

APPENDIX D13
VOC SCREENING METHODOLOGY

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Screening the volatile organic compounds (VOCs) for inclusion in the exposure assessment was a two-step process. The first step was determining that only those VOCs listed in both Appendix VIII of Title 40 of the Code of Federal Regulations (CFR) Part 261 and in the Waste Isolation Pilot Plant (WIPP) Quality Assurance Program Plan (QAPP) were eligible for inclusion in the demonstration. The second step was to score the VOCs based on the concentration-toxicity screening technique presented by the U.S. Environmental Protection Agency (EPA) in the *Risk Assessment Guidance for Superfund* (EPA 1989, p. 5-23). The scoring was performed using the weighted average VOC concentrations reported in the Idaho National Engineering Laboratory (INEL) and Rocky Flats Environmental Technology Site (RFETS) headspace sampling (Appendix C2, Table C2-1). The methodology used in calculating the average VOC headspace concentrations is described in Appendix C2.

The listing in Appendix VIII and/or the QAPP was used as a rough screening. VOCs that were to be analyzed on a site-specific basis (i.e., formaldehyde and hydrazine) were also screened out. VOCs listed in these sources are presented in Table D13-1; VOCs selected from this listing are as follows:

- Benzene 18
 - Bromoform 19
 - Carbon disulfide* 20
 - Carbon tetrachloride 21
 - Chlorobenzene 22
 - Chloroform 23
 - 1,2-Dichloroethane 24
 - (cis)-1,2-Dichloroethylene 25
 - 1,1-Dichloroethylene 26
 - Isobutanol* 27
 - Methyl ethyl ketone 28
 - Methylene chloride 29
 - 1,1,2,2-Tetrachloroethane 30
 - Tetrachloroethylene 31
 - Toluene 32
 - 1,1,1-Trichloroethane 33
 - 1,1,2-Trichloroethane* 34
 - Trichloroethylene 35
 - Trichlorofluoromethane* 36
 - Vinyl chloride* 37
- * No headspace data available 38

TABLE D13-1
 Chemicals in 40 CFR Part 261 Appendix VIII and WIPP QAPP

Compound	Synonyms	CAS Number	Appendix VIII Constituent	QAPP
Acetone	2-Propanone	67-64-1		+
Antimony		7440-36-0		+
Arsenic		7440-38-2	+	+
Barium		7440-39-3	+	+
Benzene		71-43-2	+	+
Beryllium		7440-41-7	+	+
Bromoform	Tribromomethane	75-25-2	+	+
n-Butyl alcohol	Butanol, 1-Butanol	71-36-3		+
Cadmium		7440-43-9	+	+
Carbon disulfide	Carbon bisulfide	75-15-0	+	+
Carbon tetrachloride		56-23-5	+	+
Chlorobenzene		108-90-7	+	+
Chloroform		67-66-3	+	+
Chromium		7440-47-3	+	+
Cresol	Cresylic acid	1319-77-3	+	+
Cyclohexane		110-87-7		+
1,4-Dichlorobenzene	p-Dichlorobenzene	106-46-7	+	+
ortho-Dichlorobenzene	1,2-Dichlorobenzene	95-50-1	+	+
1,1-Dichloroethane	Ethylidene chloride	75-34-3		+
1,2-Dichloroethane	Ethylene dichloride	107-06-2	+	+
(cis)-1,2-Dichloroethylene	(cis)-1,2-Dichloroethene, sym-Dichloroethylene	540-59-0	+	+
1,1-Dichloroethylene	1,1-Dichloroethene, Vinylidene chloride	75-35-4	+	+
2,4 Dinitrophenol		51-28-5	+	+
2,4-Dinitrotoluene		121-14-2	+	+
Ethyl benzene		100-41-4		+
Ethyl ether	Diethyl ether, Ether	60-29-7		+
Formaldehyde		50-00-0	+	SS
Hexachlorobenzene		118-74-1	+	+
Hexachloroethane		67-72-1	+	+
Hydrazine		302-01-2	+	SS
Isobutanol	Isobutyl alcohol	78-83-1	+	+
Lead		7439-92-1	+	+
Mercury		7439-97-6	+	+
Methanol	Methyl alcohol	67-56-1		+
Methyl ethyl ketone	2-Butanone	78-93-3	+	+
Methyl isobutyl ketone	4-Methyl-2-pentanone	108-10-1		+
Methylene chloride	Dichloromethane	75-09-2	+	+
Nickel		7440-02-0	+	+
Nitrobenzene		98-95-3	+	+
Pentachlorophenol		87-86-5	+	+
Polychlorinated Biphenyls (PCBs)		1336-36-3	+	+
Pyridine		110-86-1	+	+
Selenium		7782-49-2	+	+
Silver		7440-22-4	+	+
1,1,1,2-Tetrachloroethane		79-34-5	+	+
Tetrachloroethylene	Tetrachloroethene, Perchloroethylene	127-18-4	+	+
Thallium		7440-28-0	+	+
Toluene		108-88-3	+	+
1,1,1-Trichloroethane	Methyl chloroform	71-55-6	+	+
1,1,2-Trichloroethane		79-00-5	+	+
Trichloroethylene	Trichloroethene	79-01-6	+	+
Trichlorofluoromethane	Freon-11	75-69-4	+	+
1,1,2-Trichloro-1,2,2-trifluoroethane	Freon-113	76-13-1		+
1,2,4-Trimethylbenzene	Pseudocumene	95-63-6		+
1,3,5-Trimethylbenzene	Mesitylene	108-67-8		+
Vanadium Pentoxide	Vanadium Oxide	1314-62-1	+	+
Vinyl chloride	Chloroethylene	75-01-4	+	+
m-Xylene	1,3-Dimethylbenzene	108-38-3		+
o-Xylene	1,2-Dimethylbenzene	95-47-6		+
p-Xylene	1,4-Dimethylbenzene	106-42-3		+
Zinc		7440-66-0		+

