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Project Summary

Response Factors of VOC Analyzers at a Meter Reading of 10,000 PPMV for Selected Organic Compounds

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The report summarizes results of a reinterpretation of data generated in a laboratory study of the sensitivity of two types of portable hydrocarbon detectors to a variety of organic compounds. (A previous report, EPA-600/2-81-002 [NTIS PB 81-136194], describes and gives original results of the laboratory study.) Detector sensitivity is quantified by a response factor for each compound where the response factor equals the actual concentration of the compound divided by the observed concentration from the detector. The previous report estimated response factors at 10,000 ppmv actual concentration of the compound. This report presents response factors estimated for a 10,000 ppmv detector reading. The instruments were calibrated to 7993 ppmv methane gas.

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).

Introduction

Portable hydrocarbon analyzers are used to detect fugitive VOC emissions from petroleum refinery and chemical plant process units. The sensitivity of the analyzers varies, depending on the chemical and concentration detected. The detector sensitivity is quantified by a "response factor" for each compound where:

$$\text{Response Factor} = \frac{\text{Actual Concentration of Compound}}{\text{Observed Concentration from Detector}}$$

Results

This summary presents response factors for two types of portable hydrocarbon analyzers, the "OVA-108" and the "TLV sniffer," for 168 different chemical compounds. The response factor is defined as the ratio of the actual concentration to the observed concentration (or instrument response) The response factor varies with concentration. In a previous report (EPA-600/2-81-002), the response factors were presented at 10,000 ppmv actual concentration of the compound. In this summary, the response factors are computed at a meter reading of 10,000 ppmv.

Table 1 presents response factors for compounds on both types of instruments along with the 95 percent confidence intervals.

Two statistical methods were used here to compute estimates and associ-

Table 1. *Response Factors with 95% Confidence Intervals Estimated at 10,000 PPMV Response*

