



Project Summary

Theoretical Investigation of Selected Trace Elements in Coal Gasification Plants

A. H. Hill, G. L. Anderson, and D. K. Fleming

Results of a theoretical investigation of the disposition of five volatile trace elements—arsenic, boron, lead, selenium, and mercury—in SNG-producing coal gasification plants are reported. Three coal gasification processes—dry-bottom Lurgi, Koppers-Totzek, and HYGAS—were investigated to examine the possible effects of gasifier operation conditions on speciation of the volatile trace elements. Dispositions of these volatile trace elements in a general gas processing scheme (consisting of gas quench, acid-gas removal, and combined shift methanation) were then projected. A different acid-gas removal process was used in each process. The Rectisol process was used for the Lurgi projection; the Benfield, for the Koppers-Totzek; and the Selexol, for the HYGAS. Results of this theoretical investigation suggest that none of the trace elements considered in this study will be present in the product SNG from a coal gasification plant, but will be removed from the fuel gas by various unit operations. Results also suggest that the speciation of these volatile trace elements is not significantly affected by gasifier conditions.

This Project Summary was developed by EPA's Industrial Environmental Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Results of a theoretical investigation of the disposition of five volatile trace elements—arsenic, boron, lead, selenium, and mercury—in SNG-producing coal

gasification plants are reported. Three distinct coal gasification processes—dry-bottom Lurgi, Koppers-Totzek, and HYGAS—were investigated to examine the possible effects of gasifier operating conditions on the speciation of the volatile trace elements. The dispositions of these volatile trace elements in a general gas processing scheme (Figure 1)—consisting of gas quench, acid-gas removal, and combined shift-methanation—were then projected. A different acid-gas removal process was used in each process. The Rectisol process was used for the Lurgi projection; the Benfield, for the Koppers-Totzek; and the Selexol, for the HYGAS.

Results of this theoretical investigation suggest that none of the trace elements considered in this study will be present in the product SNG from a coal gasification plant, but will be removed from the fuel gas by various unit operations. Results also suggest that the speciation of these volatile trace elements is not significantly affected by gasifier conditions. Arsenic is expected to appear in the raw fuel gas from the gasifier as a combination of the elemental forms and the hydride, arsine (AsH_3). Boron is expected to appear as boric acid, B(OH)_3 . Selenium is expected to exist as the hydride, hydrogen selenide (H_2Se). Mercury is expected to appear as the elemental form. Contrary to expectations, the projection also indicated that only a minor fraction of the lead is expected to be present in the raw fuel gas. The range of concentration for these volatile trace elements in the raw fuel gas from the gasifiers was projected to be AsH_3 , 0.02 to 0.5 ppmv; As_4 , 0 to 4 ppmv; H_2Se , 0.02 to 1.4 ppmv; B(OH)_3 , 1 to 300 ppmv; PbS , $<1 \times 10^{-4}$ ppmv; PbCl_2 , $<2 \times$

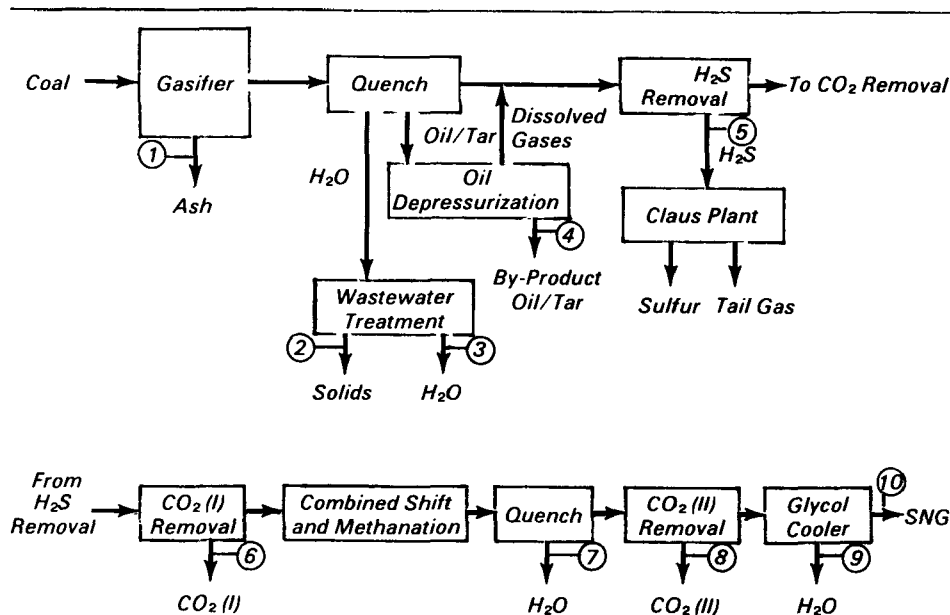


Figure 1. Typical gas processing configuration for producing SNG. (Arabic numerals in circles are identified in Table 1.)

10^{-5} ppmv; Pb, $<6 \times 10^{-4}$ ppmv; and Hg, 0.001 to 0.1 ppmv. The ranges of these projections reflect the entire range of concentrations at which these trace elements exist in U.S. coals as reported by Ruch, *et al.** The concentration ranges assumed for this study were 0.5 to 14 ppmw arsenic, 0.45 to 7.7 ppmw selenium, 2 to 224 ppmw boron, 1 to 200 ppmw lead, and 0.02 to 1.6 ppmw mercury.

