

Supplementary Materials: Application of Infrared Spectroscopy in Prediction of Asphalt Aging Time History and Fatigue Life

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Table S1. Basic physical performance indices of asphalt for the four samples.

Test Parameter		Unit	TPC70#	JL70#	SBS-1	SBS-2	Test Method
Penetration (25 °C, 100 g, 5 s)		mm	62.1	61.3	55.2	54.6	T0604
Ductility (5 °C, cm/min)		cm	19.5	20.8	34.6	35.2	T0605
Softening point		°C	49.4	50.6	77.8	78.2	T0606
Brookfield viscosity (135 °C)		Pa·s	0.492	0.486	1.38	0.486	T0625
Rotating film heating test (RTFOT) residue 163 °C, 85 min	Mass loss	%	0.08	0.07	0.07	0.08	T0610
	Ductility (5 °C, cm/min)	cm	13.7	14.3	17.2	17.6	T0605
	Penetration ratio	%	84.4	82.8	79.2	78.9	T0604

Table S2. Aging asphalt samples.

Asphalt Brand	Aging Simulation Method	Aging Temperature (°C)	Aging Time (min)	Aging Asphalt Samples
Matrix asphalt	JL70#	RTFOT	163	0 JL-A
				85 JL-B
				120 JL-C
				240 JL-D
				360 JL-E
	TPC70#	RTFOT	163	0 TPC-A
				85 TPC-B
				120 TPC-C
				240 TPC-D
				360 TPC-E
Modified asphalt	SBS-1	RTFOT	163	0 SBS1-A
				85 SBS1-B
				120 SBS1-C
				240 SBS1-D
				360 SBS1-E
	SBS-2	RTFOT	163	0 SBS2-A
				85 SBS2-B
				120 SBS2-C
				240 SBS2-D
				360 SBS2-E

Table S3. The values of spectral peak area under each benchmark.

Peak Range of Reference Spectrum (cm ⁻¹)	The Sum of Peak Area
650~1400	$\sum A_1 = A_{699} + A_{721} + A_{744} + A_{807} + A_{863} + A_{965} + A_{1030} + A_{1159} + A_{1306} + A_{1376}$
1400~4000	$\sum A_2 = A_{1456} + A_{1599} + A_{1700} + A_{2850} + A_{2920}$
650~4000	$\sum A_3 = A_{699} + A_{721} + A_{744} + A_{807} + A_{863} + A_{965} + A_{1030} + A_{1159} + A_{1306} + A_{1376} + A_{1456} + A_{1599} + A_{1700} + A_{2850} + A_{2920}$
2920, 2850	$\sum A_4 = A_{2850} + A_{2920}$

Table S4. Functional group index of aged asphalt.

Asphalt Samples	I _{C=O}	I _{S=O}	I _{B,a}	I _B	I _{Ar}
JL-A	0	0.048	1.248	2.141	0.091
JL-B	0.005	0.083	1.210	2.114	0.111
JL-C	0.007	0.094	1.242	2.048	0.084
JL-D	0.011	0.107	1.210	2.127	0.085
JL-E	0.031	0.115	1.167	2.105	0.108
TPC-A	0	0.049	1.390	2.037	0.131
TPC-B	0.007	0.061	1.404	1.919	0.138
TPC-C	0.010	0.062	1.415	1.976	0.142
TPC-D	0.017	0.077	1.403	1.938	0.118
TPC-E	0.026	0.119	1.342	1.901	0.132
SBS1-A	0	0.061	0.849	1.368	0.103
SBS1-B	0.002	0.067	0.848	1.418	0.100
SBS1-C	0.003	0.070	0.858	1.429	0.092

SBS1-D	0.014	0.076	0.841	1.378	0.091
SBS1-E	0.029	0.082	0.815	1.317	0.089
SBS2-A	0	0.038	0.885	1.604	0.089
SBS2-B	0.005	0.050	0.875	1.638	0.101
SBS3-C	0.007	0.054	0.889	1.700	0.098
SBS2-D	0.011	0.061	0.865	1.640	0.085
SBS2-E	0.015	0.072	0.853	1.627	0.078

Table S5. Fitting results of the recovery rate R model.

Temperature, °C	Stress, kPa	Fitting Parameters		
		R^2	MS	Sig
64	0.1	0.8954	264.27	2.12×10^{-6}
	3.2	0.8959	234.77	1.62×10^{-6}
70	0.1	0.8994	245.93	1.62×10^{-6}
	3.2	0.8988	215.81	1.69×10^{-6}
76	0.1	0.8898	250.48	3.01×10^{-6}
	3.2	0.8605	212.27	1.51×10^{-6}
82	0.1	0.8743	238.96	7.43×10^{-6}
	3.2	0.7419	129.50	9.27×10^{-6}
88	0.1	0.8607	224.36	8.43×10^{-6}
	3.2	0.6538	108.31	10.32×10^{-6}

Table S6. Correlation matrix of five characteristic functional group indices.

Functional Group Indices	$I_{C=O}$	$I_{S=O}$	$I_{B,a}$	I_B	I_{Ar}
$I_{C=O}$	1	0.84	0.18	0.14	0.16
$I_{S=O}$	0.84	1	0.36	0.40	0.13
$I_{B,a}$	0.18	0.36	1	0.95	0.82
I_B	0.14	0.40	0.95	1	0.48
I_{Ar}	0.16	0.13	0.82	0.48	1

Table S7. Total variance explanation.

Component	Initial Eigenvalue		
	Total	Variance Percentage, %	Cumulative Contribution Rate, %
1	2.47	49.35	49.35
2	1.60	32.08	81.43
3	0.67	13.32	94.74
4	0.21	4.12	98.87
5	0.06	1.14	100

Table S8. Rotating component matrix.

Functional Group Index	PCA1	PCA2
$I_{C=O}$	0.36	0.86
$I_{S=O}$	0.53	0.78
$I_{B,a}$	0.94	−0.30
I_B	0.84	−0.22
I_{Ar}	0.70	−0.37



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