

SUPPLEMENTARY MATERIAL

Compounds Manufactured in Combustion

Except for molybdenum, any compounds of the 17 listed metals in Table 1 (main text) that are manufactured in amounts totaling more than 25,000 lb/yr are reportable to the Toxics Release Inventory (TRI). In addition, specific forms of aluminum, molybdenum and vanadium also are listed. These are the fibrous (man-made) form of aluminum oxide, aluminum dust or fume, vanadium dust or fume, and molybdenum trioxide. Since aluminum and vanadium are converted during combustion to natural oxides rather than elemental metal, these two substances are not reportable for power plants. Though chemical forms of molybdenum in power plant wastes are not routinely measured, experience in the molybdenum industry indicates that MoO_3 is the principal compound formed at typical combustion temperatures in an oxidizing atmosphere (25). Although other compounds involving Mo in coal combustion cannot be ruled out, a conservative assumption is that all Mo converts to molybdenum trioxide, and would therefore be reportable if the threshold is exceeded.

As noted in the text, EPA has stated that in the absence of better site-specific information, other metals that take part in the combustion process may be assumed to convert completely into the lowest weight metal oxide per unit of the metal possible for each metal. Table S1 lists the lowest weight oxides per unit of metal for TRI metals (26). The last column gives the TRI threshold release in terms of equivalent elemental emissions, which is the quantity reportable for chemical categories. If the total quantity oxidized (or otherwise converted) at a given facility exceeds this amount, then *all* releases of that substance at the facility must be reported, whether

“manufactured” or not. However, trace chemicals in power plant air and water intake streams are excluded from TRI reporting.

Formation of Acid Aerosols

HCl and HF are formed from chlorides and fluorides in fuel and emitted in gaseous form. Sulfuric acid is formed in the flue gas stream from the reaction of sulfur trioxide and water vapor. At typical flue gas temperatures (below 200 C), SO₃ is converted completely to H₂SO₄ (although flue gas concentrations are typically reported as SO₃). Sulfuric acid mist or condensation (i.e., a true aerosol) can be expected whenever the flue gas temperature falls below the acid dewpoint, which is a function of the SO₃ and H₂O content of the flue gas. Dewpoint temperatures for coal plants typically are in the range of 127-149°C (27). For stack gas exit temperatures above the acid dewpoint, H₂SO₄ exists in gaseous form (28, 29). Releases of H₂SO₄ thus occur in aerosol or gaseous form, depending upon the dewpoint temperature. However, as noted in the text, the TRI defines an aerosol to include gases and vapors. Thus, all gaseous HCl and H₂SO₄ emissions are reportable TRI releases for power plants if thresholds are exceeded.

Trace Element Removal Efficiency

Table S2 summarizes the removal efficiency data used to partition total releases between air and land. Stack gas data indicate that 99.3% of the chlorides and 98.6% of the fluorides are in the gaseous phase.

Trace Element Variability in Coal

Table S3 shows the range of total annual release values for the 650 MW case study plant based on a 90% probability interval for coal properties. This interval is defined by the 5th and

95th percentile values for coal trace species concentration, as illustrated in Figure 2 (main text) for chromium. The ranges in Table S3 (based on the PISCES Model database) provide the basis for the intervals shown in Figure 3 of the text. These data are for bituminous coals used for power generation. For any particular coal seam or coal supply, a much smaller variation can be expected than the ranges for all bituminous coals shown in Table S3.

Reportable TRI Compounds

Table 4 (main text) showed that HCl, H₂SO₄ and barium compounds are likely to always be reportable at plants burning bituminous coal, based on the median trace element concentrations shown in Table 2. On the other hand, releases of mercury and silver compounds are well below current reportable levels for all U.S. plants (e.g., the 650 MW case study plant had total Hg releases of 350 lb/yr). Releases of combustion-generated organic compounds also are well below current reporting thresholds, ranging from zero to several hundred pounds for the case study plant.

Because a number of chemical compounds that are not currently reportable to the TRI are of environmental concern, EPA recently proposed lowering the TRI reporting threshold to 10 lbs/yr for a number of substances including mercury and several organic compounds (30). Dioxins also would be added to the list of TRI chemicals at a reporting threshold of 0.1 gram. These proposed thresholds would take effect beginning in 2000. At the proposed new threshold, mercury would become reportable for most coal-fired plants.

National Estimates

Table S4 summarizes the range of estimated TRI emissions from all coal-fired plants in 1995, based on a site-specific analysis of reported coal use and quality. Details are reported in Ref. (21).

