

Supplementary materials:

Determination of chemical speciation of arsenic and selenium in high-As coal combustion ash by X-ray photoelectron spectroscopy: Examples from a Kentucky stoker ash

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Table S1. Chemical analyses of whole-sample and sized fly ash samples. Moisture on as-determined basis; ash, C, H, N, S, and O as percent on dry basis (O by difference); major oxides as % of 750°C ash; Hg and Se on whole-ash basis; minor and trace elements on ppm ( $\mu\text{g/g}$ ) basis of 750°C ash; and rare earth elements on ppm ( $\mu\text{g/g}$ ) basis of 500°C ash. REE = total rare earth elements; REY = REE+Y; REYSc = REE+Y+Sc; LREE = sum of La through Sm; HREE = sum of Eu through Lu; and LREE/HREE is the light to heavy REE ratio.

Sample number	wt. %	Mois.	Ash	C	H	N	S	O	SiO <sub>2</sub>	TiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	Fe <sub>2</sub> O <sub>3</sub>	MgO	CaO	MnO	Na <sub>2</sub> O	K <sub>2</sub> O	P <sub>2</sub> O <sub>5</sub>
93259 whole ash		2.92	73.73	17.66	0.58	0.32	1.42	6.29	39.50	1.31	20.71	31.52	0.56	1.35	0.17	0.51	1.32	3.04
93260 whole ash		3.43	74.75	17.61	0.76	0.30	1.50	5.08	39.66	1.33	20.26	29.87	0.54	1.32	0.19	0.64	1.36	4.85
93261 whole ash		4.22	61.28	25.42	0.78	0.39	2.13	10.00	52.25	2.26	26.13	11.81	0.67	2.03	0.04	1.03	2.18	1.59
93259 >60 mesh	10.8	1.94	89.12	4.07	0.61	0.10	1.18	4.92	3.24	0.08	2.12	89.12	0.13	0.11	0.54	0.25	0.21	4.17
93259 60x100 mesh	11.1	2.49	77.42	14.25	0.69	0.33	1.09	6.22	15.72	0.37	10.43	65.52	0.29	0.28	0.32	0.25	0.57	6.25
93259 100x200 mesh	19.9	2.56	75.57	18.57	0.67	0.44	0.88	3.87	31.30	0.90	19.23	41.84	0.47	0.74	0.16	0.29	0.92	4.16
93259 200x325 mesh	18.8	2.10	78.96	15.07	0.53	0.30	0.64	4.50	44.84	1.66	24.39	23.25	0.56	1.49	0.07	0.27	1.28	2.20
93259 325x500 mesh	13.4	1.84	82.68	12.87	0.47	0.24	0.51	3.23	48.91	1.99	25.48	18.02	0.59	1.86	0.05	0.27	1.40	1.43
93259 <500 mesh	26.0	3.71	66.48	23.16	0.77	0.32	0.85	8.42	51.23	2.29	24.88	15.99	0.50	1.12	0.03	0.22	1.65	2.08

	Li	Be	V	Cr	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Rb	Sr	Zr	Nb	Hg
93259 whole ash	101	20	192	277	121	304	532	262	111	163	4876	256	38	523	155	20	0.15
93260 whole ash	99	19	185	285	125	320	685	321	143	239	8450	230	38	479	139	18	0.39
93261 whole ash	135	26	248	200	177	298	556	404	204	203	1378	200	54	652	218	26	0.30
93259 >60 mesh	20	3	38	508	45	289	671	166	59	165	8022	222	7	47	13	3	0.06
93259 60x100 mesh	45	10	95	319	63	246	550	184	80	194	9379	305	22	257	63	9	0.16
93259 100x200 mesh	66	22	205	247	95	249	421	179	91	169	5768	321	38	490	146	20	0.20
93259 200x325 mesh	78	30	283	206	115	254	324	141	88	104	2856	288	46	782	230	29	0.21
93259 325x500 mesh	84	37	350	227	144	304	329	126	92	89	1663	225	50	996	307	36	0.23
93259 <500 mesh	57	25	264	219	99	215	722	166	194	171	2033	260	46	502	255	29	0.72

