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Assessment of Antistripping Agents on Adhesion of Damaged Asphalt by Neural Network

Sanjida Ahsan

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ASSESSMENT OF ANTISTRIPPING AGENTS ON ADHESION OF DAMAGED

ASPHALT BY NEURAL NETWORK

BY

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THESIS

Submitted in Partial Fulfillment of the

Requirements for the Degree of

MASTER OF SCIENCE

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DEDICATION

To my family

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ASSESSMENT OF ANTISTRIPPING AGENTS ON ADHESION OF DAMAGED ASPHALT BY NEURAL NETWORK

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ABSTRACT

In this study, Neural Network (NN) model is developed to quantify nano-level adhesion force of moisture damaged asphalt binder using Atomic Force Microscopy (AFM) test data. AFM data contains five point force-distance values determined for some specific asphalt chemical functional groups. Asphalt binder samples contain different types and percentages of polymer modifiers and antistripping agents (ASA). Due to complex and nonlinear interaction between the asphalt properties and adhesion force of asphalt, it is difficult to assess the effects of asphalt binder properties on the adhesion forces using laboratory AFM testing. NN has the ability to recognize and trace the complex relationship trend existing between inputs and outputs; therefore NN is chosen to be used for the development of the model in this study.

Two neural network models are developed, one for lime treated and another for chemical antistripping agent treated asphalt samples. To train the network, AFM tip-sample distance data, percentage of lime, type and percentage of polymer and asphalt chemical functional groups are considered as inputs and AFM force as an output. On the basis of performance, 12-9-16-3 and 11-25-25-5 NN are selected as the final structure of models for lime and chemical antistripping agents treated asphalt samples respectively. The models show good agreement with the laboratory data for both models.

v

To this end, the developed models are used to predict adhesion of both lime treated and chemical antistripping agents treated dry and wet asphalt for same inputs. This allows observing the effect of lime and chemical additives in resisting adhesion loss due to moisture conditioning thus moisture damage of bond forces of asphalt. NN induced results show that lime performs better in resisting moisture effect for samples containing 3% SB polymer compared to other polymer modified samples. Also, lime fails to resist the degradation of adhesion force in wet sample determined by silicon nitride tip for all types of modified asphalt samples. Among all the chemical ASAs, Morlife shows best performance in presence of 3% SB and 3 and 5% SBS in reducing moisture effect on adhesion and cohesion bond forces of asphalt at nano-level. In all cases, increase in percentage of additives above 1% does not aid in resistance to moisture damage.

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CHAPTER 1 INTRODUCTION

1.1 Background

The effect of water on the performance of Hot Mix Asphalt (HMA) pavement is a complex issue that has been a prime topic to the researches for last six decades. In presence of water, asphalt concrete pavements experience loss in durability and strength. Divito and Morris (1982) specify three attributes to be related to pavement strength. Those are: cohesive resistance of binder, adhesive bond between binder-aggregate and the aggregate interlock and the frictional resistance between aggregate particles. Cheng et al. (2002) mentioned that strength loss subjected to moisture conditioning can be predicted by comparing wet and dry adhesive bond strength between asphalt and aggregate. In addition, Huang et al. (2002) stated that moisture sensitivity of HMA can be better understood by quantifying the effect of water on both adhesion and cohesion of asphalt. Therefore, moisture damage can be defined as the loss of strength and durability of the adhesion bond between asphalt and aggregate and cohesion bond within the asphalt binder by the action of water.

The bond exists between the aggregate and asphalt at the interface of asphalt-aggregate is known as adhesion and the intermolecular bond force present within asphalt is defined as cohesion of asphalt. When water intrudes at the interface of the asphalt-aggregate system, it weakens or breaks the bond between asphalt and aggregate. This phenomenon is known as stripping action of water. Stripping eventually leads to breaking the adhesion bond completely and finally towards the failure of pavement. Cohesion failure due to moisture occurs when water interacts with the asphalt that results in damage in integrity of the molecules with asphalt. Cohesion

failure eventually leads to the adhesion failure of HMA due to reducing the strength of bond of asphalt film to stick together.

Asphalt has a complex chemical structure. Chemical composition of asphalt varies significantly among asphalt of different sources (Robertson 2000). Therefore, mostly, measurement of moisture sensitivity in terms of adhesion and cohesion of asphalt has been done based on laboratory tests (Canestrari et al. 2010). Researchers have related the adhesion and cohesion of asphalt to mechanical properties of asphalt and have developed numerous laboratory techniques such as hamburg wheel tracking (Aschenbrener 1995), asphalt pavement analyzer (West et al. 2004), original Lottman indirect tension tests (Lottman 1982) and so on to determine moisture damage of asphalt. However, empirical nature of test methods used for the evaluation of moisture damage and inherent variability of asphalt property impede the reliable characterization and assessment of water effect on pavement deterioration (Yilmaz and Sargin 2012).

Cheng et al. 2002 state that cohesion and adhesion of asphalt aggregate system are directly related to the surface energy of the asphalt. Therefore, efforts have been made to quantify moisture damage by determining surface energy of asphalt with the help of Atomic Force Microscopy test (Al-Rawashdeh and Sargand 2013), dynamic Wilhelmy plate test (Wasiuddin and Zaman 2008), Microcalorimeter test (Bhasin and Little 2009) etc. These tests improve the understanding of microscale to nanoscale behavior of asphalt with different asphalt binder properties undergoing moisture damage. Quantification of adhesion from surface energy measurement is now accepted as a more fundamental way of approach to predict moisture susceptibility (Arabani and Hamedi 2011). On-going efforts are being made by researchers to develop more reliable and improved methodologies to identify and quantify fundamentals of the moisture susceptibility phenomena of asphalt binder.

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There are some measures that are proved to be effective by laboratory tests and field performances in lowering the propensity of moisture damage. The use of hydrated lime or other liquid and chemical anti-stripping agents (ASA) is the most common method to improve the moisture susceptibility of asphalt binders (Putman and Amirkhanian 2006). ASA improves the resistance to moisture damage by increasing the bond strength of asphalt. Laboratory tests are done to prove the effectiveness of ASA on the adhesion and cohesion of asphalt undergoing moisture damage. However, moisture damage in asphalt concrete is influenced by many factors such as asphalt grade, modifiers, phenol group concentrations, aggregate surface chemistry, minerals and so on (Hicks et al. 2004). Thus, chemical interaction between different additives and asphalt also depends on the mentioned factors. So, moisture damage is expected to be mitigated by the use of ASA but the performance of ASA on asphalt cannot be predicted thus moisture damage problem cannot be fully resolved. Therefore, water effect on pavement deterioration is an open ended problem which is yet to be understood. Also, the performance of ASA for different asphalt chemical and mix properties under moisture effect is needed to be assessed to identify better and more effective ASAs in resisting moisture related damage.

1.2 Motivation

Adhesion and cohesion loss are two prime issues that are used to define and quantify moisture damage. Therefore, determination of factors and their extents in affecting cohesion and adhesion loss can be useful in evaluating moisture damage. However, due to complex interaction of all the factors involved influencing adhesion and cohesion of conditioned asphalt, it is difficult to observe the effect of individual and combined effect of the factors on adhesion and cohesion of asphalt. Therefore a model can be developed that can trace the intricate relationship between asphalt adhesion/cohesion of asphalt and the factors those have impact on adhesion/cohesion of

asphalt. The model can be used in predicting adhesion and cohesion of wet and dry conditioned asphalt undergoing moisture effect. Comparing the predicted value of dry and wet conditioned adhesion and cohesion can be utilized to assess the influence of the asphalt properties on adhesion and cohesion loss of asphalt so as moisture damage of asphalt.

Atomic Force Microscopy (AFM) test was conducted to measure the adhesion and cohesion forces of wet and dry conditioned asphalt using functionalized tips. The tips were functionalized so that both cohesion and adhesion of asphalt can be resembled by the tip and asphalt surface interaction on AFM test. AFM test provides nano-level adhesion and cohesion forces for some prominent chemical functional groups present in asphalt binder and is conducted on dry and wet asphalt samples with varying contents of polymer and ASAs. An attempt is made to construct a Neural Network (NN) model to predict adhesion and cohesion of asphalt by addressing the functional relationship exists between the chemical mix properties of asphalt (inputs) and adhesion forces (output) determined by AFM test. NN has been successfully used in many civil engineering application to analyze complex relationship exists among multiple variables and proved to be better performed technique in comparison to other conventional models (Xiao and Amirkhanian 2008). Therefore, NN is chosen to develop the model in this study. In addition, effects of ASA on the adhesion and cohesion loss of asphalt can be assessed using the relationship developed by NN comparing bond force of wet and dry conditioned asphalt sample.

1.3 Objectives

The main objectives of the study are to

- Develop Neural Network (NN) model that predicts asphalt adhesion force of dry and wet asphalt samples using Atomic Force Microscopy (AFM) laboratory test data. The model is to be constructed to map the nonlinear complex relationship between the asphalt chemical and mix properties and nano level adhesion forces of asphalt on the basis of AFM laboratory test factors and force measurements.
- Use the developed NN to predict adhesion force of asphalt samples having different type and percentages of antistripping agents to examine the effect of ASA on the adhesion loss of asphalt due to moisture conditioning.

1.4 Organization of the Study

The study is divided into five chapters based on the specific objectives. Chapter 1 provides the incentives to perform the study. Literature review on determination of adhesion and cohesion of asphalt to assess moisture damage of asphalt are covered in Chapter 2. Use of NN in developing prediction model in pavement materials and a brief description of the AFM test data to be used to develop model are also included in Chapter 2. Chapter 3 provides the fundamentals of the NN. Also types, algorithm and tool associated to develop the NN prediction model are incorporated in Chapter 3. In Chapter 4, stepwise development of NN model based on the lime treated asphalt samples is provided. In addition, use of developed NN model to predict adhesion of dry and wet asphalt to compare and discuss the performance of lime in reducing moisture damage is provided in Chapter 4. Chapter 5 has the same content as Chapter 4 but all analyses are performed and

explained for chemical ASAs instead of lime. Finally, the conclusions and recommendations based on this study are presented in Chapter 6.

CHAPTER 2 LITERATURE REVIEW

2.1 Importance of Quantification of Adhesion and Cohesion of Asphalt

Moisture damage has been a major concern to asphalt technologies. It accelerates premature failures and degrades pavement performance by inducing different pavement distresses including rutting, fatigue cracking, thermal cracking etc. It is acknowledged that distress resistance of asphalt pavement depends on the asphalt-aggregate interfacial bonding strength that could be highly deteriorated by moisture (Moraes et al., 2011). Three mechanisms are mentioned by Copeland et al. (2007) that cause moisture degradation of asphalt mixture: (1) loss of cohesion within the asphalt mastic (2) failure of the adhesive bond between aggregate and asphalt and (3) degradation of the aggregate.

Probable mechanism behind loss of adhesion can be described by the greater affinity of aggregate to water than asphalt. When water intrudes at the interface of asphalt-aggregate, aggregate attract more to water than asphalt film. This causes bond failure of asphalt and aggregate. This phenomenon is known as stripping. Loss of cohesion mechanism can lead to two different types of failure (Graf, 1986). The first involves softening of asphalt by the interaction of water that weakens the cohesion bond between the molecules within asphalt. This drives toward the disintegration of asphalt film to stick together. The other involves reduction in adherence capacity of asphalt to the surface of aggregate that leads towards the separation of asphalt film from aggregate surface.

Correlation between adhesion and cohesion bond of asphalt with moisture damage is well established in many literature (Bhasin and Little 2009, Majidzadra and Brovold 1968). Therefore, a better understanding of the moisture sensitivity of HMA can be achieved with a

quantitative measurement of the influence of water on both adhesion and cohesion, performed directly on the asphalt-aggregate system (Youtcheff and Aurilio, 1997; Huang et al., 2002; Kanitpong and Bahia., 2003).

Hence, association of cohesion and adhesion mechanisms with moisture damage makes these parameters so important in moisture damage behavior and quantification related studies in asphalt technology. Not only determination of adhesion and cohesion useful in understanding behavior of moisture damage, but also it plays vital role in assessing performance of different modifiers and additives added to moisture conditioned asphalt to improve adhesion loss so as moisture damage.

2.2 Past Studies on Quantification of Adhesion and Cohesion of Asphalt

Adhesion and cohesion of asphalt mix have been determined by developing methodologies laboratory tests and by modeling based on empirical theories for wet and dry conditioned asphalt.