OCPDB* ID No	Compound Name	Volatility Class**	OVA Response Factor	OVA Confidence Intervals	TLV Response Factor	TLV Confidence Intervals
70	Acetic Acid	LL	1.64	(1.11, 2.65)	15.60	(7.05, 46.20)
80	Acetic Anhydride	LL	1.39	(1 09, 1.86)	5.88 I	(2.71, 12.80)
90	Acetone	LL	0.80	(0.57, 1.20)	1.22	(0.81, 2 00)
100	Acetone Cyanohydrin	HL	3.51	(0.69, >100.00)	21 00 N	(1.09, >100 00)
110	Acetonitrile	LL	0.95	(0 85, 1.06)	1 18	(0.94, 1.52)
120	Acetophenone	HL	18.70	(5.52, >100.00)	B	
125	Acetyl Chloride	LL	2.04	(1.72, 2.48)	2.72	(1.65, 5 32)
130	Acetylene	G	0.39	(0.36, 0.43)	B	
150	Acrylic Acid	LL	4.59	(3.38, 6.57)	B	
170	Acrylonitrile	LL	0.97	(0.80, 1 20)	3.49 I	(0.44, 27.90)
	Allene	G	0.64	(0.60, 0.69)	15.00	(9.68, 26.50)
200	Allyl Alcohol	LL	0.96	(0.76, 1.27)	X	
250	Amyl Alcohol, N-	HL	0.75	(0.57, 1.04)	2.14	(0.45, >100.00)
2855	Amylene	LL	0.44	(0.34, 0.61)	1.03	(0.59, 2.59)
330	Anisole	LL	0.92	(0.65, 1.46)	3.91	(0.52, >100.00)
360	Benzaldehyde	HL	2.46	(1.38, 5.62)	B	
380	Benzene	LL	0.29	(0.28, 0.31)	1.07	(0 96, 1.20)
450	Benzonitrile	HL	2.99	(1.18, 15.30)	B	
490	Benzoyl Chloride	HL	22.10 D	(3.43, >100.00)	B	
530	Benzyl Chloride	HL	15.30 D	(3.96, >100.00)	B	
570	Bromobenzene	LL	0.40	(0.34, 0.48)	1.19	(0.27, >100.00)
590	Butadiene, 1,3-	G	0.57	(0.54, 0.60)	10.90	(8.11, 15.40)
	Butane, N-	G	0 50	(0.46, 0.55)	0.63	(0.58, 0.70)
640	Butanol, N-	LL	1.44 I	(0.89, 2.34)	4.11 I	(2.16, 7.83)
650	Butanol, SEC-	LL	0.76	(0.70, 0.83)	1.25	(0.99, 1 66)
660	Butanol, Tert-	S	0.53	(0.38, 0.81)	2.17	(1.34, 4 43)
592	Butene, 1-	G	0.56	(0.51, 0.62)	5.84	(4.20, 8.89)
600	Butyl Acetate,	LL	0.66	(0.54, 0.83)	1.38	(1.15, 1.70)
630	Butyl Acrylate, N-	LL	0.70	(0.63, 0.78)	2.57 I	(1.17, 5.68)
	Butyl Ether, N-	LL	2.60	(0.81, 95.60)	3.58 I	(1.82, 7.04)
	Butyl Ether, Sec-	LL	0.35	(0.21, 0.95)	1.15	(0.75, 2.17)
670	Butylamine, N-	LL	0.69	(0.53, 0.98)	2.02	(1 14, 4.97)
680	Butylamine Sec-	LL	0.70	(0.58, 0.87)	1.56	(0.77, 5 24)
690	Butylamine, Tert-	LL	0.63	(0.58, 0.70)	1.95	(1.42, 2.91)
	Butylbenzene, Tert-	HL	1.32	(0.89, 2 20)	B	
750	Butyraldehyde N-	LL	1.29	(1.07, 1.61)	2.30	(0.96, 12.80)
760	Butyric Acid	HL	0.80	(0.38, 3.14)	10.70 I	(6.53, 17.60)
780	Butyronitrile	LL	0.52	(0.40, 0.74)	1.47 I	(0.62, 3.48)
790	Carbon Disulfide	LL	B		3.92	(1.87, 12.60)
830	Chloroacetaldehyde	LL	9.10	(5.73, 16.20	5.07	(3.08, 9 79)
890	Chlorobenzene	LL	0.38	(0.32, 0.47)	0.88	(0 77, 1.00)
1740	Chloroethane	G	5.38 I	(1.87, 26.40)	3.90 P	(1.58, 14.10)
930	Chloroform	LL	9.28	(5.19, 20.00)	B	
960	Chlorophenol, O-	HL	4.56	(1.72, 27.20)	18.30 I	(6.50, 51.50)
	Chloropropene, 1-	LL	0.67	(0.61, 0.73)	0.87	(0.69, 1.16)
210	Chloropropene, 3-	LL	0.80	(0.72, 0.90)	1.24	(1.08, 1.42)
970	Chlorotoluene, M-	LL	0.48	(0.45, 0.51)	0.91	(0.40, 7 47)
980	Chlorotoluene, O-	LL	0.48	(0.42, 0.55)	1.06	(0.33, >100 00)
990	Chlorotoluene, P-	LL	0.56	(0.52, 0 61)	1.17 I	(0.77, 1.77)
1010	Cresol, O-	S	0.96	(0.70, 1.45)	4.36 I	(0.40, 47.40)
1040	Crotonaldehyde	LL	1.25	(0.82, 2.24)	B	
1060	Cumene	LL	1.87	(1.10, 3.71)	B	
1120	Cyclohexane	LL	0.47	(0.39, 0.58)	0.70	(0.62, 0 80)
1130	Cyclohexanol	HL	0.85	(0.65, 1.20)	B	
1140	Cyclohexanone	LL	1.50	(0.97, 2.76)	7.04	(1.59, >100.00)
1150	Cyclohexene	LL	0.49	(0.42, 0.57)	2.17	(1.78, 2.74)

