FINAL REPORT

ORGANIC VAPOR RESPIRATOR SERVICE LIFE PREDICTION

by

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Launch Support Division
Cocoa Beach, Florida

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16. Abstract (Limit: 200 words)

The service life of an average organic vapor respirator cartridge was estimated for 231 compounds listed in 29 Code of Federal Regulations (CFR) 1910.1000. The study was requested by NIOSH to aid in determining substances with possible marginal service lives for laboratory testing. Calculations were performed on a computer using the Dubinin equation to determine adsorption capacity and the modified Wheeler equation to estimate service life. A computer print out tabulation provided the threshold limit value, density, vapor pressure, adsorption capacity, and predicted cartridge service life for each compound. Fifty additional compounds are listed for which cartridge service life was not estimated because of insufficient density and vapor pressure data. The author suggests that the estimates of cartridge service life may be helpful to industrial health professionals in administering industrial respiratory programs.

17. Document Analysis a. Descriptors

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ABSTRACT

To aid NIOSH in determining organic compounds with marginal respirator cartridge service lives, the service lives of 231 compounds listed in 29 CFR 1910.1000 were estimated mathematically. The calculations were performed on a computer using the Dubinin equation to calculate adsorption capacity and the modified Wheeler equation to estimate service life.

I. INTRODUCTION

The purpose of this task was to estimate the service life of an average organic vapor respirator cartridge against each of the organic compounds listed in 29 CFR 1910.1000. This information was requested by NIOSH as an aid in determining substances with possible marginal service lives for laboratory testing. By publication of this information, it is hoped that industrial health professionals may find the data helpful in administering industrial respirator programs. Although data are presented for a wide variety of substances listed in 29CFR 1910.1000, it should be recognized that NIOSH does not recommend the use of sorbent type respirators for all of these substances. Service lives (10 percent breakthrough time) were estimated for 231 organic compounds; service lives for another 50 compounds were not calculated because of insufficient density and vapor pressure data. The calculations were performed on a computer using Fortran IV program language.

II. TASK SPECIFICATIONS

The task order specified the use of the Dubinin equation [1] for calculation of adsorption capacity and the modified Wheeler equation [2] for prediction of service life. The Dubinin equation is as follows:

$$W_S = \rho W_O \exp\left[-\frac{BT^2}{\beta^2}\log^2(p_s/p)\right]$$

where W_S = adsorption capacity (gram/gram)

ρ = solvent density (grams/cc)

W_O = maximum adsorption space (cc)

B = microporosity constant

T = temperature (°K)

β = affinity coefficient

p_s = saturation vapor pressure at temperature T (torr)

p = partial pressure (torr)

and the Wheeler equation is:

$$t_b = \frac{w_s}{C_o Q}\left[W - \frac{\rho_c Q \ln (C_o/C)}{k}\right]$$

where t_b = breakthrough time (min.)

w_s = adsorption capacity (gram/gram)

C_o = input concentration (grams/liter)

Q = flowrate of contaminated air (liters/min.)

W = weight of charcoal in cartridge (gram)

ρ_c = charcoal density (grams/liter)

C = breakthrough concentration

k = adsorption rate constant

The following conditions were specified in the task order:

Carbon weight	average of commercially available cartridges
Carbon type	petroleum base
Flowrate	30 liters/min./cartridge
Temperature	303° K
Wheeler rate constant	4,094 min^{-1}
Input concentration	10 X TLV, with a maximum of 1,000 ppm
Affinity coefficient (β)	to be calculated from molar volumes

III. TASK PARAMETERS

Based on these specifications and work performed on a previous contract [3], the following parameters were chosen:

Carbon weight (W) = 34 grams/cartridge

Microporosity constant (B) = 1.1×10^{-6}

Maximum adsorption space (W_o) = 0.53 cc/gram

Carbon density (ρ_c) = 400 grams/liter

In addition to the Dubinin and Wheeler equations, the following mathematical relationships were used in the computer program.

$$V_m = \frac{M}{\rho}$$

where V_m = molar volume (cc/mole)

M = molecular weight (grams/mole)

ρ = compound density (grams/cc),

$$\beta = \frac{V_m}{V_m \text{ ref}}$$

where V_m = molar volume (cc/mole)

V_m ref= molar volume of carbon tetrachloride (96.49 cc/mole)

β = affinity coefficient

$$C_o = \frac{C_i \times M}{24.863 \times 10^6}$$

where C_o = input concentration (grams/liter)

M = molecular weight (grams/mole)

C_i = input concentration (ppm)

$$p = \frac{760\ C_i}{10^6}$$

where p = partial pressure (torr)

C_i = input concentration (ppm)

and C_o/C = 10 (since all calculations are for 10% breakthrough).

IV. DATA SOURCES

The computer program required as input the following: compound name, molecular weight, density, and vapor pressure. The program calculates and prints out affinity coefficient, adsorption capacity, and service life. In addition, the input data is printed out along with the calculations.