Adhesion is measured with the pull-off tensile strength test by using the pneumatic adhesion tensile tester. (Youtcheff and Aurilio, 1997; Kanitpang and Bahia, 2005). They carried out the test on the basis that adhesion and cohesion of asphalt-aggregate system are closely related to the indirect tension strength of asphalt mixture. Kanitpong and Bahia (2005) also performed tact test to measure cohesion strength of asphalt binder. They accomplished these tests to evaluate effects of modifiers and antistripping additives on adhesion and cohesion of asphalt under moisture conditioning.

Wasiuddin et al. 2008 conducted dynamic Wilhelmy plate test using the concept of surface free energy concept to investigate the effect of additives on the adhesion of asphalt. The adhesion

force between two different materials depends on the surface free energy value. (Al-Rawasdeh and Sargand 2013). Therefore adhesion loss thus moisture damage is characterized by surface free energy in this paper.

Yang and Al-Qadi (2009) performed tests using Scanning electron microscope with energy dispersive spectroscopy to investigate the adhesion interface between asphalt and aggregate.

Atomic force microscopy test was performed to measure adhesion/cohesion pull of forces of moisture conditioned asphalt. (Tarefder and Zaman 2010). They used functionalized tips to simulate cohesion and adhesion of asphalt aggregate system. Also, they evaluated the effect of polymer modification on asphalt undergoing moisture damage.

Adhesion and cohesion of warm mix asphalt in terms of surface energy is determined by performing AFM laboratory test (Al-Rawasdeh and Sargand 2013). In this study, real aggregate tips are used to measure adhesion instead of industrial tip. They also used a functionalized tip to determine cohesion of asphalt. They observed effect of some additives on adhesion and cohesion of wet and dry conditioned asphalt.

Bhasin and Little (2009) developed a methodology to quantify adhesion by application of microcalorimeter. They evaluated effects of different types of aggregate and asphalt binder on adhesion of asphalt using microcalorimeter.

In addition to laboratory tests, modeling of asphalt using empirical theories are developed by researchers to observe adhesion and cohesion damage of moisture conditioned asphalt pavements. Hossain and Tarefder (2012) developed a finite element model to determine adhesive and cohesive damages in asphalt concrete under both dry and wet conditions based on surface based traction separation damage law and maximum stress criteria respectively.

All the studies quantified adhesion and cohesion of asphalt by performing laboratory test or modeling developed on the basis of different methodologies. However water effect on adhesion and cohesion of asphalt is a very intricate phenomenon and depends on various factors such as chemical, mechanical and surface properties of asphalt and aggregate. The factors have complex influence on adhesion and cohesion of asphalt. Therefore, a neural network model is developed in this study using AFM laboratory test data to map the complex relationship between different asphalt mix properties of asphalt (including polymer modifiers and antistripping additives) and adhesion/cohesion of asphalt.

2.3 Use of NN in Pavement Engineering

In the past 15 years there has been an increased interest in NNs, a computational intelligence system, in pavement system applications. Past studies revealed that, there have been several successful studies that incorporated NNs to predict the pavement structural parameters such as pavement moduli, pavement layer thickness, etc. using Falling Weight Deflectometer (FWD) deflection data (Gucunski et al. 1998, Kim and Kim 1998, Lee et al. 1998, Meier et al. 1997, Meier and Rix 1995, Williams and Gucunski 1995, Saltan and Terzi 2004, Ceylan et al. 2008). The researchers concluded NNs to be more efficient and a better technique compared to conventional and traditional tools in this regard. In addition, a NN proved to a better prediction tool in predicting low temperature performance of modified asphalt mixtures in comparison to a general linear model (Tasdemir 2009) due to its versatile and complex pattern tracing and computational capabilities. Different state Departments of Transportation (DOT) developed models on the basis of NNs to compute pavement related parameters. For example, Illinois DOT successfully used NNs with low average error in comparison to ILLI-PAVE analysis in estimating pavement moduli, maximum stress and strain from FWD data (Ceylan et al. 2004).

Texas DoT also developed a methodology to calculate remaining life of flexible pavement with the help of NN (Ferregut et al. 1999).

NNs are not only used in predicting pavement structural parameters, they are also used in determining pavement performance parameters by researchers. Owusu-Ababio (1998) developed a NN based model to predict cracking performance of pavement. Pavement cracking depends on many parameters. Though cracking maintained complex and critical relationships with the parameters, NN was able to pick the trend of the relationship and predict cracking on the basis of those parameters. Yang et al. (2003) applied a NN in predicting the pavement crack index and pavement condition rating, which was very difficult to forecast using traditional techniques and tools. Alsugair (1995) and Huang and Moore (1997) utilized a NN technique to develop a module that suggested suitable maintenance strategies on the basis of distress data and corresponding maintenance offered for pavement.

From the laboratory test data for bituminous materials, NN was used to predict dynamic modulus of Hot mix asphalt (HMA) (Ceylan et al. 2008) and fatigue life (Huang et al. 2007). Xiao and Amirkhanian (2008) involved NN to predict stiffness behavior of rubberized asphalt concrete mixtures with reclaimed asphalt pavement. They also developed a neural network model to predict the resilient modulus of rubberized mixtures containing recycled asphalt pavement (RAP). On the basis that the resilient modulus can be characterized by the pulse loading and strain, the input variables selected for modeling were percentage of rubber and RAP, viscosity value, shear loss modulus, binder stiffness, m value and testing temperature. NN model results were compared to results obtained from regression analysis. The relationship between the dependent and independent parameters is complex in nature and NN model predicted better accurate result rather than regression model. Tarefder et al. 2005 used NN to determine asphalt

rutting. They also determined permeability from asphalt mix properties using NN. All NN models showed satisfactory performance, better efficiency compared to traditional regression models and so, were being accepted by researchers.

All of the past studies imply that a NN is capable of tracing the complicated relationships existing between the input and output parameters of a model. However, a NN has not been used extensively in determining pavement material characterization. The AFM laboratory data used in this study has an intricate relationship between the test parameters and adhesion value of asphalt. Therefore, a NN model is chosen to develop a model that is capable to predict adhesion of asphalt on the basis of test factors provided to the model.

2.4 Fundamentals of AFM testing

2.4.1 Basics of AFM Testing

AFM is a scanning probe technique that measures force as a function of distance between two molecules or atoms. It uses a laser beam deflection system along with a probe and sample. A probe is a sharp tip placed on a cantilever. Laser is reflected from the reflective surface of the cantilever and onto a position sensitive detector. Using this system, beam position can be determined. When a tip with the cantilever comes in close distance to a sample surface, an attraction or repulsion force occurs in between the surface and probe depending on the distance between them. This force is not directly measured by AFM, rather the deflection of the cantilever due to the attractive or repulsive force is recorded. Knowing the stiffness of the cantilever, force is determined from Hooke's law as follows:

$$
F = -kz \tag{2.1}
$$

$$
\lim_{\omega\rightarrow\infty}\mathbf{Z}=\mathbf{I}
$$

Where, F is the force, k is the stiffness of the lever, and ζ is the distance the lever is bent.

Fig. 2.1 shows schematic five point force-distance curve that can be attained from the AFM test. It can be seen that, initially, when the tip is far away from the sample's surface, there is no attraction or repulsion between the tip and surface. Then, the tip approaches to a distance when at first the tip jumps onto the sample's surface due to some attraction (position B). Pushing the tip further toward the sample's surface then produces a strong repulsive force (position C). Now, retracting the tip from the sample's surface decreases the repulsion and increases the attraction force. On the retraction path, there is a distance beyond which the attraction tends to decrease. A "pull off" force is needed at position D to completely remove the tip from the influence of the strong attraction force. The force value at position D is commonly regarded as the adhesion or cohesion force of that particular sample. Finally, the tip is fully retracted from the force influence zone at position E.

2.4.2 Tip Functionalization

Asphalt is a mixture of highly condensed polycyclic aromatic hydrocarbons. Asphalt chemical structure is yet not fully explored. However, presence of some compounds in asphalt has been detected such as carboxyl (-COOH), methyl $(-CH_3)$, ammine $(-NH_3)$ and hydroxyl $(-OH)$ groups (Testa 1995). AFM tips were functionalized with these functional groups to measure cohesion within the asphalt. Another tip, made of silicon nitride $(Si₃N₄)$ is used to probe the asphalt surface to measure adhesion between asphalt and aggregate.

2.4.3 Laboratory AFM Data Processing

AFM test is conducted on an asphalt sample using five different types of AFM tips to probe the sample. A force distance curve attained from the AFM test is shown in Fig. 2.2. The figure is for an asphalt sample probed with a tip modified with the –OH functional group. Fig. 2.2 has the same characteristic as the schematic force-distance curve shown in Fig. 2.1. Indeed, force and distance values are tabulated corresponding to the points A, B, C, D, E in Fig. 2.1 and Fig. 2.2. From the force-distance curve, the force value corresponding to point D is considered as the adhesion or cohesion force. On the basis of what type of tip is used to probe the asphalt surface, the force can be named as adhesion or cohesion.

2.4.4 AFM Test Data

The AFM laboratory test data chosen to develop NN model contains five point force-distance values (including adhesion/cohesion force) of modified asphalt sample measured by five different tips for dry and wet conditions. Two types of modifications techniques are incorporated in asphalt sample: polymer modification and addition of antistripping agent (ASA). AFM tests were done to acquire the force distance curve for a sample with the variables illustrated below.

2.4.5 Wet/Dry

Asphalt sample is conditioned both wet and dry to observe the effect of moisture on bond force of asphalt.

2.4.6 Polymer Type and Percentage

Polymer modification on asphalt is commonly done to improve the resistance of rutting, fatigue and thermal cracking of asphalt pavements. Two elastomer types of polymers are used to modify

asphalt sample used in AFM test. They are Styrene Butadiene Styrene (SBS) and Styrene Butadiene (SB). Elastometric polymer is useful in enhancing the elastic component and reducing viscous component of asphalt binder. (Robinson 2004). SB and SBS type polymers have emerged as effective polymers to be used in asphalt with optimum performance, reliability, ease of use and economy. This allows the modified binder to have reduced permanent deformation. In addition, modified binder becomes less susceptible to temperature and more resistive to thermal cracking and rutting. Also, polymer modified asphalt showed better performance under moisture effect. Polymers effect viscosity of asphalt in a way that improves the adhesion ability of asphalt binder to aggregate surface. Therefore, asphalt sample modified with 3, 4 and 5% of SB and SBS modified samples are used to determine bond force of asphalt in AFM test.

2.4.7 Tip Type

Force distance curve results are recorded for five different tips that are used to probe asphalt sample in the laboratory test. Among the tips, four tips are functionalized with asphalt functional groups such as carboxyl (-COOH), methyl (-CH3), ammine (-NH3) and hydroxyl(-OH). These tips are used to facilitate the measurement of cohesion force exists between two asphalt molecules. Another tip silicon nitride Si3N4 (Silica is the most naturally occurring aggregate mineral) is used to measure adhesion force of asphalt-aggregate. Among the tips, COOH and OH are hydrophilic that is they have affinity to water. All other tips are hydrophobic type.

2.4.8 Antistripping Agent Type and Percentage

Lime and four different types of chemical antistripping agents are used to conduct AFM test. They are Unichem, Morlife, Wetfix and Klingbeta. General composition of chemical ASA includes proprietary surfactant blend. Surfactants modify the interfacial tension of aggregate-

asphalt and reduce the contact angle and allow the aggregate to be wetted by the asphalt. Typical dosage of ASA is between 0. 25% to 1.0% by the weight of the binder. Some general description of chemical ASAs provided by the supply companies are given below

Wetfix

Wetfix is a liquid anti-strip for hot-mix asphalt. According to Idaho Department of transportation it shows good heat stability, requires only low dosages and has low volatility. It is liquid aminebased surfactant additive for asphalt mixes. It can be pre-blended with the asphalt binder or it can be injected into the asphalt line at the hot-mix plant.

Morlife

Morlife is a premium performance product based on a proven chemistry for use as an adhesion promoter in hot-mix asphalt pavements. Morlife improves the bond between asphalt and aggregates, overcoming problems associated with poor adhesion and water suspectability. HMA mixes treated with Morlife exhibit superior resistance to moisture-related damage and stripping, resulting in longer lasting pavements. The heat stability of Morlife is a dramatic improvement over many additives in HMA applications.

