were highly correlated with the performance characteristics. However, computational models such as, Artificial Neural Networks (ANN) and Adaptive Neuro- Fuzzy Inference System (ANFIS) models were implemented were used by several researchers. In the other hand, this thesis proposes the application of three different data-driven algorithms, including Back Propagation Neural network (BPNN) Support vector machine (SVM) and multi-linear regression (MLR) analysis to predict complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen using different model input combinations.

1.2 Problem Statement

In the field of pavement construction, to improve the quality of asphalt mixture varies modifiers like polymers and Nano-materials were used. Due to the high cost of some materials and leakage in laboratory equipment which has a high cost as well. That leads to a limited number of studies that have been acknowledging the performance of modified bitumen with nanomaterial (Firouzinia & Shafabakhsh, 2018; Ziari et al., 2018). It can be noticed that the field of nanomaterial in the bitumen modification still requires significant amount of research before field application, while most of the studies which have beendone to asphalt binders modified with polymer nanocomposite materials are limited to be addressed by experimental investigations of ANN and ANFIS modeling in this matter requires further study. Therefore, these computational models were implemented in this study using physical properties of, bitumen modified with polymer and polymer nanocomposites at various concentrations and test conditions as predictor and the performance characteristics indicator, complex modulus (G*) as the predicted variable to find out the behavior of Bitumen modified with polymer and polymer nanocomposite materials.

1.3 The objective of the study

The objectives of the study are to:

- To have a brief understanding on the application of data driven model viz: SVM, BPNN and traditional Multilinear Regression analysis (MLR).
- To employed the SVM, BPNN and MLR model to predict the complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen

- To develop a comparison study between the SVM, BPNN and traditional Multilinear Regression analysis (MLR) and the experimental results.

1.4 Significant of study

Due to the outflow of the studies that have been discussed the performance of modified bitumen with nanomaterial and the studies which have been conducted to asphalt binders modified with polymer nanocomposite materials are limited to be addressed only by experimental test therefor the results of the study will be of great benefit to the pavement field by finding the viscoelastic properties of modified asphalt cement at elevated temperatures and frequencies using Support Vector Machine (SVM), Back Propagation Neural Network (BPNN) and traditional Multilinear Regression analysis (MLR) models in the prediction process and showing the capability and efficiency of this applications to deal with Complex behavior of pavement materials.

1.5 Thesis Organization

- Chapter one is explaining the introduction about the topic, problems statement as well as the objectives of the research
- Chapter two is addressing the previous researches that were conducted on or related to the study area
- Chapter three is providing in detail the methods and procedures that carried on to achieve the objectives of the study
- Chapter for discusses the results of the research
- Chapter five is about the conclusion, recommendation and future studies

CHAPTER 2
LITERATURE REVIEW

2.1 Introduction

Bituminous materials are a hydrocarbon which obtained as a product of the distillation of crude petroleum or found in natural deposits (Read & Whiteoak, 2003).All bituminous materials consist primarily of bitumen and have strong adhesive properties, it has the capacity adhere to a solid surface in a fluid stat depending on the surface's nature, while the adhesion could be prevented by adding water to surface, therefore the Bitumen is water resistant, the flow or viscous properties of bitumen change according to stress and temperature conditions. The failure, or loss of the desirable properties of bitumen, can be noticed it takes the form of hardening. Resultantly, a decrease in flow and adhesive properties and an increase in the coefficient of thermal expansion and the softening point temperature (Mochinaga et al., 2006). All bituminous materials have colors ranging from dark brown to black. Also, asphalts are thermoplastic materials, meaning that they liquefy when heated and solidify when cooled (Ali et al., 2017). To check the efficiency of the Asphalt in the site, designing the physical properties of the binders is very fundamental. There to find out the properties of Asphalt the following testing methods are carried out: Direct Tension (DTT), Pressure aging vessel (PAV), Rolling Thin film Oven (RTFO), and Bending Beam Rheometer (BBR) etc.

2.2 Classification Of Different Types Of Bitumen

Bitumen has been used since the old civilization until now due to its natural resources, it can be used in the different field for humans needs such as waterproofing in sealing flat roofs and roofing felt, while most of the Bitumen produced used in pavement field due to the following reasons (Yildirim, 2007):

- Production of Bitumen is economical
- Rheological and Physical Properties of it bring Versatility
- Bitumen melts at a low point

- Bitumen can be Recycled
- Bitumen increase Adhesive Nature
- Bitumen has a diversity Colors

The specification of Bitumen to displays the safety, disparity with the durability, physical properties, and the solubility. The Bitumen can be categorized into the following grade types:

2.2.1 Penetration grade bitumen

Penetration grade Bitumen, these is a kind of refinery bitumen which is manufactured at various viscosity. Usually the penetration analysis is done in order to characterize the bitumen according to its hardness. And hence called penetration bitumen. Penetration grades ranges from 15-450 for road asphalt. Though, the commonly used range is between 25-200. This can be achieved through the distillation procedure control test. The needed hardness may be acquired through the application of partial control fluxing the residual Bitumen with the oils (Read & Whiteoak, 2003).

2.2.2 Oxidized bitumen

The filter Bitumen is further managed by inserting the produced air. The way the oxidized Bitumen is produced. By preserving an adjusted temperature, the air is inserted under pressure into smooth Bitumen.by the reaction of the components of Bitumen and this introduced oxygen, a Compounds of higher molecular weight are formed. The Maltenes and the Asphaltenes content helps in increasing the harder mix. The mix which has a temperature sensitivity and a less ductility. This type of Bitumen is commonly used in manufacturing fields such as covering forpipes and ceiling. By this way of producing, the Bitumen which has a less penetration can be produced, it can be used in the pavement(Loeber, Muller, Morel, & Sutton, 1998).

2.2.3 Cutback bitumen

This type is called to the Bitumen when it has a grade less than penetration grade, it has a decreased viscosity for a specific time by inserting of volatile oil. the Bitumen gain back its normal viscosity when the volatile materials are evaporated after the application. The penetration grade Bitumen can be classified as a thermoplastic material. It demonstrates the various value of viscosity for various temperature. In the site of the road industry, it is requisite for the materials to be a liquid shape in surface dressing phase. By cutback asphalt, the material can earn back its normal rigidity after casting. By increasing the temperature, the liquidity can be for any Bitumen. cutback Bitumen is used when there is a need to have fluidity for any Bitumen at lower temperatures in the surface dressing phase (Lamperti, 2011).

2.2.4 Bitumenemulsion

This kind of Bitumen has 2 phase system with 2 immiscible fluids. The first one is scattered like specific globules included in the other fluid. This kind of Bitumen is obtained once the separate globules of bitumen are separated from a continuous form of water. An emulsifier having a long hydrocarbon series with an anionic or cationic ending is applied for receding the Bitumen globules. This type supplies an electrochemical climate. The ionic section of the series has an attraction to the water and the Bitumen is attracted by hydrocarbon section. This Bitumen is conducted by using sprays also the viscosity has the main attention. when the content of the Bitumen is increased, the viscosity of the mixture increased. The stability of emulsions relies on the Water evaporation rate, the types of Bitumen emulsifier and its quantity, the Mechanical forces, and the Bitumen globules size (Brown & Needham, 2000).

2.3 Pavement Distresses

The pavement may face Too many distress some of them may occur according to the chemical and physical properties of the asphalt binder, while the other may occur by the weather conditions and the loads which applied by the tracks. the distresses are as the following:

2.3.1 Fatigue

(Alligator) Cracking: is the principal structural distress, the layer materials and thicknesses of pavement, applied loads the consistency of the asphalt cement, the Bitumen content and the air voids and aggregate characteristics of the asphalt concrete mix are the factors which affect the development of fatigue(El-Basyouny & Witczak, 2005).

2.3.2 Bleeding

This refers to the accumulation of asphalt cement material around the surface of pavement. It starts accumulating by an individual drop and subsequently aggregate into a sticky and shiny film. Bleeding shows surface friction which can be considered as a potential safety hazard. Bleeding occurs as a result of insufficient mixing between the cement and air which creates a void as the asphalt cement is expanding (Xu & Huang, 2012).

2.3.3 Block cracking

Block Cracking is a crack of an asphalt pavement which takes a rectangular shape. It is related to the use of an asphalt cement which is or has become too stiff for the climate. Block cracking caused by shrinkage of the asphalt concrete in response to low temperatures, and progress from the surface of the pavement downward (Adlinge & Gupta, 2013).

2.3.4 Frost heave

Frost heave It happens in freezing climates, in frost-susceptible soils when enough water is available. When the temperature in the soil reaches the freezing point, this water freezes and becomes ice lenses, which will be thicker. The progressive growth process of these ice lenses is still continuing as additional water is drawn to the freezing front that produces the dramatic raising of the road surface known as frost heave(Johanneck & Khazanovich, 2010).

2.3.5 Pothole

Pothole: is a bowl-shaped hole through one or more layers of the asphalt pavement structure, between 15 cm to 90 cm in diameter. Potholes start to form when crumbs of asphalt concrete are displaced by traffic wheels, in fatigue-cracked areas. Potholes increase in depth and size as water present in the hole and penetrate into the base and subgrade, which increase weakness in the vicinity of the pothole (Koch, Jog, & Brilakis, 2012).

2.3.6 Raveling

Raveling is occurred by the continued infiltration of water and the break downing of an asphalt top layer. When the water is presented on the top layer of asphalt bitumen and sunlight will start to damage the asphalt surface by breaking the bond between the aggregate and asphalt bitumen. it will affect the asphalt surface losing its impermeable properties and will let water enter the surface. When water begins to enter into an asphalt surface it will lead to further cracks then the pavement failure occurs (Adlinge & Gupta, 2013).

2.3.7 Rutting

Rutting is channeled depressions in asphalt surface. When the deformation takes a place only in the asphalt concrete it may occur by plastic flow or consolidation. Asphalt cement stiffness is a big influence for rutting resistance of asphalt mixes while the Stiffer asphalt cement can increase rutting resistance (Xiao, Amirkhanian, & Juang, 2007).

2.4 Modification of Asphalt

The asphalt road’s problems have a negative impact on the safe side for humans and to the economic side for the government especially for developing countries where financial resource for pavement maintenance is often insufficient and due to the limitations of bitumen regarding the temperatures, modification of bitumen is one of the best ways to improve the properties of bitumen various types of modifiers such as polymers, plastic, still slag, glass, were added to the base asphalt to improve the performance of the asphalt mixture (Cuadri, Partal, Navarro, García-Morales, & Gallegos, 2011a).

The usage of modified asphalt gives the ability to control the limits of mechanical stability of road surfacing by enhancing the properties of some types of surfacing during a hard extremely conditions of services (Sarsam & Lafta, 2014). By using modifiers with asphalt showed increasing in performance by raising the cohesion of the bitumen, and increase the viscosity and decrease the thermal capability of the binder (Al-Khateeb & Al-Akhras, 2011). Some studies conducted that by using a minimum of 10% of modified bitumen leads to longer enduring streets with better execution (Sabadra, 2017).

Many studies conducted to modified asphalt and it concluded that by adding modifiers to asphalt its heat and strength resistance to reach the double and that leads to improving the shearing resistance it also showed that the density of modified asphalt is more than density of the base asphalt and it gains by increasing the content of modifiers so the water saturation, respectively, reduces (Kishchynskyi, Nagaychuk, & Bezuglyi, 2016). Sarsamand Lafta studied different type of modified asphalts to find out the physical properties of it and, obtained result showed that by adding the modifiers to the base asphalt, the penetration value of asphalt cement decreased, while the Softening point of asphalt cement gained and Ductility of asphalt cement decreased (Sarsam & Lafta, 2014).

2.4.1 Polymer materials modified asphalt

The polymer is a chemical compound with molecules and bond together to create a long repeating chain. It can be used in a different field due to its unique properties (Sabadra, 2017). Polymers widely used as a modifiers for binder it can be classified as the following: plastomers, thermoplastic elastomers, and reactive polymer, it has the ability to enhance the thermal capability of asphalt binders, each one of them has its particular impact according to their properties: Thermoplastic elastomers increase the resistance of the binder to fatigue by improving the elastic properties, reactive polymers and plastomers increase the resistance to deformation and also increase the stiffness, (Brasileiro, Moreno-Navarro, Tauste-Martínez, Matos, & Rubio-Gámez, 2019).

The usage of polymer modified bitumen showed the ability to increase the resistance of the mixture against rutting and thermal cracking. Furthermore, the incompatibility between the bitumen and polymers leads to phase segregation among the blends which deuced the strength of pavement (Ali et al., 2017). By modifying the bitumen with polymer, the polymers differ the viscoelastic properties and the strength of the Asphalt, by providing the ductility, improve the Fracture strength, increase the elastic response and improve the cohesive property (Yildirim, 2007).

Becker et al., (2001) reported that indications in polymers applied as modifiers in paving field because of its ability to increase the physical properties of the binders, introducing polymer improves the resistance to rutting, thermal cracking, stripping and fatigue. It is generally used if high performance and durability are necessary (Becker & Méndez, 2001).

The application of polymers generally is to enhance the elasticity of bitumen, to minimize the risk caused by permanent deformation through viscous flow beneath the loading applied. The phase angle in an unmodified bitumen is increased through an increase in temperature. But nevertheless, through introduction of the required polymers the elastic recoverable component is reinforced while the phase angle is minimized (Airey, 2003).

