

Supplementary Materials

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1. Calculation of Hg contents

1.1 Parameters and symbols

- 1) W_A – weight content of Hg in sample A (ng/L);
- 2) W_B – weight content of Hg in sample B (ng/L);
- 3) W_C – weight content of Hg in sample C (ng/L);
- 4) L_{sample} – volume of gas sample collected and measured in the real condition (L);
- 5) $L_{standard}$ – volume of gas sample, in the standard condition (L);
- 6) T – temperature measured at the inlet of the pump (°C);
- 7) W_{FA} – weight content of Hg in fly ash sample (ng/g);
- 8) W_{coal} – weight content of Hg in coal (ng/g);
- 9) $L_{gasflow}$ – volume in standard condition of gas flow of the boiler (KNm³/h). The value is 1610;
- 10) m_{coal} – mass of coal consumed in boiler, per hour (t/h). The value is 286.8;
- 11) m_{Hg^0} – total mass of Hg⁰ collected in the sample (ng);
- 12) $m_{Hg^{2+}}$ – total mass of Hg²⁺ collected in the sample (ng);
- 13) m_{Hg^P} – total mass of Hg in the fly ash sample, calculated based on the operation data (ng);
- 14) m_{Hg^T} – total mass of Hg in the flue gas collected (ng);
- 15) c_{NO} – concentration of NO in flue gas (mg/m³);
- 16) c_{NO_2} – concentration of NO₂ in flue gas (mg/m³);

- 17) c_{N_2O} – concentration of N_2O in flue gas (mg/m^3);
- 18) $c_{SO_4^{2-}}$ – concentration of SO_4^{2-} in the washing fluid sample (ppm);
- 19) c_{SO_3} – concentration of SO_3 in flue gas (mg/m^3).

1.2 Calculation formulas

1) $L_{standard} = L_{sample} \times (273 / (273 + T)) \times (\frac{96.4}{101.3}) \times ((21 - 3.6) / 21 \times 1.4)$ (where the local gas pressure is 96.4 kPa in Chongqing China, the concentration of oxygen in flue gas at SCR inlet is 3.6% and that of standard condition is 6%);

$$2) m_{Hg^0} = W_B \times 0.5L + W_C \times 1L;$$

$$3) m_{Hg^{2+}} = W_A + 1L;$$

4) $m_{Hg^P} = \frac{L_{standard}}{L_{gasflow} \times 1,000,000} \times (m_{coal} \times 1,000,000) \times 0.28 \times 0.7 \times W_{FA}$ (where 28% ash content is in coal and fly ash accounts for 70% of total ash);

$$5) m_{Hg^T} = m_{Hg^0} + m_{Hg^{2+}} + m_{Hg^P};$$

$$6) \text{Hg oxidation efficiency: } \eta_{Hg} = \frac{m_{Hg^{2+}}}{m_{Hg^0} + m_{Hg^{2+}} + m_{Hg^P}};$$

$$7) \text{Hg balance} = m_{Hg^T} / \left(\frac{m_{coal} \times 1,000,000 \times W_{coal}}{L_{gasflow}} \times L_{standard} \right);$$

$$8) c_{NOx} = (46 / 30 \times c_{NO} + c_{NO_2} + 46 / 44 \times c_{N_2O});$$

9) $c_{NOx}(standard) = c_{NOx} \times 373 / 273 \times ((21 - 6) / (21 - 3.6))$ (where temperature in the FTIR equipment is 100 °C, the concentration of oxygen in flue gas at SCR inlet is 3.6% and that of standard condition is 6%);

$$10) \text{NO}_x \text{ removal efficiency} = 1 - \frac{c_{NOx}(standard, sampling - port)}{c_{NOx}(standard, inlet)};$$

11) $c_{SO_3} = c_{SO_4^{2-}} / 96 \times 80 \times 0.001 \times 250 / L_{standard}$ (where the volume of washing fluid sample is 250 mL).

2. Coal information

Table S1 Weight content of Hg in coal

Sampling date	W_{coal} (ng/g)
Jan 11, 2024	148.7
Jan 12, 2024	149.9
Jan 14, 2024	163.8
Jan 16, 2024	151.1
Jan 18, 2024	166.9
Jan 20, 2024	128.2
Jan 22, 2024	130.1
Jan 22, 2024	130.1
Feb 27, 2024	121.5
Mar 22, 2024	145.5
Apr 19, 2024	142.8
May 23, 2024	140.6
Jun 19, 2024	169.2
Jul 22, 2024	166.6
Aug 26, 2024	155.4
Sep 25, 2024	158.3
Oct 21, 2024	138.8
Nov 26, 2024	135.2
Dec 19, 2024	140.6

*The samples of coal are collected from the conveyer belt. In each condition, at least 3 samples are collected and measured. The data shown in this Table S1 is the average value.

