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The Rapid Determination Method of Performance Parameters and PG Grade for SBS Modified Asphalt

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Abstract. This paper demonstrates the application of support vector machine (SVM) applied to ATR-FTIR data to solve classification and regression problems associated with rapid determination of PG grade for SBS modified asphalt. The modified asphalt samples were produced by mixing three kinds of matrix asphalt, two kinds of SBS and five kinds of SBS content from 2% to 6% under the same manufacture process. Therefore a total of 150 data sets were evaluated with five parallel tests for each sample. In the SVR model, the ATR-FTIR data were parameter for the input layer whereas the PG parameters of asphalt such as, rut factor, creep stiffness and creep rate were output layer. While in the SVC model, high temperature grade and low temperature grade were output layer. This new method allows rapid determination of multi-properties from a single spectrum for SBS modified asphalt and it is promising for online material monitoring of specific project.

1. Introduction

In order to improve the performance in all aspects of matrix asphalt, many kinds of additives were tried to be added into asphalt. Among them, the application of polymer is most extensive with its excellent modification effect. In recent years, the most commonly used polymer for asphalt modification is SBS followed by other polymers such as SBR and EVA [1-3]. The engineering property of asphalt can be greatly improved by adding polymer into asphalt. SBS can increase the elasticity and viscosity performance of asphalt and it is maybe the most suitable polymers for asphalt modification at present [4-7].

It is important to accurately obtain PG grade of PMA in order to evaluate the efficiency of the additives. However, it requires a large number of tests to obtain the PG grade for asphalt, including RTFOT, PAV, BBR, DSR, DTT according to the SHRP specification. During the past decade, vibrational spectroscopy such as infrared spectroscopy in combination with machine learning algorithms was powerful analytical technique which has received extensive application. The rapid determination of PG grade and other performance parameters such as complex shear modulus G^* and phase angle δ can help improve the quality control of modified asphalt.

However, the research on the rapid determination of SHRP indexes is still blank. The combined use of advanced machine learning algorithms and infrared spectroscopy technology provides the possibility for rapid and accurate prediction of the PG grade and SHRP performance parameters of asphalt. With the extensive application of SBS modified asphalt, the support vector machine regression (SVR) and classification (SVC) models were developed for rapid determination of PG grade and SHRP performance parameters for SBS modified asphalt combined with the ATR-FTIR data in this work. The optimized model can be used for online material monitoring in specific project.



2. Materials and sample preparation

The main purpose of this research was to establish SHRP performance parameter regression model and PG grade classification model by using of FTIR data combined with SVR and SVC. The rapid prediction of PG grade for asphalt performance just can be realized by plugging the infrared spectrum test data of the test into the prediction model. To achieve this objective, it was necessary to prepare various types of SBS modified asphalt. For the purpose of this research, three kinds of matrix asphalt type respectively is Sinopec 70#, Cnooc 70# and Shell 70# are prepared followed with two kinds of SBS type, respectively is linear YH791 and star BM4302 as Fig.1. SBS content is added from 2% to 6% by weight of asphalt under the same manufacture process. SBS modified asphalt is prepared by high-speed shearing equipment. Therefore a total of 30 combinations were evaluated, and 150 data sets were obtained with five parallel tests.



Figure.1 The SBS samples: (a) is linear YH791 and (b) is star BM4302 SBS

3. Test and data analysis

For the prepared 30 kinds of asphalt samples, DSR, BBR and ATR-FTIR were tested separately. The DSR and BBR test are performed according to industry standard as Tab.1 and Tab.2. G^* of all samples significantly increases with the increase of temperature, while the phase angle δ presents the opposite changing law. It can be seen from Tab.1 that the rut factor $G^*/\sin\delta$ increases with the increase of SBS content. When SBS content is 4%~6%, the high temperature performance for matrix asphalt can improve of two levels. It can be seen from Tab.2 that the low temperature performance of the asphalt can be improved for a level by adding 3%~5% SBS.

Table.1 Rut factor of Shell 70# asphalt

Temp /°C	Samples	SBS content/%					
		0	2	3	4	5	6
64	unaged	1.72	3.91	4.98	6.02	7.11	7.59
	RTFOT	2.92	4.81	5.73	6.99	7.86	8.03
70	unaged	0.82	1.11	1.76	2.42	2.87	3.23
	RTFOT	1.73	1.98	2.44	3.42	3.85	4.03
76	unaged	0.45	0.64	0.95	1.28	1.76	2.16
	RTFOT	0.73	1.02	1.54	2.31	2.43	2.71
82	unaged	0.38	0.45	0.62	0.92	1.44	1.45
	RTFOT	0.65	0.88	1.12	1.63	1.85	1.81
PG high temp grade/°C		64	64	70	76	76	76