Klingbeta

Klingbeta is a proprietary surfactant blend. It shows exceptional stability in hot asphalts, can be used at low dosage levels as it is a concentrated product. Despite its high activity, Klingbeta offers low viscosity and easy handling even at low temperatures. Recommended dosage of Klingbeta based on asphalt binder weight are 0.25-0.75% for hot mix, which should be confirmed in laboratory mix design tests. Klingbeta is preferably added to the asphalt at the mix plant by means of a specially designed injection system. Alternatively, the product can be

incorporated into the asphalt by mechanical agitation, pump circulation of the storage tank, or by injection into the asphalt loading line followed by recirculation through the truck bypass system until properly mixed.

Unichem

Unichem is a liquid antistrip additives conatains some heat stable ingredients that perform well in various heat stability evaluations. It increases the wettability of aggregate surface to allow easy coating of asphalt. Unichem is effective in concentrations ranging upward from 0.l25 percent by weight of asphalt. (Arifuzzaman 2010)

The use of hydrated lime or other liquid anti-stripping agents (ASA) is the most common method to improve the moisture susceptibility of asphalt mixes (Puttman and Amirkhanian 2006). The AFM data to be used by NN contains adhesion value of polymer modified asphalt samples added with lime and four chemical ASAs named as Unichem, Morlife, Klingbeta and Wetfix. Lime is added at three different percentages (0.5, 1 and 1.5) and chemical ASAs are mixed at a range of 0.25 to 1% by weight of base binder. Chemical ASAs are mixed at asphalt plant but polymers are mixed at laboratory. This study aims to observe the effect of lime and other chemical ASAs on the quantification of adhesion by NN using pull off force determined by AFM test. Therefore, past studies on lime and other chemical ASAs incorporated to improve the adhesion loss of asphalt so as moisture damage, are included in this chapter.

2.5 Effect of Lime and Chemical Antistipping Additives on Asphalt

A number of different methods have been used to improve the adhesion loss of asphalt under moisture damage that makes asphalt pavement more resistant to moisture damage. Some of the methods included addition of dry lime or portland **c**ement to the mix or lime-slurry treatment of

the aggregates, bitumen precoating of the aggregate, careful selection of aggregate using spe**c**ial mineral fillers or not allowing hydrophili**c** aggregates, washing or blending of aggregates, and addition of chemical antistripping agents (Divito and Morris 1982).

Lime is the most widely used antistripping additive (Little and Epps 2001). Kim et al. (2008) concluded that mixed treated with lime performed better due to increase in strength and stiffness of mastic that eventually led to better resistance to moisture damage. Kennedy and Ping (1991) conducted laboratory tests on asphalt mix containing lime and found that lime treatment was consistently effective in reducing moisture damage in terms of tensile strength property ratio. Pickering et al. (1992) observed the effect of lime on moisture damage of asphalt mix by conducting resilient modulus and tensile strength test. They concluded that lime treatment resulted in significant improvements in moisture conditioned properties of HMA mixture. Jaskula and Judycki (2005) concluded on the basis of laboratory tests that application hydrated lime improved asphalt concrete resistance to water and frost action. A report on effectiveness of antistripping additives in fields carried by Virginia transportation research council showed that projects containing hydrated lime displayed less adhesion loss thus less stripping.

Chemical antistripping agents are also used to reduce the surface tension of asphalt for more uniform wetting on the surface of aggregate. Thus it improves the adhesion between the aggregate and asphalt. Chemical antistripping agents have chemical compositions that are in general proprietary information. Mostly, ammine based chemical additives are used to reduce moisture damage of asphalt mix. Surfactant blend based chemical antistrip additives show good performance in moisture effect performance tests conducted by Department of Transportation of many states. Also, laboratory tests are done to determine the effects of antistripping agent on the determination of adhesion and cohesion of moisture conditioned asphalt. (Kanitpang and Bahia

2005). However it is difficult to generalize the effect of antistripping agent on moisture damage behavior of asphalt. Variability in the chemical composition and alteration of mechanical properties of asphalt due to change in source and various factors makes it very tough to predict the behavior of different antistripping agents on adhesion/cohesion of asphalt. Therefore research efforts are continued to be provided on this sector so that effective ASAs can be chosen for a particular type of binder.

In this study, two different neural network models are developed for lime treated and chemical ASA treated asphalt AFM laboratory test data. These two developed models are then used to assess the performance of lime and other chemical ASA in reducing moisture damage of asphalt binder.

Figure 2.1 Sample force-distance curve for AFM laboratory test

Figure 2.2 Force-distance curve obtained for asphalt sample probed with –OH tip by AFM laboratory test

CHAPTER 3 NEURAL NETWORKS

3.1 Basics of Neural Network

Neural network is a parallel distributed information processing system. It is a non-linear computational model which contains neuron that performs mathematical function. Following the basic functional system of biological neuron, neural network models are developed. Structure and task of biological neurons are extremely simplified and incorporated in terms of some mathematical functions in a neural network model.

Fig 3.1 shows the structure of a biological neuron and mathematical model neuron. A biological neuron comprises dendrites, axon and synapses. Through dendrites, neuron receives information. Then the information is sent as spikes of electrical activities through axon. Axon delivers the information transferred by axon to branches of neuron known as synapses. Synapses have excitatory and inhibitory activities that filter the significant and important information passed to next neuron dendrites. Thus, information is propagated from neuron to neuron for processing. Internal process of the brain neurons is very complex and some of the processes are still unknown. Neural network model is not a mimic of the functions of the human brain and neuron. It is just inspired from the observational studies of the human brain and neuron activities. A model neuron comprises of nodes and connection weights. Input information comes via connection weights to node. Node processed the information and passes the processed information via outputs. Basics of NN model structure and activities are illustrated in Fig. 3.2.

3.1.1 Nodes

Neural network contains inputs, outputs and intermediate (also known as hidden) layers with set of nodes and connection between nodes. Nodes can be considered as computational units. The nodes $(x_n, n = 1,2,...n)$ in input layer are passive. It means that they only receive inputs from external source and pass the input information through some connections to the next hidden layer nodes without any modification. Each connection has some connection weights (w_n , $n = 1,2,...n$) associated with it. This weight is not fixed and can be updated (depending on the learning task to perform) to address the desired pattern identification task. Nodes receive information and process to obtain output. Each node contains a summation function. Summation function accumulates the multiplication of input value (x_i) , where $i = 1, 2, \ldots n$ and weight (w_i) , where $i = 1, 2, \ldots n$ 1,2,…*n*) of the connection through which it is fed to node. Node passes the summed value of inputs through an activation function to compute output. Output of the node can serve as inputs to the nodes in next layer.

Summation function,
$$
v = x_1w_1 + x_2w_2 + x_3w_3 + \dots + x_nw_n
$$
 (3.1)

3.1.2 Activation Functions

It is also known as transfer function. Activation function limits the output of node. Summation function value calculated by node is fed to transfer function to generate output.

$$
Action function, \phi(\nu) = \frac{1}{1 + e^{-(\nu)}} \tag{3.2}
$$

Transfer function can be linear or nonlinear. Some of the most common transfer functions are depicted in Fig. 3.3.

$$
Pure-linear: \phi = n
$$

The input units use the identity function (Fig. 3.3(a)).

$$
Log-Sigmoid: \phi = \frac{1}{1 + e^{-n}}
$$
\n(3.3)

This function is useful in neural networks trained by back propagation as it introduces nonlinearity and smooth function that is differentiable. It applies to applications whose desired output values are between o and 1 (Fig. 3.3(b)).

Tangent-Sigmoid:
$$
\phi = \frac{2}{(1 + e^{-2n}) - 1}
$$
 (3.4)

This function has similar properties with the log sigmoid function. It is used to limit output values in range of [-1, 1]. It is better to use where speed is important and the exact shape of the transfer function is not (Fig. $3.3(c)$).

It can be seen that, summation function of a node in an intermediate layer depends on the connection weights and inputs of the previous layer and output depends on the activation function applied on the summation function. If more than one set of intermediate or hidden layer with neurons is used, then the activation output of first hidden layers will be used as inputs for second hidden layer nodes. Then, the same calculation will be done in each node of single hidden layer till it reaches the output layer.

$$
\phi(\phi(\nu)) \cong \phi^2(\nu) \tag{3.5}
$$

Sigmoid function is nonlinear. Therefore, addition of each hidden layer gives higher order nonlinearity to the activation output. Thus, this computational model is very suitable to establish a prediction model by addressing nonlinear higher order polynomial relation between input and output parameters.

3.2 Types of NN

There are many different types of NN models available. Neural network classification depends on the way the network is used. Some of the categories are illustrated below:

3.2.1 Organization of Information Flow

On the basis of this criterion, NN can be broadly classified into two categories: feed forward and feedback NN. In a feed-forward NN, information is allowed to flow one way. Information is passed through connections from nodes of one layer to nodes to next layer. There is no interconnection between nodes in between a layer. This type of network is extensively used for pattern recognition and prediction models. On the other hand, feedback NN is a dynamic NN which is very powerful and complicated. In this type of NN, information is propagated in both directions i.e. it allows loops in between nodes of a particular layer. Time series are modeled by this type of neural network.

3.2.2 Way of Learning

NN can be trained in two ways: supervised and unsupervised. In a supervised technique, both inputs and outputs are known. This type of network learns from examples. A number of inputs and corresponding outputs are fed to NN so that the network can learn a function that can define output variables in terms of input variables. The learning of the model is updated on the basis of error from the comparison of predicted and known output. When the NN is fully trained with given data, it can be used to predict output for a set of inputs of which, outputs are not known. Unsupervised technique requires no desired response during the training process of the network. It organizes input data present to the NN by itself according to the inherent properties of the input parameters.

3.3 Backpropagation NN

Among all the types of NN, multilayer feedforward backpropagation network is selected to attain the goal of the study. Multilayer feedforward network has been applied successfully to map nonlinear relation between input-output variables in a supervised manner using backpropagation algorithm (BPA) (Saltan et al. 2004, Tasdemir 2009). This type of NN is based on error correction rule. In a multilayer feedforward NN, input information is received through input layer nodes. Then the information is transmitted in a forward direction from layer to layer to determine the output. Association of BPA with the feedforward network helps the network to learn from the error in the determination of output from input information (see Fig. 3.4). A feed forward backpropagation NN has two steps: forward transfer and inverted transfer for error correction. Forward transfer of information is done by feed forward NN assuming some connection weights to calculate output. Then, comparing the network output and actual output, error is determined.

BPA is applied to the net to make the error information flow in backward direction. Backward pass of error information helps to modify the connection weights to minimize error and get a closer value to target. After modification of weights, input information is again propagated through the modified weights on a layer to layer basis to produce outputs. Then again on the basis of error correction, backward pass occurs. This forward and backward pass continue on till the NN predicted value falls within the tolerable limit of error in comparison to actual value.

If a NN has *i* inputs, *j* hidden nodes and *k* outputs with weight connection between input and hidden as w_{ji} and hidden nodes and output as w_{ki} , then the algorithm can be written as follows:

Step 1: Initialize weights and biases to small random values.

Step 2: Declare stopping criteria.

If stopping criteria is false, continue from step 3 to 8.

FeedForward:

Step 3: Receive inputs by each input unit and pass to the next layer (hidden) nodes through connection weights

Step 4: Calculate the summation of weighted inputs in each node of the hidden layer using the formula

$$
\nu_j = \sum_{i=1}^m w_{ji} x_i + b_{ji} \tag{3.6}
$$

Step 5: Apply the activation function to compute output for the node using

$$
\phi_j = f(v_j) \tag{3.7}
$$

Step 6: Determine output for each output node. Use the output of previous node as inputs for the output nodes and apply summation function given below to determine network outputs.

$$
\nu_{jk} = \sum_{i=1}^{p} w_{ji} \phi_j + b_{kj} \tag{3.8}
$$

Backpropagation Error:

Step 7: Calculate the error by taking the difference between target and network output. Use the error to determine local gradient of error by any optimization technique and update the weight by steepest descent method based technique to minimize the error.

$$
w_{i+1} = w_i + \eta \nabla E(w_i) \tag{3.9}
$$

The gradient vector $\nabla E(w_i)$ is computed by the backpropagation of error through layers of Feedforward network. Η is denoted as learning rate that helps to avoid convergemce to a saddle or maximum point. In practice, a small learning rate is chosen in order to secure the convergence.

Step 8: Test stopping criteria

There are many different BPAs available for error minimization. For this study, Levenberg-Marquartz algorithm is chosen to be implemented in MATLAB. This technique is fast and requires less memory use in analysis (Mathworks 2013 manual). Also, (Gopalakrishnan 2010) showed this algorithm performs better in developing prediction model in comparison with other error minimization techniques.