Table S2 Content of main components in coal (air-dry basis)

Sampling date	C	H	O	N	S	Cl	Br	Water	Ash
Jan 11, 2024	59.48%	3.06%	4.07%	0.71%	2.34%	0.045%	*N.D.	1.54%	28.80%
Jan 12, 2024	60.25%	3.42%	3.53%	0.74%	2.11%	0.045%	N.D.	2.27%	27.68%
Jan 14, 2024	61.11%	3.88%	2.79%	0.70%	2.23%	0.042%	N.D.	2.19%	27.10%
Jan 16, 2024	62.29%	3.75%	2.95%	0.66%	1.95%	0.039%	N.D.	2.89%	25.48%
Jan 18, 2024	58.19%	4.22%	3.72%	0.57%	2.67%	0.051%	N.D.	1.98%	28.60%
Jan 20, 2024	57.94%	4.12%	3.69%	0.55%	2.79%	0.047%	N.D.	2.03%	28.84%
Jan 22, 2024	58.03%	4.44%	3.94%	0.61%	2.70%	0.050%	N.D.	1.88%	28.35%
Jan 22, 2024	58.03%	4.44%	3.94%	0.61%	2.70%	0.050%	N.D.	1.88%	28.35%
Feb 27, 2024	64.36%	4.97%	3.05%	0.41%	1.87%	0.032%	N.D.	1.59%	23.72%
Mar 22, 2024	63.38%	5.02%	2.96%	0.49%	1.94%	0.033%	N.D.	1.69%	24.49%
Apr 19, 2024	60.78%	4.09%	3.66%	0.59%	1.49%	0.052%	N.D.	1.48%	27.86%
May 23, 2024	59.22%	3.91%	3.79%	0.62%	1.46%	0.044%	N.D.	1.38%	29.58%
Jun 19, 2024	59.81%	4.18%	3.70%	0.67%	1.41%	0.049%	N.D.	1.40%	28.79%
Jul 22, 2024	53.39%	5.04%	3.13%	0.48%	2.10%	0.029%	N.D.	2.05%	33.79%
Aug 26, 2024	52.95%	4.88%	3.01%	0.44%	1.89%	0.025%	N.D.	2.31%	34.50%
Sep 25, 2024	53.93%	5.09%	3.15%	0.39%	2.01%	0.022%	N.D.	2.21%	33.20%
Oct 21, 2024	57.19%	3.77%	4.10%	0.69%	2.79%	0.061%	N.D.	1.89%	29.51%
Nov 26, 2024	56.89%	3.70%	4.04%	0.72%	2.89%	0.058%	N.D.	1.72%	29.99%
Dec 19, 2024	56.90%	3.60%	4.24%	0.071%	2.65%	0.059%	N.D.	1.82%	30.66%

*N.D. means “not detected”.

Table S3 CaBr₂ addition amount into the coal

Sampling date	CaBr ₂ addition to the coal (mg/kg)	<i>W</i> _{coal} (ng/g)
Jan 11, 2024	0	148.7
Jan 12, 2024	14.14	149.9
Jan 14, 2024	21.21	163.8
Jan 16, 2024	28.29	151.1
Jan 18, 2024	35.35	166.9
Jan 20, 2024	42.42	128.2
Jan 22, 2024	49.49	130.1
Jan 22, 2024	49.49	130.1
Feb 27, 2024	49.49	121.5
Mar 22, 2024	49.49	145.5
Apr 19, 2024	49.49	142.8
May 23, 2024	49.49	140.6
Jun 19, 2024	49.49	169.2
Jul 22, 2024	49.49	166.6
Aug 26, 2024	49.49	155.4
Sep 25, 2024	49.49	158.3
Oct 21, 2024	49.49	138.8
Nov 26, 2024	49.49	135.2
Dec 19, 2024	49.49	140.6

