Article | Received 12 February 2026; Revised 11 May 2026; Accepted 13 June 2026; Published 2 September 2026
https://doi.org/10.55092/rse20260006

Supplementary data

Formation mechanism and particle size distribution optimization of large fly ash particles

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Supplementary tables

Table S1. Coal quality analysis.

Item	Symbol	Unit	Coal 1	Coal 2	Coal 3	Coal 4	Coal 5	Coal 6
Total Moisture	Mt	%	6.90	3.40	2.90	16.90	4.30	15.90
Air-dried Moisture	Mad	%	2.48	1.19	1.08	9.83	1.41	7.74
Ash Content (As-received)	Aar	%	53.37	33.66	30.99	33.33	23.10	12.12
Volatile Matter (Dry Ash-free)	Vdaf	%	45.43	35.74	35.63	42.02	11.69	34.85
Carbon (As-received)	Car	%	27.65	50.77	53.31	37.13	66.10	59.99
Hydrogen (As-received)	Har	%	2.31	3.32	3.49	2.53	2.64	3.27
Nitrogen (As-received)	Nar	%	0.44	0.76	0.79	0.40	0.93	0.60
Oxygen (As-received)	Oar	%	8.42	5.91	5.21	8.80	0.98	7.55
Total Sulfur (As-received)	St,ar	%	0.91	2.18	3.31	0.91	1.95	0.57
Gross Calorific Value (As-received)	Qgr,v,ar	MJ/kg	10.65	20.20	21.35	14.13	25.02	23.03
Net Calorific Value (As-received)	Qnet,v,ar	MJ/kg	10.02	19.44	20.56	13.22	24.38	21.99
Net Calorific Value (As-received)	Qnet,v,ar	kcal/kg	2394	4644	4912	3158	5824	5253
Hardgrove Grindability Index	HGI	–	94	66	68	73	66	66
Deformation Temperature	DT	℃	> 1500	1500	1470	1250	1360	1150
Softening Temperature	ST	℃	> 1500	> 1500	> 1500	1270	1390	1230
Hemisphere Temperature	HT	℃	> 1500	> 1500	> 1500	1280	1400	1240
Flow Temperature	FT	℃	> 1500	> 1500	> 1500	1290	1410	1250
SiO_2 in Coal Ash	SiO_2	%	52.23	45.33	40.56	59.41	52.95	53.66
Al_2O_3 in Coal Ash	Al_2O_3	%	34.71	33.16	34.02	18.28	25.96	16.35
Fe_2O_3 in Coal Ash	Fe_2O_3	%	6.40	11.23	14.70	11.27	8.64	9.69
CaO in Coal Ash	CaO	%	1.48	4.38	4.33	3.19	6.17	10.86
MgO in Coal Ash	MgO	%	0.36	0.50	0.40	1.39	0.74	0.92
Na_2O in Coal Ash	Na_2O	%	0.80	0.74	0.59	0.64	0.33	0.83
K_2O in Coal Ash	K_2O	%	0.73	0.68	0.54	2.58	0.73	1.40
TiO_2 in Coal Ash	TiO_2	%	1.27	1.17	1.29	1.23	1.26	1.19
SO_3 in Coal Ash	SO_3	%	1.38	2.25	2.60	0.85	2.10	3.85
MnO_2 in Coal Ash	MnO_2	%	0.019	0.058	0.048	0.245	0.075	0.164
P_2O_5 in Coal Ash	P_2O_5	%	0.151	0.214	0.209	0.166	0.596	0.699

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Table S2. Particle size distribution of fly ash. Bold values indicate the proportion of fly ash particles smaller than 45 μm.

Item	Size Range	Unit	Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Sample 6	Sample 5 (90% content)
Mass	> 200 mesh	g	0.1649	0.1433	0.3469	0.0279	0.044	0.1425	0.0928
	150–200 mesh	g	0.1473	0.2256	0.3749	0.0261	0.1066	0.1024	0.0629
	90–150 mesh	g	1.044	1.9769	2.3034	0.2001	1.597	0.8576	0.4067
	45–90 mesh	g	4.4199	5.0789	6.5983	1.8368	7.5959	3.512	3.7912
	< 45 mesh	g	19.2239	17.5753	15.3765	22.9091	15.6565	20.3855	20.6464
Coal Mass	—	g	18	18	18	15	5	15	—
Ash Mass	—	g	5	9	12	1	7	4	—
Proportion	> 200 mesh	%	0.66	0.57	1.39	0.11	0.18	0.57	—
	150–200 mesh	%	0.59	0.9	1.5	0.1	0.43	0.41	—
	90–150 mesh	%	4.18	7.91	9.21	0.8	6.39	3.43	—
	45–90 mesh	%	17.68	20.32	26.39	7.35	30.38	14.05	—
	< 45 μm	**%**	**76.9**	**70.3**	**61.51**	**91.64**	**62.63**	**81.54**	—

Table S3. Sulfur content and sulfur forms of the six coal samples.

No.	Item	Symbol	Unit	1	2	3	4	5	6
1	Total Sulfur (As-received)	St,ar	%	0.91	2.18	3.31	0.91	1.95	0.57
2	Total Sulfur (Air-dried)	St,ad	%	1	1.51	2.28	0.95	2.26	0.67
3	Sulfate Sulfur	Ss,ad	%	0.36	0.06	0.05	0.02	0.03	0.01
4	Pyritic Sulfur	Sp,ad	%	0.3	0.74	0.82	0.63	1.01	0.56
5	Organic Sulfur	So,ad	%	0.34	0.71	1.41	0.3	1.22	0.1

Table S4. Ignition temperatures and ignition grades of the six coal samples.

Coal Sample No.	Ignition Temperature IT	Ignition Grade
1	700	Difficult
2	720	Difficult
3	680	Middle
4	540	Extremely Easy
5	760	Difficult

Extremely Easy: IT ≤ 550 °C; Easy: 550 °C < IT ≤ 600 °C; Middle: 600 °C < IT ≤ 700 °C; Difficult: IT > 700 °C.

Table S5. Results of the full-scale boiler combustion optimization tests.

Item	Unit	Base Case 1	Base Case 2	Base Case 3
Oxygen Concentration	%	3.1	3.6	4.1
Proportion of Fly Ash Particles > 45 μm	%	52.2	50.5	48.7
Primary Air Flow Rate	t/h	High Primary Air	Low Primary Air	-
Proportion of Fly Ash Particles > 45 μm	%	65.8	49.3	-
Overfire Air Damper Opening	%	25%	50%	80%
Proportion of Fly Ash Particles > 45 μm	%	62.2	49.3	47.8
Operating O_2	%	3.1	4.1	3.6
Total coal flow	t/h	148	144	140.4
Calorific value of coal	kcal/kg	3573	3722	3573
Sulfur content of coal	%	0.97	1.41	0.97
Separator speed	rpm	5	20	5
Burn-out damper opening	%	25	25	25
Primary air flow (A/B/C/D mills)	t/h	47/52/46/40	48/52/45/40	48/52/45/40
Proportion of Fly Ash Particles > 45 μm	%	52.2	65.8	50.5