3.4 Neural Network in MATLAB

Neural Network model is developed using Neural Network Toolbox of MALAB version 2012a. There are many inbuilt optimization techniques are available in MATLAB to develop backpropagation NN. Among them, training NN with Levenberg-Marquardt Optimization is chosen for this study.

3.4.1 Levenberg-Marquardt Optimization Algorithm

Backpropagation NN involves error correction technique to learn the pattern exists between inputs and outputs.

Levenberg-Marquardt is derived from two algorithms: steepest decent algorithm based on first order Taylor series and Neuton's method based on second order Taylor series.

Like the quasi-Newton methods, the Levenberg-Marquardt algorithm was designed to approach second-order training speed without having to compute the Hessian matrix. When the performance function has the form of a sum of squares (as is typical in training feedforward networks), then the Hessian matrix can be approximated as

$$
H = J^T J \tag{3.10}
$$

and the gradient can be computed as

$$
g = J^T e \tag{3.11}
$$

where *J* is the Jacobian matrix that contains first derivatives of the network errors with respect to the weights and biases, and e is a vector of network errors. The Jacobian matrix can be computed through a standard backpropagation technique that is much less complex than computing the Hessian matrix.

Derivation of the algorithm is beyond the scope of the study. The Levenberg-Marquardt algorithm uses this approximation to the Hessian matrix in the following Newton-like update:

$$
x_{k+1} = x_k - [J^T J + \mu I]^{-1} J^T e \tag{3.12}
$$

When the scalar μ is zero, this is just Newton's method, using the approximate Hessian matrix. When μ is large, this becomes gradient descent with a small step size. Newton's method is faster and more accurate near an error minimum, so the aim is to shift toward Newton's method as quickly as possible. Thus, μ is decreased after each successful step (reduction in performance function) and is increased only when a tentative step would increase the performance function. In this way, the performance function is always reduced at each iteration of the algorithm.

3.5 Neural Network Definitions and Terms

3.5.1 Initialization

It is necessary to initialize the weights of the connections between the layers of NN. Randomly chosen weights may take more time to converge and also may be responsible to reach local minima instead of global minima.

3.5.2 Bias

Bias is used to create hyperplanes to separate the input dimensions. Without bias, all hyperplanes are constrained to go through the origin of the hyperspace defined by the inputs.

3.5.3 Epoch

An epoch is a measure of the number of the passes all the training vectors are used once to update the weights. On the basis of weight update procedure, neural network training can be divided into two types: batch training and sequential training. On the batch learning process, all the training vectors are introduced once to complete a full epoch. Then the weight is updated. For sequential training, after passing single training vector, update of weight is done. Therefore, in a single epoch of sequential training, weight is updated for n_{train} times where n_{train} stands for number of train vectors or number of input observations.

3.5.4 Stopping Criteria

In general, minimum mean squared error is considered to be the stopping criteria of the training of a NN. However, in some cases, overfitting occurs after a certain point during training when the network is trained to get as low error as possible. Due to the overfitting, network establishes

intermediate points between two observations which disrupt NN in generalization. There are various techniques available to avoid overfitting: early stopping is one of the widely used among the techniques. Hecht and Nielson (1987) suggested use of two set of data during training: training and validation set. Training set is used to update weights and validation set is used to calculate the error using the updated network. If the error calculated by validation set decreases, training continues on. If, error of validation set starts increasing, then the training is stopped. Also, for some further epochs, training can be continued to observe whether the validation set error starts decreasing or continue on increasing. For those specific epochs, if the validation error still continues on increasing, then the training is stopped, otherwise, training is continued on.

3.6 Methodology of Development of NN

To construct a neural network that can be used to map nonlinear and complex relation exist between input and outputs successfully, two issues are to be resolved. Those are: determination of number of hidden layers and number of nodes in each hidden layer and setting weights and biases for the connections. On the basis of inputs and output parameters chosen in the study, number of nodes in input and output layers are fixed that is number of input variables and outputs are equal to the number of nodes in input and output layers respectively. Now the numbers of layers and nodes in each layer is to be determined. This is a very important issue because if the number of hidden layers and nodes in each layer is insufficient, then the developed network is not capable of tracing the relationship between input and output. On the other hand, over estimation of numbers of nodes and layers may cost the network to lose its ability to generalize.

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There is no general rule to selecting the number of neurons in the hidden layer. Usually trial and error method is adopted in this regard. To select the NN architecture appropriate for the data on hand, the data set is divided into two parts: training and testing. Training data set is also divided into two data sets: training and validation. For random initial weight, the training and validation data is fed to the NN to train and validate the process simultaneously. At training stage, performance of the network is recorded as Mean Squared Error of the validation data.

After the learning, prediction performance of trained network is determined by test data and performance is expressed in terms of Goodness of fit, R^2 . The equations used to calculate these two mentioned performance parameters are given below

Mean Squared Error,
$$
MSE = \frac{\sum_{j=1}^{p} \sum_{i=1}^{n} (o_{ij} - t_{ij})^2}{n.p}
$$
 (3.13)

Goodness of fit,
$$
R^2 = \frac{\sum (o-t)^2}{\sum (o - o_{mean})^2}
$$
 (3.14)

Where, $n =$ total number of data sets, $o =$ network output, $p =$ number of outputs, $t =$ target output and o_{mean} = average of network output.

NN models having one and two hidden layers with varying nodes are run through this procedure. Each model is run for 100 different randomly selected weights and for each weight, data is randomized for 75 times. Performance of each model having different structure with 100 randomized weights and 75 randomization of data fed to each weight set, are recorded in terms of MSE and \mathbb{R}^2 . Then the maximum frequent value of MSE and \mathbb{R}^2 of each model is determined. The model showing minimum MSE and maximum R^2 is chosen as the structure of NN.

In addition, the selected architecture of NN with fixed number of layers and nodes in each layer is undergone trial and error of 10000 weights to fix the weights and biases, On the basis of performance parameters, 10 best performed weights are selected and stored. These weights along with the NN structure specification is now ready to be used for prediction of outputs for the data set in concern.

3.7 Calculation of Relative Contribution of Inputs

The relative contribution of the input parameters on the prediction of the output parameter can be calculated using Garson's scheme (Garson 1991, Tarefder et al. 2005). This scheme provides a technique so that the connection weights of the hidden layers and output layers can be broken into components and partitioned in an association with each input node. The connections weights gives weightage to the information transferred from layer to layer, so partitioning them related to each input parameter can infer relative contribution of the input parameters on the predicted parameter.

Suppose, a model has $i-h_1-h_2-o$ network, i.e., the input layer (*i*), two hidden layers (h_1 and h_2) with n_1 and n_2 nodes, respectively, and the output layer (o). To apply the Garson's scheme, the relative influence of the inputs on a single output (output node=1) is considered. Also, the bias weights are not involved in the calculation. At first, the connection weights between the h_1-h_2 and h_2 -*o* are taken for the calculation. Dimensions of the weight matrices in between h_1 - h_2 and h_2 -*o* are n_2 x n_1 and n_2 x 1, respectively, considering one output only.

Now, absolute product of the *wh1*-*h2* and *wh2*-*^o* are taken and stored as beta factor of each *h²* node using the following equation:

$$
\beta_{pq} = |w_{qp}.w_{po}| \tag{3.15}
$$

Where, $p =$ node identification in the second hidden layer, range from $1 - n₂$

 $q =$ node identification in the first hidden layer, range from $1 - n_l$

 w_{qp} = weight between node *q* in h_1 and node *p* in h_2

 w_{po} = weight between node p in h₂ and output node o (=1)

For each value of *p*, i.e., for each h_2 node, β_{pq} are calculated changing the *q* from 1 to n_1 . Then, theta (θ) is calculated from β using the following equation:

$$
\theta_{pq} = \frac{\beta_{pq}}{\sum_{q=1}^{n_1} \beta_{pq}}\tag{3.16}
$$

Now, theta values are summed up to calculate another variable *X*, which has a dimension of $n₁x1$. The equation to calculate *X* is as follows:

$$
X_{q1} = \sum_{p=1}^{n_2} \theta_{pq} \tag{3.17}
$$

Here, *q* is given input from 1 to n_1 at a time. Results for theta θ_{pq} and X_{q1} are recorded. This X_{q1} is used as the output connection weights and the same calculations are to be repeated. That is, for this case, instead of weights between h_1 and h_2 , weight between input and h_1 is used and instead of weights between h_2 and output, X_{q1} will be used. After calculating X_{input} for each input node, the percentage contribution of each input parameter can be calculated from the *Xinput* values.

Figure 3.1 Biological and computational neural network

Figure 3.2 A generalized NN structure

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Figure 3.3 Graphs of typical transfer functions used in NN

Figure 3.4 Backpropagation NN architecture

CHAPTER 4 DEVELOPMENT OF NN FOR LIME TREATED ASPHALT

4.1 Introduction

Hydrated lime is an additive that increases the performance and thus life of pavement through multiple ways. Literature on lime modified asphalt reveals the ability of hydrated lime to control water sensitivity and its well accepted performance as an antistrip in resisting moisture damage (Little and Epps 2001).

Schmidt and Graf (1989) state that the mechanism by which hydrated lime improves adhesion loss resistance cannot be completely explained by the reactions occur between asphalt and lime. Therefore, laboratory tests are usually conducted to observe the performance of lime on the mechanical and rheological properties of asphalt. This allows getting information on the probable performance of lime on improving the properties that helps resisting moisture damage. However, the effect of different mix variables on adhesion/cohesion of asphalt is difficult to predict due to the complexity and nonlinearity in relationship among the variables.

Atomic Force Microscopy (AFM) test is performed on lime treated as well as some other ASA treated asphalt sample to determine some major bond forces of detected to be present in wet and dry asphalt. There are also other mix properties of asphalt involved on the test asphalt sample. Using the laboratory test data, individual NN for model for lime and other ASAs are developed to map the association of mix variables with the adhesion/cohesion of moisture conditioned asphalt. Two different models are incorporated instead of one is due to the fact that input parameters and force-distance values trend for lime treated and chemical ASAs treated samples are quite different and cannot be traced using same NN. This chapter discusses the development

and application of NN model for lime treated sample data. Next chapter provides another NN development for four chemical ASA treated asphalt sample AFM data.

4.2 NN Variable Selection

Development of Neural Network prediction model using backpropagation requires input and target data. Training NN with inputs and corresponding target data aids in tracing the relationship between input and target data. To develop the NN model using AFM data, five point forces are chosen as outputs and corresponding five point distances and asphalt chemistry that is, type of polymer, percentage of polymer and lime, tip type used to probe asphalt sample and moisture condition type are selected to use as inputs. However, data trend shows that there are only four unique initial (X_1) and final distance (X_5) values are available in the laboratory test records. Also the forces corresponding to the mentioned distance are constants. If X_1 and X_5 distance corresponding constant forces are considered as outputs, these effect on the determination of other forces. Also, starting distance and corresponding force may have effect on the preceding forces and distances. Therefore, F_1 and F_5 distances are not discarded, rather the forces F_1 , F_5 corresponding to the distances X_1 and X_5 are also considered as inputs. This accounts the effect of the initial and final force distance values effect on other forces to be determined including adhesion/cohesion force in lime dataset. The selected input and output variables are shown in Table 4.1.

4.3 Selection of NN Architecture

The methodology to select Architecture of NN is described on Chapter 3. On the basis of the number of inputs and outputs chosen to conduct the analysis, number of nodes in input and output layers is fixed. Therefore, the network to be developed has 12 input nodes and 3 output

nodes (see Table 4.1). Now, the concern is the number of hidden layers and number of nodes in each hidden layer. To determine the structure of NN as described in chapter 3, a total of 677 data is involved. The data is randomly divided into 610 (90%) and 67(10%) for training and testing data set respectively. The training data is again randomly divided into 90% and 10% for training and validation respectively. One and two hidden layers containing 6-20 nodes in each layer are at a time used as a structure of NN and all model performance in terms of R^2 and MSE are recorded. Performance plot of NN with a random weight is shown in Fig. 4.1. Furthermore, regression performance plot at tranining and validation phases are shown in Fig. 4.2. For the data in concern, NN having two hidden layers with 9 and 16 nodes shows best performance (see Table 4.2). Therefore the NN structure chosen for the development of prediction model is 12-9- 16-3 and is shown in Fig. 4.3.

Another concern in NN development process is fixing the values of connection weights. The procedure taken in consideration in this study to set the connection is already described in Chapter 3. Using the process, 10 connection weights are recorded as appropriate to address the pattern between the inputs and outputs. Thus, the NN is fixed and ready to use for any prediction on the basis of the learning acquired from the training data.

