

## Supporting information

# An Optimization Method Based on Spatial Confinement and Spectra Data Screening for Laser-induced Breakdown Spectroscopy Quantitative Analysis of Coal Particle Flow

Junbin Cai,<sup>a, b</sup> Meirong Dong,<sup>a, b, \*</sup> Hongjie Chen,<sup>a, b</sup> Zihan Shang,<sup>a, b</sup> Shunchun Yao,<sup>a, b</sup> and Jidong Lu<sup>a, b</sup>

<sup>a</sup> School of Electric Power, South China University of Technology, Guangzhou 510640, P. R. China

<sup>b</sup> Guangdong Province Engineering Research Center of High Efficient and Low Pollution, Guangzhou 510640, P. R. China

**Table S1.** The proximate analysis data of coal specimens

Specimen No.	Ash(wt.%)	Fixed carbon (wt.%)	Volatile matter (wt.%)	Calorific value (MJ/Kg)
S1	2.52	37.69	40.11	20.82
S2	14.04	43.99	27.91	19.42
S3	23.96	66.57	5.05	24.22
S4	14.82	21.64	34.72	13.70
S5	26.18	65.23	4.88	22.76
S6	23.13	68.99	4.92	25.00
S7	4.06	56.03	27.93	24.05
S8	13.44	53.21	29.31	26.18
S9	17.16	48.68	26.48	22.44
S10	7.71	52.17	28.56	23.64
S11	40.43	41.64	16.42	17.66
S12	22.38	46.14	27.50	22.58
S14	12.74	49.45	28.82	23.22
S15	23.84	64.19	10.61	25.70
S16	25.70	66.63	4.84	23.40
S17	42.64	41.11	14.40	17.24
S18	15.76	45.51	25.56	21.92
S19	18.90	71.64	6.50	27.15
S20	37.45	56.67	4.06	18.99
S21	13.86	52.81	29.47	26.16
S22	19.50	46.41	27.44	22.04
S23	27.92	57.00	13.24	23.14
S24	73.96	11.68	13.10	4.62
S25	32.84	44.35	19.14	19.44
S26	15.44	37.18	32.04	18.88
S27	39.46	47.08	11.92	18.76
S28	32.78	53.04	13.49	22.48
S29	37.30	59.5	2.58	19.32
S30	38.08	50.89	9.53	19.03
S31	31.35	52.45	14.46	21.55
S32	25.61	50.68	18.81	21.84

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<b>N1</b>	14.08	43.54	29.92	20.84
<b>N2</b>	20.96	47.26	28.28	23.8
<b>N3</b>	10.83	51.64	32.11	26.04
<b>N4</b>	36.90	59.93	2.61	19.12
<b>N5</b>	30.80	61.77	5.12	20.74
<b>N6</b>	48.16	24.84	19.04	11.13
<b>N7</b>	41.08	33.08	23.72	17.16

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**Table S2.** Spectral data screening of Coal N6 and S10 without spatial confinement

<b>Threshold of SNR method</b>	<b>Elimination number/ elimination rate (%) of Coal N6</b>	<b>Elimination number/ elimination rate (%) of Coal S10</b>
4.5	383 / 36.48%	4 / 0.38%
5	434 / 41.33%	4 / 0.38%
5.5	486 / 46.29%	6 / 0.57%
6	535 / 50.95%	10 / 0.95%
6.5	586 / 55.81%	15 / 1.43%
7	622 / 59.24%	18 / 1.71%
7.5	673 / 64.10%	27 / 2.57%
8	712 / 67.81%	30 / 2.86%
8.5	753 / 71.71%	33 / 3.14%
9	789 / 75.14%	43 / 4.10%
9.5	825 / 78.57%	56 / 5.33%
10	853 / 81.24%	66 / 6.29%

  