Table 1. *(Continued)*

OCPDB* ID No	Compound Name	Volatility Class**	OVA Response Factor	OVA Confidence Intervals	TLV Response Factor	TLV Confidence Intervals
1160	Cyclohexylamine	LL	0.57	(0.42, 0.86)	1 38	(1 28, 1 48)
	Decane	HL	0.09 N	(0.05, >100.00)	0.16 I	(0 07, 0.35)
1190	Diacetone Alcohol	HL	1.45	(0.96, 2.48)	0.98	(0 44, 5 93)
	Diacetyl	LL	1.54	(1 25, 1.92)	3 28	(2.25, 5.12)
1270	Dichloro-1-Propene, 2,3-	LL	0.75	(0 56, 1.09)	1 75	(1 14, 3 18)
1215	Dichlorobenzene, M-	HL	0.64	(0 55, 0.77)	2 36	(0 58, >100 00)
1216	Dichlorobenzene, O-	HL	0.68	(0.47, 1.11)	1.26	(0 35, >100 00)
	Dichloroethane, 1,1-	LL	0 78	(0.62, 1.02)	1 86	(1 56, 2 25)
1244	Dichloroethane, 1,2-	LL	0 95	(0 77, 1 22)	2.15	(1 66, 2 92)
1235	Dichloroethylene, CIS1,2-	LL	1.27	(1.05, 1.56)	1.63	(0 99, 3 47)
1236	Dichloroethylene, TRANS 1,2-	LL	1.11	(0.98, 1.27)	1.66	(0 67, 12 60)
2620	Dichloromethane	LL	2.81	(2.13, 3.87)	3.85	(2 46, 6 88)
3110	Dichloropropane, 1,2-	LL	1 03	(0.82, 1.33)	1 65	(1.06, 3 05)
1440	Diisobutylene	LL	0.35	(0.29, 0.44)	1.41	(0 96, 2 40)
1870	Dimethoxy Ethane, 1,2-	LL	1.22	(0 64, 3.61)	1 52	(0.65, 8 38)
1490	Dimethylformamide, N,N-	LL	4.19	(2.90, 6.58)	5.29	(4 05, 7.20)
1495	Dimethylhydrazine 1,1-	LL	1.03	(0.77, 1.45)	2 70	(0 51, >100 00)
1520	Dimethylsulfoxide	HL	0.07 I	(0.05, 0.11)	8.45 I	(4 15, 17.20)
1480	Dioxane	LL	1.48	(1.04, 2 33)	1 31	(0 70, 3.60)
1650	Epichlorohydrin	LL	1.69	(1.56, 1.84)	2.03	(1 79, 2 33)
	Ethane	G	0.65	(0.44, 1.58)	0 69 I	(0 21, 2.30)
1660	Ethanol	LL	1 78	(1.59, 2.01)	X	
1910	Ethoxy Ethanol, 2-	LL	1.55	(1.26, 1.96)	1.82	(0 96, 5 12)
1670	Ethyl Acetate	LL	0.86	(0 77, 0.95)	1.43	(1.07, 2 00)
1680	Ethyl Acetoacetate	HL	3 82	(1 89, 10 70)	5 60	(1 93, 38 80)
1690	Ethyl Acrylate	LL	0.77	(0.63, 0 97)	X	