Burger et al., reported in a study that involves the use of frequency sweeps test. The results obtained from this study showed that increasing a polymer to binder also increases its performances under higher temperature and at a lower frequency. These polymer binders is more elastic when this conditions were fulfilled and satisfied While it can be noticed that the addition of polymer doesn't affect the binder response to loading in terms of the relative distribution between elastic and viscous response (Burger, Van de Ven, Jenkins, & Muller, 2001).

Studies conducted to polymer modified bitumen showed that when the polymer is added to bitumen it increases the softening point and impart a high elasticity to bitumen. On the other hand, it showed that the mixture has a lower temperature sensitivity. It has higher strength at high temperatures and lower strength at low temperatures (Kishchynskyi et al., 2016). One of the main limits of polymer modifiers is that the polymers are thermodynamically unsuited with asphalt due to the large differences of density, molecular weight, solubility and polarity between the polymer and the asphalt. This may lead to delamination of the composite during thermal storage, which cannot be noticed easily and badly affects the material (Fang, Yu, Liu, & Li, 2013). The high cost of the polymer modifiers is the reason that affects a wide use of it and to improve the bonding of polymer elements, between themselves and with bitumen, plasticizer was added in a polymer composition in some situation (Kishchynskyi et al., 2016).

2.4.2 Nanomaterials modified asphalt

Nanomaterials are of morphological features on the nanoscale, and especially have special properties stemming from their nanoscale dimensions (Fang, Yu, Liu, & Li, 2013). Many studies in airport engineering and highway field have been done to explore the utilize of nanomaterials as a modifiers for asphalt, and they found that when nanoparticles are added to the binder, the viscosity and the cohesion of asphalt can be increased, which mean the mixture may have a good performance under high-temperature conditions (Ezzat et al., 2016).

Abdelrahman et al.(2014) made an experimental on the NC-asphalt nanocomposite. The indicated results showed that Nano clay modification of asphalt enhances the physical properties of asphalt. Raising Nano Clay concentration in the binders increase the temperature susceptibility of asphalt, as well as rising the complex modulus, while decreasing phase angle (Abdelrahman, Katti, Ghavibazoo, Upadhyay, & Katti, 2014).

Jahromi and Khodaii (2009) conducted a research based on comparative test, which is done according to rheological test using dynamic shear rheometer (DSR) conducted on modified base bitumen. The result clearly shows that the presence of nanoclay has the ability of altering the rheological properties of bitumen through decreasing the phase angle as well as increasing the stiffness, it also proved the ability to increase the ageing resistance (Jahromi & Khodaii, 2009).

studies conducted to asphalt modified with nanomaterial, it found that the aging resistance, thermal storage and rheological properties of asphalt modified with nanomaterials are improved, which increase the service life of the asphalt pavement (Fang, Yu, Liu, & Li, 2013). The previous studies have reported that the performance of bitumen modified with nanomaterials shows that the complex shear modulus of modified bitumen improved while the phase angle decreased, indicating that the permanent deformation (rutting) of modified bitumen could be minimized (Ali et al., 2017).

A study conducted by Ezzat et al. (2016) to evaluate the Asphalt Binders Modified with Nanoclay and Nanosilica, it concludes that the mixture resistance to permanent deformation could be improved using the proper amount of nanomodifier and, thenanomodified asphalt binder can be stored to be used after few days it can be up to 10 days without big effect on its properties obtained by modification process in the bingeing. The nanomaterials have been introduced as another way to improve the properties of bitumen and enhance the compatibility among the bitumen and polymers. Nanomaterials have been developing and incorporated rapidly in the field of asphalt mixture as it has unique properties. These properties include high surface work, a large fraction of surface atoms, structural features, quantum effects, and spatial confinement (Saltan et al., 2018).

It was predictable that modification of bitumen with nanomaterials would improve the properties of bitumen including an increase of stiffness of bitumen which leads to be less susceptible to the temperature and improve the strength of bitumen against moisture damage. Some nanomaterials have been used to modify polymer modified bitumen such as; nanoclay, nanofibers, carbon nanotubes and nanosilica (Ali et al., 2017). It can be noticed, although Nano-materials are promising, some type of Nano-materials are expensive and demands further research to exploring and optimizing the enhancement in the binder properties before field testing and applications (Ezzat et al., 2016).

Due to the limitation of time and a high cost of the materials and experiments, also the leakage in equipment therefor some studies were conducted to predict the behavior of modified Bitumen using Adaptive Neuro-Fuzzy Inference System (ANFIS) and Artificial Neural Networks (ANN). Using the Artificial intelligence models to solve the different type of real-life procedures in engineering and environmental field shows its productivity and capabilities by dealing with a non-linear characteristic. AI applications can be used in the modeling of different real-life procedure in the field of engineering due to their predictive capacities and nonlinear characteristics (Asadi, Hassan, Nadiri, & Dylla, 2014).

It is understood that complex real-world problems may require intelligent systems that possess human-like expertise within a specific domain, adapt themselves to changing environments, and be able to explain how they make decisions or take actions (Bradshaw, 1997).

2.5 Back Propagation Neural Networks (BPNN)

ANN is a system for processing data by mimicking the idea of the way biological neurons work in a human brain. Using ANN as a research methodology, the key idea is to develop a novel model that learns from past experiences and produces new results based upon them (Naderpour & Mirrashid, 2018). BPNN is the most utilized algorithms owing to its remarkable performance in various field of environmental and water resources management (Gozen Elkiran et al., 2019a). The typical three layers (input, hidden and output) BPNN can be illustrated in Fig. 2.1. The function of hidden node is overcome the intricacy involved in the process. It important to note that in ANN modeling the choice of activation function both in the hidden and output layer is essential as it affect the efficiency of the model. In this study, Levenberg–Marquardt optimization was employed to calibrate the network owing to its fast learning and less time consuming (Hameed, Sharqi, et al., 2017).

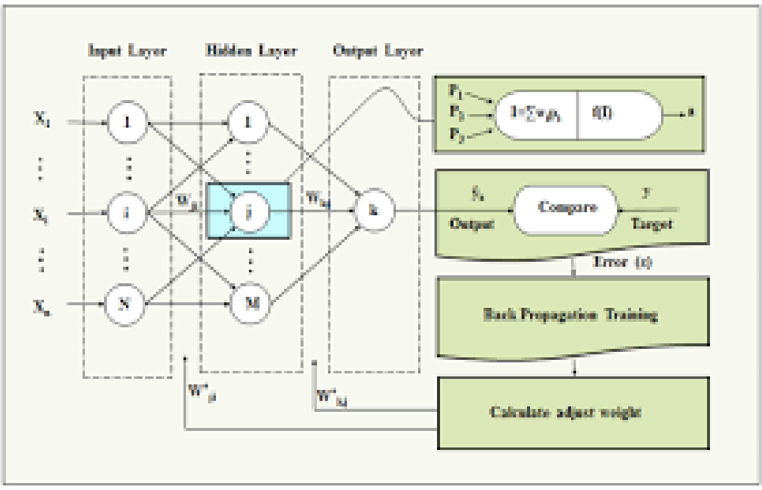


Figure 2.1: Back Propagation Neural Network structure

Luiet al. (2018) have attempted to predict the dynamic modulus of virgin asphalt mixtures and asphalt mixtures containing recycled asphalt shingles with data from four different projects. The input parameters included were sieve test results on aggregates, air voids, effective binder content, theviscosity of the asphalt binder, loading frequency, and recycled asphalt board contents. The suggested ANN model was compared with the iowa model and gave significantly higher prediction veracity than the iowa model (Liu, Yan, Liu, & Zhao, 2018).

Elbadawy et al. (2018), made a comparison study between ANN models and regression models with Witczak NCHRP 1-37A, Witczak NCHRP 1-40D, and Hirsch E* predictive models for predicting dynamic modulus of hot mix asphalt. The database contained the test results of volumetric properties, aggregate gradations, binder viscosity, complex shear modulus and phase angle experimental results obtained from mixes from KSA and Idaho State. The ANN models using the same input parameters gave better performance for 3 predictive models than regression models (El-Badawy, Abd El-Hakim, & Awed, 2018).

In a study conducted by M. Firouzinia and Gh. Shafabakhsh. (2018), it was stated that the asphalt mixtures are highly temperature susceptible and sole enhancement of binder rheological properties are not sufficiently able to overcome this problem. Thus additives should be applied in asphalt mixtures. In their study, the impact of Nano-silica addition at five different contents was investigated on the thermal sensibility of hot mix asphalt using experimental procedures and the ANN models. It was found that modifying asphalt mixtures with Nano-silica improved the temperature sensitivity and the ANN models were generated with 5 input parameters of the percentage of the void, aged sample situation, bitumen type, bitumen situation and temperature with training algorithm as Radial Basis Function (RBF) Which show the capability to give an accuracy result (Firouzinia & Shafabakhsh, 2018).

Tapkınet al. (2009) presented a study to predict the strain accumulation in polypropylene (PP) modified marshal specimens. The data observed from repeated creep tests were modeled in ANN and demonstrated positive similarities with the experimental observation results. The significance of their study was that for a specific type of asphalt mixture and predefined testing conditions the cumulative strains at the end of repeated Load creep tests could be conducted without applying destructive tests (Tapkın et al., 2009).

Abedali (2018), conducted a comparison study between the performance of Multiple Linear Regression models (MLR) and ANN with base asphalt binder considering temperature, frequency, dynamic viscosity, shear stress and strain as inputs and G* as output. Ziariet al. (2018), performed a similar study with carbon nanotube (CNT) modified the asphalt binders to predicting the rutting performance using MLR and ANN and considered the CNT content, test temperature, and loading frequency as input variables. Both studies demonstrated that the ANN prediction performance outperformed the MLR models (Abedali, 2015).

Köket al. (2010), investigated the shear modulus of base and styrene-butadiene-styrene (SBS) modified binders with ANN using the five different SBS contents, bitumen temperature, and the frequency as inputs and used Levenberg-Marquardt (LM), Scaled Conjugate Gradient (SCG), and Pola- Ribiere Conjugate Gradient (CGP) as the training algorithms. It had appeared that the LM algorithm was the most favorable topology for predicting G* (Kok et al., 2010).

Venudharan and Biligri (2017), employed an Artificial Neural Network to predict rutting performance of asphalt binder with different Crumb Rubber (CR) ranges. The input parameters were considered as five different CR gradations, base binder viscosity, frequency, and test temperature. The various combinations of neural network architectures with varying algorithms of training and transfer functions were trained, and backpropagation learning algorithm with SCG as the training algorithm in a feed forward, two hidden layers neural network with 7 and 3 neurons were found to be the optimum model (Venudharan & Biligiri, 2017).

Xiao Laboratory research performed by Tapkin (2010), predicted the fatigue of bituminous mixture and the fly ash was added as a filler and the results showed that ANN can be considered as a good tool which can be used in the prediction process. He compared the results by applying from a single, double and triple-layer networks and find out that one layer of the ANN is enough to predict the fatigue of the mixture with the introduction of fly ash (Tapkın, Çevik, & Uşar, 2010).

It has been reported by Xiao et al (2011) in one of their studies which involves the usage of a serial ANN models in order to predict the viscosity rate of a crumb rubber modified (CRM) binders. The result of the study showed that ANN models can be used in predicting the viscosity of CRM binders. Furthermore, these models can be used in prediction using other kind of rubber types (Xiao, Putman, & Amirkhanian, 2011).

In a study conducted by Cüneyt Aydin, A., et al (2006), 2 ANFIS models were used: HSC data and NSC data to predict the elastic modulus of concrete. The ANFIS results were compared with codes and some data obtained from the literature and the study was concluded that ANFIS is a good tool for modeling and predicting the complex modulus of bitumen and it showed the ability to evaluate the elements affecting complex modulus of asphalt before it moves to the site which will help to save time consumed.

A study by F. Khademi et al used three artificial intelligence techniques: Artificial Neural Network (ANN), Adaptive Neuro-Fuzzy Inference System (ANFIS) and Multiple Linear Regression (MLR) to predict the 28 days compressive strength of concrete using 14 different input variables. The obtained result that ANN and ANFIS models efficient in predicting the 28 days compressive strength of concrete and are recommended due to its high efficiency especially when high accuracy is needed. (Khademi, Jamal, Deshpande, & Londhe, 2016).

In a study of Yilmaz, M et al (2011), ANFIS was used to model the complex of base and ethylene-vinyl-acetate (EVA) polymer modified bitumen. The data was obtained from a dynamic shear rheometer (DSR) test. In the modeling process the EVA content, bitumen temperature, and frequency were the inputs data and the complex modulus was the output data. The ANFIS result was closely related to the actual the results they conclude their study that ANFIS can be used for modeling the complex modulus of bitumen under varying temperature and frequency and it is important method to evaluate the factors affecting it and Adaptive Neuro-Fuzzy Inference System can be considered as good tools which help reduce the time consumed.

2.6 Support Vector Machine (SVM)

Learning in the context of support vector machine (SVM) was proposed and introduced by Cortes and Vapnik (1995), which provides a satisfactory approach to the problems of prediction, classification, regression and pattern recognitions. SVM is based on the concept of machine learning comprises of data driven model. The structural risk minimization and statistical learning theory are two useful functions of SVM; this makes it different from ANN because of its ability to reduce the error, complexity and increases the generalization performance of the network. Generally, SVM is categorized into linear support vector regression (L-SVM) and non-linear support vector regression (N-SVM) (Elkiran et al., 2019). Therefore, support vector regression (SVM) is a form of SVM based on the two basic structural layers; first layer is kernel function weighting on the input variable while the second function is the weighted sum of kernel outputs.