<b>Threshold of RSNR method</b>	<b>Elimination number/ elimination rate (%) of Coal N6</b>	<b>Elimination number/ elimination rate (%) of Coal S10</b>
0.45	204 / 19.43%	31 / 2.95%
0.5	245 / 23.33%	45 / 4.29%
0.55	279 / 26.57%	67 / 6.38%
0.6	317 / 30.19%	99 / 9.43%
0.65	349 / 33.24%	127 / 12.10%
0.7	387 / 36.86%	180 / 17.14%
0.75	419 / 39.90%	246 / 23.43%
0.8	453 / 43.14%	309 / 29.43%
0.85	488 / 46.48%	366 / 34.86%
0.9	520 / 49.52%	433 / 41.24%
0.95	553 / 52.67%	505 / 48.10%
1.0	584 / 55.62%	578 / 55.05%

**Table S3.** Spectral data screening of Coal N6 and S10 with spatial confinement

<b>Threshold of SNR method</b>	<b>Elimination number/ elimination rate (%) of Coal N6</b>	<b>Elimination number/ elimination rate (%) of Coal S10</b>
4.5	8 / 0.76%	2 / 0.19%
5	14 / 1.33%	3 / 0.29%
5.5	20 / 1.90%	3 / 0.29%
6	30 / 2.86%	3 / 0.29%
6.5	43 / 4.10%	4 / 0.38%
7	75 / 7.14%	6 / 0.57%
7.5	109 / 10.38%	7 / 0.67%
8	163 / 15.52%	7 / 0.67%
8.5	218 / 20.76%	8 / 0.76%
9	293 / 27.90%	8 / 0.76%
9.5	375 / 35.71%	11 / 1.05%
10	454 / 43.24%	13 / 1.24%

  

<b>Threshold of RSNR method</b>	<b>Elimination number/ elimination rate (%) of Coal N6</b>	<b>Elimination number/ elimination rate (%) of Coal S10</b>
0.45	9 / 0.86%	8 / 0.76%
0.5	7 / 0.67%	12 / 1.14%
0.55	26 / 2.48%	16 / 1.52%
0.6	37 / 3.52%	29 / 2.76%
0.65	63 / 6.00%	46 / 4.38%
0.7	99 / 9.43%	71 / 6.76%
0.75	153 / 14.57%	117 / 11.14%
0.8	212 / 20.19%	186 / 17.71%
0.85	288 / 27.43%	271 / 25.81%
0.9	375 / 35.71%	358 / 34.10%
0.95	459 / 43.71%	476 / 45.33%
1.0	544 / 51.81%	574 / 54.67%

**Table S4.** Prediction results of ash content of coal specimens from test set

No.	Reference value of ash content	SNR		RSNR	
		R <sup>2</sup> =0.9225		R <sup>2</sup> =0.9334	
		Predicted value	SD	Predicted value	SD
N1	14.08	10.31	0.46	11.26	1.68
N2	20.96	21.33	0.85	20.27	0.89
N3	10.83	13.12	1.14	13.07	1.24
N4	36.9	37.42	3.68	37.31	3.17
N5	30.8	32.06	1.64	32.42	1.96
N6	48.16	44.13	1.34	44.63	0.87
N7	41.08	33.91	0.57	33.94	0.56

  

No.	Reference value of ash content	Spatial confinement + SNR		Spatial confinement + RSNR	
		R <sup>2</sup> =0.9834		R <sup>2</sup> =0.9845	
		Predicted value	SD	Predicted value	SD
N1	14.08	14.10	1.55	14.20	1.17
N2	20.96	19.39	0.54	19.29	0.23
N3	10.83	11.14	1.03	11.52	0.52
N4	36.9	36.13	0.95	36.27	1.14
N5	30.8	32.67	0.95	33.04	0.68
N6	48.16	46.03	0.90	45.81	0.95
N7	41.08	38.13	0.51	39.00	0.27