1750	Ethyl Chloroacetate	LL	1 99	(1 70, 2 36)	1 59	(0 40, >100 00)
1990	Ethyl Ether	LL	0.97	(0 77, 1.30)	1.14	(0.94, 1 42)
1710	Ethylbenzene	LL	0.73	(0.52, 1.11)	4.74 D	(1 38, 61.30)
1770	Ethylene	G	0.71	(0.63, 0.82)	1.56	(1 26, 2.06)
1980	Ethylene Oxide	G	2.46	(1.95, 3.29)	2.40	(0.96, >100.00)
1800	Ethylenediamine	LL	1.73	(1 29, 2 46)	3 26	(0.78, >100 00)
2060	Formic Acid	LL	14.20	(10.60, 19.80)	B	
2105	Glycidol	LL	6.88	(3.33, 19.70)	5.66	(2.08, 34 70)
	Heptane	LL	0.41 I	(0.28, 0.60)	0.73	(0.33, 6.10)
	Hexane, N-	LL	0.41	(0.38, 0.45)	0.69	(0.63, 0 76)
	Hexene, 1-	LL	0.49	(0.39, 0.66)	4.69 D	(0.85, >100.00)
	Hydroxyacetone	LL	6.90	(4.45, 12.10)	15.20	(6.11, 66.40)
	Isobutane	G	0.41	(0.29, 1.04)	0.55	(0.41, 0.81)
2200	Isobutylene	G	3.13	(0.90, 38.50)	B	
2350	Isoprene	LL	0.59	(0.46, 0.80)	X	
2360	Isopropanol	LL	0.91	(0.72, 1.20)	1.39	(0.94, 2.31)
2370	Isopropyl Acetate	LL	0.71	(0.62, 0.83)	1.31	(1.04, 1 72)
2390	Isopropyl Chloride	LL	0.68	(0.60, 0.77)	0.98	(0.82, 1.22)
	Isovaleraldehyde	LL	0.64	(0.57, 0.74)	2.19 D	(1.14, 6.65)
2450	Mesityl Oxide	LL	1.09	(0.94, 1.29)	3.14	(1.43, 12.00)
	Methacrolein	LL	1.20	(0.90, 1.71)	3 49 D	(1.51, 19.80)
2460	Methacrylic Acid	HL	0.82	(0.31, 14.70)	1 06 I	(0.24, 4.56)
2500	Methanol	LL	4.39 P	(3.61, 5.60)	2 01	(1.66, 2.48)
1930	Methoxy-Ethanol, 2-	LL	2.25	(1.62, 3.34)	3.13	(1.13, 27 40)
2510	Methyl Acetate	LL	1.74	(1.46, 2.13)	1.85	(1.44, 2.49)
	Methyl Acetylene	G	0.61	(0.58, 0.64)	6.79	(4.86, 10.40)
2560	Methyl Chloride	G	1.44	(1.22, 1.76)	1.84	(0.73, >100.00)
2640	Methyl Ethyl Ketone	LL	0.64	(0.51, 0.84)	1.12	(0.93, 1.38)
2645	Methyl Formate	LL	3.11	(2.42, 4.14)	1.94	(1.72, 2.21)
2665	Methyl Methacrylate	LL	0.99	(0.90, 1.10)	2.42	(1.39, 5.38)
2650	Methyl-2-Pentanol, 4-	LL	1.66	(1.27, 2.32)	2.00	(1.40, 3.15)