2.7 Multilinear Regression (MLR)

MLR is a model that is applied to evaluate the linear relationship between the dependent and independent variables. This model is based on the concept of least squares, which is the value of the predicted parameter, expressed as a linear function (Abba et al., 2017). The linear regression can be categorized into simple and multiple linear regressions. The model is assumed to be the simple linear regression (SLR), if the goal is to predict the linear relationship or correlation between one predictor and one criterion variable. The model is called multiple linear regression when the aim is to forecast the linear correlation between two or more predictors.

CHAPTER 3
MATERIALS AND METHODOLOGY

3.1 Experimental Procedures

3.1.1 Materials and properties

The base bitumen utilized was of 80/100 penetration grade. ASA in the form of white powder was used as the polymer modifier at 5% concentration to the weight of base bitumen. Two different nanomaterials, namely Nano copper and Nano calcium, were obtained from a company in China and mixed with ASA at 3% and 5% compositions to form two different binders modified with polymer composites. Samples were prepared using a high shear mixer on a constant temperature of 170 ^{o}C and at the speed of 5000 rpm for 90 minutes in order to make homogeneous mixtures. Evaluation of the physical properties of the unmodified, polymer modified and polymer nanocomposite modified binders were conducted by penetration (ASTM D5) and softening point (ASTM D36) tests. Physical properties of the binders were also used as input parameters in computational modelling. Findings are presented in Table3.1

Table 3.1: Physical properties of samples

Material	Penetration (dmm)	Softening point (^{o}C)
Bitumen 80/100	82	46
5% ASA	74	50
3% ASA-Nano copper	66.4	56
5% ASA-Nano copper	69.1	55
3% ASA-Nano calcium	75.3	55
5% ASA-Nano calcium	76.9	53

3.1.2 Dynamic shear rheometer

A Dynamic Shear Rheometer (DSR) was used to observe the rheological properties of modified binder samples mentioned in the Materials and Properties section above. The test are conducted at temperatures from 46 ^{o}C to 82 ^{o}C with increments of 6 ^{o}C as specified in Superpave PG guidelines. Temperature control of the samples was achieved by a fluid bath system and temperature control unit in order to keep temperatures constant and uniform over the range of temperatures in which the experiments were conducted. The DSR equipment shown in Figure 3.1 consists of top and bottom plates. Samples of 1-mm thickness were sandwiched between 25-mm diameter plates, where the bottom plate was fixed and the top plate was oscillating back and forth with ranging frequencies to simulate shearing action. The analysis is conducted at 9 different frequencies ranging from 0.159 Hz to 15.92 Hz. The analysis is software controlled, while measured stresses and resulting strains were obtained in terms of complex modulus (G*) and phase angle (δ), which are considered as the most significant parameters to define the rutting (G*/sin δ) and fatigue (G*.sin δ) performance of asphalt binders. The effect of temperature on the performance of asphalt binders was illustrated using isochronal plots, master curves, and rutting performance graphs. G* results are used to construct the master curves. In order to represent the results in a single curve that is known as master curve, a reference temperature of 64^{o}C was defined and frequencies were shifted relative to this temperature. Numerous shifting methods have been used in the literature, namely the Williams–Landel–Ferry (WLF) equation, the Laboratories Central des Ponts et Chaussées (LCPC) approach, viscosity–temperature-susceptibility (VTS) equation, the Arrhenius equation, modified Kaelble equation, and log-linear approach, (Ali, S.I.A., et al., 2015). The log-linear approach was adopted in this study using relevant shift factor constants at each test temperature to obtain the best fitting master curve.

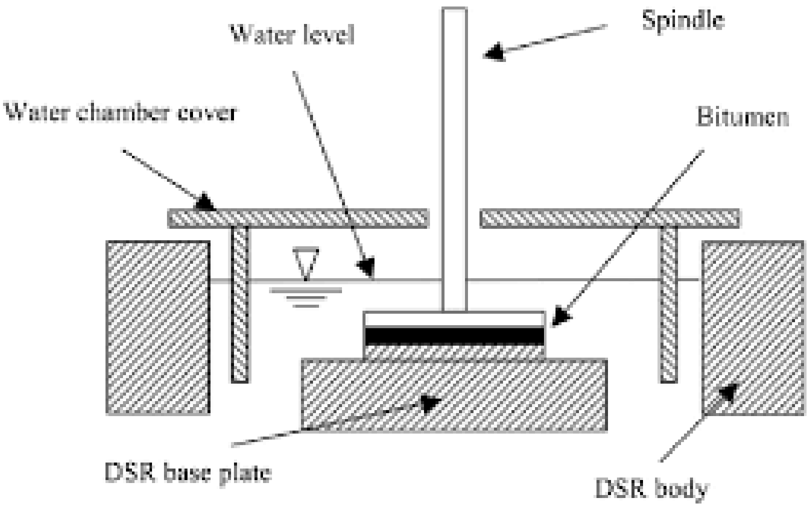


Figure 3.1: Schematic presentation of DSR

3.2Back Propagation Neural Network (BPNN)

Artificial neural networks (ANN) belong to the learning machine family, which uses a computational approach to develop predictive models for desired parameters by simulating the way biological neurons work in the human brain, (Liu, J., et al., 2018). BPNN is the most utilized algorithms owing to its remarkable performance in various field of environmental and water resources management (Elkiran et al., 2019). The typical three layers (input, hidden and output) BPNN can be illustrated in Fig 3.1. The function of hidden node is overcome the intricacy involved in the processNumerous types of ANN have been adopted in the literature. A feedforward multilayer perceptron (FFMLP) was adopted in this study. With this type of ANN, the learning is supervised, which indicates that for a given set of input vectors, the output vectors are provided to the network and the system is expected to adjust its weights using forward and backward calculations to minimize the prediction errors, which is also known as the learning phase.

The structure of MLP is divided into three layers, which are strongly interconnected with artificial neurons. The initial layer is the input layer x_i where the input signals are stored for a given set of input parameters x_{ai}. Input parameters in this study were the physical properties of the blends (penetration value and softening point) and mechanical test parameters (temperature and frequency).

$$x_i = (x_{1i}, x_{2i}, \dots \dots \dots x_{ai}) \quad i = 1, \dots \dots, n \qquad (3.1)$$

The final layer is the output layer y_i,where the targeted parameter, G*, was expected to be predicted in this study.

$$y_i = (y_{1i}, y_{2i}, \dots \dots \dots y_{bi}) \quad i = 1, \dots \dots, n \qquad (3.2)$$

The intermediate layer is called the hidden layer and it is devoted to the calculations that formally connect the input layer x_i with the output layer y_i.

A weighted sum of the values of the input variables is computed through the weights that are associated with each connection by eqn. 3.3;

$$y = \sum_{i=1}^{a} w_i x_i + w_0 \qquad (3.3)$$

Where w_i is the weight associated with the i^{th} input parameter, x_i is the data corresponding to the input parameter and w_o is the bias.

The output value is calculated in a forward pass using a transfer function. Numerous transfer functions such as the Heaviside step function, sigmoidal, or hyperbolic tangent have previously been used in the literature. Utilization of the activation function is highly dependent on the nature of the dataset and the type of model desired to be developed. In this study, a hyperbolic tangent as expressed in eqn. 3.4 was adopted.

$$f(a) = \frac{e^{a} - e^{-a}}{e^{a} + e^{-a}} = \frac{2}{1 + e^{-2a}} - 1 \qquad (3.4)$$

The abovementioned procedure is an iterative process. The network performs a series of forward and backward calculations to adjust its weights in order to achieve the most accurate predictions to the target values, which is also called the training of the neural network (Baldo, Manthos, & Pasetto, 2018).). In this study, MATLAB (MathWorksInc R2013a) was used in order to develop ANN models. Although various training algorithms are available in MATLAB, the selection of the training algorithm depends on the type of neural network to be modelled and the structure and complexity of the data to be fed to the network. The Levenberg-Marquardt (LVM) training algorithm was observed to be the most suited algorithm considering the structure of the dataset observed from the DSR oscillation tests. Figure 3.2 below showed the configuration of the neural network applied

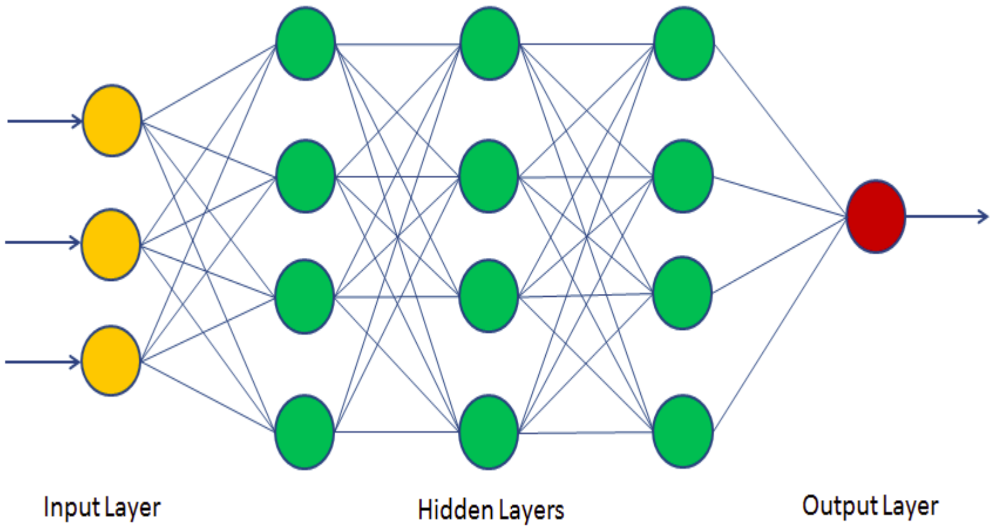


Figure 3.2: Configuration of the selected artificial neural network

3.3 Support Vector Machine (SVM)

The support vector machine (SVM) algorithm is an advanced algorithm of the standard SVM, that gives a computational advantage (it decrease the computational burden) over the standard SVM by converting the quadratic optimization problem into a system of linear equations (Nourani et al., 2018).In the LS-SVM algorithm, can get a solution by solving a linear set of equations than solving a quadratic programming problem involving the standard SVM. The LS-SVM will be used for classification and regression problems. Summary of the LS-SVM is as follows. And the structure is presented in Fig. 3.3

By considering inputs x_i and output y_i, given by LS-SVM method, the nonlinear LSSVM function will be expressed as follows.

$$f(x) = w^T \varphi(x) + b \qquad (3.2)$$

where$f$ is indicates as the relationship between climate variables (predictors) and local rainfall (predictand), and w, φ and b are the m-dimensional weight vector, mapping function and bias term, respectively.

Using the function estimation error, regression problem might be given in terms of the structural minimization principle as:

$$\min J(w,e) = \frac{1}{2} w^T w + \frac{\gamma}{2} \sum_{i=1}^{m} e_i^2 \qquad (3.6)$$

will be subjected to the following constraints:

$$y_i = w^T \varphi(x_i) + b + e_i \text{ (i=1, 2,…, m)} \qquad (3.5)$$

where γ refers to the penalty term and e_i as the training error for x_i.

To get solutions to w and e, the Lagrange multiplier optimal programming method is used to solve Equation (3). The objective function will be determined by changing the constrained problem into an unconstrained problem. The Lagrange function L is expressed as

$$L(w,b,e,\alpha) = J(w,e) - \sum_{i=1}^{m} \alpha_i \left\{ w^T \varphi(x_i) + b + e_i - y_i \right\} \qquad (3.8)$$

where α_i are the Lagrange multipliers.

Taking in account, the Karush-Kuhn-Tucker (KKT) conditions, the optimal conditions will be obtained by taking the partial derivatives of Equation (5) with respect to w, b, e and α, respectively as

$$\begin{cases} w = \sum_{i=1}^{m} \alpha_i \varphi(x_i) \\ \sum_{i=1}^{m} \alpha_i = 0 \\ \alpha_i = \gamma e_i \\ w^T \varphi(x_i) + b + e_i - y_i = 0 \end{cases} \quad (3.9)$$

Thus, the linear equations can be derived after the elimination of e_i and w as

$$\begin{bmatrix} 0 & -Y^T \\ Y & ZZ^T + I/\gamma \end{bmatrix} \begin{bmatrix} b \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (3.10)$$

where $Y = (y_1, ..., y_m), Z = (\varphi(x_1)^T y_1, ..., \varphi(x_m)^T y_m), I = (1, ..., 1), \alpha = (\alpha_1, ..., \alpha_l)$

By defining kernel function $K(x, x_i) = \varphi(x)^T \varphi(x_i), i = 1, ..., m$, which is satisfied with Mercer's condition, the LSSVM is represented as

$$f(x) = \sum_{i=1}^{m} \alpha_i K(x, x_i) + b \quad (3.11)$$

The commonly used RBF kernel function was used in this study. Given in the Equation (3.12)

$$K(x, x_i) = \exp(-\| x - x_i \|^2 / 2\sigma^2 \quad (3.12)$$

Before LSSVM is calibrated, the values ofpredictor variables and local rainfall were normalized by their respective means and standard deviations. The normalized values of predictor variables and local rainfall were then used to calibrate the LSSVM. The LSSVM will need the calibration of the two parameters: the penalty term (γ) and the kernel width (σ). During the training period of the LSSVM, the grid-search method was used to obtain the optimal parameters. The grid search method will yield an optimal parameter set and employing a cross-validation procedure can restrict the downscaling model from over-fitting.