The fixed network is then used to predict adhesion of asphalt. The model shows good prediction ability. The correlation between predicted and actual data for asphalt adhesion force (F_4) is given in Fig. 4.4. F_2 and F_3 forces show R^2 values of 0.84 and 0.96. In both training and testing phase, it is difficult to fit F_2 force as it has both positive and negative values. All other forces have either positive or negative values. For further study, only F_4 force (adhesion) is considered, other forces are not taken into concern.

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4.4 Input Contributions to Determine Output

The relative contribution of the input parameters on the prediction of the output parameter is calculated using Garson's scheme explained in Chapter 3. The model built in this chapter is a 12- 9-16-3 network i.e. the input layer (*i*) has 12 nodes, two hidden layers (h_1 and h_2) have 9 (n_1) and 16 (*n2*) nodes, respectively, and the output layer (*o*) has 3 nodes. As explained before, there are two steps involved in calculating relative percentages of inputs for networks having two hidden layers. At first, the relative contribution of second hidden layer (h_2) to calculate the output is determined. Then that calculation is taken into account to calculate the input contributions. Among the ten weight sets, one connection weight set between the h_1-h_2 and h_2-o are shown in Table 4.3 for sample calculation. Table 4.4 provides the determination of relative contribution of *h²* to output using equations 3.15, 3.16 and 3.17. Same procedure is adopted for the weight set between *i*-*h*₁ and h₁-newly calculated X_{q1} to determine the contribution of inputs (X_{input}) . Contribution of each input factors in percentages are given in Table 4.5.

From Table 4.5, it can be seen that tip type is the most significant input factor in determining the forces by NN model. Tip type, which means asphalt's chemical composition (-COOH, -OH, $NH₃$ etc.), shows the highest percent contribution that is calculated using the connection weights. Also, percentage and type of polymer and moisture conditioning of asphalt have high contribution percentages in determining the forces. On the other hand, initial and final forces have little contribution in predicting adhesion.

4.5 NN Predicted Results and Discussion

AFM test is conducted to determine adhesion/cohesion values of lime treated asphalt modified with SB and SBS polymers. Four cohesion forces within asphalt are simulated by pull-off forces

between asphalt surface and four functionalized tips. Adhesion between asphalt and aggregate represented by the interaction between asphalt surface and commercially available tip for AFM testing as the tip material is close to aggregate material type. To compare the effectiveness of lime in improving moisture effect in the determination of all bond forces of asphalt, the developed NN using AFM laboratory test data is used to predict bond forces of asphalt. As the corresponding distances to five point forces are not same, therefore it is difficult to compare between dry and wet sample forces having all other material properties same. In addition, relative effect of input variables shows that distances have influence in the determination of bond forces using NN. Hence, the distances, first and last force as well as all other input parameters are kept fixed for all input observations and adhesion/cohesion forces are determined by NN prediction. Also, two percentages above 1.5% is added to the prediction to observe the influence of extrapolated percentage of lime on the behavior of bond forces of asphalt under moisture damage.

This study is divided in two segments. At the first segment, trends of wet and dry polymer modified lime treated samples are observed and discussed for individual bond forces. Second segment provides comparison among the adhesion loss of all bond forces of lime treated asphalt under moisture conditioning. This helps to comprehend overall performance of lime on the moisture conditioned asphalt bond forces at nano-level.

4.5.1 CH³ tip

The trends depicted by CH_3 tip probed lime treated samples are shown in Fig. 4.5. SB modified samples with lime shown in Fig. 4.5(b) has very close values of dry and wet adhesion force thus it indicates reduced moisture effect. On the other hand, lime treated SBS modified samples

shows some very unusual pattern. At lower percentages of lime, SBS treated wet samples adhesion falls drastically compared to dry samples especially the samples modified with 5% SBS. It is expected in AFM test that the hard samples give low values of adhesion compared to soft samples. Therefore, wet samples are relatively softer than dry samples and in general, should provide higher values of adhesion compared to dry samples (Arifuzzaman 2010). 5% polymer modified samples adhesion in both the cases seems to have reverse effect with the increase in percent of lime above 1%.

4.5.2 NH³ tip

Fig. 4.6(a) and (b) are plotted for lime treated asphalt samples modified with 3% and 5% SBS and SB polymers respectively. Lime varies from 0.5 to 2.5% at an increment of 0.5% and adhesion forces of the asphalt are predicted by the NN model for asphalt samples probed with the NH³ functionalized tip. From both the figures, it can be seen that, 5% polymer modified lime treated wet samples have much higher adhesion values corresponding to dry samples. It means lime does not help resisting moisture damage for the mentioned samples. Below 1percent, lime seems to be activated which results is closer or lesser value of bond force of wet samples than dry samples. Increase in percentage of lime above 1% tends to reduce the performance of lime in reducing moisture effect.

4.5.3 COOH tip

Effect of lime on bond force of wet asphalt determined by COOH is shown in Fig. 4.7. Lime proved to be effective in reducing moisture effect below 1%. Addition of lime above 1% tends to increase the wet adhesion values thus moisture damage is also increased. Trend of wet samples adhesion for both SB and SBS is almost same with the increase in percent of lime. Lime seems

to resist moisture damage in 3% polymer modified samples thus the wet samples show lower value of adhesion compared to dry samples.

4.5.4 OH tip

Same as Fig. 4.7, Fig. 4.8 depicts effect of lime on the bond force of polymer modified moisture conditioned asphalt samples measured by OH tip. From the figure, it can be seen that lime performs better in presence of SB polymer compared to SBS polymer in resisting moisture effect. Also, performance of lime seems to be better in 3% polymer modified samples rather that 5% polymer modified samples. Increase in percentage of lime does not seem to effect the effectiveness in improving moisture damage.

4.5.5 Si3N⁴ tip

Adhesion force measurement between asphalt-aggregate is facilitated by using $Si₃N₄$ tip. Effect of lime on the determination of adheison force of asphalt is shown in Fig. 4.9. It can be observed that lime is ineffective in reducing moisture effect nano-level adhesion force of asphalt containing 5% polymer as 5% polymer modified wet asphalt samples have very high values of adhesion compared to dry samples. Though, a decreasing trend can be identified for both 3% SB and SBS modified samples with the increase in percentage of lime, it fails to resist moisture effect at lower percentage of lime. Thus, wet and dry adhesion differ by a large number.

Effect of increment of percentage of lime from 0.5-1.0 percent in individual wet and dry samples for different functional group adhesion values are shown in Fig. 4.10. Percent change in adhesion shown in y-axis is calculated maintaining 0.5% lime corresponding adhesion as reference. Negative change in adhesion depicts effect of lime on 1% lime samples making the sample

stronger. For both dry and wet samples, it can be observed that, with the increment of percentage of lime fro 0.5 to 1.0 percent, tip adhesions are improved except for NH₃ functionalized adhesion especially in wet samples. For all other functionalized adhesion, lime seems to work good in making the sample strong.

4.5.6 Effects of lime on Adhesion Loss

To justify overall effect of lime in reducing moisture damage of all the bond forces of asphalt determined by AFM at nano-level, Fig. 4.11 is plotted. The figure comprises two subplots. Four subplots correspond to 3% and 5% SB modified sample comparison. Each subplot contains adhesion loss vs percent of lime plots for all tips.

From the plots, it can be observed that lime activates better in resisting moisture damage in presence of 3% SB polymer than 5% SB polymer. Addition of 0.5% lime is effective in resisting moisture damage for maximum of the cohesion forces determined by functionalized tips for both 3% and 5% SB modified samples However, lime shows poor performance in reducing adhesion loss of the bond force representing adhesion force in case of 5% SB modified sample. With the increase in percentage of lime, 3% SB modified samples has a tendency to improve resistance to moisture effect by reducing adhesion loss. Whereas, 5% SB modified samples do not show any decreasing trend in adhesion due to increase in percentage of lime.

Almost similar trend in adhesion loss can be observed for lime treated SBS modified samples shown in Fig. 4.12. 3% SBS samples serves better in activating lime to resist moisture damage compared to 5% SBS samples. Also, lime does not show good performance in reducing moisture effect for adhesion force measured by $Si₃N₄$ tip.

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4.6 Conclusions

- A 12-9-16-3 feedforward NN is constructed to predict adhesion of lime treated asphalt samples. The model shows good prediction ability.
- Relative contribution determination of input parameters using connection weights reveals that, chemical functional group of asphalt is the most significant parameter to influence the prediction of adhesion. Type of polymer also has good contribution in the determination of adhesion of asphalt.
- The performance of lime in reducing moisture damage is observed by comparing wet and dry samples adhesion predicted by developed NN. Lime is effective in reducing moisture damage for adhesion forces of asphalt measured with functionalized tips but shows very poor performance in resisting adhesion loss of bond force measured by silicon nitride tip.
- Lime activates better in presence of 3% SB modifier compared to other polymers.
- Addition of 5% polymer seems to have random and in some case has reverse effect on the performance of lime in resisting moisture effect.
- Addition of percentage of lime above 1 percent has no effect in reducing adhesion loss of polymer modified asphalt samples.

Figure 4.1 Performance plot of NN during training and testing

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Figure 4.2 Regression performance of NN for a selected weight during training

Figure 4.3 Structure of fully connected NN selected for model development. Connections for first and last node are shown for convenience

Figure 4.4 Correlation between laboratory test data and model prediction output for adhesion force

Figure 4.5 Adhesion force vs percent of lime for asphalt sample probed with $CH₃$ tip

Figure 4.6 Adhesion force vs percent of lime for asphalt sample probed with NH₃ tip

Figure 4.7 Adhesion force vs percent of lime for asphalt sample probed with COOH tip

Figure 4.8 Adhesion force vs percent of lime for asphalt sample probed with OH tip

(a) SBS modified sample (b) SB modified sample

Figure 4.9 Adhesion force vs percent of lime for asphalt sample probed with $Si₃N₄$ tip

(a)

Figure 4.10 Effect of increment of % lime from 0.5-1.0% on (a) dry and (b) wet asphalt samples modified with polymer

(a) 5% SB

(b) 3% SB

Figure 4.11 Adhesion loss vs percent of lime for SB modified samples

(a) 5% SBS

(b) 3% SBS

Figure 4.12 Adhesion loss vs percent of lime for SBS modified samples

Table 4.1 Input and Output Variables for NN Model

No. of Neurons in the First Hidden Layer	No. of Neurons in the Second Hidden Layer	Validation MSE	Test R^2
9	12	2.25E-15	0.982801
9	13	2.25E-15	0.98414
9	14	2.48E-15	0.982636
9	15	1.95E-15	0.979361
9	16	1.77E-15	0.982796
9	17	2.19E-15	0.981308
9	18	1.92E-15	0.976444
9	19	2.32E-15	0.974326

Table 4.2 Sample Results for Selection of NN Structure

						W_{qp}					W_{po}
	q , p =node no. for h_1 and $h2$ respectively	$q=1$	$q=2$	$q=3$	$q=4$	$q=5$	$q=6$	$q=7$	$q=8$	$q=9$	$o=1$
	$p=1$	0.4259	2.5781	0.6504	-0.4381	-0.3945	-1.5862	-1.7546	-0.1458	-2.1225	-0.3270
	$p=2$	-0.1034	-0.6968	-0.5733	3.0228	1.3348	-1.2349	-0.0677	0.7334	-0.5514	0.4735
	$p=3$	0.2331	-0.2704	0.8037	0.2182	-0.3689	0.5061	0.3632	1.0837	-0.1399	-1.1122
	$p=4$	0.6927	1.3845	0.0460	0.9788	0.8663	0.0852	-1.1701	-1.9336	-0.5920	0.9676
	$p=5$	-0.0519	-0.4082	-1.3763	1.0626	2.1426	-1.2453	1.2705	0.6873	0.4839	-0.9629
	$p=6$	-0.4090	0.5858	0.6589	1.9193	0.0882	-0.6475	-0.3191	1.5053	-0.9593	0.2059
	$p=7$	1.1384	-0.7603	-0.0593	0.0949	-0.9647	1.5103	1.5713	2.4436	2.0744	-0.6206
$\nabla_{\mathbb{P}}$	$p=8$	0.0333	1.1147	-1.4283	-0.5558	-0.5393	0.3106	-0.5556	0.9693	0.2610	0.0583
	$p=9$	0.1057	1.6304	-1.1490	1.2086	-0.1673	0.0791	-1.1776	1.0742	0.2100	0.0725
	$p=10$	-1.5891	0.1339	-1.7805	0.1433	0.4063	0.8100	1.2954	-0.4052	-1.8543	-0.0237
	$p=11$	-0.3052	0.2292	-0.3887	0.4697	-0.2889	1.2481	1.0163	0.4307	1.4988	-0.7437
	$p=12$	0.0591	1.7326	0.5356	0.2135	0.5066	0.2300	-1.0310	-1.6742	-1.1293	-1.1258
	$p=13$	0.1467	0.5196	1.9573	0.4046	1.2640	0.9959	0.5178	-1.4582	-1.0922	0.6525
	$p=14$	0.3814	0.1380	0.8542	0.5667	-1.1200	0.1679	0.0606	0.9871	0.3347	0.5362
	$p=15$	0.5165	-0.2850	0.8336	1.2041	-0.7530	1.1610	-0.5070	-0.7634	-0.1424	-1.0812
	$p=16$	1.6426	1.2959	0.4621	0.2146	-0.2993	1.1365	0.2035	-1.2107	1.1609	0.2089