**Table S5.** Prediction results of fixed carbon content of coal specimens from test set.

No.	Reference value of fixed carbon	SNR		RSNR	
		R <sup>2</sup> =0.9264		R <sup>2</sup> =0.9579	
		Predicted value	SD	Predicted value	SD
N1	43.54	43.68	0.77	46.13	0.49
N2	47.26	47.31	1.38	46.54	1.67
N3	51.64	47.74	3.17	47.24	2.57
N4	59.93	59.17	1.36	59.54	0.86
N5	61.77	65.01	1.80	62.25	2.87
N6	24.84	26.48	1.52	24.34	0.73
N7	33.08	40.27	1.24	37.43	1.8

  

No.	Reference value of fixed carbon	Spatial confinement + SNR		Spatial confinement + RSNR	
		R <sup>2</sup> =0.9671		R <sup>2</sup> =0.9736	
		Predicted value	SD	Predicted value	SD
N1	43.54	42.89	0.99	41.74	0.86
N2	47.26	48.47	0.72	49.08	0.65
N3	51.64	46.55	1.40	47.63	0.89
N4	59.93	61.12	2.42	60.04	1.26
N5	61.77	59.77	0.91	59.90	0.86
N6	24.84	23.80	0.88	23.25	0.77
N7	33.08	34.42	1.28	33.63	1.12

**Table S6.** Prediction results of volatile matter content of coal specimens from test set

No.	Reference value of volatile matter content	SNR		RSNR	
		R <sup>2</sup> =0.9215		R <sup>2</sup> =0.9360	
		Predicted value	SD	Predicted value	SD
N1	29.92	32.13	0.30	31.56	0.46
N2	28.28	28.41	0.68	28.44	0.80
N3	32.11	28.33	0.76	28.90	0.58
N4	2.61	1.52	3.64	3.21	1.24
N5	5.12	1.20	0.76	2.25	1.48
N6	19.04	20.56	0.96	20.75	0.25
N7	23.72	18.35	0.72	18.23	0.86

  

No.	Reference value of volatile matter content	Spatial confinement + SNR		Spatial confinement + RSNR	
		R <sup>2</sup> =0.9638		R <sup>2</sup> =0.9815	
		Predicted value	SD	Predicted value	SD
N1	29.92	33.18	0.20	31.91	0.26
N2	28.28	28.34	0.86	26.99	0.83
N3	32.11	33.09	0.51	33.87	0.61
N4	2.61	2.19	0.93	2.45	0.87
N5	5.12	5.02	0.66	5.84	0.63
N6	19.04	18.26	0.58	17.79	0.48
N7	23.72	19.43	0.26	21.50	0.15

**Table S7.** Prediction results of calorific value of coal specimens from test set

No.	Reference value of calorific value	SNR		RSNR	
		R <sup>2</sup> =0.9479		R <sup>2</sup> =0.9562	
		Predicted value	SD	Predicted value	SD
N1	20.84	21.13	0.10	20.93	0.31
N2	23.8	23.28	0.37	23.45	0.43
N3	26.04	25.36	0.36	24.98	0.28
N4	19.12	18.98	0.52	18.99	0.22
N5	20.74	21.53	0.62	21.20	0.58
N6	11.13	10.99	0.51	11.31	0.45
N7	17.16	19.57	0.28	19.31	0.32

  

No.	Reference value of calorific value	Spatial confinement + SNR		Spatial confinement +RSNR	
		R <sup>2</sup> =0.9701		R <sup>2</sup> =0.9897	
		Predicted value	SD	Predicted value	SD
N1	20.84	19.95	0.34	20.31	0.28
N2	23.8	23.42	0.24	23.59	0.25
N3	26.04	25.59	0.37	25.35	0.29
N4	19.12	19.41	0.24	19.29	0.37
N5	20.74	20.01	0.42	20.04	0.24
N6	11.13	12.20	0.35	10.78	0.25
N7	17.16	18.29	0.22	17.15	0.38