3. Details of measuring and calculating Hg

Table S4 Detailed data of Hg sampling and measurement

Sampling date	Br in flue gas (ppm)	Sampling ports	Sampling times	m_{Hg^0} (ng)	$m_{Hg^{2+}}$ (ng)	m_{Hg^P} (ng)	L_{sample} (L)	η_{Hg} (%)	$\overline{\eta}_{Hg}$ (%)
Jan 11, 2024	0	IN	1	4805	1048	0.50	500.1	17.91	16.85
			2	6508	1170	159.51	487.9	14.93	
			3	8831	1907	29.82	455.7	17.71	
		MO	1	6333	4844	1.82	498.5	43.33	45.19
			2	5156	4858	266.93	447.4	47.25	
			3	2891	2846	589.18	466.9	44.99	
		UN	1	4581	3949	58.91	488.4	45.98	36.22
			2	3039	1325	61.12	496.1	29.95	
			3	8411	4152	122.53	490.5	32.73	
Jan 12, 2024	40	IN	1	5891	2937	1485.72	447.9	28.48	35.07
			2	5971	604	1084.75	480.8	7.88	
			3	3259	10699	1581.91	477.1	68.85	
		MO	1	1578	26106	0	473.9	94.30	83.33
			2	1486	308097	0	488.1	99.52	
			3	1974	2530	0	497.7	56.17	
		UN	1	1249	1222	0	459.5	49.46	58.13
			2	1648	5722	0	467.9	77.64	
			3	1439	1291	0	499.1	47.29	
Jan 14, 2024	70	IN	1	7495	6900	584.91	459.8	46.06	43.58
			2	5948	12103	1059.99	504.8	63.33	
			3	5409	1698	845.07	503.3	21.35	
		MO	1	1489	51500	0	477.9	97.19	89.16
			2	1495	99519	0	497.0	98.52	
			3	1333	3389	0	485.8	71.77	
		UN	1	1589	2939	0	488.1	64.91	66.63
			2	1348	5446	0	478.6	80.16	
			3	1954	2371	0	469.9	54.82	
Jan 16, 2024	100	IN	1	5537	3372	1102.58	449.4	33.68	47.85
			2	5729	5773	275.31	465.0	49.02	
			3	6568	11435	788.81	495.9	60.85	
		MO	1	1463	5464	0	538.9	78.88	91.08
			2	1909	126212	0	478.2	98.51	
			3	1828	42220	0	474.8	95.85	
		UN	1	1626	6468	0	476.6	79.91	74.07
			2	1580	9088	0	471.9	85.19	
			3	1756	2338	0	494.2	57.11	

(Continued) Table S4 Detailed data of Hg sampling and measurement

Sampling date	Br in flue gas (ppm)	Sampling ports	Sampling times	m_{Hg^0} (ng)	$m_{Hg^{2+}}$ (ng)	m_{Hg^P} (ng)	L_{sample} (L)	η_{Hg} (%)	$\overline{\eta_{Hg}}$ (%)
Jan 18, 2024	130	IN	1	3929	2719	572.49	451.63	37.66	52.20
			2	3850	5026	798.71	488.01	51.95	
			3	4916	12200	1095.69	478.47	66.99	
		MO	1	1376	17709	0	449.96	92.79	90.86
			2	1887	8140	0	529.01	81.18	
			3	1739	123369	0	481.26	98.61	
		UN	1	1690	9668	0	528.34	85.12	78.89
			2	1820	2870	0	487.83	61.19	
			3	1904	17847	0	538.88	90.36	
Jan 20, 2024	160	IN	1	7093	9015	1011.47	486.63	52.66	55.81
			2	7694	17656	683.48	535.41	67.82	
			3	4198	4218	567.99	485.81	46.95	
		MO	1	1666	226553	0	497.42	99.27	93.03
			2	1869	1097543	0	454.33	99.83	
			3	1889	7551	0	456.34	79.99	
		UN	1	1334	18169	0	497.80	93.16	82.72
			2	1777	7148	0	445.89	80.09	
			3	1312	3917	0	449.47	74.91	
Jan 22, 2024	190	IN	1	6669	24065	1093.7	510.06	75.61	57.77
			2	6651	8849	344.43	453.77	55.85	
			3	7631	6400	1261.84	467.58	41.85	
		MO	1	1918	6454	0	444.84	77.09	92.01
			2	1515	164969	0	440.04	99.09	
			3	1538	1023759	0	538.65	99.85	
		UN	1	1048	7225	0	514.33	83.69	84.48
			2	1527	3901	0	442.90	71.87	
			3	1531	70686	0	500.35	97.88	

(Continued) Table S4 Detailed data of Hg sampling and measurement

Sampling date	Br in flue gas (ppm)	Sampling ports	Sampling times	m_{Hg^0} (ng)	$m_{Hg^{2+}}$ (ng)	m_{Hg^P} (ng)	L_{sample} (L)	η_{Hg} (%)	$\overline{\eta}_{Hg}$ (%)
Jan 22, 2024	190	IN	1	6669	24065	1093.7	510.06	75.61	
			2	6651	8849	344.43	453.77	55.85	57.77
			3	7631	6400	1261.84	467.58	41.85	
		MO	1	1918	6454	0	444.84	77.09	
			2	1515	164969	0	440.04	99.09	92.01
			3	1538	1023759	0	538.65	99.85	
		UN	1	1048	7225	0	514.33	83.69	
			2	1527	3901	0	442.90	71.87	84.48
			3	1531	70686	0	500.35	97.88	
Feb 27, 2024	190	IN	1	6718	17709	568.21	539.46	70.85	
			2	7690	8414	1494.59	510.17	47.81	58.79
			3	6304	9893	945.28	462.35	57.71	
		MO	1	1548	3849	0	499.73	71.32	
			2	1929	2141404	0	485.61	99.91	90.04
			3	1330	118490	0	456.88	98.89	
		UN	1	1468	5563	0	455.88	79.12	
			2	1313	2688	0	539.37	67.18	80.99
			3	1758	51035	0	447.22	96.67	
Mar 22, 2024	190	IN	1	6851	4051	1358.82	470.99	33.04	
			2	5237	6425	696.22	473.00	51.99	53.87
			3	5881	22025	854.73	498.98	76.58	
		MO	1	1751	29913	0	441.84	94.47	
			2	1905	4477	0	454.58	70.15	87.87
			3	1738	170341	0	496.56	98.99	
		UN	1	1534	2957	0	491.15	65.84	
			2	1354	4082	0	479.40	75.09	76.59
			3	1479	11774	0	500.09	88.84	
Apr 19, 2024	190	IN	1	3210	4321	341.08	492.93	54.89	
			2	7222	12066	553.92	461.46	60.81	59.85
			3	7545	15303	1118.98	533.19	63.85	
		MO	1	1492	8011	0	458.67	84.30	
			2	1992	4754	0	496.66	70.47	84.44
			3	1681	114250	0	486.14	98.55	
		UN	1	1569	2065	0	513.74	56.83	
			2	1885	2696	0	469.54	58.85	71.11
			3	1795	74588	0	503.81	97.65	