Table 4.3 Weight Matrix in Between Hidden Layer h_1-h_2 and Hidden Layer h_2-o

						θ pq				
	$p,q = node$ no. for h1 and h ₂ respectivel y	$q=1$	$q=2$	$q=3$	$q=4$	$q=5$	$q=6$	$q=7$	$q=8$	$q=9$
	$p=1$	0.0422	0.2554	0.0644	0.0434	0.0391	0.1571	0.1738	0.0144	0.2102
	$p=2$	0.0124	0.0838	0.0689	0.3634	0.1605	0.1485	0.0081	0.0882	0.0663
	$p=3$	0.0585	0.0678	0.2016	0.0547	0.0925	0.1269	0.0911	0.2718	0.0351
	$p=4$	0.0894	0.1787	0.0059	0.1263	0.1118	0.0110	0.1510	0.2495	0.0764
	$p=5$	0.0059	0.0468	0.1577	0.1217	0.2455	0.1427	0.1456	0.0787	0.0554
	$p=6$	0.0577	0.0826	0.0929	0.2706	0.0124	0.0913	0.0450	0.2122	0.1353
	$p=7$	0.1072	0.0716	0.0056	0.0089	0.0909	0.1423	0.1480	0.2302	0.1954
	$p=8$	0.0058	0.1933	0.2476	0.0964	0.0935	0.0538	0.0963	0.1680	0.0453
θ pq	$p=9$	0.0155	0.2397	0.1689	0.1777	0.0246	0.0116	0.1731	0.1579	0.0309
	$p=10$	0.1888	0.0159	0.2115	0.0170	0.0483	0.0962	0.1539	0.0481	0.2203
	$p=11$	0.0519	0.0390	0.0661	0.0799	0.0492	0.2124	0.1730	0.0733	0.2551
	$p=12$	0.0083	0.2436	0.0753	0.0300	0.0712	0.0323	0.1450	0.2354	0.1588
	$p=13$	0.0176	0.0622	0.2342	0.0484	0.1513	0.1192	0.0620	0.1745	0.1307
	$p=14$	0.0827	0.0299	0.1853	0.1229	0.2429	0.0364	0.0131	0.2141	0.0726
	$p=15$	0.0838	0.0462	0.1352	0.1953	0.1221	0.1883	0.0822	0.1238	0.0231
	$p=16$	0.2154	0.1699	0.0606	0.0281	0.0393	0.1490	0.0267	0.1588	0.1522
Xq_1		1.0431	1.8263	1.9818	1.7849	1.5949	1.7191	1.6878	2.4991	1.8630

Table 4.4 Calculated Values of Theta and X Using Equation 3.15,3.16 and 3.17

Input variables	Wet/dry	SB/SBS/none	$%$ of polymer	$%$ of lime	Tip type	X1	X2	X3	X4	X5	F1	F5
Percent contribution	7 ₁ $\overline{}$	7.6	18.6	3.0	21.6	4.3		10.1	1.0	5.7	2.4	

Table 4.5 Percent Contribution of Input Factors

CHAPTER 5 DEVELOPMENT OF NN FOR CHEMICAL ADDITIVE TREATED ASPHALT

5.1 Introduction

Antistripping agent (ASA) proved to be effective in improving adhesion between the asphalt binder and aggregate surface thus the resistance to moisture damage. Many commercially available chemical ASAs are now used by Department of Transportation (DoT) of different states as per their requirements.

A common problem faced in all asphalt pavements is the deterioration of pavement strength, performance and life due to moisture effect. Moisture creates damage in asphalt pavement by breaking the bond between asphalt and aggregate. This phenomenon is known as water stripping. Chemical ASAs are used to address this issue of water stripping of asphalt by increasing the adherence property of asphalt to the surface of aggregate. Chemical ASAs, commonly used to resist moisture effect are known to be surfactant blend type chemicals. These types of chemicals act at the interface of asphalt and aggregate and improve the adhesion bond between asphalt and aggregate by reducing surface tension of asphalt. However, Anderson et al. (1982) evaluated the effects of commercially available ASAs on asphalt binder. They showed that addition of ASAs can alter the physical characteristics and composition of binder. So, ASAs may have effect on the cohesion force present within asphalt too.

To determine the effect of chemical antistrip additives on intermolecular bond within asphalt and in between asphalt aggregate, a neural model is developed. With the help of NN model, the relationship between asphalt mix properties and adhesion/cohesion of asphalt involved in Atomic Force Microscopy (AFM) is traced and using the mapped relationship, influence of chemical

antistripping agents(ASA) on adhesion at nano-level are observed. This analysis will give insight on the comparative performance of different ASAs in improving certain bond forces of asphalt undergoing moisture damage.

5.2 NN Database

The database considered in this part of the study include five point force-distance values of asphalt modified with polymers and four chemical antistripping agents and probed with four functionalized tips and one industrial tip without modification. The chemical antistripping agents are provided with their name and a brief description in Chapter 2.

To construct the NN, the variables are separated into two groups: input and output and are shown in Table 5.1. In Table 5.1, subscripts of X and F denote the positions of the probe referring to Fig. 2.1. Variables that fall under the input category are selected as inputs and five forces corresponding to five distances are selected as outputs to construct a supervised NN model. Though the initial and final distances and corresponding forces are constants, trial NN shows that including initial and final forces in the output increases the predictability of NN to determine other three forces. Therefore five forces are set as outputs for this model.

5.3 Selection of NN Architecture

A fully connected feed-forward backpropagation NN is chosen for this study. There are 11 test parameters that were incorporated in the AFM laboratory test on the determination of adhesion force of the asphalt. These are provided as inputs for the NN model. The output of the model is set as five point forces corresponding to five distances. Thus, a NN with 11 input nodes and 5 output nodes is developed. To determine the number of hidden layers and number of nodes in

each layer to successfully predict the outputs, a number of models are run for the single hidden layer with 4-20 nodes and two hidden layers each with 4-20 nodes. The total data set (1497) is split into 90% and 10% for training and testing respectively. The training data set is divided into two sets: training and validation. Initially, the network is trained using the training data, and calculating *MSE* for the validation data simultaneously to check performance of the trained network. After the network is trained, the network is tested with the test data. Goodness of fit of the model predicted data and actual data is determined. However performance of trial NN shows that two hidden layers with 4-20 nodes in each layer are not sufficient to trace the relation. Therefore, the nodes in each hidden layer is increased to 25 nodes and the model is run for two hidden layers each having nodes varying from 20-25. On the basis of R^2 and MSE, the best performed NN architecture is selected with 2 hidden layers and 25 and 25 nodes in the first and second hidden layer respectively. The performances recorded as Mean Squared error and Goodness of fit for some of the networks is shown in Table 5.2. One performance plot and one regression plot during training of NN is shown in Fig. 5.1 and Fig. 5.2 respectively.

After selection of the NN architecture, the 11-25-25-5 network is again trained but now for 10,000 randomized connection weights. From the MSE and R^2 performance of validation and testing set, respectively, the 10 best performed network connection weights are stored. These weights are further fed to the network and used in prediction. The maximum frequent value of the outputs of the prediction models for 10 connection weights will be taken as predicted output. The established NN is then tested with the test data. The model shows good correlation with the actual data for adhesion force (Fig. 5.3). Similar to the case of lime treated samples, it was really hard to fit NN model for F_2 output and it did not show that much good correlation ($R^2 = 0.72$). However, as it is not used for further study, more concentration is put on the fitted adhesion data.

5.4 Input Contributions to Outputs

Using the Garson's scheme (see chapter 3), the input contributions to outputs are determined using the connection weights in between layers. The model developed in this chapter has 11 inputs, 25 (n_1 and n_2) nodes in each hidden layer and five outputs. As the size of the weight matrices are large (25x11, 25x25 and 5x25), the matrices are not shown in this study. On the basis of weight matrices, the contribution of each input is calculated and tabulated in Table 5.3.

Form the table, it can be observed that, chemical functional groups of asphalt is the highest responsible factor in determining the nano-level forces. Also, type of ASA has high contribution in determining the outputs.

5.5 NN Induced Results and Discussions

The relationship between the adhesion force of asphalt and asphalt mix properties traced by NN is used to predict adhesion values of asphalt of different types of antistripping agents having all the input variables same. This allows performance comparison of antistripping agents to be made on reducing adhesion loss thus moisture damage.

AFM laboratory test was conducted for asphalt sample modified with SBS and SB polymer and probed with four different types of functionalized tips. Adhesion of asphalt is predicted for all types of chemical ASAs using developed NN keeping all the input parameters same. In addition, two percentages (2.0, 2.5) of ASAs are added to the data set and for 0.25-2.5 percentage of ASAs, adhesion forces of wet and dry asphalt are predicted using NN model. The general trends of bond forces with ASA content and percentages determined by functionalized tips are discussed first and then the performance of ASA on bond forces are assessed by comparative study.

5.5.1 Hydrophobic Tips

Fig. 5.4 shows adhesion force vs. antistripping agents (ASAs) for wet and dry SBS and SB modified samples respectively probed with $NH₃$ one of the three hydrophobic tips. The figure depicts that in general, dry sample adhesion force has a lower value than that of wet adhesion force. In AFM test, stronger samples give lower values of adhesion forces than the weaker samples (Arifuzzaman M., 2010). Therefore, wet samples are under moisture damage. However, small difference between wet and dry sample adhesion can be observed for some of the asphalt samples. Those samples indicate reduced effect of moisture. Morlife ASA content samples modified with 3% SB and SBS polymer show reduced moisture damage than other samples. For 3% SB and SBS modified samples, Klingbeta and Unichem samples improve moisture damage resistivity with the increase in ASA percent above 1.0%. Increase in percentage of other antistripping agents shows no effect on the moisture damage.

NN induced result for asphalt samples probed with CH_3 tip, is shown in Fig.5.5 It can be seen that wet samples have closer values and in some cases have lower values that corresponding dry samples. These trends indicate that moisture has less or negligible effect on the adhesion of $CH₃$ functionalized group present in asphalt. Increase in percentage of all ASAs above 1% has little or no significant effect on the adhesion of wet asphalt except for Unichem. Unichem samples show drastic fall in values of adhesion after the increment of ASA above 1%, especially for the samples contains 5% SBS and SB polymer. Thus, with the increase in percentage of Unichem in polymer modified samples, moisture damage is significantly reduced. All other ASAs show better performance in reducing moisture damage with ASA content ranged between 0.25-1%. Use of Morlife demonstrates closer values of wet and dry adhesion thus it is effective in reducing moisture effect.

Fig. 5.6 provides NN induced results for asphalt sample probed with $Si₃N₄$ tip. It is observed from the figure that Unichem and Morlife treated asphalt samples show very high values of adhesion force for wet samples compared to dry samples. Therefore, moisture damage is clearly noticeable in Unichem and Morlife treated samples. Wetfix and Klingbeta show better performance in in maintaining low values of wet samples compared to dry samples. Performance of ASAs does not vary much with respect to type and percentage of modifier used in asphalt binder. Though, some decreasing trend in wet adhesion can be noticed in Unichem and Morlife treated samples with the increase in percentage of ASA, overall no noticeable improvement in adhesion of wet asphalt can be depicted from the figure.

5.5.2 Hydrophillic Tips

Among the functionalized tips used to probe the asphalt sample in AFM test, COOH and OH tips are hydrophilic. However, increase in percentage of ASAs exhibit completely different patterns in asphalt samples probed with OH and COOH tips.