SS=Site Specific

The VOCs listed were further screened using the scoring technique outlined by EPA (EPA, 1989). First, the headspace concentration in parts per million by volume was converted to a concentration in micrograms per cubic meter for carcinogens and milligrams per cubic meter for noncarcinogens. Several VOCs did not have sample quantitation limits (SQLs) reported by the laboratories providing the headspace sampling data; for these VOCs (carbon disulfide, isobutanol, 1,1,2-trichloroethane, trichlorofluoromethane, and vinyl chloride), SQLs were calculated (Appendix C2), and one-half the calculated SQL (rounded to two decimal places) was used for the headspace concentration in the scoring process.

A risk factor was calculated for each VOC from the weighted average headspace concentration and the toxicity value. The risk factors for all VOCs were summed to yield a total risk factor. The contribution of each VOC to this risk factor was then calculated by dividing the individual risk factor by the total risk factor. The chemicals cumulatively responsible for approximately 99 percent of the total risk factor were selected for use in the assessments.

The conversion of headspace VOC concentration in parts per million per volume to micrograms per cubic meter (for carcinogens) was performed using the following equation:

$$HS_c = (HS)(10^{-6} \text{ mol fraction/ppmv})\left(\frac{P \times MW}{R \times T}\right)(10^6 \mu\text{g/g})(10^3 \text{ L/m}^3) \quad (\text{D13-1})$$

where

- HS_c = weighted average headspace concentration for carcinogens, $\mu\text{g/m}^3$
- P = pressure, 1 atm
- MW = molecular weight, g/mol
- R = ideal gas constant, 0.082057 L atm/mol K
- T = temperature, 298 K
- HS = weighted average headspace concentration, ppmv.

The conversion of headspace VOC concentration in parts per million per volume to milligrams per cubic meter (for noncarcinogens) was performed using the following equation:

$$HS_n = (HS)(10^{-6} \text{ mol fraction/ppmv})\left(\frac{P \times MW}{R \times T}\right)(10^3 \text{ mg/g})(10^3 \text{ L/m}^3) \quad (\text{D13-2})$$

where

- HS_n = weighted average headspace concentration for noncarcinogens, mg/m^3 .

1 The equation used to calculate the individual risk factors for carcinogens was:
2

(D13-3)

$$R_{ci} = HS_c \times UR$$

3
4 where

5 R_{ci} = risk factor for carcinogenic VOC i
6 UR = unit risk factor for VOC i , $(\mu\text{g}/\text{m}^3)^{-1}$.

7
8 The equation used to calculate the individual risk factors for noncarcinogens was:
9

(D13-4)

$$R_{ni} = \frac{HS_n}{RfC}$$

10 where

11 R_{ni} = risk factor for noncarcinogenic VOC i
12 RfC = reference concentration for VOC i , mg/m^3 .

13
14 The total risk factor was calculated using the equation:
15

(D13-5)

$$R_t = R_1 + R_2 + R_3 + \dots + R_i$$

16 where

17 R_t = total risk factor
18 $R_1 + \dots + R_i$ = risk factors for VOCs 1 through i .

19
20 Separate values of R_i were calculated for carcinogens and noncarcinogens. Finally, the ratio of
21 the individual risk to the total risk (R_{ci}/R_t or R_{ni}/R_t) was calculated for each VOC. Based on this
22 ratio, the VOCs responsible for approximately 99 percent of the total risk factor were selected
23 for inclusion in the assessments.