Table 1. *(Continued)*

OCPDB* ID No	Compound Name	Volatility Class**	OVA Response Factor		OVA Confidence Intervals		TLV Response Factor		TLV Confidence Intervals	
2660	Methyl-2-Pentanone, 4-	LL	0.56		(0.46,	0.69)	1.63		(1.22,	2.35)
2550	Methyl-3-Butyn-2-OL, 2-	LL	0.59		(0.44,	0.86)		X		
	Methylal	LL	1.37		(1.06,	1.83)	1.46		(1.24,	1.74)
2540	Methylaniline, N-	HL	4.64		(3.91,	5.57)	9.46	I	(2.55,	35.20)
2570	Methylcyclohexane	LL	0.48		(0.28,	1.39)	0.84		(0.68,	1.09)
	Methylcyclohexene, 1-	LL	0 44		(0.36,	0.54)	2.79		(1.79,	5.12)
2670	Methylpentynol	LL	1.17		(0.71,	2.48)	3.42		(1.83,	8.54)
2690	Methylstyrene, A-	LL	13.90		(9.50,	21.50)		B		
2700	Morpholine	LL	0.92		(0.67,	1.40)	2.59	I	(0.64,	10.50)
2770	Nitrobenzene	HL		B	(		0.01	I	(0.00,	82.80)
2790	Nitroethane	LL	1.40		(1.20,	1.65)	3.45		(1.56,	13.00)
2791	Nitromethane	LL	3.52		(3.03,	4.15)	7.60		(1.91,	>100.00)
2795	Nitropropane	LL	1.05		(0.80,	1.48)	2.02		(1.17,	4.47)
	Nonane-N	LL	1.54		(0.94,	2.98)	11.10		(3.13,	>100.00)
	Octane	LL	1.03		(0.89,	1.21)	2.11		(1.68,	2.75)
2851	Pentane	LL	0.52		(0.42,	0.66)	0.63		(0.57,	0.70)
2973	Picoline, 2-	LL	0.43		(0.38,	0.50)	1.18		(1.08,	1.29)
	Propane	G	0.55	I	(0.46,	0.72)	0.60	P	(0.59,	0.69)
3063	Propionaldehyde	LL	1.14		(1.00,	1.32)	1.71		(1.11,	3.06)
3066	Propionic Acid	LL	1.30		(1.03,	1.70)	5 08	D	(0.73,	>100.00)
3070	Propyl Alcohol	LL	0.93		(0.77,	1.16)	1.74		(1.06,	3.50)
	Propylbenzene, N-	LL	0.51		(0:45,	0.58)		B		
3090	Propylene	G	0.77		(0.44,	2.66)	1.74	I	(0.15,	20.30)
3120	Propylene Oxide	LL	0.83		(0 74,	0.95)	1.15		(0.69,	2.46)
3130	Pyridine	LL	0.47		(0.40,	0.55)	1.16		(1.03,	1.34)
3230	Styrene	LI	4.22		(3.45,	5.27)		B		
3290	Tetrachloroethane, 1,1,1,2-	LL	4.83	D	(1.24,	>100.00)	6.91		(3.14,	22.50)
3291	Tetrachloroethane, 1,1,2,2-	LL	7.89		(5.01,	13.80)	25.40		(8.06,	>100.00)
2860	Tetrachloroethylene	LL	2.97		(1.71,	6.11)		B		
3349	Toluene	LL	0.39		(0.36,	0.43)	2.68	D	(0.79,	>100.00)
3393	Trichlorobenzene, 1,2,4-	HL	1.21	I	(0.50,	2.94)	0.47	I	(0.32,	0.68)
3395	Trichloroethane, 1,1,1-	LL	0.80		(0.72,	0.90)	2.40		(1.81,	3.35)
3400	Trichloroethane, 1,1,2-	LL	1.25		(1.05,	1.50)	3.69		(2.77,	5.16)
3410	Trichloroethylene	LL	0.95		(0.83,	1.09)	3.93		(2.68,	6.32)
3420	Trichloropropane, 1,2,3-	LL	0.96		(0.64,	1.78)	1.99		(1.27,	3.82)
3450	Triethylamine	LL	0.51		(0.40,	0.70)	1.48		(0.96,	2.76)
3510	Vinyl Acetate	LL	1.27		(0.95,	1.82)	5.91	D	(1.26,	>100.00)
3520	Vinyl Chloride	G	0.84		(0.61,	1.38)	1.06		(0.59,	4.60)
	Vinyl Propionate	LL	1.00	I	(0.57,	1.74)	1.21	I	(0.46,	3.20)
3530	Vinylidene Chloride	LL	1.12		(0.87,	1.52)	2.41		(1.82,	3.35)
3570	Xylene, P-	LL	2.12		(1.71,	2.68)	7.87		(3.49,	24.90)
3550	Xylene, M-	LL	0.40		(0.36,	0.46)	5.87	D	(0.91,	>100.00)
3560	Xylene, O-	LL	0.43		(0.28,	0.85)	1.40		(0.61,	9.33)