Fig. 5.7 shows the adhesion force vs antistripping agent plot for wet and dry SB and SBS polymer modified asphalt samples probed with OH tip. The values of adhesion of asphalt acquired from NN model are having very random trends. Trends show that, in maximum cases, wet sample has lower values of adhesion than that of the corresponding dry samples and the difference is noticeable. With the increase in percent of ASA, wet adhesion of some of the samples fall drastically compared to dry adhesion. As, dry sample adhesions having that much high values compared to that of the wet samples in maximum cases are hard to accept from the practical point of view, these results can be considered as random. For one or two cases,

exception may happen, but most of the cases showing the same trend are not being considered as exception.

Hydrophilic tendency of the tip may have affected much in the determination of adhesion of asphalt that caused the random trends in adhesion determination. Water contamination at surface of the sample interrupted the determination of bond force of asphalt. Water may have made a thin layer at the surface of the wet asphalt sample. When the sample is probed with OH hydrophilic tip, the tip interacted with water film on the surface rather than the uncontaminated asphalt sample. As OH tip has strong affinity to water, tip and water exerts strong adhesion force between them. Therefore, wet samples especially those containing Wetfix and Klingbeta depict very low values of adhesion force than the dry samples for all mix cases.

Therefore, results of adhesion force of asphalt probed with OH tip do not provide reliable measurement of adhesion between asphalt and tip. So, this particular tip induced analysis results is not incorporated for further analysis.

Adhesion force values for dry and wet asphalt samples are quite different for asphalt sample probed with COOH tip compared to asphalt sample probed with OH tip. It shows completely opposite trend to OH tip. From Fig.5.8, it can be seen that dry polymer modified samples provide more or less constant or decreasing trend in adhesion force with the increase in percent of ASA whereas no significant improvement in resisting moisture damage is noticed for wet polymer modified samples with the increase in percentage of ASA. Wet samples have increasing trend with the increase in ASA% up to 1-1.5%. Decreasing patterns in most of the wet samples are then noticed with further increase in ASA% from 1.5%. Comparing SB and SBS samples, SB samples depict less adhesion value that corresponding SBS samples. Among all the cases 5% SB

modified wet asphalt sample with Unichem ASA gives the best performance in terms of reducing or at least maintaining least difference in adhesion force with corresponding dry sample.

5.5.3 Effect of ASAs on Adhesion Loss

This part is included in the analysis to compare the performance of ASAs in reducing adhesion loss thus moisture damage. Moisture damage is quantified in terms of adhesion loss. Adhesion loss is defined as the wet asphalt adhesion minus dry asphalt adhesion force of samples. If wet minus dry adhesion is positive, it means adhesion loss occurs thus moisture damage takes place. On the other hand lower value of wet adhesion than dry adhesion provides negative value of adhesion loss that stands for no moisture damage.

Fig. 5.9 illustrates the comparison of antistripping agents on the moisture damage of asphalt binder modified with 5% SB polymer. From the plots above, it can be seen that, Morlife and Klingbeta ASAs show significant improvement in the cohesion of asphalt determined by $CH₃$ functionalized tip. Mixing 0.25% Morlife and Klingbeta make the cohesion force stronger in wet conditioned samples compared to dry conditioned asphalt samples. Thus, adhesion loss of those samples becomes negative. Wetfix and Klingbeta help resisting moisture damage by lowering adhesion loss of asphalt probed by $Si₃N₄$ tips. With the addition of these two ASAs, asphalt sample is able to fully resist the moisture damage.

No other noticeable improvement in adhesion loss can be observed for asphalt sample probed with other two functionalized tips. Among all the ASAs, Unichem performs better with minimum adhesion loss for asphalt probed with $NH₃$ tip and COOH tip. NH3 tip probed asphalt sample behave as inert to any percentages of antistripping agent. Adhesion loss seems to remain

almost the same or varies very slightly with the addition of percentages of antisripping agents. Same trend is observed for COOH tip.

As mentioned before, most of the ASAs are surfactants. Usually, ASA comprises two tails, one has binder affinity and the other has water or polar substance affinity. (Castano et al. 2004). These tails are placed on the bitumen-aggregate surface to create a chemical bonding between the aggregate and asphalt. $Si₃N₄$ tip represents aggregate surface. Wetfix and Kingbeta may have produced the bridge properly by creating tight hydrogen bonds between asphalt molecule and Si3N⁴ tip (resembles to aggregate) in presence of water molecules. Therefore, these two ASAs are helpful in resisting moisture damage.

As, antistripping agents are additives, only the interfacial bond between asphalt and aggregate that is adhesion force was taken into concern in all literatures. Very few papers discussed the effect of antistripping agent on the binder only (Anderson et al. 1982, Kanitpong K. and Bahia H. 2005). Kanitpong K. and Bahia H. 2005 concluded that antistripping agent has effect only on the adhesion of asphalt. They performed tack test to determine the effect of the antistripping agent on the cohesion of asphalt binder and established the decision that antristripping agent has no effect on the cohesion of asphalt. On the other hand, Anderson et al. evaluated the effect of liquid antistripping agent on asphalt binder and showed that addition of liquid antistripping additives can alter the physical characteristics and composition of asphalt binder even the viscosity of the binder can be changed due to the addition of antistripping agent. However, the chemical reaction occurs within asphalt in presence of water cannot be clearly stated as the chemical composition of asphalt depends on various factors. Also, Little D. N. and Jones IV D. R. (2007) mentioned that cohesion depends not only on the binder property but also is influenced by rheology of the filler binder. Therefore, no chemical explanation can be provided from the laboratory test data. It

can only be stated that cohesion force determined by $CH₃$ tip for asphalt samples with Morlife and Klingbeta show better resistance to moisture damage. Other two cohesion forces determined by COOH and NH³ do not show good resistance to moisture effect due to addition of any of the antistripping agent. Among all the ASAs, Unichem performs better than other ASAs in reducing adhesion loss in all cases.

The same plot as Fig. 5.9 is plotted for asphalt sample modified with 5% SBS (see Fig. 5.10). The trends obtained for adhesion loss of 5% SB and SBS modified are almost same except for NH³ tip. Performance of Unichem and Morlife get worse in resisting adhesion loss measured by NH³ tip. For other bond forces, performance of ASA seems to be closely same irrespective to type of polymer type.

Fig. 5.11 depicts the comparison of antistripping agents on the moisture damage of asphalt binder modified with 3% SB polymer. 3% and 5% SB polymer modified samples have almost the same effects of ASAs on the trends of adhesion loss except for COOH tip induced results. Same as 5% SB samples, 3% SB modified samples containing Wetfix and Klingbeta show better performance in reducing moisture damage when probed with $Si₃N₄$ tip. All four ASAs yield moisture resistivity in asphalt sample probed with $CH₃$ tip. Unlike 5% SB samples results probed with COOH tip, cohesion of wet asphalt improved significantly by adding Unichem and Morlife.

Performances of ASAs for 3% SBS modified samples are quite same as that of 3% SB modified samples (see Fig. 5.12) except for Morlife. Morlife appears to improve adhesion loss due to moisture damage measured by NH³ and COOH tips in 3% SBS modified samples compared to 35 SB modified samples. Unichem seems to degrade a bit in performance on the bond force of asphalt determined by COOH tip.

5.5.4 Rank of Antistripping Agents

ASAs are ranked for each tip on the basis of their performance in reducing adhesion loss in asphalt. The ranking is done on the basis of two parameters, lowest percentage of antistripping agent at which adhesion loss due to moisture effect is started to be resisted completely and adhesion loss values corresponding to that percentage of ASA. If any ASA fails to overcome adhesion loss fully, lowest value of adhesion loss is taken into consideration. To be more specific, the starting negative value of adhesion loss and the percentage at which adhesion loss starts to be negative are the two factors based on which ranking of ASA is done. If adhesion loss for a particular case never falls below zero, then the minimum adhesion loss and corresponding ASA is chosen for ranking. Typical range of percentage of ASA suggested by ASA production companies and also by several DoTs' for better function of ASA is 0.25-1%. Also, AFM laboratory test was performed for this range. Therefore, performance of ASA is observed within this range of percent of ASA and ranked accordingly.

Table 5.4 shows the ranking of ASAs for both 3and 5% SB modified asphalt samples proved with four different tips. The procedure of ranking is illustrated below.

At first, for individual tip type, the negative maximum adhesion loss for different ASA mixed asphalt samples within 1% ASA range are identified and recorded in column 4. For example, $CH₃$ tip probed sample showed negative -11.22 nN adhesion loss due to addition of 0.25% Unichem. If there is no negative adhesion loss is appeared within 1% of ASA, then minimum adhesion loss value is recorded. Klingbeta mixed sample probed with $CH₃$ tip adhesion loss does not fall below zero for any percentage of ASA. Therefore minimum positive value of adhesion loss 18.19nN corresponding to 0.25% ASA is recorded for Klingbeta. After that, percentage of

ASA corresponding to recorded adhesion loss is entered in column 5. Now, these two factors are used to rank the ASAs according to their performance in reducing moisture effect. This is definitely the prime concern to reduce adhesion loss as much as possible by using ASA. But, how much ASA is used is also a concern from economic perspective. To incorporate the percentage of ASA on the adhesion loss, equivalent factor is calculated. Equivalent factor is determined by dividing each value in column 5 by 0.25assuming adhesion loss has linear relation with % of ASA. Asphalt sample containing Unichem probed with NH₃ has lowest value of adhesion loss at 1% of ASA addition. Therefore, equivalent factor for % of ASA is 1/0.25=4. This is done to calculate equivalent adhesion loss for 0.25% ASA. The factor is then used to determine modified adhesion loss shown in column 7. It is assumed that moisture effect is improved with the increase in ASA in all cases. Therefore, value of column 4 is multiplied with the factor if value is positive and value of column is divided by factor if value is negative. Asphalt sample containing Unichem and probed with $NH₃$ tip has equivalent factor 4 and positive adhesion loss value. Thus, modified adhesion value for this case is $36.90*4 = 147.60$ nN whereas Unichem contained 5% SB modified asphalt sample probed with $CH₃$ has negative adhesion value with value of equivalent factor of 2.4. For this case, modified adhesion is - 2.99/2.4= -1.25nN. Then on the basis of the value in column 7, ranking of ASA is made. Lowest to highest value of modified adhesion loss is ranked as 1 to 4.

The ranking is individual for different tip types. To have the combined ranking, 4 individual ranking of an ASA for four tips are summed up and showed in Table 5.5. The ASA having least sum total value is the highest performing ASA in resisting moisture damage in asphalt cohesion and adhesion.

From Table 5.5, it is clear that, Morlife performs well in reducing moisture effect on adhesion and cohesion of asphalt especially cohesion of asphalt sample modified with 3% SB polymer. On the other hand, performance of the ASAs in resisting moisture damage in 5% polymer modified samples is not consistent. For different type of tips, ASAs depict different performance and thus it is difficult to choose the highest performed ASA. Therefore, sum rank values of ASAs are so close. Among all four ASAs, Unichem has overall lowest sum rank value, so it can be taken as highest performed ASA in maintaining lower adhesion loss values due to moisture effect in asphalt sample modified with 5% SB.

Same calculations are done for SBS modified samples to rank the ASAs according to their performance in reducing moisture damage. Table 5.6 and 5.7 provide the results.

From Table 5.6 and 5.7, it can be seen that, Morlife performed better than other ASAs for both the percentages of SBS. Also, for both the percentage of polymer modified cases, overall performance rankings of ASAs are same. However, the sum rank for ASAs are close in the case of 3%SBS polymer modified samples. Therefore, overall performances of all ASAs on reducing adhesion/cohesion loss for all bond types due to moisture damage are pretty close. Also, comparison between Table 5.5 and 5.7 reveals that overall performances of ASAs on all the bond forces seem to vary due change in type of polymer present in the sample.

5.6 Conclusions

The following conclusions can be made on the basis of the analyses made in this paper:

 A Neural Network (NN) model has the capability to map the complex the relationship exists between the adhesion force of asphalt and the test factors or variables incorporated in

AFM laboratory test. Therefore, a 11-25-25-5 NN, developed in this chapter, shows good agreement with actual and model predicted adhesion force.