(Continued) Table S4 Detailed data of Hg sampling and measurement

Sampling date	Br in flue gas (ppm)	Sampling ports	Sampling times	m_{Hg^0} (ng)	$m_{Hg^{2+}}$ (ng)	m_{Hg^P} (ng)	L_{sample} (L)	η_{Hg} (%)	$\overline{\eta}_{Hg}$ (%)
May 23, 2024	190	IN	1	7284	15645	1099.54	445.56	65.11	65.19
			2	5968	21563	626.39	475.77	76.58	
			3	6446	8854	1132.92	512.10	53.88	
		MO	1	1864	9251	0	446.67	83.23	80.09
			2	1911	3143	0	491.17	62.19	
			3	1415	26061	0	496.58	94.85	
		UN	1	1774	6065	0	510.68	77.37	69.97
			2	1942	3888	0	500.65	66.69	
			3	1878	3621	0	455.01	65.85	
Jun 19, 2024	190	IN	1	6008	7325	1311.48	536.20	50.02	53.37
			2	3127	4167	875.40	539.48	51.01	
			3	7818	11886	414.31	470.28	59.08	
		MO	1	1788	3865	0	523.36	68.37	79.59
			2	1555	6582	0	524.59	80.89	
			3	1436	13824	0	522.27	90.59	
		UN	1	1324	6365	0	539.21	82.78	64.18
			2	1873	2808	0	464.60	59.99	
			3	1719	1703	0	468.27	49.77	
Jul 22, 2024	190	IN	1	6852	8383	787.62	491.20	52.32	54.93
			2	3010	4611	905.11	467.50	54.08	
			3	6518	10834	1202.31	520.33	58.39	
		MO	1	1811	2564	0	461.69	58.61	75.55
			2	1465	3601	0	507.58	71.08	
			3	1320	42101	0	487.48	96.96	
		UN	1	1870	950	0	441.16	33.68	59.82
			2	1937	2772	0	520.49	58.87	
			3	1469	9753	0	520.64	86.91	
Aug 26, 2024	190	IN	1	6751	8248	954.22	536.91	51.70	57.78
			2	5973	8015	458.46	454.13	55.48	
			3	6858	14171	390.42	444.89	66.16	
		MO	1	1673	3807	0	535.24	69.47	75.08
			2	1305	2879	0	469.17	68.81	
			3	1354	9029	0	472.06	86.96	
		UN	1	1901	1076	0	484.84	36.14	60.07
			2	1503	2461	0	451.22	62.08	
			3	1845	8399	0	521.73	81.99	

(Continued) Table S4 Detailed data of Hg sampling and measurement

Sampling date	Br in flue gas (ppm)	Sampling ports	Sampling times	m_{Hg^0} (ng)	$m_{Hg^{2+}}$ (ng)	m_{Hg^P} (ng)	L_{sample} (L)	η_{Hg} (%)	$\overline{\eta}_{Hg}$ (%)
Sep 25, 2024	190	IN	1	4472	4639	426.29	502.78	48.64	60.77
			2	7375	10989	204.94	487.71	59.18	
			3	5636	20195	1279.95	499.09	74.49	
		MO	1	1522	1990	0	456.95	56.66	71.11
			2	1435	2252	0	487.00	61.08	
			3	1674	36285	0	522.62	95.59	
		UN	1	1549	1259	0	468.21	45.55	53.49
			2	1386	1159	0	538.01	44.83	
			3	1761	4127	0	511.13	70.09	
Oct 21, 2024	190	IN	1	3985	18194	1424.97	530.55	77.08	53.33
			2	5284	5003	580.19	514.37	46.04	
			3	7986	5165	857.81	531.53	36.87	
		MO	1	1720	6428	0	532.46	78.89	65.18
			2	1911	2541	0	535.34	57.08	
			3	1489	2194	0	488.89	59.57	
		UN	1	1833	3028	0	507.82	62.29	50.55
			2	1383	982	0	518.31	41.53	
			3	1585	1453	0	470.98	47.83	
Nov 26, 2024	190	IN	1	6926	7273	294.70	523.39	50.18	57.90
			2	4039	5503	1435.39	454.79	50.13	
			3	7873	23527	657.57	474.54	73.39	
		MO	1	1956	7033	0	443.62	78.24	66.08
			2	1541	2837	0	534.36	64.80	
			3	1687	2079	0	475.13	55.20	
		UN	1	1763	960	0	514.02	35.26	45.58
			2	1616	2798	0	459.15	63.39	
			3	1599	984	0	494.38	38.09	
Dec 19, 2024	190	IN	1	3936	8996	983.03	444.95	64.65	60.92
			2	3035	3987	216.84	467.00	55.08	
			3	4382	8501	604.39	464.64	63.03	
		MO	1	1630	2558	0	471.97	61.08	62.22
			2	1661	3531	0	515.28	68.01	
			3	1607	2180	0	491.96	57.57	
		UN	1	1993	2443	0	519.80	55.07	43.08
			2	1327	714	0	518.09	34.99	
			3	1650	1034	0	491.46	39.18	