Projections on the probable disposition of these volatile trace-element-containing compounds in the gas quenching operations indicated that essentially all the $B(OH)_3$, As_4 , and lead-containing compounds, and a major fraction of the H_2Se will be removed from the fuel gas during quenching. The $B(OH)_3$ and the H_2Se should be recovered in the aqueous condensate. The lead-containing compounds should precipitate. In the Koppers-Totzek process, the arsenic should also precipitate, but in the HYGAS and Lurgi processes, where aromatic oils and tars are produced, the arsenic may be dissolved in these by-products, reaching concentrations as high as 2000 ppmw. Only AsH_3 , mercury, and part of the H_2Se were projected to remain in the quenched fuel gas. The projected concentration range for these constituents was 0.03 to 0.83 ppmv, 0.002 to 0.14 ppmv, and 0.003 to 1.35 ppmv, respectively.

* Ruch, R. R. Gluskoter, H. J., and Shimp, N. F., *Occurrence and Distribution of Potentially Volatile Trace Elements in Coal*, Environmental Geology Note Series 72, Illinois State Geological Survey, Urbana, IL, 1974.

gasifier ash, and the primary condensate streams from quenching operations and performing elemental balances. Variations in the concentration of the trace element in the feed coal make this approach imprecise. Based on IGT's theoretical projections, the volatile trace-element-containing compounds in the quenched fuel gas may represent only a small percentage ($<10\%$) of the feed. This fraction is of the same order of magnitude as the uncertainty in the elemental balances.

The projected dispositions of the five trace elements in commercial-scale versions [7.082 million m^3 (std)/d (250 million scf/d) of SNG] of the three gasification processes are summarized in Table 1.

The disposition of the mercury and H_2Se in the three acid-gas removal processes was projected to be identical to that of H_2S . The disposition of arsine was projected to be similar to that of CO_2 in the Selexol and Rectisol processes, but the AsH_3 was projected to remain with the treated gas in the Benfield process. However, these projections have considerable uncertainty associated with them: no solubility data exist for these compounds in these acid-gas removal solvents. If the above projections are indeed correct, two potential problems can be cited. First, the CO_2 -rich gas from the Selexol and Rectisol processes may have environmentally significant levels of AsH_3 . The projected concentration range for AsH_3 is 0.1 to 2.5 ppmv before additional treatment. Second, arsenic, selenium, and mercury may significantly contaminate any elemental sulfur produced from the H_2S -rich acid-gas stream from these three acid-gas removal processes. The potential concentrations range from 1 to 1000 ppmw for selenium, 0.01 to 30 ppmw for arsenic, and 2 to 200 ppmw for mercury. This degree of contamination could make the elemental sulfur unsuitable as a chemical feedstock.

These projections indicate the need for direct determination of the concentrations of volatile trace-element-containing compounds in all major gas streams of an integrated coal gasification process. The methodology used in previous environmental assessment studies has consisted primarily of analyzing the feed coal, the

Table 1. Projected Disposition Rates For Selected Trace Elements In Commercial-Scale Lurgi, Koppers-Totzek, and HYGAS Plants

Stream No. ^a	Description	Arsenic			Boron			Lead		
		L ^d	K-T ^d	H ^d	L	K-T	H	L	K-T	H
						kg/d				
1	Gasifier Residue ^b	4-850	0	4-750	18-2030	0	16-1775	72-3950	73-3960	63-3460
2	Quench Solids ^c	0	9-1700	0	0	0	0	<0.008	<0.5	<0.005
3	Wastewater	0.3-3.0	<0.001	0.2-0.3	18-2030	36-4060	16-1775	<0.0002	<0.0001	<0.0002
4	Oil/Tar ^c	0.4-740	0	0.8-700	0	0	0	0	0	0
5	H ₂ S-Rich Acid Gas	0.4-3.9	<0.02	0.3-3.6	0	0	0	0	0	0
6	CO ₂ -Rich Acid Gas (I)	3.8-38	<0.07	3.8-50	0	0	0	0	0	0
7	Methanation Condensate	0	2.0-9.5	0	0	0	0	0	0	0
8	CO ₂ -Rich Acid Gas (II)	0	0	0	0	0	0	0	0	0
9	Glycol Cooler Condensate	0	0	0	0	0	0	0	0	0
10	SNG	0	0	0	0	0	0	0	0	0

Stream No. ^a	Description	Selenium			Mercury		
		L	K-T	H	L	K-T	H
						kg/d	
1	Gasifier Residue ^b	4.1-70	0	3.5-66	0	0	0
2	Quench Solids ^c	0	0	0	0	0	0
3	Wastewater	3.8-65	2.0-31	3.5-59	<0.002	<0.001	<0.001
4	Oil/Tar ^c	<0.005	0	<0.005	0	0	0
5	H ₂ S-Rich Acid Gas	0.3-4.5	6.3-108	0.2-4.2	0.4-29	0.4-29	0.4-25
6	CO ₂ -Rich Acid Gas (I)	<0.02	<0.01	<0.02	<0.05	<0.03	<0.05
7	Methanation Condensate	0	0	0	0	0	0
8	CO ₂ -Rich Acid Gas (II)	0	0	0	0	0	0
9	Glycol Cooler Condensate	0	0	0	0	0	0
10	SNG	0	0	0	0	0	0

^a See Figure 1

^b K-T Gasifier residue includes entrained slag recovered in waste heat boiler.

^c Excludes carryover fines from gasifier.

^d L = Lurgi; K-T = Koppers-Totzek; H = HYGAS

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William J. Rhodes is the EPA Project Officer (see below).

The complete report, entitled "Theoretical Investigation of Selected Trace Elements in Coal Gasification Plants," (Order No. PB 83-250 001; Cost: \$10.00, subject to change) will be available only from:

National Technical Information Service
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Springfield, VA 22161
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