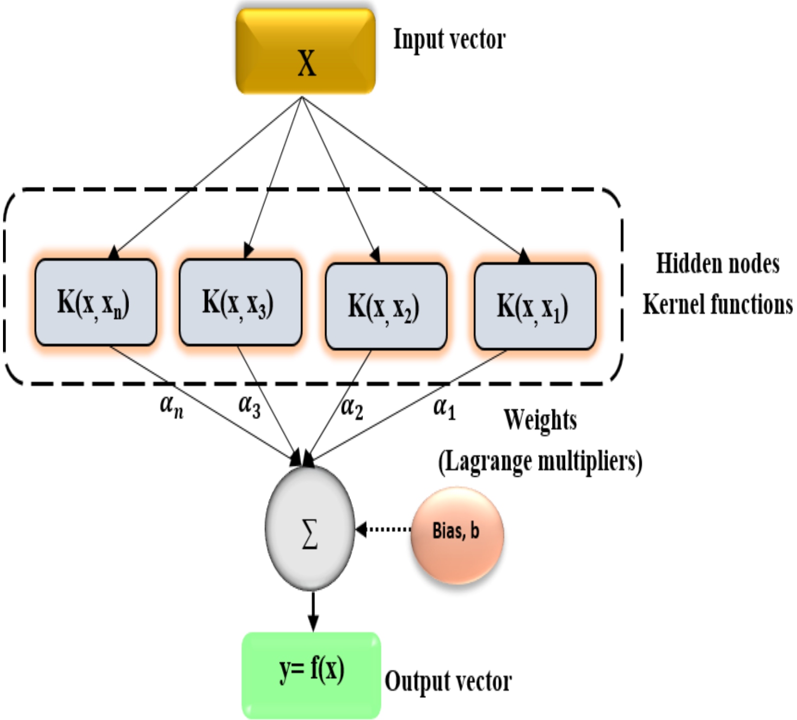


Figure 3.3: Support Vector Machine Structure

3.4Multilinear Regression (MLR)

Generally, linear regression is classified into two majors categorized of multiple and simple linear regression. Which depends on the aim of the prediction, for example if the aim involves estimating the linear correlation that exists between a single predictor and a single criterion variable such model is considered to be called simple linear regression (SLR), moreover, if the aim of predicting the linear correlation which exists between more than one predictor and still with a single criterion variable, such model is referred to as Multiple Linear Regression (MLR) (Elkiran et al., 2018). Mostly, multilinear regression (MLR) is the widely used type of linear regression involves an analysis whereby each value from the independent variables is related to a dependent variable value. Usually, MLR involves the estimation of the level of correlation that exists between a single response variable i.e. the dependent and two or more predictors i.e independent variables (Khademi and Behfarnia, 2016; (Parmar & Bhardwaj, 2015; Chen & Liu, 2015). The general form of MLR can be represented as:

$$\hat{Y} = a_o + \sum_{j=1}^{m} a_j\, X_j \tag{3.13}$$

where$\hat{Y}$ is the model 's output, X_j are the independent input variables to the model, and a_o,a_1,…a_m are partial regression coefficients?

3.5 Proposed Modeling Procedures

In this study, data driven models including Back Propagation Neural Network (BPNN), Support Vector Machine (SVM) and Multilinear regression analysis is carried out to predict the complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen. The inputs of those models are softening point, penetration, Temperature, and frequency. The data were observed from a dynamic shear rheometer (DSR) test. The resulted G* and (δ) from the three data driven approach will be compared with the experimental result. Conclusion can be drawn based on comparing their performance. The main proposed method by which the test was performed is shown in Figure 3.3 below. A set of 381 data points from six different blends of AC at different concentrations were used in the modelling of three data driven models (BPNN, SVM and MLR), the data is provided in Appendix 1. Furthermore, 285 (75%) of the data points were used for training the network, 96 (25%) of the data points were used for testing the models. The reason why checking data set for the model validation was used is in order to stop and minimized the overfitting of the training data set, therefore a validation data set is used to check and control the potential for the model overfitting the data. The testing data set has significance since it shows the prediction capacity of the network for the untrained data set.

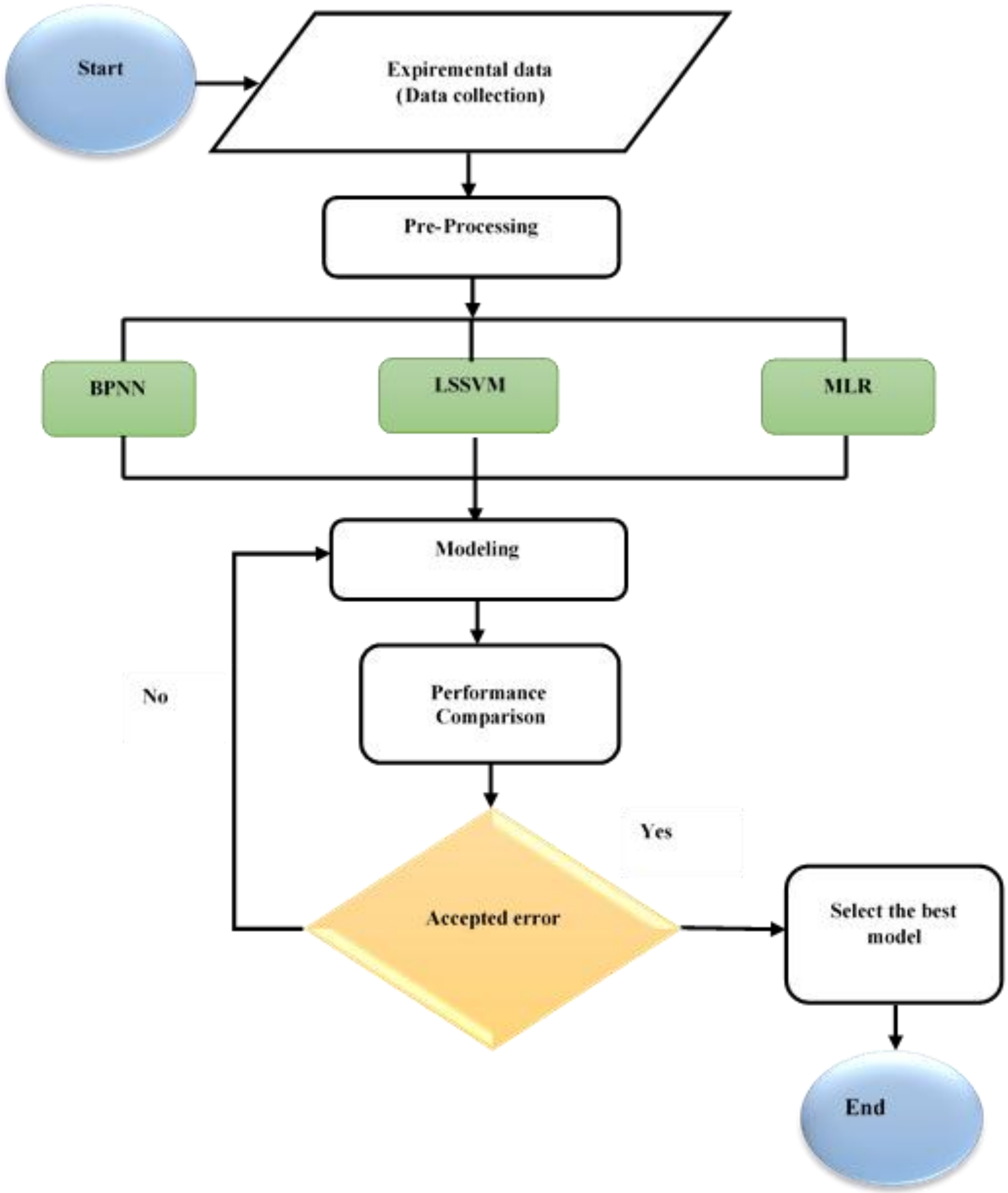


Figure 3.4: Proposed Methodology of data driven models

3.6 Data Normalization AndPerformance Evaluation

In order to maintain and make sure that equal priority and attention was given to both the input as well as the output, and also to reduce their dimensions, the data applied in this research was scaled in the range between 0 to 1. The major advantage of normalizing the data prior the introduction of Al models is to reduce data redundancy, and to reduce or minimize the larger numerical errors (Sola & Sevilla, 1997). The data employed in this research was normalized using Eqn. 3.12 prior to BPNN, SVM and MLR modelling.

$$X_n = \frac{x - x_{min}}{x_{max} - x_{min}} \quad (3.14)$$

Where X_n is the normalized data. x is the measured data, $\bar{x}$ is the mean of the measured data, x_{max} is the maximum value of the measured data and xmin is the minimum value.

The data driven models (BPNN, SVM and MLR) models developed with training and testing data sets were evaluated for their prediction capacity using the performance indicator metrics. Coefficient of determination (DC), root mean squared error (RMSE) and correlation coefficient (R)were the common statistical performance indicators adopted in various studies (El-Badawy et al., 2018; Kok et al., 2010; Liu et al., 2018).). R^2 and RMSE as expressed in Eqn. 3.13 and 3.14 were adopted in this study.

$$DC = 1 - \frac{\sum_{j=1}^{N}\left[(Y)_{obs,j} - (Y)_{com,j}\right]^2}{\sum_{j=1}^{N}\left[(Y)_{obs,j} - \overline{(Y)}_{obs,j}\right]^2} \quad (3.15)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(Y_{obsi} - Y_{comi})^2}{N}} \quad (3.16)$$

$$R = \frac{\sum_{i=1}^{N}(Y_{obs} - \bar{Y}_{obs})(Y_{com} - \bar{Y}_{com})}{\sqrt{\sum_{i=1}^{N}(Y_{obs} - \bar{Y}_{obs})^2}\sum_{i=1}^{N}(Y_{com} - \bar{Y}_{com})^2} \quad (3.17)$$

Where N, Y_{obsi}, $\bar{Y}$ andY_{comi} $a$re data number, observed data, average value of the observed data and computed values, respectively.

CHAPTER 4
RESULTS AND DISCUSSION

4.1 Experimental Results and Analysis

4.1.1 Dynamic mechanical analysis test

DSR oscillation tests were conducted on base bitumen, polymer modified bitumen (5% ASA) and polymer composite binders of (ASA-Nano copper and ASA-Nano calcium) at 3% and 5% concentrations in order to understand the effect of test parameters and the influence of modification on the performance of the modified binders. The performance of the modified binders was observed in a range of temperatures ($46^{o}C$-$82^{o}C$) and frequencies (0.159 Hz-15.92 Hz), while isochronal plots, master curves, and rutting parameter plots were used in the evaluation of performance characteristics.

a. Isochronal plots

Isochronal plots were used to represent complex modulus over a range of temperatures at constant frequencies. Isochronal plots assisted in making a comparison for G* at given temperatures. Furthermore, temperature susceptibility of asphalt cement can be interpreted using isochronal plots. On this basis, complex modulus versus a range of temperatures is plotted in Figs. 4.1 and 4.2 at two constant frequencies of 0.159 Hz and 15.92 Hz, respectively. It can be observed that all modified blends demonstrated significant enhancement in G* and reduced temperature susceptibility compared to base AC. 3% ASA-Calcium blends showed the greatest enhancement, while the 5% ASA blends showed the least. It was also noted that enhancement in the properties of the modified blends was greater at higher frequencies and lesser at lower frequencies, which is in compliance with numerous studies conducted on styrene-butadiene-styrene (SBS), natural rubber latex (NR) and epoxidized natural rubber (ENR).