Molecular weight data were either obtained from reference books or were calculated from atomic weights. Densities were obtained from reference books, primarily reference [4]. Vapor pressures at 30° C were the most difficult data to obtain. Some were found tabulated in the literature. Others were interpolated or extrapolated from data at other temperatures by plotting log p vs. 1/T, and some vapor pressures were calculated from the Antoine equation. The Antoine equation is:

$$\log p = A - B/(t + C)$$

where p = vapor pressure

A, B, and C = constants for a particular compound

t = temperature (°C)

The most extensive collection of Antoine constants is in the compilation by Dreisbach [5-7]. Some vapor pressure data was also found in the periodical literature.

V. TASK RESULTS

Tabulated below, as printed out by the computer, (Table I) are the input

data and calculation results for 231 compounds. TLV (Threshold Limit Value) is in parts per million, density is in grams/cubic centimeter, vapor pressure is in torr, adsorption capacity (w_s) is in grams of solvent/gram of carbon, and service life (t_b) is in minutes.

Following this tabulation is Table II, which lists the compounds for which calculations were not made due to insufficient vapor pressure and density data. Following Table II is the Fortran IV program.

TABLE I

INPUT DATA AND CALCULATION

RESULTS FOR 231 COMPOUNDS

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TASK ORDER 1 SORBENT SERVICE LIFE PREDICTIONS

COMPOUND NAME	MW	DENSITY	V PRESS	BETA	WS	TB
TLV PPM		G/CC	TORR		G/G	MINUTES
ACETALDEHYDE						
200.00000	44.05	0.7834	0.9877E+03	0.58	0.023	11.9
ACETIC ACID						
10.00000	60.05	1.0490	0.2060E+02	0.59	0.102	382.6
ACETIC ANHYDRIDE						
5.00000	102.09	1.0820	0.5500E+01	0.98	0.350	1549.7
ACETONE						
1000.00000	58.08	0.7920	0.2827E+03	0.76	0.132	51.4
ACETONITRILE						
40.00000	41.05	0.7830	0.1160E+03	0.54	0.042	58.4
ACETYLENE TETRABROMIDE						
1.00000	345.70	2.9600	0.4600E+00	1.21	1.260	8234.2
ACROLEIN						
0.10000	56.06	0.8410	0.3580E+03	0.69	0.000	198.0
ACRYLAMIDE						
0.10000	71.08	1.1220	0.2000E+01	0.66	0.038	12193.3
ACRYLONITRILE						
20.00000	53.06	0.7970	0.1434E+03	0.69	0.065	137.6
ALLYL ALCOHOL						
2.00000	58.08	0.8550	0.3240E+02	0.70	0.047	921.5
ALLYL CHLORIDE						
1.00000	76.53	0.9380	0.4535E+03	0.85	0.020	585.2
ALLYL GLYCIDYL ETHER						
10.00000	114.14	0.9698	0.6600E+01	1.22	0.398	788.0

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COMPOUND NAME	MW	DENSITY	V PRESS	BETA	WS	TB
TLV PPM		G/CC	TORR		G/G	MINUTES
N-AMYL ACETATE						
100.00000	130.18	0.8760	0.8000E+01	1.54	0.444	77.0
SEC-AMYL ACETATE						
125.00000	130.18	0.8600	0.1300E+02	1.57	0.428	74.3
ANILINE						
5.00000	93.12	1.0220	0.9100E+00	0.94	0.437	2118.2
O-ANISIDINE						
0.07000	165.19	1.0980	0.4000E+00	1.56	0.413	80606.1
P-ANISIDINE						
0.07000	165.19	1.0890	0.4000E+00	1.57	0.412	80395.2
BENZENE						
10.00000	78.11	0.8684	0.1180E+03	0.93	0.141	407.5
BENZYL CHLORIDE						
1.00000	126.58	1.1000	0.2670E+01	1.19	0.368	6565.5
BROMOFORM						
0.50000	252.77	2.8900	0.7000E+01	0.91	0.413	7381.5
1,3-BUTADIENE						
1000.00000	54.09	0.6210	0.2470E+04	0.90	0.071	29.8
2-BUTANONE (MEK)						
200.00000	72.10	0.8050	0.1214E+03	0.93	0.242	75.7
2-BUTOXYETHANOL						
50.00000	118.17	0.9027	0.1000E+01	1.36	0.474	181.1
BUTYL ACETATE						
150.00000	116.16	0.8820	0.1800E+02	1.36	0.422	82.0