- Input contributions determined by connection weights in between layers of NN shows that, tip type has the highest contribution in adhesion of asphalt. Also, type of ASAs also shows high influence in adhesion of asphalt.
- The model is used to predict adhesion of asphalt for four types of antistripping agent, each with 8 varying percentages to observe the effect of antistripping agent types and percentages on the adhesion loss of asphalt. The followings conclusions are derive from the results
	- o Comparing wet and dry adhesion of asphalt in presence of 4 different ASAs show that, ASAs are effective in reducing moisture effect in some of the bond forces of asphalt. Analyses on the adhesion loss of 3% and 5% SB polymer modified samples probed with four different tips are discussed below
		- All ASAs performed well in reducing adhesion loss due to moisture effect when the 3% SB modified asphalt sample is probed with $CH₃$ functionalized tip. Morlife and Klingbeta perform better in 5% SB modified samples.
		- Klingbeta and Wetfix help in resisting moisture effect on the adhesion of both 3 and 5% SB modified samples determined by Si3N4 tip.
		- However, no significant effect of ASAs is noticed on the adhesion loss of both 3% and 5% asphalt sample probed with $NH₃$ tip.
		- Adhesion loss of 5% SB modified sample probed with COOH tip shows no improvement due to addition of ASAs. However, noteworthy improvement is

observed in 3% SB modified asphalt sample adhesion loss due to addition of Unichem and Morlife.

- o Four ASAs are ranked on the basis of their performance in reducing adhesion loss of 3% and 5% SB polymer modified samples probed with four different tips. For 3% SB modified samples, the sequence of ASA from highest to lowest performance in reducing moisture damage is Morlife>Wetfix>Unichem> Klingbeta. For 5% SB modified sample, the order is Unichem>Klingbeta> Morlife/Wetfix.
- o Ranking of ASAs for both 3% and 5%SBS modified sample provides order from highest to lowest performance as Morlife>Unichem>Wetfix>Kllingbeta.
- o NN results show that 0.25-1% of antistripping agent is effective in reducing adhesion loss so as moisture damage for all type of antistripping agent except for Unichem. Unichem in SB and SBS modified asphalt samples require increase in percentage of ASA above 1% to reduce moisture effect on adhesion of asphalt determined with COOH and $CH₃$ tip. Laboratory tests conducted by different DoTs also suggest 0.25-1.0% of ASA to be the effective range of ASA in reducing moisture damage. The same result is reflected on the bond force of asphalt at nano scale.

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Figure 5.1 Performance plot at training of neural network

Figure 5.2 Regression performance of NN for a selected weight during training

Figure 5.3 Correlation between laboratory test data and model prediction output for adhesion force

Figure 5.4 Adhesion force vs percent antistripping agents plot for dry and wet SB and SBS polymer modified samples probed with NH³ tip

Figure 5.5 Adhesion force vs percent antistripping agents plot for dry and wet SB and SBS polymer modified samples probed with $CH₃$ tip

Figure 5.6 Adhesion force vs percent antistripping agent plots for dry and wet SB and SBS polymer modified samples probed with $Si₃N₄$ tip

Figure 5.7 Adhesion force vs percent antistripping agents plot for dry and wet SB and SBS polymer modified samples probed with OH tip

Figure 5.8 Adhesion force vs percent antistripping agent plots for dry and wet SB and SBS polymer modified samples probed with COOH tip

Figure 5.9 Adhesion loss vs percent of antistripping agent plot for 5% SB modified asphalt sample probed with 4 different tips

Figure 5.10 Adhesion loss vs percent of antistripping agent plot for 5% SBS modified asphalt sample probed with 4 different tips

Figure 5.11 Adhesion loss vs percent of antistripping agent plot for 3% SB modified asphalt sample probed with 4 different tips

Figure 5.12 Adhesion loss vs percent of antistripping agent plot for 3% SBS modified asphalt sample probed with 4 different tips

Table 5.1 Input and Output Variable for NN Model

No. of Neurons in the First Hidden Layer	No. of Neurons in the Second Hidden Layer	Validation MSE	Test R^2		
24	21	2.89E-15	0.981988		
24	22	2.42E-15	0.982788		
24	23	2.97E-15	0.979774		
24	24	2.31E-15	0.983984		
24	25	2.94E-15	0.98083		
25	20	2.55E-15	0.980611		
25	21	2.86E-15	0.981466		
25	22	2.73E-15	0.981784		
25	23	3.45E-15	0.980025		
25	24	2.78E-15	0.981725		
25	25	2.35E-15	0.98556		

Table 5.2 Sample Results for Selection of NN Structure

Input variables	Wet/dry	SB/SBS/none	$%$ of polymer	Type of ASA	$%$ of ASA	Tip type	X1	X2	X ₃	Χ4	
Percent contribution	8.187	8.816	9.802	11.714	3.907	16.531		9.929 7.754	7.329	9.635 6.398	

Table 5.3 Percent Contribution of Input Factors

Table 5.4 Rank of ASA on the Basis of Adhesion Loss and Percent of ASA for SB Modified Sample

% of SB	Type of ASA	Sum	Overall
polymer		rank	ranking
3	Unichem	12	3
	Morlife	6	1
	Wetfix	9	$\overline{2}$
	Klingbeta	13	4
5	Unichem	8	$\mathbf{1}$
	Morlife	11	3
	Wetfix	11	3
	Klingbeta	10	$\overline{2}$

Table 5.5 Overall Ranking of ASAs for All Four Tips for SB Modified Sample

Table 5.6 Rank of Asa on the Basis of Adhesion Loss and Percent of ASA for SBS Modified Sample

$%$ of SBS polymer	Type of ASA	Sum rank	Overall ranking
3	Unichem	10	2
	Morlife	7	
	Wetfix	11	3
	Klingbeta	12	4
5	Unichem	10	$\overline{2}$
	Morlife	7	1
	Wetfix	11	3
	Klingbeta	12	

Table 5.7 Overall Ranking of ASA for All Four Tips and for SBS Modified Sample

CHAPTER 6 CONCLUSIONS

6.1 Summary

This study attempts to develop a prediction model of nano-scale adhesion and cohesion of moisture conditioned asphalt. In addition, performance of antistrip additives on asphalt under moisture damage is assessed using the model induced results by comparing wet and dry conditioned adhesion/cohesion of asphalt.

Adhesion between asphalt-aggregate system and cohesion in between asphalt are considered to be very important mechanisms in dealing moisture damage of asphalt pavements. Due to variability and not fully explored chemical composition of asphalt, performance study based on laboratory tests are very popular in quantifying adhesion and cohesion mechanisms of asphalt under moisture conditioning. The complex interaction among the test factors involved in determination of adhesion of asphalt in laboratory tests makes prediction of asphalt adhesion and cohesion difficult using the relationship between test factors of asphalt and adhesion force of asphalt. Therefore, this study explores the utilization of the Neural Network (NN) in predicting adhesion and cohesion of asphalt having different asphalt binder properties using Atomic Force Microscopy (AFM) laboratory test data. AFM test data, incorporated in this study, provides nano-scale adhesion and cohesion of wet and dry asphalt samples modified with polymers and antistrip additives to reduce the moisture susceptibility of asphalt. AFM laboratory data consist of five point force-distance values including pull-off force (can be considered as adhesion/cohesion) measured by four representative tips for asphalt chemical functional groups and one industrial tip to simulate adhesion and cohesion of wet and dry asphalt samples. In addition, asphalt samples are modified with different type, percentages of modifiers and

additives. Due to nonlinear and complex relationships involving multiple variables in this test, it is difficult to define an appropriate relationship between the factors and predict adhesion of asphalt. NN proved to a better technique than conventional models by past literatures to map multiple variable relationships; thus it is used to predict adhesion and cohesion of asphalt in this study.

Two NN models are developed for lime treated and chemical additive treated asphalt samples to observe the performance of lime and four other chemical additives named as Klingbeta, Morlife, Wetfix and Unichem in reducing moisture effect of asphalt. Lime treated asphalt sample and chemical additive treated asphalts sample patterns are quite different thus could not be able to incorporated in single model. To develop the NN model, backpropagation NN with Levenberg-Marquardt algorithm is selected based on careful review on past studies and prediction applications of NN on pavement field. This type of NN has the ability to learn and recognize trends in the data pattern in the training phase and predict output on the basis of learned relationship in the testing phase. Two main concerns are addressed in constructing NN model: selection of input-output variables and selection of the NN architecture. The processes of selection of these two concerns are explained for both lime treated and chemical ASA treated samples. Finally, two four layer feedforward networks are developed for both the dataset. Both models show good predictability of adhesion force when tested with inputs that were not introduced during the construction of model. Furthermore, relative influences of input parameters on adhesion are calculated with the developed NN.

The established NNs are then used to predict adhesion and cohesion of asphalt for both lime and chemical ASA dataset. To assess performance of ASA in reducing moisture effect, adhesion of wet and dry damaged asphalt are predicted using NN model having all the input variables same. Having same inputs helps to create a comparison ground for all ASAs. Trends of bond forces are initially observed and then taking the difference between wet and dry conditioned adhesion of asphalt, adhesion loss is determined. Comparison of dry and wet samples adhesion provides adhesion loss thus moisture damage of asphalt samples. This procedure is applied to both lime and chemical ASA dataset. In case of lime treated sample, performance of lime in reducing moisture effect adhesion forces measured by different tips are compared. The same comparison is made for chemical ASA treated samples. However, an addition analysis is done in case of chemical ASA sample to rank the ASAs according to their performance in resisting moisture damage on asphalt adhesion at nano-level. Comparison between lime and other ASAs are not done in this study as two different models are incorporated to predict the bond forces that are not comparable in terms of inputs.

6.2 Conclusions

Based on the findings of the study, the following conclusions are made:

• In this study, two NN models are constructed that can be fitted to AFM data to predict adhesion for lime treated and chemical ASA treated asphalt samples. Four layer feedforward neural networks are developed to predict adhesion of asphalt binder using testing parameters involved in AFM test data for both lime treated and chemical ASA treated asphalt samples. Both the models show good prediction ability for the test input variables that were not introduced to the network before.

- The relative influence of each input on adhesion of asphalt is determined using the connection weights in between the layers of developed network. According to the input contribution analysis, the most significant parameter affecting adhesion is the asphalt chemical functional groups represented by tip types in the AFM testing for both the models. In case of chemical ASA treated sample, type of ASA has high influence on adhesion of asphalt.
- The developed models are utilized to observe the effect of lime and chemical ASA on the adhesion loss so as the moisture damage of asphalt. NN induced results indicate that lime helps to reduce moisture damage in some of the asphalt samples and activates better in reducing moisture effect at presence of 3% polymer modifier irrespective of the type of the modifier. Presence of 5% polymer seems to have random and in some case has reverse effect on the performance of lime in resisting moisture effect. Also, lime shows very poor performance in improving resistivity to moisture damage of asphalt adhesion measured by silicon nitride tip for all the polymer modified asphalt samples. In case of four chemical ASA treated sample, NN results show that ASAs are effective in reducing moisture effect on the adhesion forces of asphalt of some of the asphalt chemical functional groups. Analyses on the adhesion loss of 3% and 5% SB polymer modified samples probed with four different tips are discussed below
	- All ASAs performed well in reducing adhesion loss due to moisture effect when the 3% SB modified asphalt sample is probed with $CH₃$ functionalized tip. Morlife and Klingbeta perform better for 5% SB modified samples.
	- Klingbeta and Wetfix help in resisting moisture effect on the adhesion of both 3 and 5% SB modified samples determined by Si3N4 tip.

- However, no significant effect of ASAs is noticed on the adhesion loss of both 3% and 5% asphalt sample probed with $NH₃$ tip.
- Adhesion loss of 5% SB modified sample probed with COOH tip shows no improvement due to addition of ASAs. However, noteworthy improvement is observed in 3% SB modified asphalt sample adhesion loss due to addition of Unichem and Morlife.
- Comparative study is made on NN model induced result based on chemical ASA data set and all chemical ASAs are ranked on the basis of their performance in reducing moisture damage. The analysis displays that Morlife chemical additives shows better performance compared to other ASAs in reducing moisture related damage on adhesion of asphalt modified with SBS polymers. Also, it proves to be better in case of 3% SB modified samples in reducing moisture damage. However, the improvement in resistance of adhesion loss due to addition of Morlife is more in 3% SB samples compared to 3 and 5% SBS samples.
- Increase in percentage of lime above 1.5 % has no effect and in some case has worse effect on the enhancement of resistivity to moisture damage. Also, increase in percentage of ASA above 1% does not have noticeable effect in reducing adhesion loss of asphalt in case of chemical ASA treated samples.

6.3 Recommendations

The following points are recommended for future studies

 Chromatography of wet and dry asphalt samples can be done to determine the concentration of surface functional groups present in asphalt. This may help in explaining

the adhesion and cohesion trend of asphalt and tip chemically and relate the chemical theory with the NN induced results.

• Instead of using industrialized tip to determine the adhesion, aggregate tip can be used in AFM testing. The NN model constructed using the modified AFM test data will help to predict adhesion force more oriented to actual surface interaction of asphalt-aggregate.

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