Additional Literature Cited

25. W. Kennelly, Climax Molybdenum Corp., Ypsilanti, MI, personal communication, 1997.
26. *Handbook of Chemistry and Physics*; The Chemical Rubber Co.: Cleveland, OH, 1997; 78th Edition.
27. Pierce, R.R., "Estimating Acid Dewpoints in Stack Gases," *Chemical Engineering*, April 11, 1977; p. 125-128.
28. Lodge, J.P., Ed., *Methods of Air Sampling and Analysis*; Lewis Publishers, 1989; 3rd Edition, p. 523.
29. Krigmont, H., "Flue Gas Conditioning," in *Applied Electrostatic Precipitation*; Parker, K.R., Ed.; Blackie Academic and Professional, 1997; p. 437.
30. *Federal Register*, 40 CFR Part 372, 64 (2), January 5, 1999; p. 687.

Table S1. Elemental Threshold Release Values for TRI Metal Compounds Manufactured During Combustion

Metal	Lowest Weight Oxide per Unit of Metal	Ratio ^a	Adjusted Threshold ^b (lbs/yr)
Antimony	Sb ₂ O ₃	1.200	20,833
Arsenic	As ₂ O ₃	1.320	18,939
Barium	BaO	1.117	22,391
Beryllium	BeO	2.775	9,009
Cadmium	CdO	1.142	21,891
Chromium	CrO	1.308	19,113
Cobalt	CoO	1.271	19,670
Copper	Cu ₂ O	1.126	22,202
Lead	PbO	1.077	23,213
Manganese	MnO	1.291	19,365
Mercury	Hg ₂ O	1.040	25,000 ^c
Molybdenum	MoO ₃ ^d	1.500	16,663 ^d
Nickel	NiO	1.273	19,645
Selenium	SeO ₂	1.405	17,790
Silver	Ag ₂ O	1.074	23,273
Thallium	Tl ₂ O	1.039	24,058
Zinc	ZnO	1.245	20,080

^aRatio of molecular weight of oxide to weight of metal in that compound.

^bEqual to 25,000 lbs/yr divided by the ratio in the previous column.

This is the threshold quantity of the metals. Only the amount of elemental metal is reported, except for Mo where the amount of MoO₃ is reported.

^cThe EPA rule states that the threshold in this case can be increased to 25,000 lbs/yr since mercury is believed to be manufactured primarily in elemental form.

^dOnly molybdenum trioxide is a listed TRI chemical.

**Table S2. Trace Element Removed Efficiency
for Case Study Plant**

Trace Element	Removal Efficiency (%) ^a	
	Furnace ^b	ESP ^c
Antimony	6.8	99.0
Arsenic	1.4	97.4
Barium	17.7	99.6
Beryllium	16.6	99.3
Cadmium	8.8	96.6
Chloride	0.1	0.005
Chromium	16.3	99.0
Cobalt	17.1	99.4
Copper	12.7	99.1
Fluoride	0.2	0.060
Lead	9.4	99.3
Manganese	21.5	99.0
Mercury	0.8	25.4
Molybdenum	11.0	98.8
Nickel	14.4	99.5
Selenium	1.5	60.4
Silver	16.7	99.7
Thallium	1.1	99.7
Zinc	10.1	99.5

^aMass of element in collected ash solids divided by total mass into device.

^bComposite for all pulverized coal furnaces.

^cAll units with total particulate emissions rates below 0.1 lb/MBtu. Values for Ag and Th estimated based on total particulate removal efficiency.

Table S3. 90 Percent Probability Intervals for the Manufacture of TRI Chemicals for the Case Study Power Plant (650 MW net, 67% capacity factor) (all figures in thousand lbs/yr)

Chemical	90% Range for All		TRI
	Bituminous Coals		Threshold ^a
Antimony	0.6	- 8	21
Arsenic	3	- 160	19
Barium	75	- 860	22
Beryllium	0.8	- 7	9
Cadmium	0.1	- 16	22
Chromium	7	- 81	17
Cobalt	3	- 43	20
Copper	14	- 136	22
Hydrochloric acid	66	- 7000	24
Hydrogen fluoride	11	- 360	24
Lead	6	- 110	23
Manganese	18	- 240	19
Mercury	0.1	- 2	25
Molybdenum ^b	0.5	- 37	17
Nickel	13	- 130	20
Selenium	2	- 48	18
Silver	0.05	- 3	23
Thallium	1	- 10	24
Zinc	26	- 250	20

^aAdjusted TRI threshold values from Table S1, rounded to nearest thousand.

^bMultiply all values by 1.50 to get reportable molybdenum trioxide.

Table S4. Uncertainty Estimates for Total 1995 Releases from Coal-Fired Power Plants (millions of pounds) (From Ref. 21)

Substance	Air Releases		Total Releases	
	Base^a	Bound^b	Base^a	Bound^b
HCl aerosol	553	1147	553	1147
H ₂ SO ₄ aerosol	130	287	130	287
Hydrogen fluoride	55	135	55	135
Metal compounds	< 2	2	249	311
Total	740	1541	987	1880

^aBase case estimates. ^bUpper bound estimate.