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COMPOUND NAME	TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
SEC-BUTYL ACETATE	200.00000	116.16	0.8648	0.2900E+02	1.39	0.402	78.2
TERT-BUTYL ACETATE	200.00000	116.16	0.8960	0.3050E+02	1.34	0.411	80.0
BUTYL ALCOHOL	100.00000	74.12	0.8098	0.9520E+01	0.95	0.375	114.2
SEC-BUTYL ALCOHOL	150.00000	74.12	0.8080	0.2390E+02	0.95	0.333	101.6
TERT-BUTYL ALCOHOL	100.00000	74.12	0.7887	0.6360E+02	0.97	0.282	85.9
BUTYLAMINE	5.00000	73.14	0.7401	0.1164E+03	1.02	0.122	751.8
N-BUTYL GLYCIDYL ETHER	50.00000	130.21	0.9087	0.4000E+01	1.49	0.459	159.3
N-BUTYL MERCAPTAN	10.00000	90.18	0.8350	0.5810E+02	1.12	0.226	567.0
P-TERT-BUTYLTOLUENE	10.00000	148.24	0.8600	0.9500E+00	1.79	0.439	668.5
CAMPHOR	2.00000	152.23	0.9900	0.3700E+00	1.59	0.486	3605.8
CARBARYL	0.60000	201.22	1.2320	0.1000E-01	1.69	0.650	12164.6
CARBON DISULFIDE	20.00000	76.14	1.2500	0.4353E+03	0.63	0.032	47.5

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COMPOUND NAME	MW	DENSITY	V PRESS	BETA	WS	TB
TLV PPM		G/CC	TORR		G/G	MINUTES
CHLORINATED CAMPHENE						
0.03000	413.84	1.6600	0.3000E-06	2.58	0.776	141161.3
CHLORINATED DIPHENYL OXIDE						
0.05000	238.90	1.3200	0.7000E-03	1.88	0.698	132007.3
CHLOROACETALDEHYDE						
1.00000	78.50	1.1900	0.1000E+01	0.68	0.239	6876.1
ALPHA-CHLOROACETOPHENONE						
0.05000	154.59	1.3240	0.4000E-01	1.21	0.529	154642.4
CHLOROBENZENE						
75.00000	112.56	1.1066	0.1545E+02	1.05	0.487	130.2
CHLOROBROMOMETHANE						
200.00000	129.40	1.9114	0.1834E+03	0.70	0.316	55.2
CHLOROFORM						
50.00000	119.39	1.4840	0.2460E+03	0.83	0.250	94.4
CHLOROPICRIN						
0.10000	164.39	1.6920	0.3110E+02	1.01	0.108	14807.8
CHLOROPRENE						
25.00000	88.54	0.9583	0.2600E+03	0.96	0.172	175.4
M-CRESOL						
5.00000	108.10	1.0340	0.2500E+00	1.08	0.517	2161.7
O-CRESOL						
5.00000	108.10	1.0511	0.6800E+00	1.07	0.485	2024.6
P-CRESOL						
5.00000	108.10	1.0390	0.2900E+00	1.08	0.515	2150.4

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COMPOUND NAME TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
CROTONALDEHYDE 2.00000	70.09	0.8530	0.3200E+02	0.85	0.097	1564.5
CUMENE 50.00000	120.19	0.8640	0.1645E+02	1.44	0.402	151.1
CYCLOHEXANE 300.00000	84.16	0.7791	0.1217E+03	1.12	0.279	74.9
CYCLOHEXANOL 50.00000	100.16	0.9449	0.2600E+01	1.10	0.472	213.0
CYCLOHEXANONE 50.00000	98.14	0.9478	0.6500E+01	1.07	0.440	202.3
CYCLOHEXENE 300.00000	82.14	0.8102	0.1111E+03	1.05	0.280	76.9
CYCLOPENTADIENE 75.00000	66.10	0.8048	0.4500E+03	0.85	0.132	60.3
DDT 0.07000	354.49	1.5500	0.2500E-06	2.37	0.673	61270.6
DEMETON 0.01000	256.31	1.1230	0.1000E-02	2.37	0.582	512724.8
DIACETONE ALCOHOL 50.00000	116.16	0.9306	0.2300E+01	1.29	0.475	184.8
DIBUTYL PHTHALATE 0.40000	278.30	1.0450	0.2900E-04	2.76	0.525	10644.6
O-DICHLOROBENZENE 50.00000	147.00	1.3070	0.1790E+01	1.17	0.670	205.8

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COMPOUND NAME	TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
P-DICHLOROBENZENE	75.00000	147.00	1.4581	0.1070E+01	1.04	0.767	157.2
DICHLORODIFLUOROMETHANE	1000.00000	120.92	1.4860	0.5320E+04	0.84	0.097	18.0
1,1-DICHLOROETHANE	100.00000	98.96	1.1740	0.2777E+03	0.87	0.261	59.5
1,2-DICHLOROETHYLENE(CIS)	200.00000	96.94	1.2820	0.2500E+03	0.78	0.240	55.8
1,2-DICHLOROETHYLENE(TRANS)	200.00000	96.94	1.2570	0.3890E+03	0.80	0.209	48.6
DICHLOROETHYL ETHER	15.00000	143.00	1.2220	0.2600E+01	1.21	0.571	600.8
DICHLOROMONOFLUOROMETHANE	1000.00000	102.92	1.4800	0.1520E+04	0.72	0.094	20.7
1,1-DICHLORO-1-NITROETHANE	10.00000	143.96	1.4210	0.2000E+02	1.05	0.440	690.9
DICHLOROTETRAFLUOROETHANE	1000.00000	170.93	1.4550	0.2050E+04	1.22	0.346	45.7
DICHLORVOS	0.10000	221.00	1.4150	0.1000E-01	1.62	0.715	73027.1
DIELDRIN	0.02000	381.00	1.7500	0.2000E-06	2.26	0.787	233171.3
DIETHYLAMINE	25.00000	73.10	0.7108	0.2927E+03	1.07	0.153	188.7