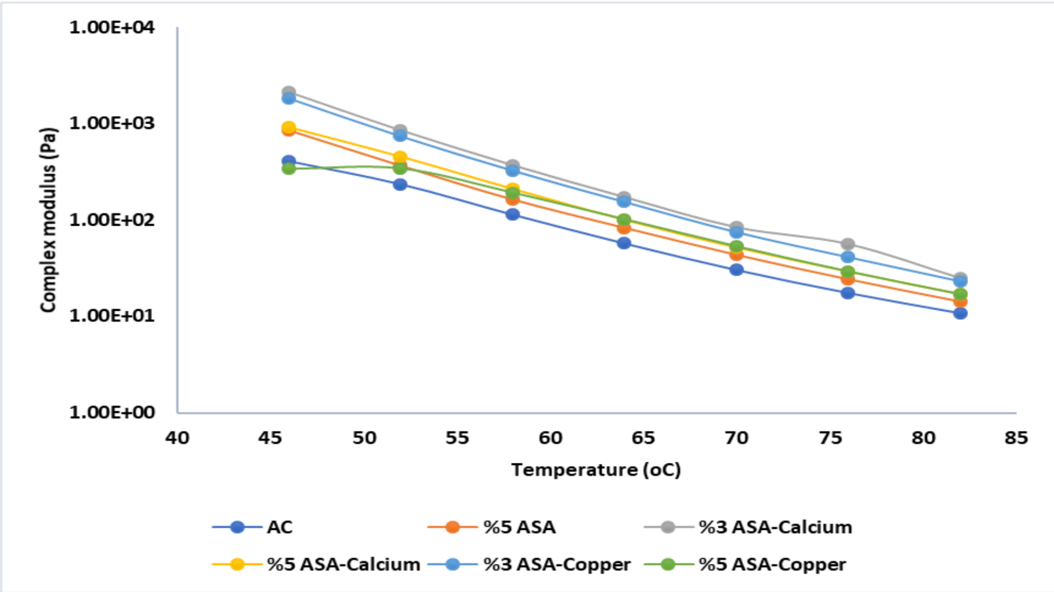


Figure 4.1: Isochronal plot of G* at 0.159 Hz

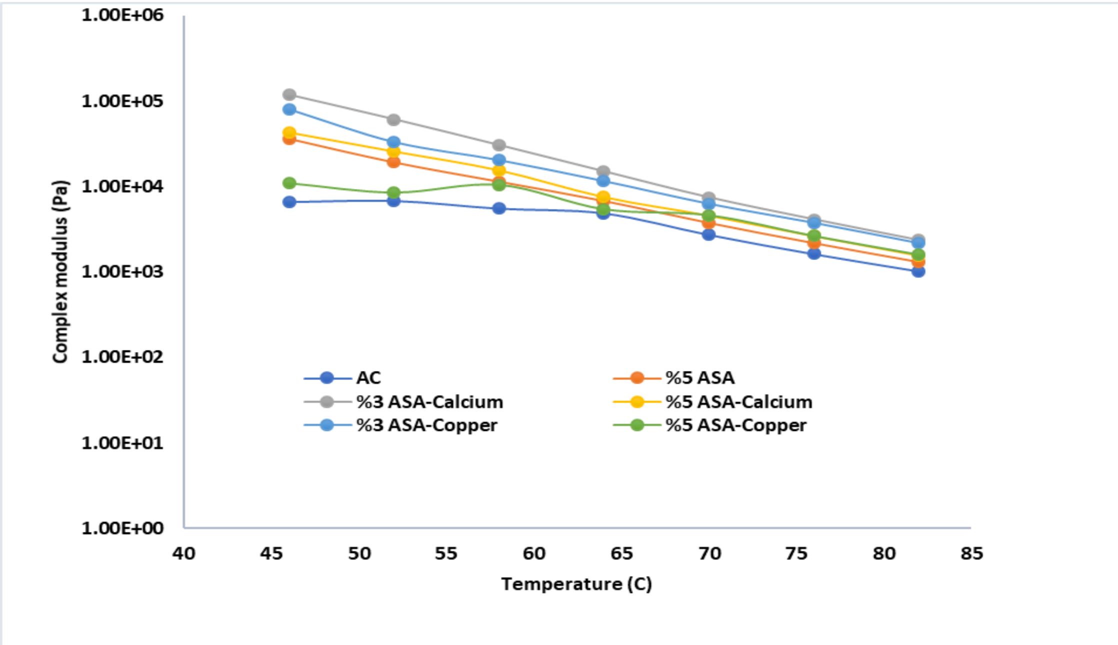


Figure 4.2: Isochronal plot of G* at 15.92 Hz

b. Rheologicalmaster curves

Master curves allow the representation of rheological measurements such as G* and δ to be plotted on a single curve at a range of temperatures and frequencies. In order to construct the master curves, a reference temperature of 64 ^{o}C was selected and all other temperatures were shifted horizontally with respect to time to obtain a smooth curve. Shifting was performed using constant numerical shift factors at each elevated temperature between 46^{o}C-82^{o}C. Fig. 4.3 presents the complex modulus master curve for different blends.

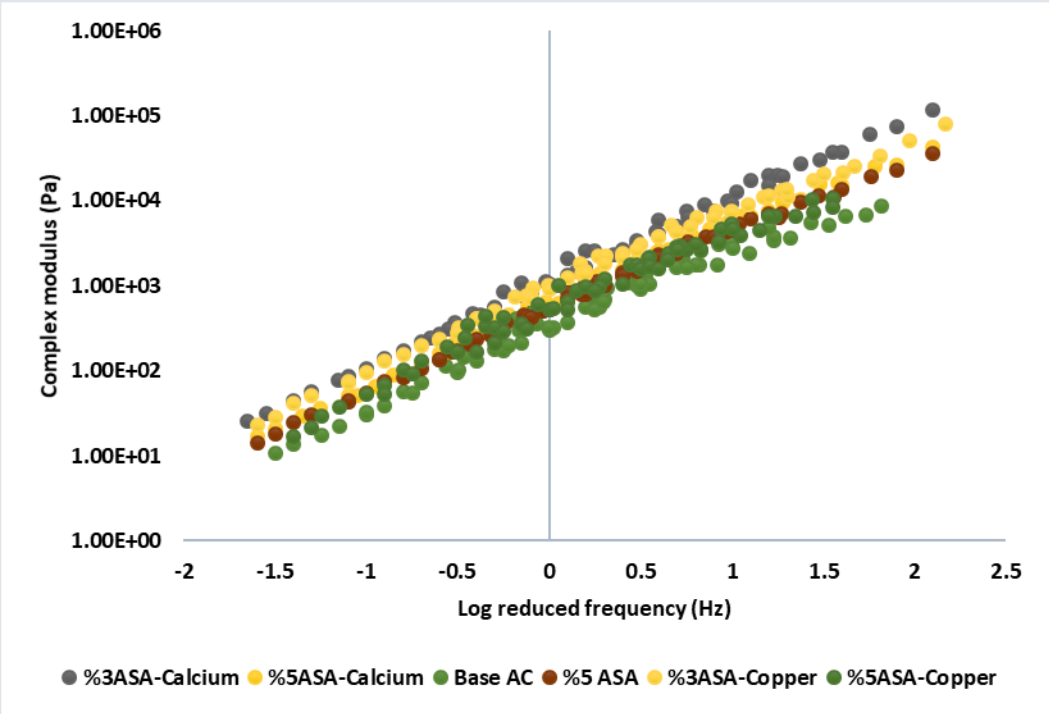


Figure 4.3: Complex modulus master curves at 64 ^{o}C reference temperature

It can be observed that consistent improvements in the complex modulus with polymer and polymer composite modified samples were achieved. An increase in the complex modulus slightly larger than 1kPa was noted between base AC and ASA-Calcium at 3% concentration. It can further be observed that up to 3% concentrations, both polymer composite blends showed significant improvement in rheological properties; however, at 5% concentrations, reduction in the enhancement of complex modulus was observed. The cause for the different behaviour could be linked to inhomogeneity of blends and the potential of particles to form clusters at higher concentrations of modification. Blends of 5% ASA-Copper and 5% ASA-Calcium are therefore not considered preferable blends to modify asphalt cement as the enhancement in complex modulus was insignificant compared to 5% polymer (ASA) modified AC. It is also noteworthy to mention that in a study conducted by Ali et al., (2015), complex modulus of 10^8 Pa was achieved with 5% ASA modified asphalt cement with a bitumen penetration grade of 60/70. In this study, bitumen grade 80-100 was used in the blends and complex modulus results yielded were slightly above 10^5 Pa, indicating that together with the type and concentration of modifier used, the penetration value of base bitumen had a significant influence on the rheological behaviour of modified asphalt cement.

c. Rutting parameter

The failure of bitumen at high temperatures was related to the rutting resistance performance of AC. Rutting parameter known as $G^*/\sin\delta$ can be evaluated from DSR oscillatory test results. In order to resist rutting, AC is preferred to be stiff and elastic. As can be deduced from the formula, higher G^* (stiffness) and lower δ (elasticity) would lead to higher rutting resistance. On this basis, as specified in the ASTM standards, the rutting parameter should not be less than 1kPa for unaged samples. The effects of rutting on base and modified binders are shown in Figure 4.4. It can be observed that all blends including base AC have passed the ASTM specification of a minimum rutting parameter of 1kPa at 82 ^oC. It is also noted that polymer nanocomposite blends have performed better in terms of temperature susceptibility compared to base AC and 5% ASA modified binders. Polymer composite blends for ASA- Nano calcium and ASA- Nano copper at 3% has been shown to have higher rutting $G^*/\sin\delta$ than at 5%. This might be explained by the occurrence of agglomeration due to poor dispersion of particles in the asphalt matrix during the mixing progress.

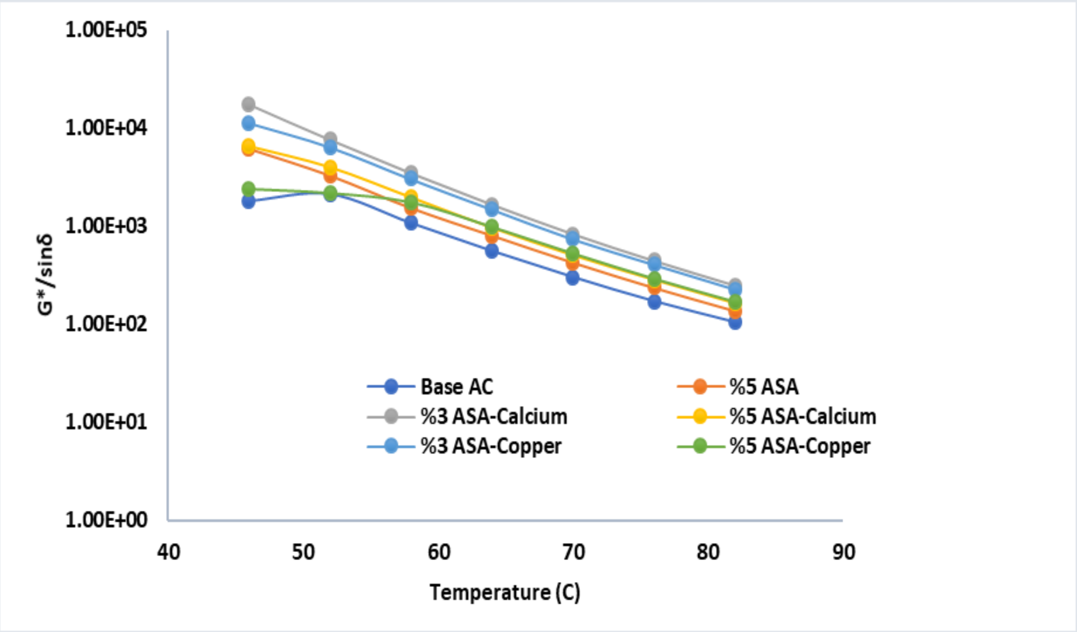


Figure 4.4: Effect of temperature on the rutting parameter

4.2Results of Data-Driven Models

In this study, data driven models including Back Propagation Neural Network (BPNN), Support Vector Machine (SVM) and Multilinear regression analysis is carried out to predict the complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen. For this purpose, all the models (BPNN, SVM, and MLR) were develop using MATLAB 9.3 (R2017a), the model input selection was done out based on the correlation analysis.

For the pre-analysis of the data, Table 4.1 gives the daily statistical analysis of the variables involved in the prediction. These statistical properties include mean (X_{mean}), minimum (X_{min}), maximum (X_{max}), standard deviation (S_x) and skewness (C_{sx}). The considered experimental data were sufficient to cover all the reasonable prediction. According to (Elkiran et al., 2019) a very high C_{sx} can affect the performance of ANN considerably, while a low C_{sx} is more appropriate for modelling. This justify our prediction performance results especially for phase angle (δ). Further analysis was carried out using the correlation matrix to measure the strength and direction associated between the multiple stations. For the development of any predictive model approaches, determination of the correlation coefficient is crucial, because the directional sign (+ or -) indicates the relationship between the stations and also shows the proportionality of independent and dependent variables (Table 4.2). Based on Table 2, the correlation results demonstrated a positive relationship between the variables. From the correlation analysis it can be seen that frequency and temperature are more correlated and therefore considered as M1, while in M2 contained the addition of softening point and penetration as shown in Table 4.3.

Table 4.1 Statistical Analysis of the variables

Variables	X_{mean}	S_x	C_{sx}	X_{min}	X_{max}
Penetration	73.97023	5.106135	-0.00243	66.4	82
Softening point	52.50131	3.504578	-0.84627	46	56
Temperature (^{o} C)	64.14099	12.11252	-0.0092	46	82
Frequency (Hz)	4.359014	5.153004	1.290405	0.159	15.92
|G*| (Pa)	4830.918	12235.1	6.031041	10.86	117800
δ	86.43951	2.816648	-2.13366	69.47	89.08709

Table 4.2. Correlation Analysis between the experimental variables

Variables	Penetration	Softening point	Temperature (^{o} C)	Frequency (Hz)	|G*| (Pa)	δ
Penetration	1					
Softening point	-0.80263	1				
Temperature (^{o} C)	0.005546	0.0039	1			
Frequency (Hz)	0.006705	0.00552	0.02205	1		
|G*| (Pa)	-0.06858	0.158232	-0.39143	0.434764	1	
δ	0.047332	-0.00292	0.624596	-0.50164	-0.66742	1

Table 4.3 Input variable combination

Model Type	Model Input combination

BPNN	M1 (Frequency +Temperature)
	M2 (Frequency +Temperature+ Softening point+ Penetration)
SVM	M1 (Frequency +Temperature)
	M2 (Frequency +Temperature+ Softening point+ Penetration)
MLR	M1 (Frequency +Temperature)
	M2 (Frequency +Temperature+ Softening point+ Penetration)

4.2.1 Results of Back Propagation Neural Network (BPNN)

In BPNN modelling, the model's network was calibrated using 1,000 iterations, 0.0001 mean square error, 0.01 was set to be the initial learning rate using the Levenberg–Marquardt algorithm and a momentum coefficient of 0.9. optimum number of hidden nodes was identified using trial and error and the best one was reported. For modeling BPNN, a total of 381 experimental data were obtained and portioned in to training and testing phase. Based two model combination (M1 and M2) the network was obtained as in Fig 4.1and the tangent sigmoid activation function was employed due to promising ability in various science and engineering research (Nourani et al., 2018).