24
25 Table D13-2 presents the VOC screening results using the headspace concentrations of the
26 VOCs. The following chemicals were selected to be included in the no-migration demonstration:
27

- 28 • Carcinogens
 - 29 - Carbon tetrachloride
 - 30 - Chloroform
 - 31 - 1,1-Dichloroethylene
 - 32 - Methylene chloride
 - 33 - 1,1,2,2-Tetrachloroethane
- 34
- 35 • Noncarcinogens
 - 36 - Carbon disulfide
 - 37 - Chlorobenzene
 - 38 - Methyl ethyl ketone
 - 39 - Toluene.

TABLE D13-2
Results of the VOC Screening Using Headspace Concentrations

Carcinogen	Molecular Weight (grams per mole)	Headspace Concentration (parts per million by volume)	Headspace Concentration (micrograms per cubic meter)	Chemical Class	UR (cubic meters per microgram)	Calculated Score	Absolute Score	Percent of total
Benzene	78.11	9.25 a	2.95e+04	A	8.30e-06 c	0.245241838	0.245241838	0.0033066001
Bromoform	252.77	9.38 a	9.70e+04	B2	1.10e-06 c	0.106656948	0.106656948	0.0014380576
Carbon tetrachloride	153.84	375.5 a	2.36e+06	B2	1.50e-05 c	35.43550059	35.43550059	0.4777774952 *
Chloroform	119.39	25.33 a	1.24e+05	B2	2.30e-05 c	2.844455073	2.844455073	0.0383518392 *
Methylene chloride	84.94	368.5 a	1.28e+06	B2	4.70e-07 c	0.601610915	0.601610915	0.0081115309 *
1,1-Dichloroethylene	96.95	11.46 a	4.54e+04	C	5.00e-05 c	2.271802306	2.271802306	0.0306307516 *
1,2-Dichloroethane	98.96	9.07 a	3.67e+04	B2	2.60e-05 c	0.954351636	0.954351636	0.0128675404 *
1,1,2,2-Tetrachloroethane	167.86	9.35 a	6.42e+04	C	5.80e-05 c	3.722673296	3.722673296	0.0501928714 *
Tetrachloroethylene	165.85	9.4 a	6.38e+04	C-B2	5.80e-07 c	0.036977659	0.036977659	0.0004985705
1,1,1-Trichloroethane	133.4	317.1 b	1.73e+06	C	1.60e-05 c	27.67834734	27.67834734	0.3731876576 *
1,1,2-Trichloroethane	133.42	0.07 b	3.82e+02	C	1.60e-05 c	0.006110926	0.006110926	0.0000823937
Trichloroethylene	131.4	25.1 a	1.35e+05	C-B2	1.70e-06 c	0.229290525	0.229290525	0.0030915283
Vinyl chloride	62.5	0.16 b	4.09e+02	A	8.40e-05 d	0.034351633	0.034351633	0.0004631637
Total=							46.3959077	1.00000
*VOCs account for approximately 99 percent of total score.								
Noncarcinogen	Molecular Weight (grams per mole)	Headspace Concentration (parts per million by volume)	Headspace Concentration (milligrams per cubic meter)	Chemical Class	RfC (milligrams per cubic meter)	Calculated Score	Absolute Score	Percent of total
Carbon disulfide	76.14	0.13 b	4.05e-01	ND	7.00e-01 d	0.578264172	0.578264172	0.0001886173
Chlorobenzene	112.56	12.52 a	5.76e+01	D	2.00e-02 d	2881.552379	2881.552379	0.9399003669 *
(cis)-1,2-Dichloroethylene	96.95	8.97 a	3.56e+01	D	ND	—	0	0
Isobutanol	74.12	0.13 b	3.94e-01	ND	ND	—	0	0
Methyl ethyl ketone	72.1	63.66 a	3.83e+01	D	1.00e+00 c	0.383306971	0.383306971	0.0001250265
Toluene	92.13	19.4 a	7.31e+01	D	4.00e-01 c	182.7304444	182.7304444	0.0596027381 *
Trichlorofluoromethane	137.38	0.07 b	3.93e-01	ND	7.00e-01 d	0.561812778	0.561812778	0.0001832512
Total=							2136.94983	1.00000
*VOCs account for approximately 99 percent of total score.								

^aMeasure data from INEL and RFETS sampling.
^bOne-half the calculated sample quantitation limit.
 ND = No data available.

^cToxicity data from *Integrated Risk Information System*.
^dToxicity data from *Health Effects Assessment Summary Tables, Annual Update*.

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