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COMPOUND NAME	TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
DIFLUORODIBROMOMETHANE	100.00000	209.80	2.2880	0.1000E+04	0.95	0.409	44.0
DIGLYCIDAL ETHER	0.50000	130.10	1.2420	0.1000E+00	1.09	0.554	19226.5
DIETHYLAMINOETHANOL	10.00000	117.20	0.8857	0.4000E+01	1.37	0.400	771.5
DIISOBUTYL KETONE	50.00000	142.24	0.8100	0.3600E+01	1.82	0.417	132.4
DIISOPROPYLAMINE	5.00000	101.19	0.7220	0.1200E+03	1.45	0.213	950.5
DIMETHYL ACETAMIDE	10.00000	87.12	0.9440	0.2000E+01	0.96	0.400	1038.1
DIMETHYLAMINE	10.00000	45.08	0.6804	0.1850E+04	0.69	0.006	29.3
N,N-DIMETHYLANILINE	5.00000	121.18	0.9557	0.1000E+01	1.31	0.450	1678.0
DIMETHYLFORMAMIDE	10.00000	73.10	0.9445	0.5560E+01	0.80	0.290	896.3
1,1-DIMETHYL HYDRAZINE	0.50000	60.10	0.7820	0.1800E+03	0.80	0.013	959.8
DIMETHYL PHTHALATE	0.60000	194.18	1.1890	0.3000E+00	1.69	0.561	10871.8
DIMETHYL SULFATE	1.00000	126.13	1.3322	0.1000E+00	0.98	0.619	11086.1

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COMPOUND NAME	TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
DI-SEC-OCTYL PHTHALATE	0.30000	390.60	0.9650	0.1400E-06	4.19	0.462	8903.2
DIOXANE	100.00000	88.10	1.0353	0.5120E+02	0.88	0.355	91.1
DIPHENYL	0.20000	154.20	0.9910	0.1600E-01	1.61	0.504	36933.6
DIPROPYLENE GLYCOL METHYL ETHER	100.00000	148.20	0.9500	0.4000E+00	1.62	0.502	76.5
EPICHLOROHYDRIN	5.00000	92.52	1.1751	0.2150E+02	0.82	0.197	962.4
EPN	0.04000	323.30	1.2680	0.5000E-02	2.64	0.658	114881.9
ETHANOLAMINE	3.00000	61.08	1.0180	0.7000E+00	0.62	0.303	3732.1
2-ETHOXYETHANOL	200.00000	90.12	0.9360	0.7700E+01	1.00	0.448	112.2
2-ETHOXYETHYL ACETATE	100.00000	132.17	0.9748	0.2500E+01	1.41	0.510	87.1
ETHYL ACETATE	400.00000	88.10	0.8946	0.1187E+03	1.02	0.297	76.2
ETHYL ACRYLATE	25.00000	100.11	0.9230	0.6000E+02	1.12	0.297	267.9
ETHYL ALCOHOL	1000.00000	46.07	0.7808	0.7880E+02	0.61	0.138	67.7

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COMPOUND NAME	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
TLV PPM						
ETHYLAMINE						
10.00000	45.08	0.7059	0.1280E+04	0.66	0.006	30.5
ETHYL SEC-AMYL KETONE						
25.00000	128.20	0.8220	0.3000E+01	1.62	0.412	290.4
ETHYLBENZENE						
100.00000	106.16	0.8669	0.2375E+02	1.27	0.399	85.0
ETHYL BROMIDE						
200.00000	108.98	1.4510	0.5640E+03	0.78	0.195	40.4
ETHYL BUTYL KETONE						
50.00000	114.20	0.8198	0.2200E+01	1.44	0.422	167.1
ETHYL CHLORIDE						
1000.00000	64.52	0.9214	0.6280E+04	0.73	0.026	9.0
ETHYLENE CHLORIDE						
50.00000	98.96	1.2570	0.1000E+03	0.82	0.274	125.0
ETHYLENE CHLOROHYDRIN						
5.00000	80.52	1.1970	0.1000E+02	0.70	0.188	1053.7
ETHYLENEDIAMINE						
10.00000	60.10	0.8994	0.1700E+02	0.69	0.149	560.1
ETHYLENE DIBROMIDE						
20.00000	187.88	2.1707	0.1740E+02	0.90	0.676	406.2
ETHYLENE GLYCOL DINITRATE						
0.20000	152.06	1.4890	0.8000E-01	1.06	0.604	44867.8
ETHYLENE OXIDE						
50.00000	44.05	0.8711	0.1559E+04	0.52	0.004	3.9