4. Details of measuring NO_x

Table S5 Detailed data of NO_x sampling and measurement

Sampling date	Br in flue gas (ppm)	Sampling times	c_{NO_x} (<i>standard</i>) at different sampling ports (mg/m ³)			NO _x removal efficiency at different sampling ports (%)			
			IN	MO	UN	MO	\overline{MO}	UN	\overline{UN}
Jan 11, 2024	0	1	371.87	16.99	10.04	95.43	96.22	97.30	95.79
		2	326.39	5.52	14.88	98.31		95.44	
		3	338.52	17.20	18.80	94.92		94.63	
Jan 12, 2024	40	1	340.00	8.47	15.57	97.51	95.98	95.42	95.72
		2	405.58	23.28	10.18	94.26		97.49	
		3	435.88	16.69	25.06	96.17		94.25	
Jan 14, 2024	70	1	384.32	27.52	16.14	92.84	95.51	95.80	95.03
		2	393.86	15.44	20.28	96.08		94.85	
		3	412.25	9.85	22.92	97.61		94.44	
Jan 16, 2024	100	1	385.06	32.19	27.11	91.64	93.65	92.96	94.68
		2	401.20	23.19	19.82	94.22		95.06	
		3	311.98	15.32	12.42	95.09		96.02	
Jan 18, 2024	130	1	338.19	28.27	23.81	91.64	93.65	92.96	94.68
		2	364.64	21.08	18.01	94.22		95.06	
		3	428.16	21.02	17.04	95.09		96.02	
Jan 20, 2024	160	1	338.21	29.39	31.35	91.31	92.18	90.73	93.39
		2	446.34	34.86	26.07	92.19		94.16	
		3	362.68	25.24	17.12	93.04		95.28	
Jan 22, 2024	190	1	290.58	16.88	16.68	94.19	91.71	94.26	92.60
		2	292.75	22.95	19.06	92.16		93.49	
		3	390.81	43.85	38.89	88.78		90.05	

***Special attention:** although it seems that the concentration of NO_x in the sampling ports of MO or UN at some sampling dates might exceed the limit of 35.00 mg/m³ as required by the ultra-low emission standard in China, there are in fact other SCR reactors after the sampling ports to further lower the concentration of NO_x and make it qualified before its emission to subsequent treatment processes.