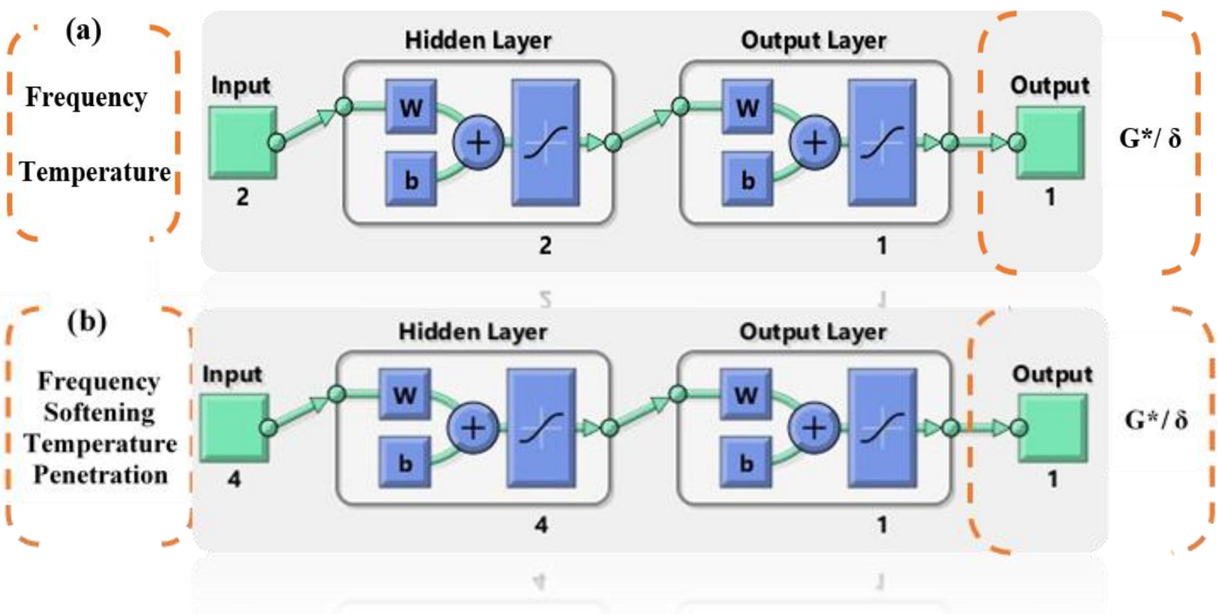


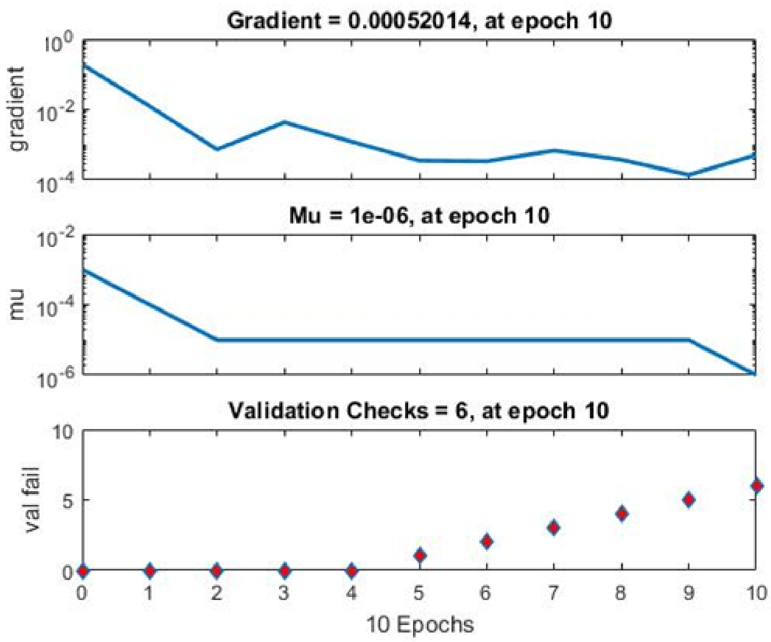
Figure 4.5: Network topology for M1 and M2 model combination

Table 4.4 show the results performance of BPNN for modeling the complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen. From the table it can be seen that seen that BPNN us capable of predicting (G*) using model combination of M2 that contained four input combination with the high accuracy in term of DC.

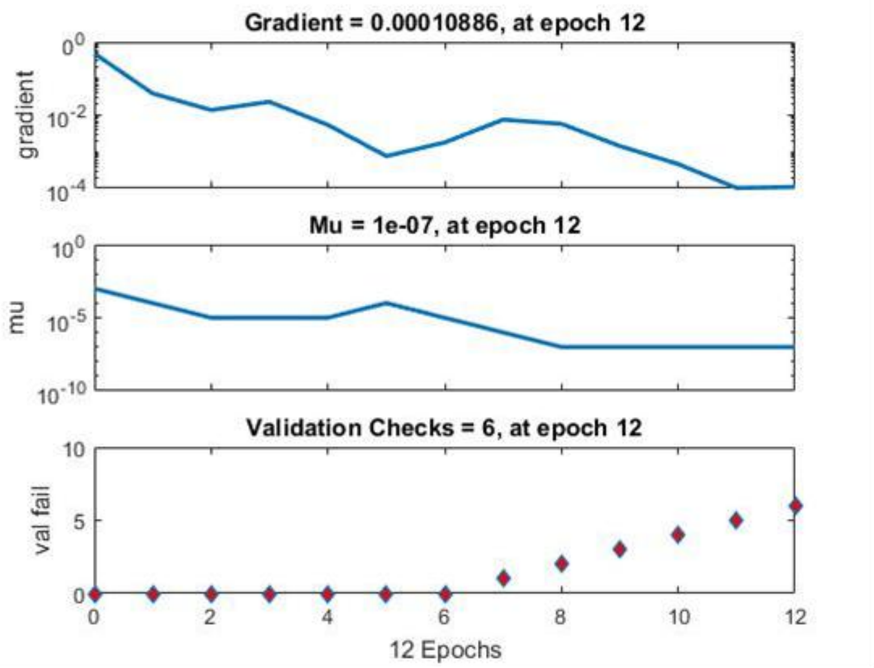
Table 4.4 Performance results of BPNN model for (G*) and (δ)

			Training			Testing		
	Outputs	Model	DC	RMSE	R	DC	RMSE	R
BPNN	(G*)	M1	0.5239	0.0697	0.7238	0.5062	0.0164	0.7520
		M2	0.9435	0.0240	0.9713	0.9631	0.0103	0.9814
	(δ)	M1	0.9971	0.0444	0.9985	0.9427	0.0262	0.9709
		M2	0.9977	0.0393	0.9989	0.9553	0.0231	0.9774

Similarly, the results demonstrated the ability if BPNN model in modeling and predicting (δ) with both the model combination M1 and M2. This can be proved by considering all the performance criteria in both training and testing phased. It can be seen that the computed correlation using formula and software are approximately the same. The training function graph for both M1 and M2 ((G*) and (δ)) can be can be presented in Fig. 4.6 and 4.3 respectively.

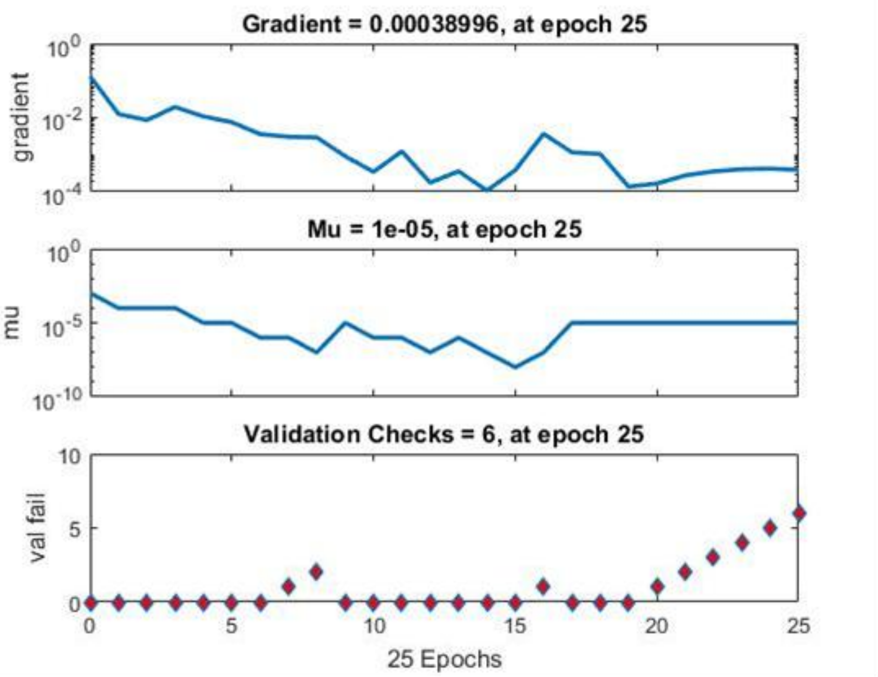


(a)

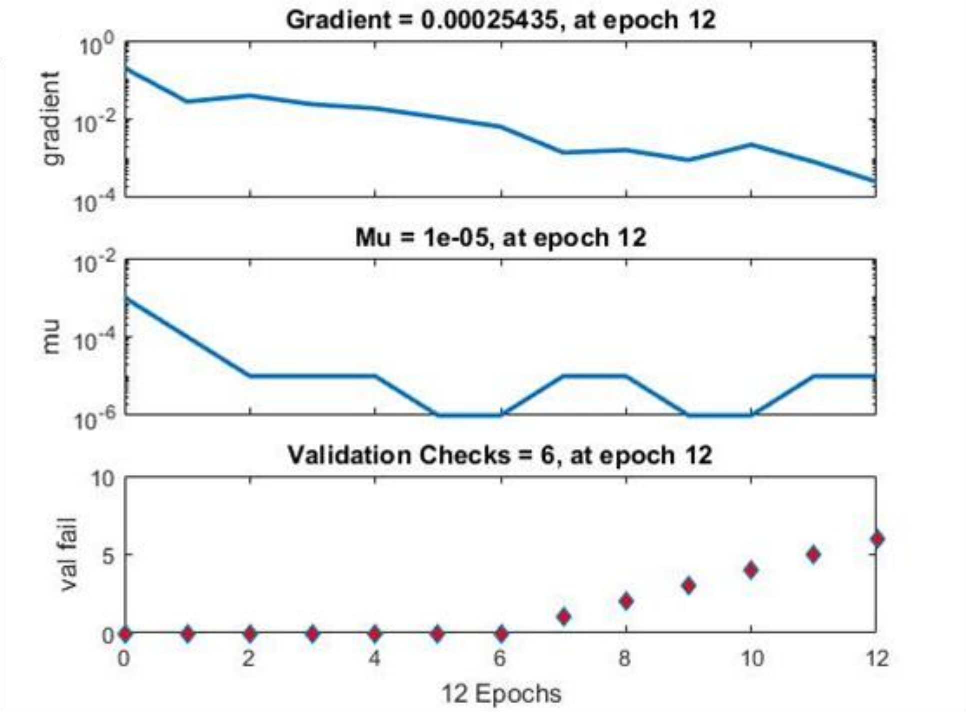


(b)

Figure 4.6: Training function of BPNN for (a) M1 and (b)M2 for (G*)



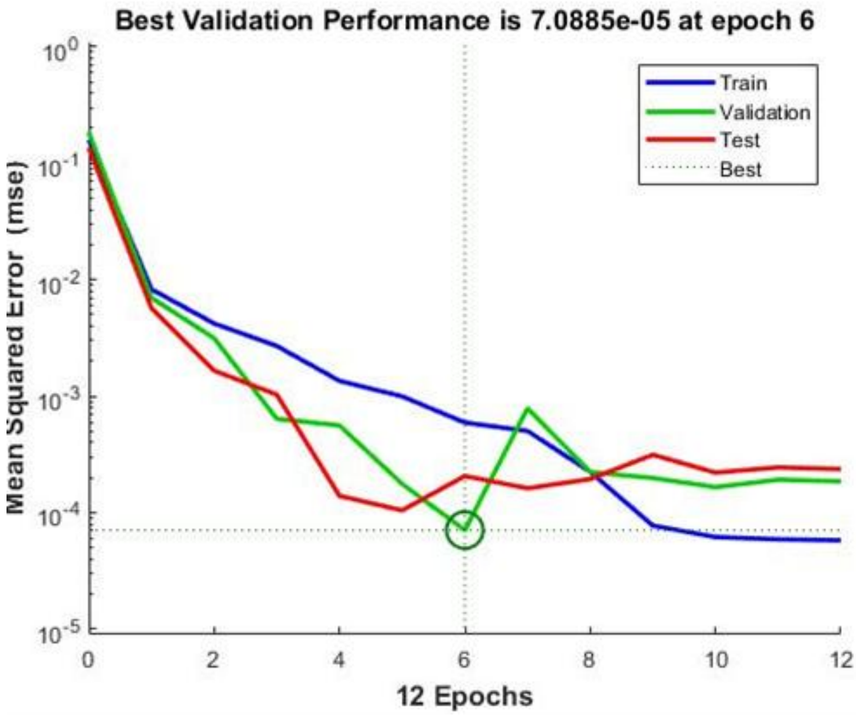
(a)



