

Desulfurization Behavior of Cerium-Iron Mixed Metal Oxides

Sorbent in Hot Coal Gas

Bo Guo^{1,2}, Liping Chang^{1*}, Kechang Xie¹

1. Key laboratory of Coal Science and Technology, Taiyuan University of Technology, Ministry of

Education and Shanxi Province, Taiyuan, Shanxi, 030024, P.R. China

2. College of Environmental Science and Engineering, Taiyuan University of Technology, Taiyuan,

Shanxi, 030024, P.R. China

* Corresponding author: lpchang@tyut.edu.cn, Tel./Fax: +86-351-6010482 (L. P. Chang)

Table S1. Compositions of red mud (wt %)

Sample	Fe ₂ O ₃ %	CaO %	MgO %	Al ₂ O ₃ %	SiO ₂ %	SiO ₂ /Al ₂ O ₃
Red mud	78.64	9.52	2.01	4.14	4.57	1.12

Table S2. Energy positions in XPS Ce 3d5/2 and Ce 3d3/2 spectra of C2F3B850 sorbent at different conditions

C2F3B850	Ce ⁴⁺						Ce ³⁺			
	V ₀	V ₁	V ₂	V ₀ '	V ₁ '	V ₂ '	U ₀	U ₁	U ₀ '	U ₁ '
fresh sorbent	882.1	888.3	897.7	900.8	907.2	916.1	885.0	880.6	903.8	899.2
1st- sul	882.3	888.6	897.9	901.1	907.3	916.4	885.0	880.7	904.1	899.6
8th-sul	882.5	889.1	898.0	901.4	907.4	916.7	885.0	881.0	904.1	899.6
8th- reg	882.3	888.6	897.8	900.8	907.5	916.3	885.0	880.5	904.1	898.9

Table S3. Energy positions in XPS Fe 2p3/2, the relative contents of Fe, Ce and the ratio of Fe to Ce of sorbent C2F3B850 at different conditions

C2F3B850	Fe 2p3/2	at% [Fe]	at% [Ce]	Fe / Ce
Fresh sorbent	710.45	0.99	3.63	0.273
1st- sul	710.3	1.33	2.97	0.448
8th- sul	710.2	1.67	1.44	1.16
8 th - reg	710.4	1.07	3.35	0.319

Table S4. BET surface area (S_{BET}), pore specific volume (V) and pore diameter distribution of sorbent C2F3B850 at different conditions

Sorbent	S_{BET} (m ² /g)	V (cm ³ /g)	Pore diameter distribution (%)			
			<20 Å	20-90 Å	90-200 Å	200-1000 Å
Fresh	10.69	0.053	1.08	13.67	21.11	64.14
1 st -sul	9.59	0.033	1.19	10.63	25.61	62.57
8 th -sul	6.77	0.030	0.71	13.77	22.25	63.27
8 th -reg	9.95	0.049	0.14	21.59	29.38	48.89