(Continued) Table S5 Detailed data of NO_x sampling and measurement

Sampling date	Br in flue gas (ppm)	Sampling times	c_{NO_x} (standard) at different sampling ports (mg/m ³)			NO _x removal efficiency at different sampling ports (%)			
			IN	MO	UN	MO	\overline{MO}	UN	\overline{UN}
Jan 22, 2024	190	1	290.58	16.88	16.68	94.19	91.71	94.26	92.60
		2	292.75	22.95	19.06	92.16		93.49	
		3	390.81	43.85	38.89	88.78		90.05	
Feb 27, 2024	190	1	335.92	30.84	41.18	90.82	89.03	87.74	90.68
		2	421.63	53.63	37.74	87.28		91.05	
		3	284.46	31.32	19.20	88.99		93.25	
Mar 22, 2024	190	1	380.49	61.14	66.66	83.93	85.66	82.48	84.51
		2	326.57	45.16	48.92	86.17		85.02	
		3	414.98	54.45	57.97	86.88		86.03	
Apr 19, 2024	190	1	328.48	57.09	60.93	82.62	83.33	81.45	81.52
		2	355.54	63.25	53.62	82.21		84.92	
		3	316.73	47.00	69.08	85.16		78.19	
May 23, 2024	190	1	375.52	58.43	92.30	84.44	80.88	75.42	77.77
		2	359.50	68.27	75.10	81.01		79.11	
		3	337.37	76.95	71.59	77.19		78.78	
Jun 19, 2024	190	1	350.81	87.39	84.26	75.09	78.13	75.98	74.94
		2	288.23	56.98	75.55	80.23		73.79	
		3	320.22	67.02	79.89	79.07		75.05	
Jul 22, 2024	190	1	327.92	89.13	93.72	72.82	72.92	71.42	68.99
		2	373.96	105.19	125.61	71.87		66.41	
		3	303.00	78.57	93.51	74.07		69.14	
Aug 26, 2024	190	1	286.03	90.39	96.71	68.40	70.87	66.19	67.51
		2	372.82	110.62	126.16	70.33		66.16	
		3	342.71	89.52	102.20	73.88		70.18	
Sep 25, 2024	190	1	363.55	107.36	139.71	70.47	68.17	61.57	63.79
		2	323.88	104.58	116.47	67.71		64.04	
		3	443.19	149.22	151.75	66.33		65.76	
Oct 21, 2024	190	1	321.41	95.01	129.75	70.44	65.88	59.63	58.96
		2	372.73	140.22	163.70	62.38		56.08	
		3	427.74	150.48	166.09	64.82		61.17	
Nov 26, 2024	190	1	321.33	109.09	149.48	66.05	64.44	53.48	53.13
		2	281.01	106.25	151.97	62.19		45.92	
		3	396.01	138.53	182.53	65.08		53.99	
Dec 19, 2024	190	1	315.85	116.36	185.34	63.16	61.10	41.32	43.92
		2	372.37	145.63	212.06	60.89		43.05	
		3	402.46	164.00	211.73	59.25		47.39	

Supplementary explanation of economic feasibility for large-scale application of Ce-modified SCR catalysts in coal-fired power plants

In Chinese coal-fired power plants, expense on pollutant emission is charged only by the first three most emitted pollutants. For now, the first two most emitted pollutants are always NO_x & SO_x and the third one is Hg or particulate matter (PM). The expense on Hg is around 1 US dollar per pollutional equivalent and that on PM is about 0.1 US dollar per pollutional equivalent. Therefore, it would be much more economical if the third most emitted pollutant is shifted from Hg to PM.

Based on the preparation method of Ce-modified SCR catalysts and Hg⁰ oxidation efficiency in this study, the average cost for Ce modification is about 0.3-0.7 US dollar per pollutional equivalent. Thus, expense on PM emission plus cost of Ce modification is about 0.4-0.8 US dollar, which is still lower than expense on Hg emission.

With above direct calculation, it is easily concluded that large-scale application of Ce-modified SCR is feasible in coal-fired power plants when all preparation and expense on pollution emission are taken into consideration.

5. Details of measuring SO₃

Table S6 Detailed data of SO₃ measurement

Sampling date	Br in flue gas (ppm)	Sampling times	Sampling port-IN			Sampling port-MO			Sampling port-UN					
			$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)
Jan 11, 2024	0	1	461.20	0.11	0.05	5673.66	403.82	5.95	3.07	6083.83	467.67	5.09	2.27	5368.76
		2	438.55	0.15	0.07	5460.35	549.83	6.78	2.57	6157.98	480.32	6.29	2.73	5445.93
		3	462.80	0.13	0.06	5755.00	521.71	7.14	2.85	4612.13	536.60	6.21	2.41	5977.09
		Average	454.18	0.13	0.06	5629.67	491.79	6.62	2.83	5617.98	494.80	5.86	2.47	5597.26
Jan 12, 2024	40	1	420.93	0.51	0.25	5650.43	485.17	4.12	1.77	5757.92	497.14	2.65	1.11	5724.81
		2	546.86	0.73	0.28	5059.79	406.72	3.61	1.85	5564.70	434.49	2.13	1.02	6203.17
		3	410.48	0.55	0.28	6356.06	483.49	3.37	1.45	5508.70	436.98	2.64	1.26	4929.62
		Average	459.42	0.60	0.27	5688.76	458.46	3.70	1.69	5610.44	456.20	2.47	1.13	5619.20
Jan 14, 2024	70	1	450.62	0.45	0.21	5562.50	494.08	4.48	1.89	5324.30	408.17	3.15	1.61	5965.63
		2	459.60	0.46	0.21	5354.03	542.15	5.28	2.03	6118.66	443.58	3.70	1.74	5537.84
		3	455.96	0.39	0.18	6427.04	506.05	5.71	2.35	5724.84	416.64	3.62	1.81	5585.67
		Average	455.39	0.43	0.20	5781.19	514.09	5.16	2.09	5722.60	422.80	3.49	1.72	5696.38
Jan 16, 2024	100	1	520.82	0.05	0.02	5486.38	524.06	4.73	1.88	5420.94	401.48	4.30	2.23	4854.52
		2	503.42	0.05	0.02	5787.12	535.36	4.57	1.78	5198.39	412.84	4.66	2.35	5024.52
		3	410.98	0.04	0.03	4984.31	441.83	3.82	1.80	5616.34	541.39	5.48	2.11	6190.97
		Average	478.41	0.05	0.02	5419.27	500.42	4.37	1.82	5411.89	451.90	4.81	2.23	5356.67