Table.2 BBR results of Shell 70# asphalt

Temp /°C	Indexes	SBS content/%					
		0	2	3	4	5	6
-6	m	83	99	92	87.4	106	112
	s	0.38	0.36	0.37	0.34	0.36	0.33
-12	m	225	231	199	183	291	299
	s	0.28	0.29	0.32	0.35	0.3	0.28

-18	m	355	368	365	398	421	433
	s	0.27	0.28	0.27	0.28	0.27	0.27
PG low temp grade/°C		-16	-16	-22	-22	-22	-16

The mixing of modifiers will absorb light components in the asphalt, the complex modulus G^* of asphalt will increase, and the phase angle δ will decrease. But it must be considered that the ratio of the four components is discrepant for different matrix asphalt. When the same proportion of modifier is added, the asphalt containing more lightweight components will be less affected by the modifier. The test data shows that the difference of G^* and δ among the modified asphalt prepared by three different matrix asphalt is obvious. Therefore, it can be concluded that the type and performance of matrix asphalt is an important aspect of modification effect.

Comparing the two different types of SBS, the effect of star modifier on G^* was significantly less than that of linear modifier from Fig.2. The reason may be that the modifier can absorb part of the light component in the matrix asphalt and then swelling. The molecular structure of the star SBS is relatively complex, and it also has large molecular weight to make it more difficult to dissolve in matrix asphalt. So the effect of star SBS on G^* of modified asphalt is less than linear SBS. Although star SBS are more difficult to dissolve in matrix asphalt, star SBS has better modification effect than linear SBS as a whole.

The variety of modifier, the type of matrix asphalt and the preparation technology of modified asphalt all have great influence on the properties of modified asphalt. The preparation technology is not considered in this study, it is easy to see that the effect of matrix asphalt type is more obvious than SBS type.

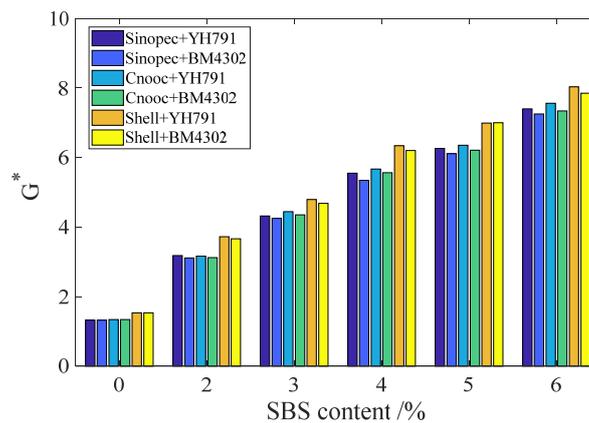


Figure.2 G^* at 64°C of all samples

4. Support Vector Machine Prediction Model

4.1 Preprocessing methods of IR data

Preprocessing of IR data can eliminate the random error in the process of data collection. At present there are many kinds of preprocessing method for infrared spectrum. In this study, several different preprocessing methods were test as Tab.3. After the optimization, the first derivative and smoothing algorithm were selected to deal with the original spectrum by contrast and analysis. The spectral data before and after preprocessing is shown in Fig.3. Among them, the first derivative is advantageous to the analysis of overlapping peak, erase the disturbance of baseline, and increase resolution of the spectrum. Smoothing algorithm can remove the effect of noise.

Table 3. Comparison of different preprocessing methods

Methods	R_{MSE}	R^2	COV
1 st derivative	0.032	0.922	0.8
2 nd derivative	0.041	0.861	1.03
Smoothing	0.027	0.945	0.68

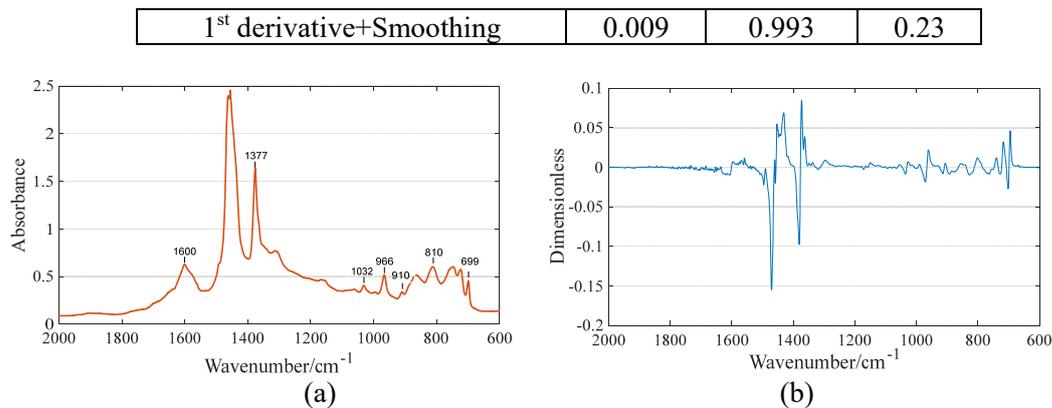


Figure 3. SBS (5% content) modified asphalt infrared spectrum. (a) The original spectrum, (b) The preprocessing spectrum.