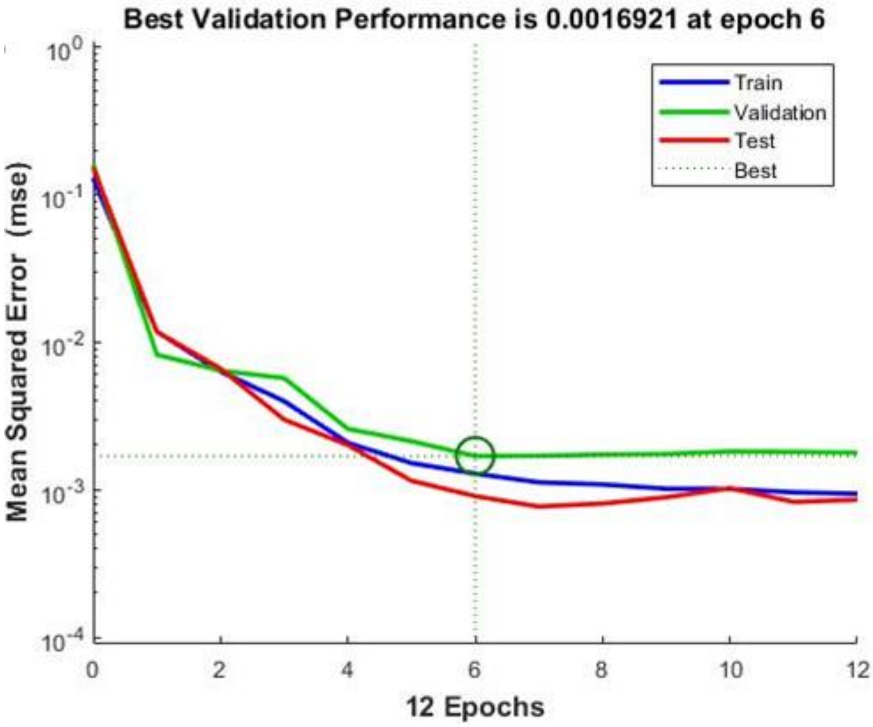
(b)

Figure 4.7: Training function of BPNN for (a) M1 and (b)M2 for (δ)

Further examination of the experimental versus predicted results can be shown in the performance graph obtained from Matlab software (Fig. 4.8). This plot was obtained based on mean square error calculated by the considering the observed and computed values. According the plots it can be justify that for the prediction of the complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen, M2-BPNN model outperformed models M1 and can served as the reliable prediction model. Meanwhile, the outcomes also showed that using four combination of variable as in M2 will increased the performance efficiency and thereby recommended to includes the softening point and penetration particularly for modeling complex modulus but in case of angle phase both M1 and M2 can served the prediction expectation. Fig. 4.9 shows the scatter plot of the best models for predicting and modeling complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen.

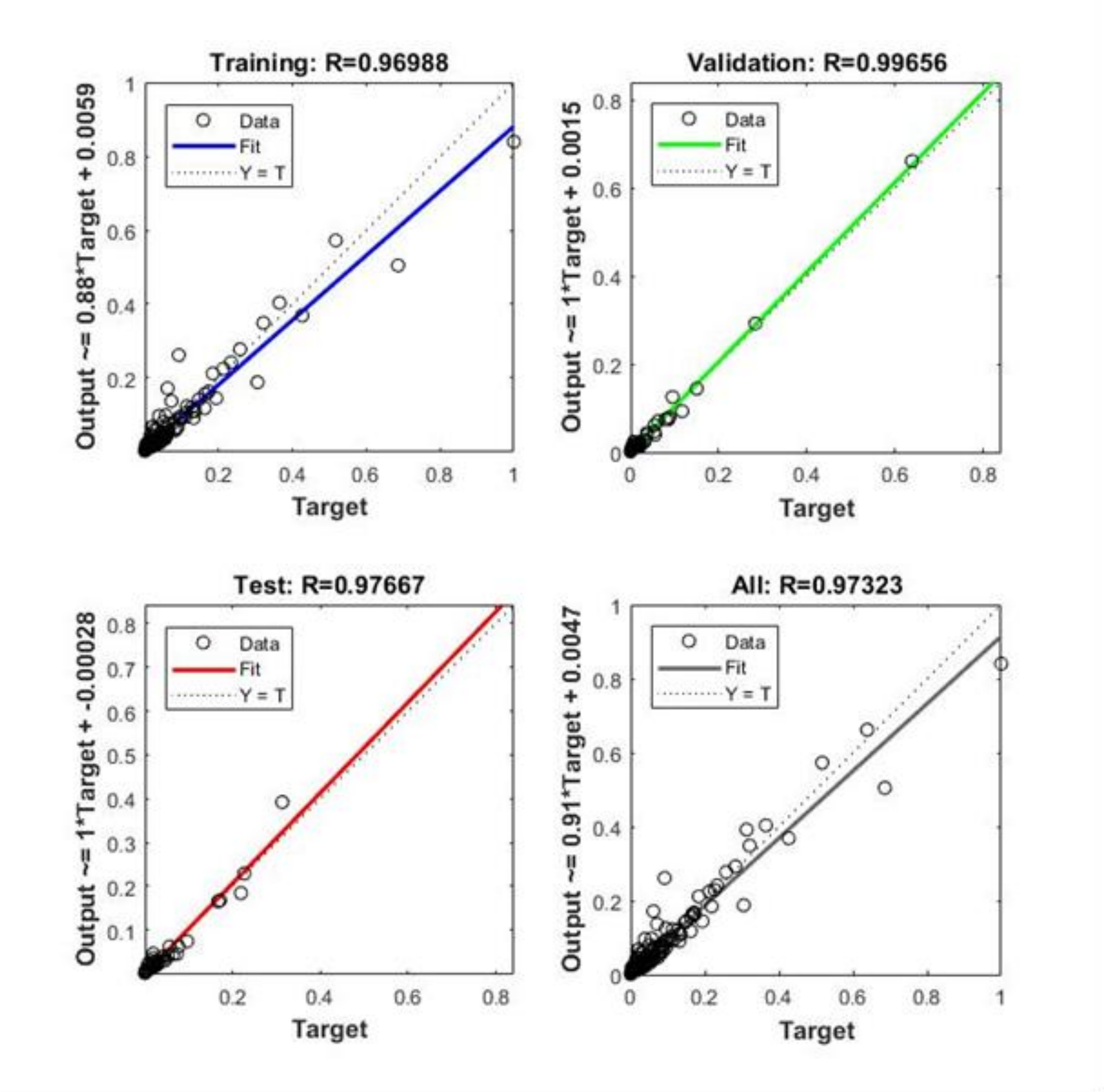


(a)

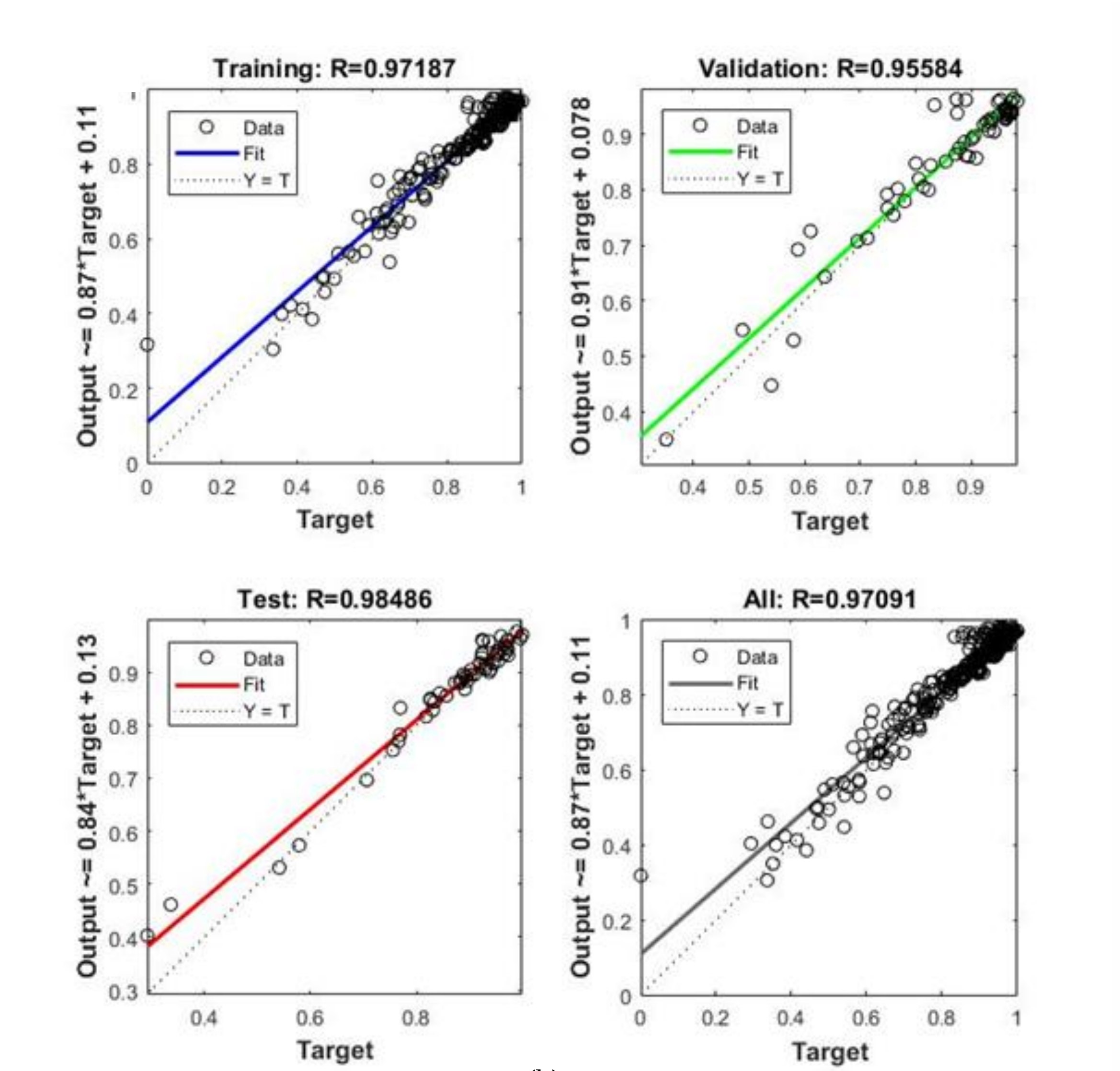


(b)

Figure. 4.8: Performance training function of BPNN for (a) (G*) and (b) (δ)


Training: R=0.96988
Output ~= 0.88*Target + 0.0059
Target
Data
Fit
Y = T
Validation: R=0.99656
Output ~= 1*Target + 0.0015
Test: R=0.97667
Output ~= 1*Target + -0.00028
All: R=0.97323
Output ~= 0.91*Target + 0.0047

(a)



(b)

Figure 4.9: Scatter plots showing the experimental versus predicted for (a) G* (b) (δ)

4.2.2 Results of support vector machine (SVM)

In SVM modeling, optimal and appropriate determination of parameters (C, ε, γ) in the LSSVM model is highly crucial for selecting the best model structure. support vector regression (SVM) is a form of SVM based on the two basic structural layers; first layer is kernel function weighting on the input variable while the second function is the weighted sum of kernel outputs. However, the results in **Table 4.5** shows the performance efficiency of SVM for the prediction of G* and (δ) of nanocomposite modified bitumen. From the results it can be seen that SVM model, as BPNN was trained using two different models M1 and M2. Among the combination models of SVM, M2 has the highest values of DC and the lowest values of RMSE both in training and testing data, therefore emerged the best models. Fig 4.10 shows point to point plots between the experimental and computed values for the best model of G* and (δ) (M2).

Table 4.5 Performance results of SVM model for (G*) and (δ)

			Training			**Testing**		
	Outputs	Models	DC	RMSE	R	DC	RMSE	R
	(G*)	M1	0.4373	0.0821	0.6613	0.3964	0.0617	0.6296
SVM		M2	0.5839	0.0791	0.7641	0.4510	0.0627	0.6715
	(δ)	M1	0.6596	0.0887	0.8122	0.5384	0.0745	0.7338
		M2	0.6649	0.0880	0.8154	0.5376	0.0742	0.7332

From the Table 4.2 can be concluded that SVM model is not capable of predicting both G* and (δ) of nanocomposite modified bitumen. This is proved by considering the valued of DC, RMSE and R coefficients. It is worth mentioning that the higher value of DC and R the better the performance analysis results and vice versa. On the other hand, the lower the value of RMSE the better the prediction accuracy. Even though the values of RMSE are low but the goodness of fit in all th model combination is low and there marked the results unreliable. The results indicated that the SVM model need to be finetune using some parameters or there is need of introducing optimization approach to improve the results of SVM model before being put in to application.