(Continued) Table S6 Detailed data of SO₃ measurement

Sampling date	Br in flue gas (ppm)	Sampling times	Sampling port-IN				Sampling port-MO				Sampling port-UN			
			$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)
Jan 18, 2024	130	1	542.92	0.26	0.10	5121.99	451.81	4.62	2.13	6010.95	462.39	3.84	1.73	4998.08
		2	517.89	0.25	0.10	6178.13	499.09	5.20	2.17	5525.14	537.16	4.43	1.72	6142.99
		3	507.07	0.32	0.13	5584.54	466.13	5.88	2.63	5245.22	540.66	4.83	1.86	5395.59
		Average	522.63	0.28	0.11	5628.22	472.34	5.23	2.31	5593.78	513.40	4.38	1.77	5512.22
Jan 20, 2024	160	1	539.08	2.07	0.80	5303.65	476.29	4.07	1.78	5283.14	528.09	5.68	2.24	5716.66
		2	503.95	2.18	0.90	5830.03	535.88	4.89	1.90	5977.52	450.66	4.50	2.08	5843.10
		3	423.80	1.73	0.85	6012.88	519.75	5.56	2.23	5737.82	432.08	5.29	2.55	5296.85
		Average	488.94	1.99	0.85	5715.52	510.64	4.84	1.97	5666.16	470.34	5.16	2.29	5618.87
Jan 22, 2024	190	1	485.64	0.91	0.39	5402.29	544.24	7.45	2.85	5330.77	471.47	7.45	3.29	5143.05
		2	450.45	0.93	0.43	6447.14	409.37	6.64	3.38	5303.00	509.48	7.26	2.97	5316.26
		3	408.54	0.86	0.44	5618.73	457.23	6.61	3.01	6524.04	405.37	6.73	3.46	6590.23
		Average	448.21	0.90	0.42	5822.72	470.28	6.90	3.08	5719.27	462.11	7.15	3.24	5683.18

(Continued) Table S6 Detailed data of SO₃ measurement

Sampling date	Br in flue gas (ppm)	Sampling times	Sampling port-IN			Sampling port-MO			Sampling port-UN					
			$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)
Jan 22, 2024	190	1	485.64	0.91	0.39	5402.29	544.24	7.45	2.85	5330.77	471.47	7.45	3.29	5143.05
		2	450.45	0.93	0.43	6447.14	409.37	6.64	3.38	5303.00	509.48	7.26	2.97	5316.26
		3	408.54	0.86	0.44	5618.73	457.23	6.61	3.01	6524.04	405.37	6.73	3.46	6590.23
		Average	448.21	0.90	0.42	5822.72	470.28	6.90	3.08	5719.27	462.11	7.15	3.24	5683.18
Feb 27, 2024	190	1	428.49	0.16	0.08	5721.02	466.49	8.84	3.95	5874.74	461.23	6.53	2.95	5740.92
		2	468.63	0.22	0.10	5427.99	482.50	7.78	3.36	5311.78	420.64	5.90	2.92	5041.13
		3	470.13	0.20	0.09	5971.99	403.47	7.17	3.70	5682.12	482.16	7.31	3.16	6007.12
		Average	455.75	0.19	0.09	5707.00	450.82	7.93	3.67	5622.88	454.68	6.58	3.01	5596.39
Mar 22, 2024	190	1	540.53	0.78	0.30	5410.37	483.29	8.49	3.66	5894.63	408.69	9.04	4.61	5229.74
		2	467.14	0.76	0.34	6171.74	454.85	9.28	4.25	5173.40	459.51	10.87	4.93	6017.34
		3	457.57	0.64	0.29	5907.86	527.00	9.51	3.76	6090.32	493.88	10.53	4.44	5690.17
		Average	488.41	0.73	0.31	5829.99	488.38	9.09	3.89	5719.45	454.03	10.15	4.66	5645.75
Apr 19, 2024	190	1	408.91	0.10	0.05	5950.45	456.70	9.32	4.25	4844.47	451.06	9.66	4.46	5361.65
		2	491.50	0.12	0.05	5659.12	408.13	10.23	5.22	5261.78	438.08	11.57	5.50	5624.45
		3	472.70	0.11	0.07	4723.78	546.56	11.91	4.54	5851.41	400.30	9.17	4.77	4898.66
		Average	457.70	0.11	0.05	5444.45	470.46	10.49	4.67	5319.22	429.81	10.13	4.91	5294.92