*Organic Chemical Producers Data Base

**G=Gas; LL=Light Liquid; HL=Heavy Liquid.

Definition of Explanatory Data Codes:

I Inverse Estimation Method
D Possible Outliers in Data
N Narrow Range of Data
X No Data Available
B 10,000 PPMV Response Unachievable
P Suspect Points Eliminated

ated confidence intervals: the classical regression method and the inverse regression method. Both methods of estimation essentially involve the fitting of a line to the actual and instrument observed concentrations. The interpolated or extrapolated actual concentration at 10,000 ppmv observed concentration is calculated based on the fitted line. The response factor is computed as he ratio of this estimated actual concentration to the specified 10,000 ppmv "observed" concentration.

Most of the response factors and associated confidence intervals were calculated using the classical method; those computed using the inverse method are noted in Table 1 with the explanatory code "I." Other explanatory codes used in Table 1 indicate data availability, data applicability, and possible data uncertainties such as the presence of outliers

In most cases the data fell very nearly on a straight line, but sometimes they did not When outliers were clearly defined they were removed from the data and the response factor recomputed This could not always be done. Often it was not clear which data points were valid and which were not. Additional data would be necessary to clarify these situations. Since it was not clear which points should be removed in these cases, all points were included.

Table 2 lists compounds tested which do not appear to respond at a 10,000 ppmv reading at any concentration. The data and the fitted line showed that the response appears to be well below 10,000 ppmv for feasible actual concentrations Sometimes it was not possible to distinguish between this situation and the problem of unresolved outliers mentioned above. Questionable or borderline cases are included in Table 1 rather than Table 2. Some of these compounds have large estimated response factors and wide confidence intervals

Table 2. *Tested Compounds which Appear to be Unable to Achieve an Instrument Response of 10,000 ppmv at any Feasible Concentration*

OVA		TLV	
OCPDB*	Compound Name	OCPDB	Compound Name
-	Acetyl-1-propanol,3-	120	Acetophenone
790	Carbon disulfide	-	Acetyl-1-propanol,3-
810	Carbon tetrachloride	130	Acetylene
-	Dichloro-1-propanol,2,3-	160	Acrylic Acid
-	Dichloro-2-propanol,1,3-	360	Benzaldehyde
-	Diisopropyl benzene,1,3-	450	Benzonitrile
-	Dimethylstyrene,2,4-	490	Benzoyl chloride
1221	Freon 12	530	Benzyl chloride
2073	Furfural	-	Butylbenzene, tert-
-	Methyl-2,4-Pentanediol,2-	810	Carbon tetrachloride
1660	Monoethanolamine	930	Chloroform
2770	Nitrobenzene	1040	Crotonaldehyde
2910	Phenol	1060	Cumene
-	Phenyl-2-Propanol,2-	1130	Cyclohexanol
		-	Dichloro-1-propanol,2,3-
		-	Dichloro-2-propanol,1,3-
		-	Diisopropyl benzene,1,3-
		-	Dimethylstyrene,2,4-
		2060	Formic acid
		1221	Freon 12
		2073	Furfural
		2200	Isobutylene
		-	Methyl-2,4-pentanediol
		2690	Methylstyrene, A-
		1660	Monoethanolamine
		2910	Phenol
		-	Phenyl-2-propanol,2-
		-	Propylbenzene,N-
		3230	Styrene
		2860	Tetrachloroethylene

* *Organic Chemical Producers Data Base ID Number*

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Bruce A. Tichenor *is the EPA Project Officer (see below)*

The complete report, entitled "Response Factors of VOC Analyzers at a Meter Reading of 10,000 PPMV for Selected Organic Compounds," (Order No PB 81-234 817, Cost. $6 50, subject to change) will be available only from.

National Technical Information Service
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