	Mo	Ag	Cd	In	Sn	Sb	Cs	Ba	Hf	Ta	W	Tl	Pb	Bi	Th	U										
93259 whole ash	52	1.56	1.3 5	0.54	53	29	3.2 4	510	4.3	7	13.9	13.7	266	3.8	17. 1	12. 2										
93260 whole ash	65	2.02	1.5 9	0.63	38	40	3.6 9	459	3.8	2	15.7	16.6	376	5.2	15. 0	12. 2										
93261 whole ash	47	2.41	2.2 8	0.84	28	40	4.5 8	598	6.1	6	22.6	18.4	503	7.6	18. 0	14. 6										
93259 >60 mesh	94	0.95	0.7 9	0.39	52	30	0.7 1	42	0.4	6	9.9	10.8	171	2.3	1.3	2.5										
93259 60x100 mesh	68	1.13	1.0 5	0.44	48	34	1.9 9	244	1.9	6	10.5	13.8	204	2.8	7.4	6.1										
93259 100x200 mesh	45	1.16	1.0 8	0.41	39	30	3.1 3	532	4.3	1	13.2	13.1	191	2.3	4	9.9										
93259 200x325 mesh	28	1.13	0.9 4	0.42	64	20	3.8 0	784	6.8	8	15.4	8.8	137	1.5	22. 0	12. 9										
93259 325x500 mesh	26	1.38	0.9 2	0.35	46	17	3.8 4	105	8.7	3	15.8	7.4	136	1.2	26. 4	15. 1										
93259 <500 mesh	50	2.85	1.3 5	1.05	97	38	3.7 3	632	7.1	3	22.2	17.1	519	8.5	22. 9	17. 5										
	Sc	Y	La	Ce	Pr	Nd	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	RE E	RE Y	REYS c	LRE E	HRE E	LREE/HRE E				
93259 whole ash	28	90	55	125	14	59	13. 4	3.1	15.6	2.4	14.8	3.0	8.8	1.1 8	7.5	1.0 9	324	414	442	267	57	4.65				
93260 whole ash	25	78	50	112	13	52	11. 5	2.6	13.4	2.0	12.4	2.5	7.2	0.9 7	6.3	0.9 1	286	364	389	237	48	4.91				
93261 whole ash	34	111	72	165	18	75	16. 6	3.7	19.3	2.9	18.0	3.6	3	10. 8	8.9	1.2 8	416	527	561	346	70	4.98				
93259 >60 mesh	3	7	5	10	1	5	0.0 1.1	0.2	1.3	0.2	1.2	0.2	0.8	0.0 9	0.7	0.0 9	27	34	37	22	5	4.59				
93259 60x100 mesh	12	34	24	52	6	26	5.6 13.	1.2	6.5	1.0	6.0	1.3	3.6	0	3.2	7	137	171	183	113	24	4.78				
93259 100x200 mesh	28	87	54	122	14	58	3 20.	3.0	15.6	2.4	14.3	2.9	8.6	1.1 7	7.5	1.0 7	318	405	433	262	56	4.63				
93259 200x325 mesh	43	135	83	195	22	89	5 25.	4.6	23.6	3.6	22.2	4.5	0	13. 6	11. 0	1.6 2	495	631	673	409	86	4.76				
93259 325x500 mesh	53	172	102	241	26	9	10 25.	5.6	29.1	4.5	27.4	5.6	0	16. 0	2.1 5	2.0 0	608	781	834	503	106	4.75				
93259 <500 mesh	39	112	75	172	19	78	17. 4	3.8	19.6	3.0	18.4	3.8	8	10. 0	1.5 9.4	1.3 7	433	545	583	361	72	5.05				

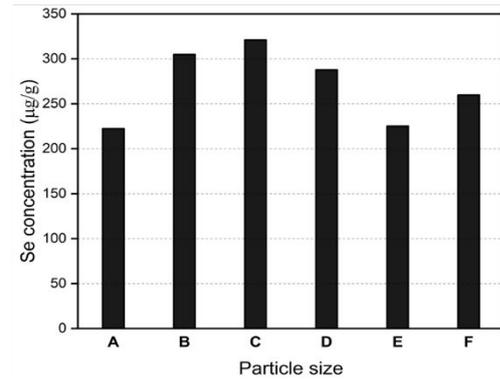
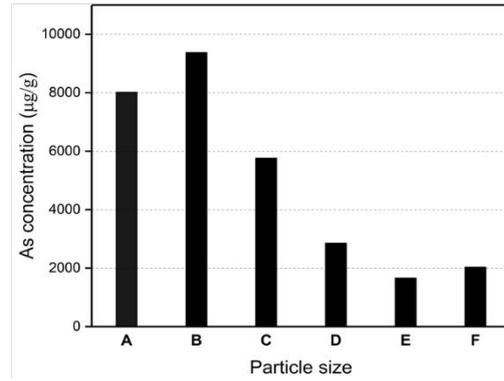
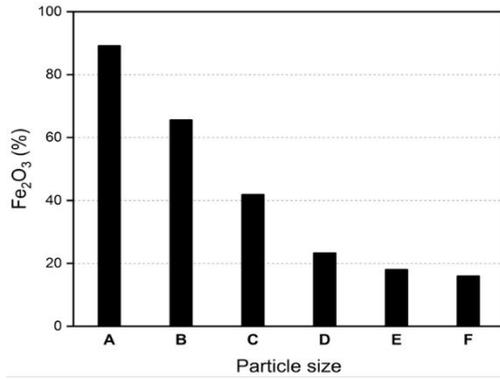


Figure S1. The contents of Fe oxides, As, and Se as a function of particle size in fly ash 93259. A: + 60 mesh; B: 60 × 100 mesh; C: 100 × 200 mesh; D: 200 × 325 mesh; E: 325 × 325 mesh; F: minus 500 mesh.