(Continued) Table S6 Detailed data of SO₃ measurement

Sampling date	Br in flue gas (ppm)	Sampling times	Sampling port-IN				Sampling port-MO				Sampling port-UN			
			$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)
May 23, 2024	190	1	444.45	0.28	0.13	5926.12	474.40	14.78	6.49	6112.43	453.51	14.35	6.59	5293.84
		2	482.59	0.28	0.12	5220.22	489.31	15.31	6.52	5097.07	487.16	15.88	6.79	5112.53
		3	484.16	0.26	0.11	5740.24	506.06	18.10	7.45	5538.09	405.97	14.21	7.29	5867.91
		Average	470.40	0.27	0.12	5628.86	489.92	16.06	6.82	5582.53	448.88	14.81	6.89	5424.76
Jun 19, 2024	190	1	537.70	1.06	0.41	5940.71	511.76	18.52	7.54	5699.55	500.03	24.36	10.15	5318.06
		2	469.56	0.95	0.42	5879.53	503.55	20.59	8.52	5846.82	422.20	21.54	10.63	5542.63
		3	405.89	0.66	0.34	5275.05	545.85	21.67	8.27	5461.47	525.35	21.51	8.53	5883.09
		Average	471.05	0.89	0.39	5698.53	520.39	8.11	8.11	5669.28	482.53	22.47	9.77	5581.26
Jul 22, 2024	190	1	503.77	0.07	0.03	5302.54	433.77	24.78	11.90	5033.11	443.85	29.95	14.06	5342.27
		2	464.56	0.07	0.04	5498.98	528.69	31.75	12.51	5463.10	457.28	35.05	15.97	4894.14
		3	536.63	0.08	0.03	6001.12	495.07	24.40	10.27	6159.67	476.11	36.13	15.81	6226.54
		Average	501.65	0.07	0.03	5600.88	485.84	26.98	11.56	5551.96	459.08	33.71	15.28	5487.65
Aug 26, 2024	190	1	546.30	0.71	0.27	5939.31	493.56	34.80	14.69	5971.81	474.26	48.35	21.24	5444.87
		2	487.38	0.58	0.25	5909.50	462.18	36.58	16.49	6325.34	549.06	66.76	25.33	5207.90
		3	405.89	0.45	0.23	5813.57	474.72	40.17	17.63	5040.51	506.59	52.43	21.56	6394.94
		Average	479.86	0.58	0.25	5887.46	476.82	37.18	16.27	5779.22	509.97	55.85	22.71	5682.57

(Continued) Table S6 Detailed data of SO₃ measurement

Sampling date	Br in flue gas (ppm)	Sampling times	Sampling port-IN				Sampling port-MO				Sampling port-UN			
			$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)	$L_{standard}$ (L)	$c_{SO_4^{2-}}$ (ppm)	c_{SO_3} (mg/m ³)	c_{SO_2} (mg/m ³)
Sep 25, 2024	190	1	405.02	0.37	0.19	5671.01	422.66	43.64	21.51	6492.08	469.30	83.82	37.21	5884.12
		2	473.85	0.45	0.20	5871.36	425.79	37.16	18.18	5247.94	501.83	85.90	35.66	5560.78
		3	548.23	0.47	0.18	6755.44	457.14	41.67	18.99	6013.14	539.01	80.41	31.08	6010.51
		Average	475.70	0.43	0.19	6099.27	435.20	40.82	19.56	5917.72	503.38	83.38	34.65	5818.47
Oct 21, 2024	190	1	511.52	0.22	0.09	5068.31	532.71	63.26	24.74	5499.25	430.94	89.61	43.32	5416.99
		2	479.01	0.18	0.08	4899.72	531.66	69.36	27.18	5478.53	515.03	125.29	50.68	5487.20
		3	543.87	0.26	0.10	6707.14	459.53	54.35	24.64	5487.33	504.62	115.88	47.84	5054.82
		Average	511.47	0.22	0.09	5558.39	507.97	62.32	25.52	5488.37	483.53	110.26	47.28	5319.67
Nov 26, 2024	190	1	424.88	0.37	0.18	5884.14	454.80	79.72	36.52	5732.27	549.35	171.03	64.86	5352.29
		2	547.76	0.45	0.17	6567.50	542.31	92.83	35.66	6120.20	423.74	142.54	70.08	5326.74
		3	466.21	0.36	0.16	5936.37	472.44	63.07	27.81	6232.97	498.89	145.19	60.63	6780.91
		Average	479.62	0.39	0.17	6129.67	489.85	78.54	33.33	6028.48	490.66	152.92	65.19	5819.98
Dec 19, 2024	190	1	542.65	0.23	0.10	6764.05	465.70	97.57	43.65	6166.36	519.11	250.54	100.55	6072.51
		2	422.60	0.18	0.09	6178.71	439.35	91.84	43.55	5776.09	495.73	228.10	95.86	6570.63
		3	402.97	0.17	0.09	5580.05	535.28	97.99	38.14	6446.86	534.66	244.99	95.46	5324.34
		Average	456.07	0.19	0.09	6174.27	480.11	95.80	41.78	6129.77	516.50	241.21	97.29	5989.16

6. The on-site photographs for catalysts and sampling



Fig. S1 Modified catalyst modules and sampling ports