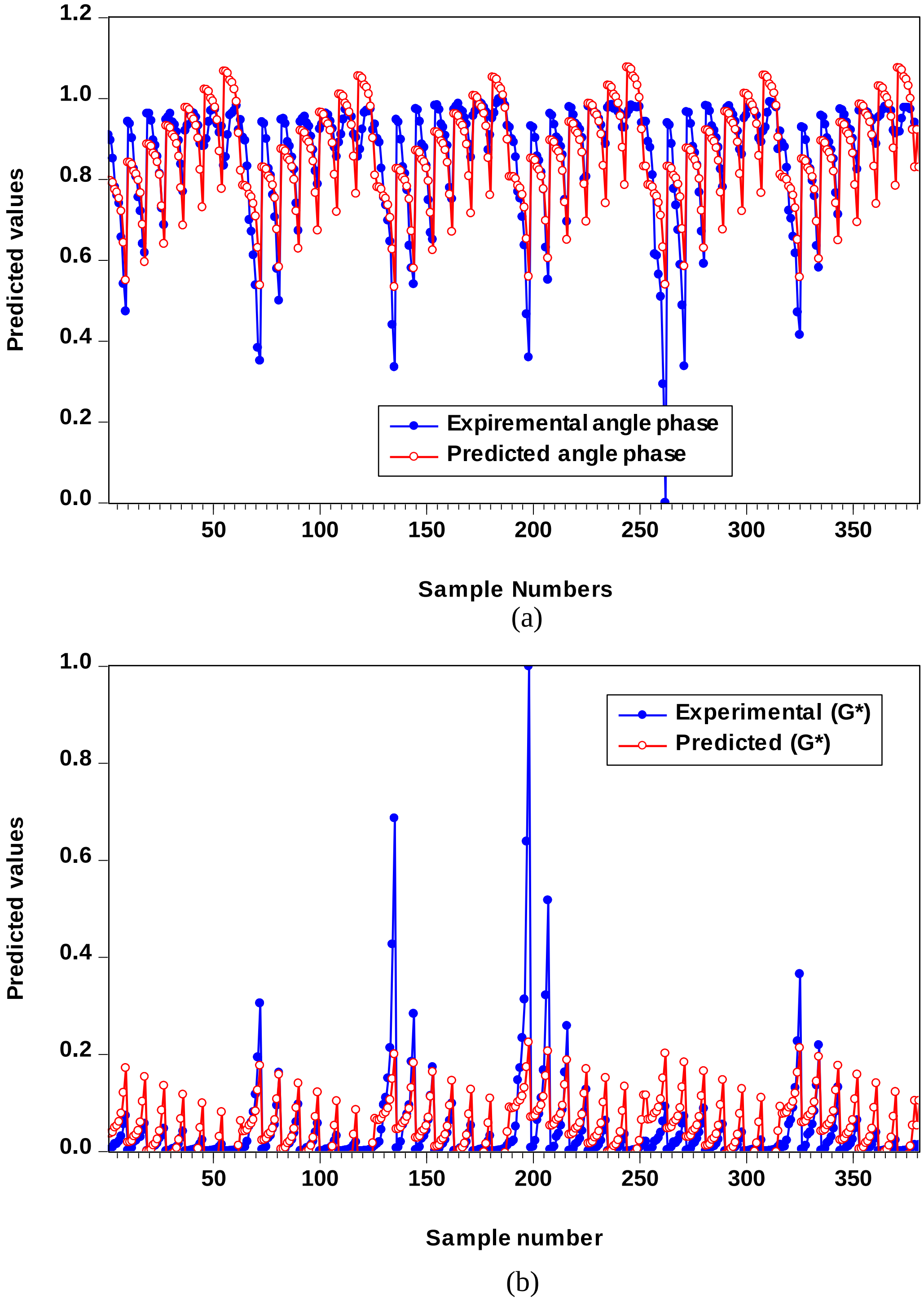


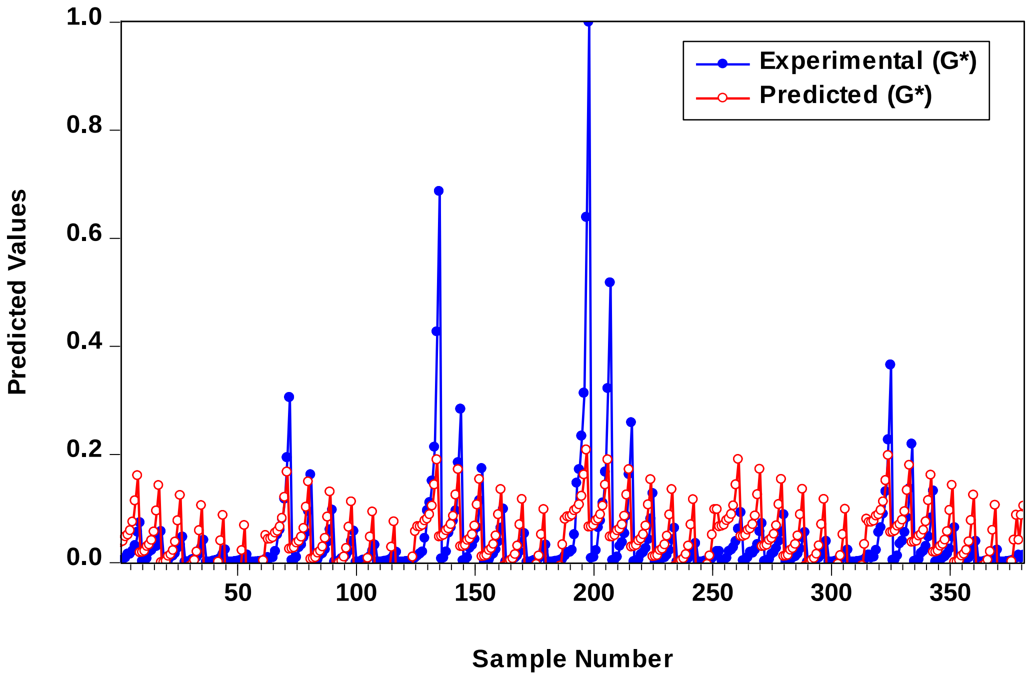
Figure 4.10: Point to point plots of the experimental vs predicted value for (a) G* (b) (δ)

4.2.3 Results of multilinear regression analysis (MLR)

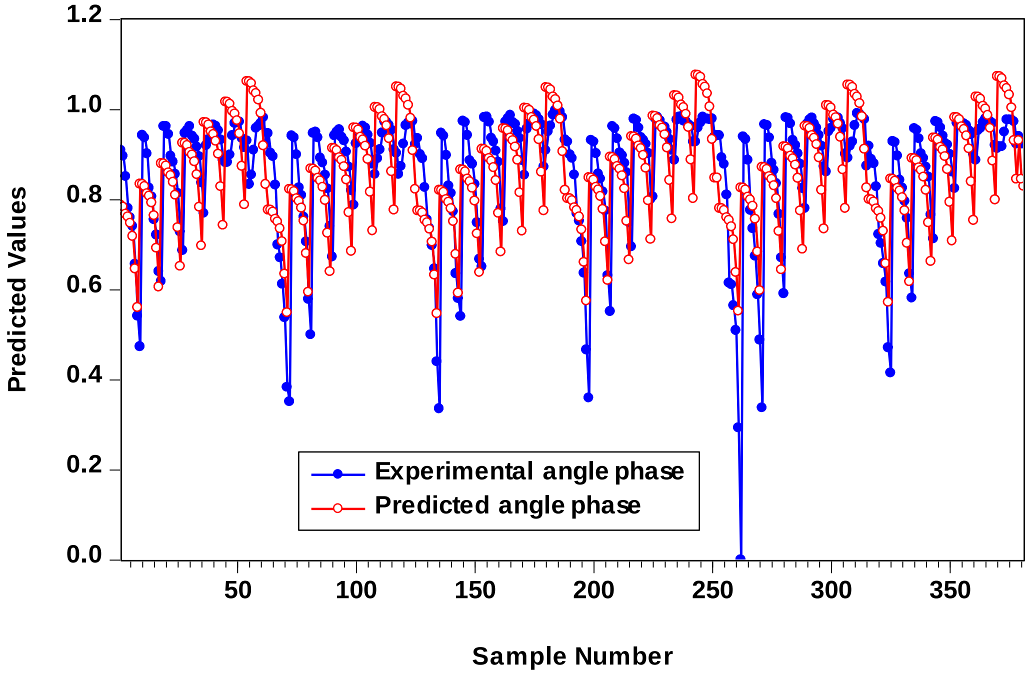
As in the case of other AI-based models, the classical MLR model were also determined using two different input combinations as stated above. For the MLR Model, the analysis was carried out in SPSS software (2018) and the performance results were computed in Microsoft excel as can be seen in Table 4.3. From the Table 4.6, it can be observed that, M2 outperformed M2 in term of DC, RMSE and R. The linear model was employed to investigate the linear relationship with the materials. The results also explained that the MLR model is not fit for the prediction of G* and (δ) of nanocomposite modified bitumen. From the result we can conclude that MLR is not reliable model for both the two combination Fig 4.11 shows point to point plots between the experimental and computed values for the best model of G* and (δ) (M2).

Table 4.6: Performance results of MLR model for (G*) and (δ)

			Training			Testing		
	Outputs	**Models**	**DC**	**RMSE**	**R**	**DC**	**RMSE**	**R**
	(G*)	M1	0.3408	0.0844	0.5838	0.3183	0.0305	0.5642
MLR		M2	0.3849	0.0816	0.6204	0.3674	0.0320	0.6061
	(δ)	M1	0.6568	0.0760	0.8104	0.6477	0.0721	0.8048
		M2	0.6671	0.0374	0.8168	0.6555	0.0495	0.8096



(a)



(a)

Figure 4.11: Point to point plots of the experimental vs predicted value for (a) G* (b) (δ)

CHAPTER 5
CONCLUSIONS AND RECOMMENDATION

5.1 Conclusions

The study employed three different data driven models including Back Propagation Neural Network (BPNN), Support Vector Machine (SVM), and Multilinear Regression (MLR) models to to predict the complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen. The outcomes of all the models where compare with the experimental models. For the data driven purpose, the used data were obtained from the experimental studies conducted on the polymer nanocomposite modified bitumen. Four different variables were carried out using two different input combination. The obtained results showed that BPNN model outperformed the two models in both the prediction of complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen. The results also indicated that the SVM model need to be finetune using some parameters or there is need of introducing optimization approach to improve the results of SVM model before being put in to application. Similarly, the results also explained that the MLR model is not fit for the prediction of G* and (δ) of nanocomposite modified bitumen. From the result we can conclude that MLR is not reliable model for both the two combination. For all the analysis three performance criteria were used which includes determination coefficient, correlation coefficients and root mean square error. The predictive skill of the models could be in order of BPNN>SVM> MLR.

The physical properties, stiffness (G*) and rutting resistance of unmodified, polymer modified and polymer Nano composite materials of Nano copper and Nano calcium modified at 3% and 5% concentrations to the weight of bitumen were investigated under a range of temperatures and frequencies using DSR. According to the test results and analytical models' performance evaluation, the following conclusions can be drawn:

I. According the BPNN model it can be justified that for the prediction of the complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen, M2-BPNN model outperformed models M1 and can served as the reliable prediction model. Meanwhile, the outcomes also showed that using four combination of variable as in M2 will increased the performance efficiency and thereby recommended to includes the softening point and penetration particularly for modeling complex modulus but in case of angle phase both M1 and M2 can served the prediction expectation

II. SVM model is not capable of predicting both G* and (δ)of nanocomposite modified bitumen. This is proved by considering the valued of DC, RMSE and R coefficients. It is worth mentioning that the higher value of DC and R the better the performance analysis results and vice versa.

III. The linear model (MLR) was employed to investigate the linear relationship with the materials. The results also explained that the MLR model is not fit for the prediction of G* and (δ) of nanocomposite modified bitumen. From the result we can conclude that MLR is not reliable model for both the two combination.

IV. Maximum enhancement in G* and (δ) was observed to be slightly above 1.00 E+05 Pa with 3% ASA-Nano calcium modified binder. Increasing the polymer nanocomposite material content enhanced the properties of the asphalt binder up to 3% concentration. However further use of modifier at 5% concentration to the weight of bitumen resulted in lower G* and rutting resistance, which is considered to be due to incompatibility of bitumen with the modifier. It was observed that 5% ASA modified and 5% ASA-Nano calcium and 5% ASA-Nano copper modified blends demonstrated almost equal enhancement in the rheological properties of asphalt binder.

5.2 Recommendation

According to a study conducted by Ali et al., (2015) the ASA modified bitumen with base 60/80 grade provided higher G* and (δ)values and therefore, it is significant that among the types of modifier materials, the penetration grade of base bitumen significantly influences the performance of asphalt binders. However, based on data driven models, it is also suggested that more algorithms and optimization methods should be introduce and practice in order to prediction of the complex modulus (G*) and phase angle (δ) of polymer nanocomposite modified bitumen. As such, genetic algorithms, particle swam optimization, extreme learning machine, deep learning algorithms should use in future studies.

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