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COMPOUND NAME TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
ETHYLENIMINE 0.50000	43.07	0.8320	0.2700E+03	0.54	0.000	12.0
ETHYL ETHER 400.00000	74.12	0.7135	0.6472E+03	1.08	0.179	54.5
ETHYL FORMATE 100.00000	74.08	0.9236	0.2975E+03	0.83	0.183	55.9
ETHYLIDENE CHLORIDE 200.00000	98.96	1.1740	0.2800E+03	0.87	0.260	59.4
ETHYL MERCAPTAN 10.00000	62.13	0.8391	0.6446E+03	0.77	0.032	114.6
N-ETHYLMORPHOLINE 20.00000	115.20	0.9160	0.1000E+02	1.30	0.399	391.0
ETHYL SILICATE 100.00000	208.30	0.9330	0.3000E+01	2.31	0.491	53.3
FLUOROTRICHLOROMETHANE 1000.00000	137.38	1.4940	0.9950E+03	0.95	0.269	44.2
FORMALDEHYDE 3.00000	30.03	0.8150	0.8100E+04	0.38	0.000	0.0
FORMIC ACID 5.00000	46.03	1.2200	0.5220E+02	0.39	0.001	9.5
FURFURAL 5.00000	96.10	1.1610	0.5300E+01	0.86	0.327	1538.6
FURFURYL ALCOHOL 50.00000	98.10	1.1290	0.1000E+01	0.90	0.585	269.5

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TASK ORDER 1 SORBENT SERVICE LIFE PREDICTIONS

COMPOUND NAME TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
GLYCIDOL 50.00000	74.10	1.1150	0.1300E+01	0.69	0.556	339.0
HEPTACHLOR 0.03000	375.30	1.5800	0.4000E-03	2.46	0.837	167808.4
HEPTANE 500.00000	100.20	0.6840	0.5835E+02	1.52	0.310	69.9
HEXACHLOROETHANE 1.00000	236.76	2.0910	0.1000E+01	1.17	0.797	7604.9
HEXANE 500.00000	86.17	0.6603	0.1834E+03	1.35	0.256	67.0
2-HEXANONE 100.00000	100.16	0.8300	0.6000E+01	1.25	0.418	94.2
HEXONE 100.00000	100.16	0.8030	0.9000E+01	1.29	0.397	89.5
SEC-HEXYL ACETATE 50.00000	144.21	0.8598	0.6500E+01	1.74	0.433	135.7
HYDROQUINONE 0.04000	110.10	1.3320	0.2000E-01	0.86	0.448	229707.0
ISOAMYL ACETATE 100.00000	130.20	0.8760	0.9000E+01	1.54	0.442	76.7
ISOAMYL ALCOHOL 100.00000	88.15	0.8160	0.5000E+01	1.12	0.410	105.0
ISOBUTYL ACETATE 150.00000	116.20	0.8685	0.2400E+02	1.39	0.409	79.5

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TASK ORDER 1 SORBENT SERVICE LIFE PREDICTIONS

COMPOUND NAME	TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
ISOBUTYL ALCOHOL	100.00000	74.12	0.8050	0.1500E+02	0.95	0.354	107.9
ISOPHORONE	25.00000	138.10	0.9229	0.8000E+00	1.55	0.481	314.8
ISOPROPYL ACETATE	250.00000	102.13	0.8740	0.8700E+02	1.21	0.346	76.5
ISOPROPYL ALCOHOL	400.00000	60.09	0.7854	0.5300E+02	0.79	0.241	90.6
ISOPROPYL AMINE	5.00000	59.11	0.6940	0.6957E+03	0.88	0.035	266.7
ISOPROPYL GLYCIDYL ETHER	50.00000	116.16	0.9186	0.1200E+02	1.31	0.427	165.9
ISOPROPYL ETHER	500.00000	102.17	0.7190	0.2030E+03	1.47	0.290	64.0
KETENE	0.50000	42.04	0.8100	0.8900E+04	0.54	0.000	0.0
MALATHION	0.01000	330.00	1.2300	0.4000E-04	2.78	0.651	445695.8
MALEIC ANHYDRIDE	0.25000	98.10	1.4800	0.7000E+00	0.69	0.192	17644.7
MESITYL OXIDE	25.00000	98.14	0.8539	0.1200E+02	1.19	0.359	330.8
METHYL ACETATE	200.00000	74.08	0.9244	0.2658E+03	0.83	0.190	57.9