4.2 Screening of modeling spectrum interval

Initially the prediction model was built using the full length of the spectra from the preprocessed data, but the precision of the prediction model is not satisfactory. In this section, in order to reduce the modeling training time, eliminate the spectrum interval which has excessive noise pollution, and determine the characteristic spectrum interval of specific component, it is very necessary to choose appropriate wavelength range for modeling.

The wavelength range selection should take into account the chemical knowledge such as the relationship between the PG parameters and characteristic functional group. In the IR spectrum, 966cm^{-1} and 910cm^{-1} are the structure characteristic peak of trans butadiene. 699cm^{-1} is the single replace peak of styryl benzene ring. So it can be concluded that these three wavenumber are the characteristic peak of SBS modified materials. Afterwards, 1032cm^{-1} is stretching vibration absorption peak of sulfoxide base S=O. 720cm^{-1} is bending vibration peak of alkanes that represent saturated hydrocarbon component of asphalt. $740\sim 840\text{cm}^{-1}$ is vibration peak of benzene that represent aromatic hydrocarbon component of asphalt. Comprehensive consideration of chemical knowledge and correlation coefficient, the feature area at $680\sim 720\text{cm}^{-1}$ and $880\sim 1050\text{cm}^{-1}$ should be determined for PG parameter prediction model.

Although the complex shear modulus G^* and creep stiffness m of asphalt are physical properties, they are closely related to the chemical composition and constituent content. Therefore, it is theoretically feasible to detect asphalt properties by using infrared spectrum as the information carrier for quantitative analysis. The incorporation of SBS has an important influence on asphalt performance. So, the characteristic peak of SBS in infrared spectrum must be considered when choosing the modeling interval of the G^* and m prediction model. Finally, the feature interval for G^* prediction model should be determined at $3400\sim 2700\text{cm}^{-1}$, $1700\sim 1100\text{cm}^{-1}$ and $1000\sim 680\text{cm}^{-1}$. Meanwhile, the feature area for creep stiffness m prediction model should be determined at $3400\sim 2700\text{cm}^{-1}$, $1700\sim 1300\text{cm}^{-1}$ and $1000\sim 680\text{cm}^{-1}$.

5. Results and Discussion

5.1 PG parameter prediction model

In this section, regression analysis is carried out to establish the prediction model by SVR algorithm. The principal component analysis method (PCA) was used for data dimensionality reduction. The accuracy of the prediction model is tested by the means of five-fold cross validation. In the SVR model, the ATR-FTIR data was parameter for the input layer whereas the PG performance parameters of modified asphalt such as G^* and rut factor at 64°C , creep stiffness and creep rate at -6°C were output layer.

In order to obtain the optimal model, different kernel function were used. The specific results of the regression model are shown in Tab.4. It can be seen that Quadratic kernel gained more promising results compared with other kernel function. Among them, the highest R^2 of the G^* prediction model can be reached 0.986 as shown in Fig.4.

The prediction accuracy of DSR parameter is enough high which can meet the requirements for application. Meanwhile, the modeling process of new method uses multiple types of asphalt, so it has more extensive applicability. However, the prediction effect of BBR test parameter is more general especially the creep rate s . This may be related to the discreteness of the test data.

Table 4. Regression result for PG parameter model

Parameter	Kernel function	R^2	R_{MSE}
G^*	Linear kernel	0.981	0.24
	Quadratic kernel	0.986	0.22
	Cubic kernel	0.985	0.23
	Guassian kernel	0.983	0.23
Rut factor $G^*/\sin\delta$	Linear kernel	0.972	0.27
	Quadratic kernel	0.978	0.25
Creep stiffness m	Linear kernel	0.89	34.1
	Quadratic kernel	0.90	29.8
Creep rate s	Linear kernel	0.72	0.08
	Quadratic kernel	0.77	0.07

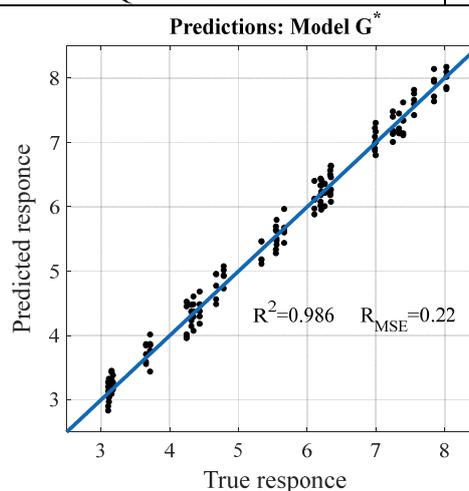


Figure 4. The G^* Regression model results of Quadratic SVM

5.2 The PG grade classification model

The predicted values of G^* , δ , m , s and other parameters can be obtained through the prediction model established in the previous section. However, in order to get the PG grade of SBS asphalt, it is necessary to establish a few models under different test temperature through this method. Meanwhile, the prediction model of low temperature parameters can not provide high accuracy. Therefore, it is difficult to judge the PG grade of asphalt by predicting the parameters of DSR and BBR. This article takes a different approach. The classification model of PG grade was established directly with IR spectral data.