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TASK ORDER 1 SORBENT SERVICE LIFE PREDICTIONS

COMPOUND NAME TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
METHYLACETYLENE 1000.00000	40.06	0.6600	0.4810E+04	0.63	0.009	4.9
METHYL ACRYLATE 10.00000	86.10	0.9490	0.1100E+03	0.94	0.161	421.5
METHYLAL 1000.00000	76.10	0.8640	0.4700E+03	0.91	0.178	52.9
METHYL ALCOHOL 200.00000	32.04	0.7913	0.1600E+03	0.42	0.019	13.4
METHYLAMINE 10.00000	31.06	0.6220	0.3160E+04	0.52	0.000	0.8
METHYL N-AMYL KETONE 100.00000	114.18	0.8166	0.6000E+01	1.45	0.416	82.4
METHYL BROMIDE 20.00000	94.45	1.7320	0.1920E+04	0.57	0.004	5.4
METHYL CELLOSOLVE 25.00000	76.09	0.9660	0.1340E+02	0.82	0.305	362.2
METHYL CELLOSOLVE ACETATE 25.00000	118.13	1.0050	0.4800E+01	1.22	0.466	356.3
METHYL CHLORIDE 100.00000	50.49	0.9180	0.4970E+04	0.57	0.005	2.4
METHYL CHLOROFORM 350.00000	133.42	1.3492	0.1570E+03	1.02	0.427	72.3
METHYLCYCLOHEXANE 500.00000	98.18	0.7864	0.5870E+02	1.29	0.336	77.3

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TASK ORDER 1 SORBENT SERVICE LIFE PREDICTIONS

COMPOUND NAME	TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
METHYLCYCLOHEXANOL	100.00000	114.19	0.9130	0.1500E+01	1.30	0.481	95.2
O-METHYLCYCLOHEXANONE	100.00000	112.17	0.9250	0.4000E+01	1.26	0.474	95.5
METHYLENE BISPHENYL ISOCYANATE	0.02000	250.25	1.1900	0.1000E-02	2.18	0.622	280575.8
METHYLENE CHLORIDE	500.00000	89.94	1.3070	0.5114E+03	0.71	0.142	35.5
METHYL FORMATE	100.00000	60.05	0.9750	0.7079E+03	0.64	0.058	21.9
METHYL IODIDE	5.00000	141.95	2.2790	0.4834E+03	0.65	0.020	64.8
METHYL ISOBUTYL CARBINOL	25.00000	102.18	0.8079	0.4500E+01	1.31	0.383	338.8
METHYL MERCAPTAN	10.00000	48.10	0.8680	0.1620E+04	0.57	0.001	7.0
METHYL METHACRYLATE	100.00000	100.11	0.9360	0.4800E+02	1.11	0.380	85.7
ALPHA-METHYLSTYRENE	100.00000	118.17	0.9018	0.3400E+01	1.36	0.467	89.3
MONOMETHYLANILINE	2.00000	107.15	0.9890	0.9000E+00	1.12	0.408	4295.1
MONOMETHYLHYDRAZINE	0.20000	46.07	0.8740	0.6000E+02	0.55	0.000	89.2

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COMPOUND NAME TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
MORPHOLINE 20.00000	87.12	0.9980	0.1350E+02	0.90	0.331	429.2
NAPHTHALENE 10.00000	128.16	1.1620	0.1400E+00	1.14	0.613	1079.4
NICOTINE 0.03000	162.23	1.0092	0.6000E-01	1.67	0.463	80537.5
P-NITROANILINE 1.00000	138.13	1.4240	0.1000E-01	1.01	0.754	12322.3
NITROBENZENE 1.00000	123.11	1.2050	0.7000E+00	1.06	0.451	8276.3
P-NITROCHLOROBENZENE 0.15000	157.60	1.5200	0.2000E-01	1.07	0.704	67218.8
NITROETHANE 100.00000	75.07	1.0520	0.2560E+02	0.74	0.362	109.0
NITROGLYCERIN 0.20000	227.09	1.6010	0.8300E-03	1.47	0.846	42058.2
NITROMETHANE 100.00000	61.04	1.1300	0.4676E+02	0.56	0.214	79.0
1-NITROPROPANE 25.00000	89.09	1.0030	0.1400E+02	0.92	0.351	355.7
2-NITROPROPANE 25.00000	89.09	0.9920	0.2000E+02	0.93	0.326	331.0
M-NITROTOLUENE 5.00000	137.20	1.1570	0.4200E+00	1.23	0.570	1877.1

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COMPOUND NAME TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
O-NITROTOLUENE 5.00000	137.20	1.1630	0.4000E+00	1.22	0.574	1891.0
P-NITROTOLUENE 5.00000	137.20	1.2990	0.3600E+00	1.09	0.635	2091.5
OCTANE 500.00000	114.23	0.7036	0.1840E+02	1.68	0.348	68.9
OXALIC ACID 0.02000	126.10	1.6530	0.2000E-04	0.79	0.773	692113.8
PARATHION 0.01000	291.30	1.2600	0.4000E-03	2.40	0.662	513031.8
PENTACHLOROPHENOL 0.05000	266.40	1.9780	0.2000E-03	1.40	1.044	177035.5
PENTANE 1000.00000	72.15	0.6260	0.6148E+03	1.19	0.182	57.1
2-PENTANONE 200.00000	86.13	0.8060	0.2480E+02	1.11	0.354	92.8
PHENOL 5.00000	94.11	1.0720	0.8000E+00	0.91	0.459	2202.4
PHENYL ETHER 1.00000	170.20	1.0700	0.3000E-01	1.65	0.560	7426.3
PHENYL GLYCIDYL ETHER 10.00000	150.17	1.1090	0.2000E-01	1.40	0.578	868.9
P-PHENYLENEDIAMENE 0.02000	108.14	1.1390	0.4000E-01	0.98	0.328	342177.3

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COMPOUND NAME	TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
PHENYLHYDRAZINE	5.00000	108.14	1.0900	0.1400E+00	1.03	0.560	2340.2
PHOSDRIN	0.01000	224.10	1.2300	0.5000E-02	1.89	0.594	598255.8
PHOSGENE	0.10000	98.92	1.3700	0.1649E+04	0.75	0.001	118.8
PHTHALIC ANHYDRIDE	2.00000	148.11	1.5270	0.4600E-01	1.01	0.791	6029.4
PROPANE	1000.00000	44.09	0.4861	0.8100E+04	0.94	0.040	20.7
PROPARGYL ALCOHOL	1.00000	56.10	0.9715	0.1740E+02	0.60	0.021	859.6
N-PROPYL ACETATE	200.00000	102.13	0.8870	0.4300E+02	1.19	0.378	83.6
PROPYL ALCOHOL	200.00000	60.10	0.8044	0.2760E+02	0.77	0.283	106.3
PROPYLENE DICHLORIDE	75.00000	112.99	1.1800	0.2380E+02	0.99	0.478	127.3
PROPYLENE OXIDE	100.00000	58.08	0.8304	0.6310E+03	0.72	0.086	33.3
PROPYL NITRATE	25.00000	105.10	1.0500	0.2400E+02	1.04	0.368	316.0
PYRIDINE	5.00000	79.10	0.9820	0.3000E+02	0.83	0.154	880.5

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TASK ORDER 1 SORBENT SERVICE LIFE PREDICTIONS

COMPOUND NAME	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
TLV PPM						
STYRENE						
100.00000	104.14	0.8964	0.7940E+01	1.20	0.442	95.8
1,1,2,2-TETRACHLORO-1,2-DIFLUOROETHANE						
500.00000	203.85	1.6440	0.7300E+02	1.29	0.685	75.9
TETRACHLOROETHYLENE						
100.00000	165.83	1.6059	0.2402E+02	1.07	0.698	95.1
TETRACHLOROMETHANE						
10.00000	153.84	1.5843	0.1430E+03	1.01	0.288	423.1
TETRAETHYLLEAD						
0.00600	323.50	1.6240	0.5700E+00	2.06	0.578	672853.6
TETRAHYDROFURAN						
200.00000	72.12	0.8880	0.2004E+03	0.84	0.204	63.9
TETRAMETHYLLEAD						
0.00600	267.33	1.9950	0.4050E+02	1.39	0.166	233420.3
TETRANITROMETHANE						
1.00000	196.04	1.6500	0.1500E+02	1.23	0.424	4887.8
TOLUENE						
200.00000	92.13	0.8576	0.3670E+02	1.11	0.361	88.4
TOLUENE DIISOCYANATE						
0.02000	176.16	1.2200	0.2500E-01	1.50	0.518	332143.0
O-TOLUIDINE						
5.00000	107.15	1.0040	0.9000E+00	1.11	0.455	1919.2
TRIBUTYL PHOSPHATE						
0.46000	266.32	0.9727	0.3000E-01	2.84	0.510	9400.6

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COMPOUND NAME	TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
1,1,2-TRICHLOROETHANE	10.00000	133.42	1.4242	0.2940E+02	0.97	0.368	623.6
TRICHLOROETHYLENE	100.00000	131.40	1.4550	0.9400E+02	0.94	0.466	80.0
1,2,3-TRICHLOROPROPANE	50.00000	147.44	1.3832	0.5000E+01	1.10	0.661	202.5
1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE	1000.00000	187.39	1.5702	0.4000E+03	1.24	0.510	61.5
TRI-O-CRESYL PHOSPHATE	0.00700	368.36	1.1700	0.4000E-06	3.26	0.594	520381.1
TRIETHYLAMINE	25.00000	101.19	0.7229	0.7310E+02	1.45	0.278	248.2
2,4,6-TRINITROTOLUENE	0.16000	227.13	1.6540	0.2000E-04	1.42	0.748	46485.5
TRIPHENYL PHOSPHATE	0.22000	326.28	1.2680	0.1000E-02	2.67	0.672	21129.4
TURPENTINE	100.00000	126.16	0.8700	0.7000E+00	1.50	0.461	82.5
VINYLTOLUENE	100.00000	118.17	0.8894	0.2310E+01	1.38	0.466	89.0
M-XYLENE	100.00000	106.16	0.8556	0.1143E+02	1.29	0.417	88.6
O-XYLENE	100.00000	106.16	0.8717	0.1555E+02	1.26	0.414	88.1