Currently, the PG grade of asphalt is judged by industry standard. The analysis process is not complicated, but the analysis tests will cost lengthy time because of that the sample needs to be processed and produced. The infrared spectrum of asphalt is related to the basic properties of asphalt. Based on the machine learning method, the infrared spectral data is correlated with basic asphalt property parameters. The prediction model can realize the PG grade rapid determination of asphalt.

The amount of asphalt type contained in the data set has an important influence on the accuracy of the classification model. The three samples selected in this paper are all 70# asphalt. The classification model whose data set contains more asphalt types will be more widely applied. But the accuracy of the model will decrease with the increase of asphalt type modeling in modeling data set. Among them, the highest accuracy of the high temperature grade prediction model established by three kinds of asphalt is 96.7% in Tab.5. The high temperature grade classification model is less affected by the increase of asphalt type than the low temperature grade classification model.

Table 5. The results of PG grade Classification model

Model type	Modeling interval(cm^{-1})	Types of asphalt	Sample size	Kernel function	Accuracy /%
High temperature grade	3000~2700, 1700~1400, 1000~680	1	50	linear	98.0
		1	50	Quadratic	98.0
		3	150	Linear	95.3
		3	150	Quadratic	96.7
		3	150	Cubic	96.0
		3	150	Fine Gaussian	95.3
Low temperature grade	3300~2700, 1700~1100, 1000~680	1	50	linear	88.0
		1	50	Quadratic	90.0
		3	150	Linear	81.3
		3	150	Quadratic	83.3
		3	150	Cubic	86.0
		3	150	Fine Gaussian	82.0

By comparison with Fig.5 and Fig.6, it can be concluded that the accuracy of high temperature grade classification model is significantly higher than the low temperature grade classification model. SBS content is highly correlated with SBS feature peak in infrared spectrum. High temperature performance is greatly influenced by SBS content. Therefore, the modeling interval can be effectively reduced according to the SBS feature peak. As to low temperature performance, it is relatively less affected by modifier content which is more correlated with the performance of matrix asphalt. Moreover, creep stiffness m and creep rate s are test indicators, test error and system error will be accumulated in the experiment. In addition, there are more characteristics interval related to these two indexes in the infrared spectrum. The increase of modeling interval will introduce more system noise which will affect the prediction accuracy of model. Even so, the accuracy of low temperature grade classification model established by one kind of asphalt is also enough high which can meet the prediction requirements.

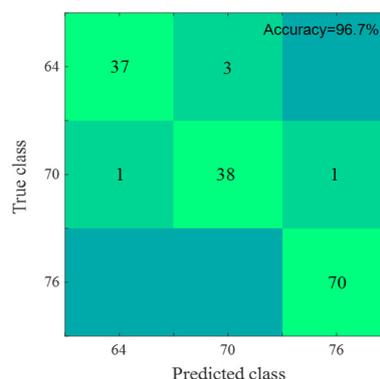


Figure 5. The accuracy of High temperature grade classification models

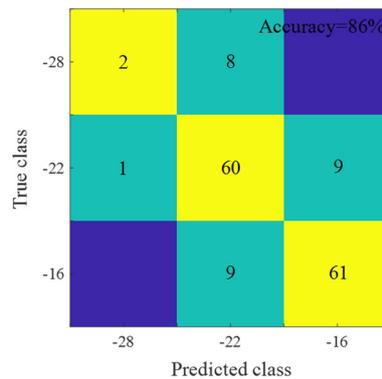


Figure 6. The accuracy of Low temperature grade classification models

6. Conclusion

This research demonstrates the application of support vector machine (SVM) applied to ATR-FTIR data to solve regression and classification problems associated with rapid determination of PG grade and performance parameters for SBS modified asphalt. The results show that SVR and SVC can provide satisfactory regression and classification models between the high temperature performance and infrared spectrum data sets, and the accuracy of low temperature performance regression and classification model established by same kind of asphalt is enough high which can meet the prediction requirements. This new method allows rapid determination of multi-properties from a single spectrum for SBS modified asphalt and can be used for online material monitoring of specific project.

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