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COMPOUND NAME	TLV PPM	MW	DENSITY G/CC	V PRESS TORR	BETA	WS G/G	TB MINUTES
P-XYLENE	100.00000	106.16	0.8523	0.2352E+02	1.29	0.395	84.0
2,4-XYLIDINE	5.00000	121.24	0.9740	0.3000E+00	1.29	0.492	1831.5
2.6-XYLIDINE	5.00000	121.24	0.9820	0.5000E+00	1.28	0.482	1794.8

TABLE II

COMPOUNDS FOR WHICH CALCULATIONS

WERE NOT MADE

1. aldrin
2. allyl propyl disulfide
3. 2-aminopyridine
4. alpha-naphthylthiourea
5. azinphos-methyl
6. benzoyl peroxide
7. tert-butyl chromate
8. chlordane
9. o-chlorobenzylidenemalonitrile
10. (tri) chlorodiphenyl
11. (penta) chlorodiphenyl
12. 1-chloronitropropane
13. Crag^{R} herbicide
14. 2,4-D
15. diazomethane
16. 1,3-dichloro-5,5-dimethylhydantoin
17. dimethyl-1,2-dibromo-2,2-dichloroethyl phosphate
18. o-dinitrobenzene
19. m-dinitrobenzene
20. p-dinitrobenzene
21. dinitro-o-cresol
22. endrin
23. Ferbam

24. hexachloronaphthalene
25. lindane
26. methoxychlor
27. methyl isocyanate
28. octachloronaphthalene
29. paraquat
30. pentachloronaphthalene
31. perchloromethyl mercaptan
32. picric acid
33. pival
34. propyleneimine
35. quinone
36. RDX
37. ronnel
38. rotenone
39. strychnine
40. 2,4,5-T
41. TEDP
42. TEPP
43. terphenyl
44. 1,1,1,2-tetrachloro-2,2-difluoroethane
45. tetrachloronaphthalene
46. tetramethyl succinonitrile
47. tetryl
48. thiram
49. trichloronaphthalene
50. trifluorobromomethane

VI. FORTRAN IV PROGRAM

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FORTRAN IV VER13/MOD00

/ READ DEVICE-MFCU1
      C WHEELER EQUATION EVALUATION-RESPIRATOR CARTRIDGES
      C CN  210-76-0108  CHG   997501
  1         REAL*8 Z1,Z2,Z3,Z4,Z5
  2         REAL MW,K
      C  CONSTANTS ASSIGNMENT STATEMENTS
  3         WO=.53
  4         T=303.
  5         B=1.1E-6
  6         W=34.
  7         COC=10.
  8         Q=30.
  9         K=4094.
 10         PC=400.
 11         N=0
 12         L=12
 13         VMREF=96.49
      C VARIABLES INPUT
 14       80 READ(1,10,END=110)(Z1,Z2,Z3,Z4,Z5,RHO,TLV,PS,MW)
 15       10 FORMAT(5A8,F10.5,F10.2,E10.4,F10.2)
 16         VM=MW/RHO
 17         BETA=VM/VMREF
 18         CI=TLV*10.
 19         IF(CI-1000.)250,250,240
 20      240 CI=1000.
 21      250 P=CI*760./10.**6
 22         CO=CI*MW/24.863/10.**6
 23         WS=RHO*WO*EXP((-B*T**2/BETA**2)*((ALOG10(PS/P))**2))
 24         TB=((WS/CO/Q)*(W-(PC*Q/K)*ALOG(COC)))
 25         N=N+1
 26         IF(N-1)20,20,25
 27       25 IF(N-L)70,70,90
 28       90 L=L+12
 29       20 IPAGE=L/12
 30         WRITE(3,120)IPAGE
 31      120 FORMAT('1' /T71,'PAGE ',I3)
 32         WRITE(3,50)
 33       50 FORMAT(////T30,' CONTRACT NUMBER 210-76-0108'//T27,' QUICK RESPONS
           BE ENGINEERING REPORT'//T19,'TASK ORDER  1  SORBENT SERVICE LIFE PR
           CEDICTIONS'///T6,'COMPOUND NAME'/11X,'TLV',7X,'MW',6X,'DENSITY',3X,
           D'V PRESS',8X,'BETA',7X,'WS',8X,'TB'/11X,'PPM',17X,'G/CC',5X,'TORR'
           E,21X,'G/G',5X,'MINUTES'//)
 34       70 WRITE(3,60)Z1   ,Z2   ,Z3   ,Z4,Z5,TLV   ,MW   ,RHO   ,PS   ,BETA,
           EWS,TB
 35       60 FORMAT(4X,5A8/6X,F10.5,F10.2,F10.4,2X,E10.4,F10.2,F10.3,F10.1//)
 36         GO TO 80
 37      110 STOP
 38         END
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